# Low Temperature Physics Division
# Fachverband Tiefe Temperaturen (TT)

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## Overview of Invited Talks and Sessions

(Lecture Rooms H2, H6, H9, H17, H18, H19, H20, H21, H24, and H41; Poster D)

### Invited and Topical Talks except for Focused Sessions

| | | | | |
|---|---|---|---|---|
| TT 17.7 | Mon | 16:45–17:15 | H19 | **Magnetic Frustration in a Quantum Spin Chain: The Case of Linarite $PbCuSO_4(OH)_2$** — •Anja U.B. Wolter |
| TT 25.7 | Tue | 11:15–11:45 | H9 | **One-dimensional fermion systems beyond the Luttinger Liquid paradigm** — •Thomas L. Schmidt |
| TT 27.1 | Tue | 9:30–10:00 | H18 | **Hydrostatic-Pressure Tuning of Magnetic, Nonmagnetic and Superconducting States in Annealed $Ca(Fe_{1-x}Co_x)_2As_2$** — •Elena Gati |
| TT 29.5 | Tue | 10:30–11:00 | H20 | **Nano-Conductors as Measurement Devices and Driving Sources** — •Sigmund Kohler |
| TT 42.8 | Wed | 17:00–17:30 | H18 | **Orbitronics in Silicon** — •Gabriel Aeppli |
| TT 48.1 | Wed | 16:45–17:15 | H19 | **Transport as a sensitive indicator for quantum criticality** — •Gernot Schaller |
| TT 59.7 | Thu | 16:45–17:15 | H6 | **Electron Spin Resonance (ESR) close to a Quantum Phase Transition: Probing $YbRh_2Si_2$ at mK Temperatures** — •Marc Scheffler |
| TT 61.1 | Thu | 15:00–15:30 | H18 | **Correlation Effects in Quantum Spin Hall Insulators** — •Martin Hohenadler |
| TT 62.5 | Thu | 16:00–16:30 | H19 | **Condensation Energy of $CeCu_2Si_2$ and Theoretical Implications** — •Stefan Kirchner |

### Tutorial "Topological Insulators and Majorana-Fermion Physics"

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|---|---|---|---|---|
| TT 1.1 | Sun | 16:00–16:45 | H20 | **Topological Insulators and Superconductors** — •Andreas Schnyder |
| TT 1.2 | Sun | 16:50–17:35 | H20 | **Proximity Induced Superconductivity in Topological Insulators** — •Hartmut Buhmann |
| TT 1.3 | Sun | 17:40–18:25 | H20 | **Majorana Fermions in Hybrid Nanosystems** — •Michael Wimmer |

### Invited and Topical Talks of the Focused Session "Correlations in Topological Bands"

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|---|---|---|---|---|
| TT 18.1 | Mon | 15:00–15:30 | H20 | **Designer Dirac Fermions, Topological Phases, and Gauge Fields in Molecular Graphene** — •Hari C. Manoharan |
| TT 18.2 | Mon | 15:30–16:00 | H20 | **Fractional Topological Insulators** — •Claudio Chamon |
| TT 18.3 | Mon | 16:00–16:30 | H20 | **Hierarchy of Fractional Chern Insulators and Competing Compressible States** — •Andreas Läuchli |
| TT 18.4 | Mon | 16:45–17:15 | H20 | **Designing Topological Bands for Ultracold Atomic Gases** — •Nigel Cooper |
| TT 18.5 | Mon | 17:15–17:45 | H20 | **Probing Topological Bloch Bands Using Ultracold Quantum Gases** — •Immanuel Bloch |

## Invited and Topical Talks of the Focused Session "Majorana Fermions in Condensed Matter"

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|---|---|---|---|---|
| TT 44.1 | Wed | 15:00–15:30 | H20 | **Subgap States in Majorana Wires** — •Piet Brouwer |
| TT 44.2 | Wed | 15:30–16:00 | H20 | **New Measurements on Nanowire Majorana Systems** — •Charles Marcus |
| TT 44.3 | Wed | 16:00–16:30 | H20 | **Adaptive Tuning of Majorana Fermions in a Quantum Dot Chain** — •Anton Akhmerov |
| TT 44.4 | Wed | 16:45–17:15 | H20 | **Majorana Fermions in Disordered Quantum Wires** — •Alexander Altland |
| TT 44.5 | Wed | 17:15–17:45 | H20 | **Parity Effects and Crossed Andreev Noise in Transport through Majorana Wires** — •Bernd Rosenow |

## Invited and Topical Talks of the Focused Session "Magnetism and Superconductivty in Fe-based Pnictides and Chalcogenides"

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|---|---|---|---|---|
| TT 54.1 | Thu | 9:30–10:00 | H20 | **Fermiology and Order Parameter of Iron-based Superconductors from ARPES** — •Sergey Borisenko |
| TT 54.2 | Thu | 10:00–10:30 | H20 | **Electron Correlations in Solids from the Dynamical Mean Field Perspective and the Origin Anomalous State of Matter in Iron Chalchogenides** — •Kristjan Haule |
| TT 54.3 | Thu | 10:30–11:00 | H20 | **A Light Scattering Study of the Evolution of Pairing in Fe-based Superconductors** — •Rudi Hackl |
| TT 54.4 | Thu | 11:15–11:45 | H20 | **Theory of Magnetism and Superconductivity for Iron-Chalcogenides** — •Jiangping Hu |
| TT 54.5 | Thu | 11:45–12:15 | H20 | **Charge Dynamics in 122 Iron Pnictides** — •Aliaksei Charnukha |

## Invited and Topical Talks of the Focused Session "Dynamical Mean-Field Approach to Correlated Electron Materials"

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|---|---|---|---|---|
| TT 63.1 | Thu | 15:00–15:30 | H20 | **How Bad Metals Turn Good: Spectroscopic Signatures of Resilient Quasiparticles** — •Antoine Georges |
| TT 63.2 | Thu | 15:30–16:00 | H20 | **Correlation Effects in Organic Superconductors** — •Roser Valenti |
| TT 63.3 | Thu | 16:00–16:30 | H20 | **Photoemission Study of Correlated Oxides at High Temperatures** — •Hao Tjeng |
| TT 63.4 | Thu | 16:45–17:15 | H20 | **Dynamical Mean Field Theory of Collective Excitations** — •Alexander Lichtenstein |
| TT 63.5 | Thu | 17:15–17:45 | H20 | **Electronic Correlations beyond Dynamical Mean Field Theory** — •Karsten Held |

## Invited Talks of the Joint Symposium SYSC

(jointly organized by DY, HL, MA, TT; coordination: TT)

| | | | | |
|---|---|---|---|---|
| SYSC 1.1 | Tue | 9:30–10:00 | H1 | **Exploring the Physics of Superconducting Qubits Strongly Coupled to Microwave Frequency Photons** — •Andreas Wallraff |
| SYSC 1.2 | Tue | 10:00–10:30 | H1 | **Hybrid Quantum Circuit with a Superconducting Qubit Coupled to an Electron Spin Ensemble** — •Yuimaru Kubo |
| SYSC 1.3 | Tue | 10:30–11:00 | H1 | **Hybrid Quantum Systems with Rare-Earth Ion Spin Ensemble** — •Pavel Bushev |
| SYSC 1.4 | Tue | 11:00–11:30 | H1 | **Quantum Coherent Coupling between a Mechanical Oscillator and an Optical Mode** — •Tobias Kippenberg |
| SYSC 1.5 | Tue | 11:30–12:00 | H1 | **Exploring Quantum Light-Matter Interactions of Quantum Dots in Photonic Crystal Nanostructures** — •Jonathan Finley |

## Invited Talks of the Joint Symposium SYTS

(jointly organized by DF, DS, HL, MA, MI, MM, TT; coordination: DF)

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|---|---|---|---|---|
| SYTS 1.1 | Wed | 9:30–10:00 | H1 | **Transport in Old and New Thermoelectric Materials** — •David Singh |

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| SYTS 1.2 | Wed | 10:00–10:30 | H1 | **Binary oxide structures as model systems for thermoelectric transport** — •Peter J. Klar |
| SYTS 1.3 | Wed | 10:30–11:00 | H1 | **Functional oxides films: from single crystals to polycrystalline substrates** — •Wilfrid Prellier |
| SYTS 1.4 | Wed | 11:00–11:30 | H1 | **The Planar Nernst Effect and the Search for Thermal Spin Currents in Ferromagnetic Metals** — •Barry Zink |
| SYTS 1.5 | Wed | 11:30–12:00 | H1 | **Tunneling magneto thermopower in magnetic tunnel junction nanopillars** — •Hans Werner Schumacher |

## Invited Talks of the Joint Symposium SYQP

(jointly organized by HL, O, TT; coordination: HL)

| | | | | |
|---|---|---|---|---|
| SYQP 1.1 | Wed | 15:00–15:30 | H1 | **Quantum plasmonics and applications in light harvesting** — •Peter Nordlander |
| SYQP 1.2 | Wed | 15:30–16:00 | H1 | **Deterministic quantum plasmonics with single nanodiamonds** — •Serge Huant |
| SYQP 1.3 | Wed | 16:00–16:30 | H1 | **Optically-active hybrid nanostructures: Exciton-plasmon interaction, Fano effect, and plasmonic chirality** — •Alexander Govorov |
| SYQP 1.4 | Wed | 17:00–17:30 | H1 | **Quantum nano-optics: Interaction of metallic nano-particles with quantum emitters** — •Salvatore Savasta |
| SYQP 1.5 | Wed | 17:30–18:00 | H1 | **Non-dipolar & magnetic interactions with optical antennas** — •Niek van Hulst |

## Invited Talks of the Joint Symposium SYES

(jointly organized by O, DS, HL, MA, MM, TT; coordination: O)

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|---|---|---|---|---|
| SYES 1.1 | Fri | 9:30–10:00 | H1 | **Molecular dynamics simulation of nucleation and growth of crystals from solution** — •Michele Parrinello |
| SYES 1.2 | Fri | 10:00–10:30 | H1 | **Describing, understanding, and discovering hybrid materials from first principles** — •Claudia Draxl |
| SYES 1.3 | Fri | 10:30–11:00 | H1 | **Mapping the Electronic Structure Landscape for Materials Discovery** — •Krishna Rajan |
| SYES 1.4 | Fri | 11:00–11:30 | H1 | **New ferroelectrics and antiferroelectrics by design** — •Karin Rabe |
| SYES 1.5 | Fri | 11:30–12:00 | H1 | **The Materials Project: The design of materials using high-throughput ab initio computations** — •Gerbrand Ceder |

## Sessions

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|---|---|---|---|---|
| TT 1.1–1.3 | Sun | 16:00–18:25 | H20 | **Tutorial: Topological Insulators and Majorana-Fermion Physics** |
| TT 2.1–2.10 | Mon | 9:30–12:00 | H3 | **Multiferroics 1 (jointly with DF, DS, KR, and MA)** |
| TT 3.1–3.13 | Mon | 9:30–13:00 | H9 | **Correlated Electrons: Low-Dimensional Systems - Models 1** |
| TT 4.1–4.4 | Mon | 9:30–10:45 | H10 | **Topological Insulators 1 (jointly with DS, HL, MA, and O)** |
| TT 5.1–5.7 | Mon | 9:30–11:15 | H17 | **Graphene - Magnetic Fields (jointly with DS, HL, MA, O)** |
| TT 6.1–6.13 | Mon | 9:30–13:00 | H18 | **Superconductivity: Tunnelling & Josephson Junctions** |
| TT 7.1–7.13 | Mon | 9:30–13:00 | H19 | **Correlated Electrons: Spin Systems, Itinerant Magnets 1** |
| TT 8.1–8.13 | Mon | 9:30–13:00 | H20 | **Transport: Quantum Dots, Wires, Point Contacts 1 (jointly with HL and O)** |
| TT 9.1–9.13 | Mon | 9:30–13:00 | H21 | **Quantum Liquids, Miscellaneous 1** |
| TT 10.1–10.10 | Mon | 10:30–13:15 | H36 | **Focused Session: Frontiers of Electronic Structure Theory 1 (jointly with HL and O)** |
| TT 11.1–11.9 | Mon | 11:30–13:45 | H17 | **Graphene -Spin-Orbit Interaction (jointly with DS,HL,MA,O)** |
| TT 12.1–12.57 | Mon | 15:00–19:00 | Poster D | **Poster Session Superconductivity** |
| TT 13.1–13.13 | Mon | 15:00–18:30 | H3 | **Multiferroics 2 (jointly with DF, DS, KR, and MA)** |
| TT 14.1–14.13 | Mon | 15:00–18:30 | H9 | **Correlated Electrons: Low-Dimensional Systems - Models 2** |
| TT 15.1–15.10 | Mon | 15:00–18:00 | H10 | **Topological Insulators 2 (jointly with DS, HL, O, and MA)** |
| TT 16.1–16.9 | Mon | 15:00–17:30 | H18 | **Transport: Quantum Dots, Wires, Point Contacts 2 (jointly with HL)** |

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|---|---|---|---|---|
| TT 17.1–17.9 | Mon | 15:00–17:45 | H19 | **Correlated Electrons: Spin Systems, Itinerant Magnets 2** |
| TT 18.1–18.5 | Mon | 15:00–17:45 | H20 | **Focused Session: Correlations in Topological Bands (jointly with DS, HL, MA, and O)** |
| TT 19.1–19.6 | Mon | 15:00–16:30 | H21 | **Quantum Liquids, Miscellaneous 2** |
| TT 20.1–20.14 | Mon | 15:00–18:45 | H22 | **Transport: Spincaloric Transport (jointly with MA)** |
| TT 21.1–21.12 | Mon | 16:00–19:00 | H17 | **Graphene - Electronic Properties and Transport 1 (jointly with DS, HL, MA, and O)** |
| TT 22.1–22.13 | Mon | 16:00–19:15 | H36 | **Focused Session: Frontiers of Electronic Structure Theory 2 (jointly with HL and O)** |
| TT 23.1–23.4 | Mon | 16:45–17:45 | H21 | **Superconductivity: Fe-based Superconductors - 1111** |
| TT 24.1–24.5 | Tue | 9:30–12:15 | H2 | **Focused Session: Dirac Fermions in Solid-State Systems (jointly with HL)** |
| TT 25.1–25.13 | Tue | 9:30–13:15 | H9 | **Correlated Electrons: Low-Dimensional Systems - Models 3** |
| TT 26.1–26.12 | Tue | 9:30–12:45 | H17 | **Graphene - Electronic Properties and Transport 2 (jointly with DS, HL, MA, and O)** |
| TT 27.1–27.13 | Tue | 9:30–13:15 | H18 | **Superconductivity: Fe-based Superconductors - 122** |
| TT 28.1–28.12 | Tue | 9:30–12:45 | H19 | **Correlated Electrons: Spin Systems, Itinerant Magnets 3** |
| TT 29.1–29.10 | Tue | 9:30–12:30 | H20 | **Transport: Quantum Dots, Wires, Point Contacts 3 (jointly with HL)** |
| TT 30.1–30.13 | Tue | 9:30–13:00 | H21 | **Correlated Electrons: Quantum Impurities, Kondo Physics** |
| TT 31.1–31.10 | Tue | 9:30–12:15 | H41 | **Correlated Electrons: Low-Dimensional Systems -Materials 1** |
| TT 32.1–32.10 | Tue | 10:30–13:15 | H36 | **Focused Session: Frontiers of Electronic Structure Theory 3 (jointly with HL and O)** |
| TT 33.1–33.14 | Wed | 9:15–13:00 | H16 | **Topological Insulators 3 (jointly with HL, MA, and O)** |
| TT 34.1–34.12 | Wed | 9:30–12:45 | H2 | **Transport: Molecular Electronics (jointly with CPP, HL, MA)** |
| TT 35.1–35.13 | Wed | 9:30–13:00 | H17 | **Graphene - Characterization and Devices (jointly with DS, HL, MA, and O)** |
| TT 36.1–36.13 | Wed | 9:30–13:00 | H18 | **Superconductivity: Fe-based Superconductors - Fe(Se,Te), LiFeAs, and other Materials** |
| TT 37.1–37.14 | Wed | 9:30–13:15 | H19 | **Quantum Coherence, Quantum Information Systems 1** |
| TT 38.1–38.14 | Wed | 9:30–13:15 | H20 | **Correlated Electrons: Metal-Insulator Transition 1** |
| TT 39.1–39.11 | Wed | 10:30–13:30 | H36 | **Focused Session: Frontiers of Electronic Structure Theory 4 (jointly with HL and O)** |
| TT 40.1–40.89 | Wed | 15:00–19:00 | Poster D | **Poster Session Correlated Electrons** |
| TT 41.1–41.14 | Wed | 15:00–18:45 | H2 | **Spintronics / Quantum Information: Materials and Methods (jointly with HL)** |
| TT 42.1–42.14 | Wed | 15:00–19:15 | H18 | **Quantum Coherence, Quantum Information Systems 2** |
| TT 43.1–43.6 | Wed | 15:00–16:30 | H19 | **Correlated Electrons: Metal-Insulator Transition 2** |
| TT 44.1–44.6 | Wed | 15:00–18:00 | H20 | **Focused Session: Majorana Fermions in Condensed Matter (jointly with DS, HL, MA, and O)** |
| TT 45.1–45.7 | Wed | 15:00–16:45 | H21 | **Superconductivity: (General) Theory** |
| TT 46.1–46.13 | Wed | 16:00–19:15 | H17 | **Graphene - SiC Substrates and Intercalation (jointly with DS, HL, MA, and O)** |
| TT 47.1–47.13 | Wed | 16:00–19:30 | H36 | **Focused Session: Frontiers of Electronic Structure Theory 5 (jointly with HL and O)** |
| TT 48.1–48.7 | Wed | 16:45–18:45 | H19 | **Correlated Electrons: Quantum-Critical Phenomena - Theory** |
| TT 49.1–49.8 | Wed | 17:00–19:00 | H21 | **Superconductivity: SQUIDs & Cryodetectors** |
| TT 50.1–50.10 | Thu | 9:30–12:15 | H2 | **Exciton Polaritons and their Condensates (jointly with HL)** |
| TT 51.1–51.11 | Thu | 9:30–12:30 | H6 | **Correlated Electrons: General Theory 1** |
| TT 52.1–52.13 | Thu | 9:30–13:00 | H18 | **Transport: Spintronics, Magnetotransport 1 (jointly with HL and MA)** |
| TT 53.1–53.13 | Thu | 9:30–13:00 | H19 | **Correlated Electrons: Heavy Fermions** |
| TT 54.1–54.7 | Thu | 9:30–12:45 | H20 | **Focused Session: Magnetism & Superconductivity in Fe-based Pnictides and Chalcogenides (jointly with MA)** |
| TT 55.1–55.13 | Thu | 9:30–13:00 | H21 | **Correlated Electrons: Low-Dimensional Systems -Materials 2** |
| TT 56.1–56.11 | Thu | 10:30–13:15 | H17 | **Graphene - Preparation and Characterization 1 (jointly with DS, HL, MA, and O)** |
| TT 57.1–57.10 | Thu | 10:30–13:15 | H36 | **Focused Session: Frontiers of Electronic Structure Theory 6 (jointly with HL and O)** |
| TT 58.1–58.51 | Thu | 15:00–19:00 | Poster D | **Poster Session Transport & Matter at Low Temperature** |

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| TT 59.1–59.12 | Thu | 15:00–18:30 | H6 | **Correlated Electrons: Quantum-Critical Phenomena - Experiments** |
| TT 60.1–60.9 | Thu | 15:00–17:30 | H17 | **Graphene - Theory (jointly with DS, HL, MA, and O)** |
| TT 61.1–61.10 | Thu | 15:00–18:00 | H18 | **Topological Insulators 4 (jointly with DS, HL, MA, and O)** |
| TT 62.1–62.11 | Thu | 15:00–18:15 | H19 | **Superconductivity: Properties, Electronic Structure, Order Parameter** |
| TT 63.1–63.5 | Thu | 15:00–17:45 | H20 | **Focused Session: Dynamical Mean-Field Approach to Correlated Electron Materials (jointly with MA)** |
| TT 64.1–64.12 | Thu | 15:00–18:15 | H21 | **Superconductivity: Heterostructures, Andreev Scattering, Vortex Physics** |
| TT 65.1–65.12 | Thu | 16:00–19:00 | H36 | **Focused Session: Frontiers of Electronic Structure Theory 7 (jointly with HL and O)** |
| TT 66.1–66.12 | Fri | 9:30–12:45 | H14 | **Spintronics / Quantum Information: Vacancies in Diamond and SiC (jointly with HL)** |
| TT 67.1–67.13 | Fri | 9:30–13:00 | H18 | **Topological Insulators 5 (jointly with DS, HL, MA, and O)** |
| TT 68.1–68.4 | Fri | 9:30–10:30 | H20 | **Transport: Spintronics, Magnetotransport 2 (jointly with HL and MA)** |
| TT 69.1–69.10 | Fri | 9:30–12:15 | H21 | **Superconductivity: Fe-based Superconductors - Theory** |
| TT 70.1–70.6 | Fri | 9:30–11:00 | H24 | **Correlated Electrons: General Theory 2** |
| TT 71.1–71.10 | Fri | 10:30–13:00 | H17 | **Graphene - Preparation and Characterization 2 (jointly with DS, HL, MA, and O)** |
| TT 72.1–72.4 | Fri | 10:45–11:45 | H20 | **Nanomechanics (jointly with BP, DF, and DY)** |
| TT 73.1–73.3 | Fri | 11:45–12:30 | H20 | **Fluctuations and Noise** |

## Annual General Meeting of the Low Temperature Physics Division

Thu 18:30 H19

## TT 1: Tutorial: Topological Insulators and Majorana-Fermion Physics

Topological insulators form a new class of quantum matter, with a bulk gap and exotic conducting surface states. When coupled to superconductors, so-called Majorana bound states are expected to exist under certain conditions. In this Tutorial, an introduction into the basic theoretical ideas is given, and the relevant experimental signatures and results are discussed.

Time: Sunday 16:00–18:25 Location: H20

**Tutorial** TT 1.1 Sun 16:00 H20

**Topological Insulators and Superconductors** — •Andreas Schnyder — Max Planck Institut für Festkörperforschung, D-70569 Stuttgart, Germany

The recent discovery of new topological electronic phases in insulating materials with strong spin-orbit coupling has lead to a renewed interest in topological states of matter. These topological materials have a full insulating gap in the bulk and support exotic metallic surface states, which are a consequence of bulk topological invariants. Topological insulating states have been observed in HgTe/(Hg,Ce)Te semiconductor quantum wells, in BiSb alloys, in $Bi_2Se_3$, and in other Bi-based compounds. Topological superconductor are fully gapped superconductors that exhibit zero-energy Majorana surface states. Here we review the theoretical foundations for topological insulators and superconductors, discuss topological band theory, and survey recent experimental findings on three-dimensional topological insulators and superconductors.

**5 min. break**

**Tutorial** TT 1.2 Sun 16:50 H20

**Proximity Induced Superconductivity in Topological Insulators** — •Hartmut Buhmann — Physikalisches Institut, EP3, University Würzburg, Würzburg, Germany

The discovery of Dirac-like surface states on a topological insulator (TI) and their qualitative relation to Cooper-pairs in superconducters inspired the exploration of interactions between those two states. In 2008 L. Fu and C.L. Kane [1] showed that so-called Majorana bound states are expected to exists under certain conditions in the proximity of those interfaces. Since then many ideas for experimental investigations have been published but unfortunately none of those has been realized so far.

In this presentation I will summarize the important signature for the search for Majorana bound states in connection with topological insulators and I will report on recent results on proximity induced superconductivity in TI surface states.

[1] Liang Fu and C. L. Kane, Phys. Rev. Lett. **100**, 096407 (2012)

**5 min. break**

**Tutorial** TT 1.3 Sun 17:40 H20

**Majorana Fermions in Hybrid Nanosystems** — •Michael Wimmer — Instituut-Lorentz, Universiteit Leiden, The Netherlands

Majorana fermions are particles that are their own anti-particle. To our current knowledge, they do not exist as elementary particles in nature. In the recent years it was however realized that quasi-particle excitations in solid state systems can mimic Majorana fermions. In particular, they appear in topological superconductors.

In the tutorial, I will show the basic properties of these "solid state Majoranas", and discuss how topological superconductors can be engineered in hybrid nanosystems consisting of ordinary superconductors and semiconductors. I will also briefly review the recent experiments that have found strong hints for the evidence of Majorana fermions in such hybrid systems. Finally, I will discuss some of the more exotic properties of Majorana fermions and how they are related to topological quantum computing.

## TT 2: Multiferroics 1 (jointly with DF, DS, KR, and MA)

Time: Monday 9:30–12:00 Location: H3

TT 2.1 Mon 9:30 H3

**Magnetoelectric coupling at the $n$-doped interface $BaTiO_3/SrTcO_3$ studied from first principles** — •Vladislav Borisov[1], Sergey Ostanin[1], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Antiferromagnetically induced magnetoelectric coupling at the interface $BaTiO_3/SrTcO_3$, which combines a robust ferroelectric and a stable antiferromagnetic perovskite, is studied from first principles. For the $BaO/TcO_2$-terminated interface, the magnetic order may change from G- to C-type antiferromagnetism upon the electric polarization reversal in the ferroelectric side. By inspecting the two-dimensional band structure and orbital occupation of the Tc 4$d$-states we conclude that the polarization-dependent charge transfer is responsible for a two-dimensional electron gas at the interface between two insulating perovskites. The case of paraelectric $BaTiO_3$ is also discussed in the context of the effect.

TT 2.2 Mon 9:45 H3

**Observation of novel multiferroic-like effect in C60-Co nanocomposites** — •Masashi Shiraishi[1], Eiiti Tamura[1], Yutaka Sakai[1], Toyokawa Shuhei[1], Eiji Shikoh[1], Vlado Lazarov[2], Atsufumi Hirohata[3], Teruya Shinjo[1], and Yoshishige Suzuki[1] — [1]Graduate School of Engineering Science, Osaka Univ., Japan — [2]Department of Physics, Univ. York, UK — [3]Department of Electronics, Univ. York, UK

A novel magnetoelectric effect is found to appear in a C60-Co nanocomposite. Although Co is well-known as a ferromagnet, its nanoparticles embedded in a C60 matrix can exhibit enhancement of magnetoresistance ratio due to a combination of Coulomb-blockade and higher order co-tunneling [1], and also multiferroic-like behavior [2], i.e., an electric field controls magnetic alignment of the nanoparticles and a magnetic field controls their charged states. This novel effect enables a strong magnetic switching effect for which the on/off ratio is ca. 1e4. Such an effect has been expected to exist and these findings show this magnetoelectric coupling for the first time.

[1] D. Hanataka, M. Shiraishi et al., Phys. Rev. B79, 235402 (2009). [2] Y. Sakai, E. Tamura, M. Shiraishi et al., Adv. Func. Mat. 22, 3845 (2012).

TT 2.3 Mon 10:00 H3

**Investigation of magnetic ordering in $Eu_{1-x}Y_xMnO_3$ using full polarization analysis at P09 beamline** — •Arvid Skaugen, Dinesh K. Shukla, Helen Walker, Sonia Francoual, and Jörg Strempfer — Deutsches Elektronen-Synchrotron, Harmburg, Germany

Varying multiferroic properties with strong ME coupling have been reported for $Eu_{1-x}Y_xMnO_3$ [1]. The crystal structure of $Eu_{1-x}Y_xMnO_3$ is similar to the one of $TbMnO_3$ with comparable lattice distortions. However, the effect of rare earth magnetism is eliminated since $Eu^{3+}$ ($4f^6$) and $Y^{3+}$ ($4f^0$) ions both are non-magnetic. The compound $Eu_{0.8}Y_{0.2}MnO_3$ first shows a phase transition at $T_N$ = 45K from a paramagnetic to an antiferromagnetic and paraelectric state with a presumably sinusoidal collinear AFM structure, in analogy to $TbMnO_3$. At $T_C$ = 30K the magnetic structure changes to weak ferromagnetism, attributed to a cone-like structure that breaks inversion symmetry and gives rise to ferroelectricity with the polarization along the a-axis.

We have investigated $Eu_{0.8}Y_{0.2}MnO_3$ using resonant x-ray diffraction as function of temperature, magnetic field and incident polarization at beamline P09 at PETRA III. The method of full polarization

analysis has been used to investigate the different resonances showing up at the Mn K-edge. From the polarization scans, it is possible to draw conclusions on the complex magnetic order. Preliminary results suggest a helicoidal SDW structure of the Mn moments rather than a cone-like structure.

[1] J. Hemberger et al., Phys. Rev. B 75, 035118 (2007)

TT 2.4 Mon 10:15 H3

**Electrostatic tuning of large-distance sputtered LSMO/PZT heterostructures** — •Philipp Moritz Leufke, Ajay Kumar Mishra, Wang Di, Robert Kruk, and Horst Hahn — Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

In order to obtain a physical picture and quantitative characteristics of a magnetoelectric coupling at ferromagnetic/ferroelectric interfaces, epitaxial $La_{0.87}Sr_{0.13}MnO_3$/Pb(Zr,Ti)$O_3$ (LSMO/PZT) heterostructures were deposited by large-distance magnetron sputtering[1,2]. The remarkably high lateral uniformity achieved in such films allowed for a ferroelectric device area of more than 6 $mm^2$.

This has enabled for the first time *in-situ* SQUID measurements of the magnetic response to the systematically varied remanent ferroelectric polarization. Temperature dependence of the magnetic modulation upon charging and the magnetic response to the ferroelectric stimulation indicates a field-effect dominated coupling mechanism and generally confirms the concept of electrostatic hole ($h^+$) doping of LSMO.

For small charge modulations at low temperature, a linear tuning coefficient of $\approx 3.6\,\mu_B/h^+$ has been determined. This suggests the activation of an antiferromagnetic coupling, even for very small surface charge densities. Simultaneously a shift in the magnetic transition temperature at higher surface charge concentration indicates the presence of a ferromagnetic phase at the LSMO/PZT interface.

[1] P. M. Leufke *et al.*, *Thin Solid Films* **520**, 5521 (2012).
[2] P. M. Leufke *et al.*, *AIP Advances* **2**, 032184 (2012).

TT 2.5 Mon 10:30 H3

**Optimized magnetoelectric interface coupling** — •Igor Maznichenko[1], Arthur Ernst[2], 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, Weinberg 2, D-06120 Halle (Saale), Germany

It was shown that magnetoelectric coupling occurs at interfaces between a magnetic and a ferroelectric material. Our idea is to construct heterostructures with a particularly strong magnetoelectric coupling. We concentrate on the optimization of the magnetic layer. We demonstrate that a small magnetic moment at the interface can still transfer the magnetoelectric coupling to a strong ferromagnet and could cause significant response. The idea is supported by numerical simulations within density functional theory using the self-consistent KKR Green function method.

TT 2.6 Mon 10:45 H3

**Role of electron correlation of FeO at Fe/ferroelectric oxide/Fe interface for magnetic transport properties** — •Andrea Neroni, Daniel Wortmann, Ersoy Sasioglu, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Fe/ferroelectric oxide/Fe is a nanoferronic tunnel junction with exciting electronic magneto-conductive transport properties. FeO layers at the interface of Fe/oxide/Fe barriers seems to significantly alter these properties as indicated by several experiments. In order to understand the role of electron correlations in FeO at the interface on the tunneling properties of a Fe/$BaTiO_3$/Fe barrier we use an embedded Green-function approach [1] implemented within the framework of the full-potential linearized augmented plane-wave (FLAPW) method `FLEUR` [2]. Conductances are obtained for different oxidation conditions and for different magnetic configurations of the contacts. Strong correlations are taken into account employing the LDA+U approach within the framework of the density functional theory (DFT) with a Hubbard U parameter determined by constrained random phase approximation (cRPA) [3]. Work is supported by Helmholtz Young Investigators Group Program VH-NG-409.

[1] www.flapw.de
[2] D. Wortmann, H. Ishida, and S. Blügel, PRB **65**, 165103 (2002)
[3] E. Şaşıoğlu, C. Friedrich, and S. Blügel, PRB **83**, 121101(R) (2011)

TT 2.7 Mon 11:00 H3

**Multiferroic Aurivillius Phases: the Case of $Bi_5FeTi_3O_{15}$ by *ab initio*** — •Yael Birenbaum, Nicola Spaldin, and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

The Aurivillius phases form a family of naturally-layered perovskite-related materials with good ferroelectric properties. $Bi_5FeTi_3O_{15}$ (BFTO) is perhaps the simplest known member of this family that also incorporates magnetic degrees of freedom. Using *ab initio* electronic structure calculations, we establish the ferroelectric and magnetic properties of BFTO. We then discuss a possible site preference of the $Fe^{3+}$ cation, which so far has not been found experimentally, and quantify the magnetic coupling between adjacent Fe cations. In addition, we analyse the different structural distortions, in order to relate BFTO to other members of the Aurivillius phases.

TT 2.8 Mon 11:15 H3

**Strain effect on magnetic properties of $La_{0.7}Ca_{0.3}MnO_3$/$SrRuO_3$ Superlattices** — •Sujit Das[1,2], Andreas Herklotz[1,2], and Kathrin Doerr[1,2] — [1]IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [2]Institute for Physics, MLU Halle-Wittenberg, 06099 Halle, Germany

Coherent interfaces between magnetic oxides such as $La_{0.7}$ $Sr_{0.3}MnO_3$ and $SrRuO_3$ may induce an intense magnetic coupling [1]. Recent work indicated an impact of elastic strain on the strength and even the sign of the coupling [2]. Superlattices (SL) of $La_{0.7}$ $Ca_{0.3}MnO_3$/$SrRuO_3$ with layer thicknesses below 10 unit cells were grown by pulse laser deposition simultaneously on $SrTiO_3$(001) (STO), $LaAlO_3$(001) (LAO) and piezoelectric 0.72Pb($Mg_{1/3}Nb_{2/3}$)$O_3$-0.28$PbTiO_3$ (001) (PMN-PT) substrates and structurally characterized by X-ray diffraction (XRD). On LAO, the SL assumes a compressive strain state, i. e. the lattice parameter is larger out-of-plane than in-plane, whereas on PMN-PT it shows a tensile strain state and on STO an intermediate strain value. Magnetization measurements demonstrate a strong antiferromagnetic (AFM) coupling in SLs on STO and LAO substrates which is due to superexchange interaction between Ru and Mn ions. The AFM coupling seems to decrease under tensile strain. The coupling is much weaker on PMN-PT, probably because of higher interface roughness. In order to probe the effect of elastic strain directly, magnetization loops in reversibly controlled strain states have been recorded for SLs on PMN-PT. [1] M. Ziese et al., PRL 104, 167203 (2010), [2] J. W. Seo et al., PRL 105, 167206 (2010) .

TT 2.9 Mon 11:30 H3

**Tuning the multiferroic phase of CuO with impurities** — •Johan Hellsvik[1], Marcello Balestieri[1], Alessandro Stroppa[2], Anders Bergman[3], Lars Bergqvist[4], Olle Eriksson[3], Silvia Picozzi[2], and José Lorenzana[1] — [1]ISC-CNR, Rome, Italy — [2]CNR-SPIN, L'Aquila, Italy — [3]Uppsala University, Uppsala, Sweden — [4]KTH, Stockholm, Sweden

The discovery that CuO is a multiferroic with a high antiferromagnetic transition temperature of 230 K opened a possible route to room-temperature multiferroicity with a strong magnetoelectric coupling [1]. CuO belongs [2] to a new class of multiferroic materials where the so called 'order by disorder mechanism' [3] plays a crucial role. In this work we study the effect of different impurities on the phase diagram of CuO aiming at engineering the multiferroic properties. Extensive density functional theory (DFT) calculations were performed for a large number of fixed spin configurations in pure CuO and CuO doped with a small fraction of the Cu atoms substituted with the nonmagnetic elements Mg, Zn or Cd, or the magnetic elements Ni or Co. Our computations established that the energy difference between the low-temperature collinear AF1 phase and the intermediate temperature multiferroic AF2 phase decreased monotonously with increasing doping level confirming that impurities favour the multiferroic phase. The magnetic phase diagram has been mapped out in Monte Carlo simulations for classical Heisenberg spins. [1] T. Kimura et al., Nature Mat. 7, 291 (2008); [2] G. Giovannetti et al., Phys. Rev. Lett. 106, 026401 (2011); [3] C. L. Henley, Phys. Rev. Lett. 62, 2056 (1989)

TT 2.10 Mon 11:45 H3

**Charge-mediated magnetoelectric coupling in patterned multiferroic heterostructures** — •daniele preziosi[1], dietrich hesse[1], marin alexe[1], martin wahler[2], and georg schmidt[2] — [1]Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, 06120 Halle(Saale) Germany — [2]Martin-Luther-Universität Halle-Wittenberg Von-Danckelman-Platz 3, 06120 Halle(Saale) Germany

Several studies on single phase multiferroics demonstrate that the coupling between the ferroelectric and the (ferro)magnetic order parameters tends to be small. Engineering of artificially structured systems could provide a reliable way to improve the MagnetoElectric (ME) coupling. Devices based on charge-mediated ME effect represent a viable alternative. The electric field produced by the polarization of the ferroelectric material can induce, at the interface with an ultrathin strongly correlated magnetic oxide, a change in the magnetization. The ME coupling would be in this case the consequence of the spin-dependent screening of the electric field. Patterned hetero-structures of La1-xSrxMnO3 (LSMO) and PbZr0.2Ti0.8O3 (PZT) have been fabricated. Transport and magnetic measurements show that the switching of the PZT polarization influences significantly the competing electronic ground states of the LSMO, modulating the resistivity as well as the magnetization value.

## TT 3: Correlated Electrons: Low-Dimensional Systems - Models 1

Time: Monday 9:30–13:00 Location: H9

TT 3.1 Mon 9:30 H9

**Charge and Spin Fractionalization of 1D Strongly Correlated Systems** — Alexander Moreno[1], •Alejandro Muramatsu[1], and José M. P. Carmelo[2] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Germany — [2]Center of Physics, University of Minho, Braga, Portugal

By means of time-dependent DMRG numerical simulations, we observe charge and spin fractionalization[1] of an electron injected into a 1D strongly correlated system, namely the t-J model, which is not expected on the basis of the Luttinger Liquid (LL) theory[2]. Our results for the supersymmetric (SUSY) point, $J = 2t$, are consistent with the Bethe-Ansatz exact solution[3] that we use as framework to explain the origin of the different fractions. Our method is able to identify more features related to fractionalization in comparison to those observed in the one-particle spectral function[4].

[1] A. Moreno, J. M. P Carmelo and A. Muramatsu, arXiv:1210.1398
[2] K.-V. Pham, M. Gabay, and P. Lederer, Phys. Rev. B **61**, 16397 (2000)
[3] P. A. Bares, G. Blatter, and M. Ogata, Phys. Rev. B **44**, 130 (1991); P. A. Bares, J. M. P. Carmelo, J. Ferrer, and P. Horsch, Phys. Rev. B **46**, 14624 (1992)
[4] C. Lavalle, M. Arikawa, S. Capponi, F. F. Assaad, and A. Muramatsu, Phys. Rev. Lett. **90**, 216401 (2003)

TT 3.2 Mon 9:45 H9

**Luttinger liquid universality in the time evolution after an interaction quench** — Christoph Karrasch[1], Jan Rentrop[2], •Dirk Schuricht[2], and Volker Meden[2] — [1]Department of Physics, University of California — [2]Institute for Theory of Statistical Physics, RWTH Aachen University

We provide evidence that the relaxation dynamics of one-dimensional, metallic Fermi systems resulting out of an abrupt amplitude change of the two-particle interaction has aspects which are universal in the Luttinger liquid sense: The leading long-time behavior of certain observables is described by universal functions of the equilibrium Luttinger liquid parameter and the renormalized velocity. We analytically derive those functions for the Tomonaga-Luttinger model and verify our hypothesis of universality by considering spinless lattice fermions within the framework of the density matrix renormalization group.

[1] C. Karrasch et al., Phys. Rev. Lett. 109, 126406 (2012).

TT 3.3 Mon 10:00 H9

**Quench dynamics of the Tomonaga-Luttinger model with momentum-dependent interaction** — •Jan Rentrop[1,2], Dirk Schuricht[1,2], and Volker Meden[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [2]JARA Fundamentals of Future Information Technology, 52056 Aachen, Germany

We study the relaxation dynamics of the one-dimensional Tomonaga-Luttinger model after an interaction quench, paying particular attention to the momentum dependence of the two-particle interaction. Several potentials of different analytical forms are investigated that all lead to universal Luttinger liquid (LL) physics in equilibrium. The steady-state fermionic momentum distribution shows universal behavior in the sense of the LL phenomenology. For generic regular potentials, the large time decay of the momentum distribution function toward the steady-state value is characterized by a power law with a universal exponent that depends only on the potential at zero momentum transfer. The commonly employed ad hoc procedure fails to give this exponent.

TT 3.4 Mon 10:15 H9

**Low-energy local density of states of the 1D Hubbard model** — Stefan Söffing[1], Imke Schneider[2], and •Sebastian Eggert[1] — [1]Fachbereich Physik und Forschungszentrum Optimas, TU Kaiserslautern — [2]Institut für theoretische Physik, TU Dresden

We examine the local density of states (DOS) at low energies numerically and analytically for the Hubbard model in one dimension. The eigenstates represent separate spin and charge excitations with a remarkably rich structure of the local DOS in space and energy. The results predict signatures of strongly correlated excitations in the tunneling probability along finite quantum wires, such as carbon nanotubes, atomic chains or semiconductor wires in scanning tunneling spectroscopy (STS) experiments. However, the detailed signatures can only be partly explained by standard Luttinger liquid theory. In particular, we find that the effective boundary exponent can be negative in finite wires, which leads to an increase of the local DOS near the edges in contrast to the established behavior in the thermodynamic limit.

TT 3.5 Mon 10:30 H9

**Density Oscillations in the 1D Hubbard Model in a Harmonic Trap at Finite Temperature** — •Denis Morath, Stefan Söffing, and Sebastian Eggert — Department of Physics, Univ. Kaiserslautern, Erwin Schrödinger Str. , 67663 Kaiserslautern, Germany

We are investigating the Hubbard-Chain in a harmonic trapping-potential at finite temperatures which is an appropriate model to describe cold atoms in a trap. Depending on the interaction strength one observes $2k_F$- and $4k_F$-oscillations of the density. Here we show the temperature dependence of these oscillations using QMC and analyze them within the bosonization scheme. With increasing temperatures the amplitude of the oscillations is decreased. We will give an estimation at which temperature it will be possible to resolve the oscillations.

TT 3.6 Mon 10:45 H9

**DMRG study of the optical conductivity of the 1D Hubbard model** — •Alexander C. Tiegel, Piet E. Dargel, and Thomas Pruschke — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

The zero-temperature optical conductivity of the Hubbard model in one dimension is studied for various values of the on-site repulsion $U$ and the electronic filling $n$ by means of frequency-resolved density-matrix renormalization group (DMRG) methods. The focus of this work is the determination of the optical gap $E_{opt}$ and the investigation of the leading frequency dependence at the onset of the finite-frequency conductivity. At half-filling, our data is compatible with a square-root increase above the band threshold, which is in agreement with conformal field theory and DDMRG results in the literature. Away from half-filling, we find an increasing pseudogap $E_{opt}$ with the amount of doping. These results as well as the extracted exponents at the onset for $n < 1$ are directly compared to existing field-theoretical values.

**15 min. break**

TT 3.7 Mon 11:15 H9

**Real-time dynamics of charge and spin densities in one-dimensional systems** — •Michael Sekania and Arno P. Kampf — Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, Germany

In the last decade great effort has been devoted to investigations of the real-time dynamics in strongly correlated systems. We present a theoretical investigation of the space-time evolution of the charge and spin perturbations induced by a local quench of the ground state of the one-

dimensional Hubbard model. Employing the time-dependent Density-Matrix Renormalization Group methods we find that induced charge and spin perturbations expand ballistically in the Mott-insulating host system. The expansion velocities in the charge and spin sector are also found to be different as expected for the spin-charge separation scenario. For the metallic hosts close to the half filling, however, the character of the charge expansion changes from ballistic to diffusive and finally to subdiffusive regimes.

TT 3.8 Mon 11:30 H9

**Phase diagram of frustrated ladder and 2D antiferromagnets** — •Alexandros Metavitsiadis, Daniel Sellmann, and Sebastian Eggert — University of Kaiserslautern, Kaiserslautern, Germany

We investigate the low energy properties of the frustrated two leg diagonal ladder exhibiting both intra- and inter-chain frustration. The renormalization group is used to obtain the phase diagram while varying the microscopic lattice parameters. We particularly emphasize the role of the in-chain marginal operators, which is tuned by the in-chain frustration and can promote a dimer phase in the system. Finally, the physics of the quasi one dimensional diagonal ladder is incorporated into a two dimensional square lattice since the former is used as the primary structure to build up the square lattice. Within the validity of our method, the classical phases—a Néel antiferromagnet and a collinear antiferromagnet—are predicted. The results are compared to numerical DMRG calculations.

TT 3.9 Mon 11:45 H9

**Thermodynamics of the Two-Dimensional Hubbard Model** — •James LeBlanc[1] and Emanuel Gull[2] — [1]Max Planck Institute For the Physics of Complex Systems, Dresden Germany — [2]University of Michigan, Ann Arbor MI

The application of a numerically exact continuous time impurity solver with the DCA dynamical mean field theory has allowed us to study the thermodynamics of the two-dimensional Hubbard model for finite, but large cluster sizes. Variation in cluster size, upwards of 50-sites, allows for extrapolation to the thermodynamic limit. We present results relevant to cold gas systems, such as entropy, double occupancy and nearest-neighbour spin correlations as well as discuss the implications of these calculations on pseudogap physics of the High-$T_c$ Cuprate superconductors away from half filling.

TT 3.10 Mon 12:00 H9

**Shear viscosity in a two-dimensional Fermi gas** — •Carolin Küppersbusch[1], Tilman Enss[2], and Lars Fritz[1] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Physik Department, Technische Universität München

We consider a two-component, two-dimensional, interacting Fermi gas which is experimentally realized in ultra cold atomic systems. An experimentally accessible quantity that has received a lot of interest recently as a measure of the interaction strength is the shear viscosity. This quantity describes the resistance of the system towards establishing a flow gradient and is lowest for strongly interacting systems. Using a Boltzmann equation we calculate the viscosity in all temperature and interaction ranges. In contrast to earlier studies we include medium scattering which lowers the viscosity by a factor of about three.

TT 3.11 Mon 12:15 H9

**Wigner Crystal in a Two-Dimensional Electron Gas with Strong Spin-Orbit Interaction** — •Peter Silvestrov[1], Ora Entin-Wohlman[2], and Yoseph Imry[3] — [1]Dahlem Center for Complex Quantum Systems, Freie Universitaet Berlin, 14195 Berlin, Germany — [2]Physics Department, Ben Gurion University, Beer Sheva 84105, Israel — [3]Department of Condensed Matter Physycs, Weizmann Institute of Science, Rehovot 76100, Israel

The Wigner crystal phase of a two-dimensional electron gas with unscreened Coulomb repulsion and Rashba spin-orbit interaction is investigated. We assume that the electron density is sufficiently low such that the spin-orbit interaction dominates over the electrons kinetic energy. In this limit the degeneracy of the minimum of the lower spin-orbit-split subband results in a strong change of the crystals properties. We predict a spontaneous breaking of the ground state symmetry, where all electrons have a finite momentum corresponding to one point at the bottom of a Mexican-hat shaped subband. In this phase electrons in the Wigner crystal become in-plane polarized and the plasmon dispersion acquires a strong angular dependance. The symmetry breaking results also in a (slight) squeezing of the triangular lattice.

TT 3.12 Mon 12:30 H9

**Topological characterization of fractional quantum Hall ground states from microscopic Hamiltonians** — •Frank Pollmann[1], Michael P. Zaletel[2], and Roger S. K. Mong[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Department of Physics, California Institute of Technology, Pasadena, California 91125, USA

We show how to numerically calculate several quantities that characterize topological order starting from a microscopic fractional quantum Hall (FQH) Hamiltonian. For finding the ground state, we employ the infinite density matrix renormalization group (iDMRG) method which is based on the matrix-product state (MPS) representation of FQH states on an infinite cylinder. From the MPS representation, we compute the topological entanglement entropies and the quasiparticle charges. We furthermore show that the wave function obtained on the infinite cylinder geometry can be adapted to a torus of arbitrary modular parameter, which allows us to explicitly calculate the non-abelian Berry connection associated with the modular T-transformation. As a result, the topological spins, central charge, and Hall viscosity of the phase can be obtained using data contained entirely in the entanglement spectrum.

TT 3.13 Mon 12:45 H9

**Characterization of Topological Phase Transitions: A Tensor-Product State Approach** — •Siddhardh Chandra[1], Frank Pollmann[1], and Norbert Schuch[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]RWTH Aachen University, Aachen, Germany

We investigate phase transitions between phases with non-trivial topological order. Topological order is a kind of order that cannot be explained with the traditional approach of Landau's symmetry breaking and local order parameters. However, it can be characterized by other quantities such as the braiding statistics of the excitations in the model. Due to recent advances in numerical techniques, it has become possible to extract these statistics from the ground-state wavefunction of a model. We consider simple string-net models, which are known to have topological order, and analyze the behavior of various quantities as we move from one topological phase to another. The useful formalism of tensor-product states allows us to create a tunable representation which helps us to study the behavior of the entanglement spectrum and modular matrices which characterize the statistics of the anyonic excitations in the two phases. We identify some of the defining components of a topological phase transition as opposed to a symmetry breaking transition and discuss the possible extensions to other models with topological order.

## TT 4: Topological Insulators 1 (jointly with DS, HL, MA, and O)

Time: Monday 9:30–10:45 Location: H10

**Invited Talk** TT 4.1 Mon 9:30 H10

**Breaking time reversal symmetry in topological insulators** — •Jagadeesh Moodera — Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Breaking time reversal symmetry in a topological insulator (TI) can lead to many exotic properties, such as image magnetic monopole, topological magneto-electric effects as well as Majorana Fermions in superconducting TIs (STI). Recently Gedik*s group in MIT demonstrated that manipulating the magnetic properties via ultrashort light pulses, selectively exciting the spin states of the surface state by exploiting its spin texture to induce a transient magnetic state. Using linearly polarized light in a pump-probe experiment unusual behavior was seen by Muenzenberg group in Gottingen University. The TI surface state can be magnetically manipulated by proximity effect. The proximity-induced ferromagnetism in a TI/ferromagnetic insula-

tor heterostructure breaks the time reversal symmetry in the TI: a large uniformly induced surface exchange gap appears on the TI without introducing scattering centers, thus keeping intact the transport of spin-momentum locked surface electrons as well as the superconducting pairing in an STI. This TI/ferromagnetic insulator bilayer system showed an induced interface magnetic moment accompanied by an unusual planar hysteresis magnetoresistance demonstrating the magnetic manipulation of the surface channel. This research is supported by ONR, NSF.

TT 4.2 Mon 10:00 H10

**Magnetic properties of the Mn doped topological insulator $Bi_2Te_3$ probed by ESR** — •S. Zimmermann[1], V. Kataev[1], Huiwen Ji[2], R.J. Cava[2], and B. Büchner[1] — [1]IFW Dresden, 01171 Dresden, Germany — [2]Dept. Chem., Princeton Univ., NJ 08544, USA

Doping of a topological insulator (TI) with magnetic elements can break the time reversal symmetry and thus open a gap in the protected spin polarized conducting surface states, driving the system into a quantum spin Hall regime [1]. Understanding of the interactions between localized magnetic moments of dopants via delocalized electrons that give rise to ferromagnetism in TIs is therefore of significant interest. Such interactions can be of a long-range character and can also be mediated by surface conducting states [2]. Electron Spin Resonance (ESR) spectroscopy is a sensitive local technique that can probe interactions of localized spins with conduction electrons as well as spin-spin interactions in semiconductors and metals. In this contribution we report an ESR study of the Mn spin dynamics and magnetic interactions in high-quality single crystals of the Mn doped 3-dimensional TI $Bi_2Te_3$ [3]. We have observed a well-defined ESR signal from Mn spins and have studied the temperature dependences of the ESR parameters for a set of $Bi_2Te_3$ crystals with different Mn doping levels. The experimental ESR data will be presented in detail and the doping dependence of the Mn spin relaxation via conducting states and the establishment of ferromagnetic order as seen by ESR will be discussed. [1] R. Yu et al., Science **369**, 61 (2010); [2] L.A. Wray et al., Nature Physics **7**, 32 (2011); [3] Y.S. Hor et al., PRB **81**, 195203 (2010)

TT 4.3 Mon 10:15 H10

**Investigation of the relation between surface band gaps and magnetism in the magnetic topological insulator $(Bi_{1-x}Mn_x)_2Se_3$** — •Jaime Sánchez-Barriga[1], Andrei Varykhalov[1], Gunther Springholz[2], Hubert Steiner[2], Raimund Kirchschlager[2], Günther Bauer[2], Ondrei Caha[3], Enrico Schierle[1], Eugen Weschke[1], Akin Ünal[1], Sergio Valencia[1], Florian Kronast[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Johannes Kepler Universität Linz — [3]Masaryk University, Brno

The Dirac cone at the surface of a magnetic topological insulator is expected to open a band gap when ferromagnetically magnetized perpendicularly to the surface plane. Angle-resolved photoemission from epitaxial films of $(Bi_{1-x}Mn_x)_2Se_3$ shows for $x > 0.02$ a band gap at the Dirac point of a size that varies with Mn concentration, is much larger than theoretically predicted ($\sim 100$ meV), and does not change with temperature from 7 to 300 K. Based on our measurements with x-ray magnetic circular dichroism (XMCD) we can exclude that the surface band gap is due to ferromagnetic order in the bulk or at the surface. In addition, we investigate by XMCD in photoemission microscopy the reported proximity magnetization induced by a ferromagnetic overlayer.

TT 4.4 Mon 10:30 H10

**Mapping the influence of cobalt atoms on the topological states of Bi2Te3** — •Paolo Sessi, Thomas Bathon, Lydia El-Kareh, and Matthias Bode — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg

Topological insulators are characterized by linearly dispersing gapless topological surface states protected by time-reversal symmetry. For these states, spin is perpendicularly locked to its momentum by spin-orbit interaction resulting in a chiral spin structure that forbids backscattering. However, this is predicted to not be the case when magnetic impurities are introduced into the system. Here, by means of scanning tunneling microscopy we investigate the robustness of the surface states of Bi2Te3 when single Co atoms are deposited on the surface. By analyzing the energy dependence of the quasi particle interference pattern produced by coherent scattering of surface states, we will examine the influence of Co atoms on scattering channels and energy dispersion relation.

## TT 5: Graphene - Magnetic Fields (jointly with DS, HL, MA, O)

Time: Monday 9:30–11:15 Location: H17

TT 5.1 Mon 9:30 H17

**Quantum interference in an electron-hole graphene ring system** — •Dmitri Smirnov, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2 30167 Hannover, Germany

We analyze the electronic properties of a topgated monolayer graphene ring. Micro-mechanical cleavage was used to place a flake on a Si/SiO2 substrate. The structuring and contacting was done via plasma etching and electron beam lithography. An additional gate was placed on top of one arm of the ring which allows us to control the charge carrier concentration locally and additionally to create a pnp- (npn-) junction inside the ring. The sample was measured in a He3 cryostat and is identified as single layer graphene via magnetotransport measurements.

We observe Aharonov Bohm (AB) effect by sweeping the magnetic field around 0 T. The period of the oscillations is approx. 16 mT which fits the size of the ring well. The AB-oscillations are measured for different temperatures and the amplitude shows a saturation for lower temperatures. We also observe the AB-oscillations when a pnp-junction is created inside the ring. The period is independent of the existence of a pnp-junction and stays constant in all situations. We analyze the amplitude in dependence of the charge carrier concentration. The absolute amplitude is constant in the bipolar and unipolar region [1].

[1] D.Smirnov. et. al, Appl. Phys. Lett. 100, 203114 (2012).

TT 5.2 Mon 9:45 H17

**Experiments on Superlattice Graphene Structures with Patterned Top Gates** — •Franz-Xaver Schrettenbrunner, Martin Drienovsky, Bastian Birkner, Sebastian Ringer, Dominik Koch, Dieter Weiss, and Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

We report on fabrication, finite element modelling (FEM), and the measurements of single- and bilayer graphene with structured top gates. By using micromechanically exfoliated graphene on $SiO_2$ surface, a $Al_2O_3$ dielectric was fabricated on top of the structure by either atomic layer deposition (ALD), evaporating thin aluminum films, or by combination of both methods. A digitated, patterned top gate electrode out of an AuPd alloy was fabricated by electron beam lithography (EBL). FEM yields that form and strength of the modulation strongly depend on thickness of the top gate dielectric, periodicity of the gate fingers, and applied voltage. Using both, the planar $SiO_2$ back gate and the patterned $Al_2O_3$ top gate the electric field effect creates variable modulations of the charge carrier concentration like pnp, nn'n, n0n, etc. along the whole underlying graphene. Measurements on these structures show typical behaviour for Klein-Tunneling resulting in an asymmetric curve of the Dirac Point. At high magnetic fields up to 14T unusual plateaus were observed when filling factors are mixing up in the top gated and the non top gated areas of the graphene samples.

TT 5.3 Mon 10:00 H17

**Weak Localization and Raman Study of Graphene Antidot Lattices Obtained by Crystallographically Anisotropic Etching** — •Florian Oberhuber, Stefan Blien, Stefanie Heydrich, Tobias Korn, Christian Schüller, Dieter Weiss, and Jonathan Eroms — Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

We report the crystallographically anisotropic etching of exfoliated

graphene on $SiO_2$ substrates by applying an etching mechanism that was demonstrated to eliminate carbon atoms located on armchair sites thus leading to zigzag edges [1]. Before exposing samples to this carbothermal reaction, they were patterned with circular antidots (diameter ≈40nm) by EBL and RIE. In the subsequent carbothermal etching step the predefined holes evolved into hexagonal antidots (≈100nm).

We investigated a set of samples patterned with square lattices of hexagonal antidots and compare them to graphene patterned with lattices of circular holes investigated previously [2]. First, we compare samples by analyzing the weak localization peak in electron transport from which we obtain the phase coherence length and lengths for inter- and intravalley scattering. Second, samples were characterized by Raman spectroscopy focusing on G, D and D* peaks. In addition to the above mentioned comparison we demonstrate the influence of the etching reaction on graphene's properties by showing a series of Raman maps acquired between consecutive sample preparation steps.

[1] Nemes-Incze et al., Nano Res. (2010)
[2] Eroms et al., New J. Phys. (2009), Heydrich et al., APL (2010)

TT 5.4 Mon 10:15 H17

**Electronic structure of graphene twist flakes** — •Wolfgang Landgraf, Sam Shallcross, Karla Türschmann, Dominik Weckbecker, and Oleg Pankratov — Lehrstuhl für Theoretische Festkörperphysik, Staudtstraße 7, D-91058 Erlangen

We study the electronic structure of bilayer graphene flakes with mutually rotated layers. The twist induces a large scale superstructure, a so called moiré pattern, which is a regular array of AA and AB stacked regions. We find that at low energies the electrons are trapped in the AA regions. This feature is visible even for a flake hosting a single AA moiré spot, which is thus acting as a quantum well. The electron density fluctuations induced by the moiré lattice are significant, being an order of magnitude greater than those generated by the rippling of a suspended graphene sheet. Finally, we determine the electronic properties of the twisted graphene flakes in the presence of an external magnetic field. We find a novel "zero-mode" structure, as well as Landau states that exhibit an electron current circulating between two graphene layers of the flake. The current distribution can be visualized as an electron flow on a torus circumventing the AA spot of the moiré lattice.

TT 5.5 Mon 10:30 H17

**Functionalized Graphene in Quantizing Magnetic Field: The case of bunched impurities** — •Peter Silvestrov — Dahlem Center for Complex Quantum Systems, Freie Universitaet Berlin, 14195 Berlin, Germany

Covalent bonding of impurity atoms to graphene, in many cases leads to creation of unusual (singular) zero energy localized electron states. Existence of such states would lead to interesting phenomena, actively discussed recently.

In this talk I consider the behavior of localized impurity levels in graphene in quantizing magnetic field. In the magnetic field the impurity level effectively hybridizes with one of the n=0 Landau level states and splits into two close opposite-energy states. In turn, mixing of localized and Landau levels changes a spin content of a quantum Hall ferromagnet and modifies, via the exchange interaction, the spectrum of electrons surrounding the impurity.

Existing theories investigate graphene uniformly covered by adatoms, though some experiments indicate the tendency towards their clusterization. To address this "unpleasant" possibility, I consider the case of a dense bunch of the impurity atoms, and show how such bunch changes dynamics and spin polarization of a large dense electron droplet surrounding it.

TT 5.6 Mon 10:45 H17

**Quantum Hall measurements on epitaxial graphene with oxygen adsorption** — •Emiliano Pallecchi[1], Mohamed Ridene[1], Dimitris Kazazis[1], Felicien Schopfer[2], Wilfrid Poirier[2], Mark Goergig[3], and Abdelkarim Ouerghi[1] — [1]Laboratoire de Photonique et de Nanostructures (LPN-CNRS), 91460 Marcoussis, France — [2]Laboratoire National de Métrologie et d'Essais, 78197 Trappes — [3]Laboratoire des Physique de Solides, F-91505, Orsay

In this contribution we present quantum transport, ARPES, and LEED investigations of molecular oxygen-adsorbed epitaxial graphene grown on SiC. We show that the carrier concentration can be significantly reduced by exposing the sample to molecular oxygen. From Hall measurements we obtain a carrier concentration on the order of 1.2 x $10^{12}$ $cm^{-2}$, about one order of magnitude smaller than typical values of intrinsic epitaxial graphene. The reduction of electron doping is consistent with estimates from ARPES measurements. At high magnetic field, we find a fully developed quantum Hall effect, with a plateau at filling factor around 2, and a vanishing longitudinal resistance. Such a plateau is the hallmark of single layer graphene and suggests that the buffer layer is not fully decoupled from the substrate. This is further confirmed by LEED study. We then discuss the intermediate field regime, where we analyze the transition between a localized state observed at low fields and the quantum Hall regime at high fields. Finally, we compare these findings to the results obtained on epitaxial graphene exposed to atomic oxygen. We find that atomic oxygen is a more violent process that can damage significantly the graphene flake.

TT 5.7 Mon 11:00 H17

**Splitting of the Zero-Energy Landau Level and Universal Dissipative Conductivity at Critical Points in Graphene** — •Frank Ortmann[1] and Stephan Roche[1,2] — [1]Catalan Institute of Nanotechnology, Barcelona (Spain) — [2]ICREA, Barcelona (Spain)

In graphene, the interaction of electrons with disorder impacts on their transport signature in a variety of experiments. Magnetotransport experiments can serve as an additional tool to probe this interaction with magnetic fields ranging from the low-field limit of weak antilocalization (∼mT) [1,2] to high fields defining the quantum Hall regime (∼10T). Being under study ever since the discovery of graphene, magnetic fields may unveil some interesting physics hidden otherwise or may generate new effects [3]. We are calculating the Kubo conductivity of graphene $\sigma_{xx}$ and $\sigma_{xy}$ in the presence of both weak and strong disorder and magnetic fields using a linear scaling method. This allows us to model realistic graphene samples up to micrometer size. Here we present our recent work on charge transport in the quantum-Hall regime and discuss our findings of universal conductivities. Particular emphasize is put on the non-trivial interference of disorder and magnetic-field and results from our novel order-N Hall-transport code.

[1] F.V. Tikhonenko et al. Phys. Rev. Lett. 103, 226801 (2009)
[2] F. Ortmann et al. EPL 94, 47006 (2011)
[3] D.A. Abanin et al. Science 332, 328 (2011)

## TT 6: Superconductivity: Tunnelling & Josephson Junctions

Time: Monday 9:30–13:00 Location: H18

TT 6.1 Mon 9:30 H18

**Strain Spectroscopy and Decoherence of Two-Level Systems** — •Jürgen Lisenfeld, Grigorij Grabovskij, Georg Weiss, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institut für Technologie (KIT), Karlsruhe

Two-level systems (TLSs) are believed to originate in individual atoms which may tunnel between two metastable positions of a disordered-lattice. Recently, TLSs have been identified as a source of noise and decoherence in nanofabricated devices such as MOSFETs, electromagnetic and nanomechanical resonators, detectors, SQUIDs, and superconducting qubits. Despite this ubiquitous importance, the microscopic nature of TLSs has remained obscure until today and is subject of current debate.

We perform novel experiments which allow us to obtain high-resolution images of the TLS distribution in a Josephson junction's tunnel barrier by operating a superconducting phase qubit as a sensitive TLS detector. Using a piezo actuator, we are able to control the mechanical strain in the sample in-situ and find that it strongly affects the TLS frequency and asymmetry energy. We will present data on the characteristic strain dependence of individual TLS's coherence times. These results are relevant for verification of TLS theoretical models within the long-standing effort of revealing the nature of TLS in disordered solids.

TT 6.2 Mon 9:45 H18

**Direct observation and characterization of two coherent and strongly coupled TLS using a superconducting phase qubit** — •Grigorij J. Grabovskij[1], Jürgen Lisenfeld[1], Jared H. Cole[2], Clemens Müller[3], Georg Weiss[1], and Alexey V. Ustinov[1] — [1]Karlsruhe Institute of Technology, Physikalisches Institut, 76131 Karlsruhe, Germany — [2]Chemical and Quantum Physics, School of Applied Sciences, RMIT University, Melbourne, 3001, Australia — [3]Département de Physique, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1

Atomic two-level tunneling systems (TLS) are known to be present in amorphous dielectrics. The use of a superconducting phase qubit allows one to study the quantum mechanical properties of individual and coherent TLS in detail. Recently, we demonstrated that controlled flexing of the substrate with a piezo actuator changes the TLS resonance frequency. Some TLS show a hyperbolic frequency dependence [1]. In further measurements, we found and investigated in detail two interacting TLS. The spectroscopically observed frequency-strain dependence exhibits a characteristic S-like shape with clearly visible avoided level crossings, both being clear signatures of the coherently coupled TLS. By measuring and analyzing this 4-level system we determine energies of the states, coupling constants and coherence times. From these data, we estimate the spatial separation between these two interacting TLS.

[1] G. J. Grabovskij *et al.*, Science **338**, 232 (2012)

TT 6.3 Mon 10:00 H18

**Superconductivity induced by carrier injection into non-superconducting $Bi_2Sr_2CaCu_2O_8$** — •Yilmaz Simsek[1], Yuri Koval[1], Irina Lazareva[1], Christian Steiner[1], Xiaoyue Jin[2], and Paul Müller[1] — [1]Department of Physics, Universität Erlangen — [2]Department of Electrical Engineering and Computer Science, MIT, Cambridge, Massachusetts, USA

The doping-induced phase transition from the antiferromagnetic to the superconducting state is still one of the fascinating subjects of high-Tc superconductors. Unlike doping by oxygen excess, we are able to change the carrier concentration of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) single crystals by injecting large currents along the c-axis. The injected electrons are trapped in the BiO and SrO layers which is compensated by increasing the hole concentration in the CuO layers. The goal of our contribution is to induce superconductivity in non-superconducting Bi2212. To eliminate the contact resistance, we have fabricated double cross-bar crystal stacks of fully oxygen depleted Bi2212 single crystal which was not superconducting above 4.2 K. Therefore we were able to investigate the evolution of c-axis transport properties from the antiferromagnetic to the superconducting state exclusively by carrier injection. We have also investigated the doping mechanism by carrier injection depending on the number of intrinsic Josephson junction, ambient temperature and doping level of the sample.

TT 6.4 Mon 10:15 H18

**Tunable qubit based on a molecule of two fractional Josephson vortices** — •Dennis Manuel Heim[1], Karl Vogel[1], Wolfgang Peter Schleich[1], Dieter Koelle[2], Reinhold Kleiner[2], and Edward Goldobin[2] — [1]Institut für Quantenphysik and Center for Integrated Quantum Science and Technology ($IQ^{ST}$), Universität Ulm, D-89069 Ulm, Germany — [2]Physikalisches Institut and Center for Collective Quantum Phenomena in $LISA^+$, Universität Tübingen, D-72076 Tübingen, Germany

We propose a concept of a qubit based on two coupled fractional vortices pinned at two artificially created $\kappa$ discontinuities of the Josephson phase in a long Josephson junction. Each discontinuity can be created by a pair of tiny current injectors with the current $I_{\rm inj}$ applied. We map the dynamics of the system to the dynamics of a single particle in a double-well potential and calculate the effective parameters of this potential. By tuning the discontinuities $\kappa \propto I_{\rm inj}$ during the experiment we are able to control the parameters of the effective double-well potential as well as to initialize the fractional vortex molecule to a desired state. The system can be used to study macroscopic quantum phenomena involving tailored vortex matter.

TT 6.5 Mon 10:30 H18

**Tripartite GHZ generation scheme in presence of bosonic baths** — •Samuele Spilla[1], Rosanna Migliore[2], Matteo Scala[1], and Anna Napoli[1] — [1]Dipartimento di Fisica, Università di Palermo, via Archirafi 36, 90123 Palermo, Italy — [2]Institute of Biophysics, National Research Council, via U. La Malfa 153, 90146 Palermo, Italy

We analyse an entangling protocol to generate tripartite Greenberger-Horne-Zeilinger (GHZ) states in a system consisting of three superconducting qubits with pairwise coupling. The dynamics of the open quantum system is investigated by taking into account the interaction of each qubit with an independent bosonic bath with an ohmic spectral structure. To this end, a microscopic master equation is constructed and exactly solved. We find that the protocol discussed here is stable against decoherence and dissipation due to the presence of the external baths.

TT 6.6 Mon 10:45 H18

**$\varphi$ Josephson junctions with a tunable current-phase relation** — •Hanna Sickinger[1], Adi Lipman[2], Roman Mints[2], Martin Weides[3], Hermann Kohlstedt[4], Dieter Koelle[1], Reinhold Kleiner[1], and Edward Goldobin[1] — [1]Universität Tübingen, Germany — [2]Tel Aviv University, Israel — [3]KIT Karlsruhe, Germany — [4]Universität zu Kiel, Germany

Josephson junctions (JJs) with a ferromagnetic interlayer can be used to fabricate $\pi$ JJs, which have a phase drop of $\pi$ in the ground state in comparison to conventional JJs having a phase drop of 0 (0 JJs). One can use these $\pi$ JJs in superconducting circuits as a device that provides a constant phase shift, i.e. as a $\pi$ phase battery. A generalization of a $\pi$ JJ is a $\varphi$ JJ, which has the phase $\pm\varphi$ in the ground state. The value of $\varphi$ can be chosen by design and tuned in the interval $0 < \varphi < \pi$. The $\varphi$ JJs we used in our experiment are fabricated as 0-$\pi$ JJs with asymmetric current densities in the 0 and $\pi$ facets [1]. This system can be described by an effective current phase relation [1], which is tunable by an externally applied magnetic field. We present the experimental evidence of such a $\varphi$ JJ [2]. In particular we demonstrate that: (a) a $\varphi$ JJ has two states $-\varphi$ and $+\varphi$, (b) the unknown state can be detected (read out) by measuring $I_c$ ($I_{c+}$ or $I_{c-}$), and (c) we can prepare a particular state by applying a magnetic field or a special bias sweep sequence. The experimental data are in good agreement with the theoretical predictions.

[1] E. Goldobin, et al., Phys. Rev. Lett. **107**, 227001 (2011)
[2] H. Sickinger, et al., Phys. Rev. Lett. **109**, 107002 (2012)

TT 6.7 Mon 11:00 H18

**Towards $\pi$ Josephson Junctions with Fe, Si based Barriers** — •Nico Ruppelt[1], Ondrej Vavra[1], Hanna Sickinger[2], Edward Goldobin[2], Dieter Koelle[2], Reinhold Kleiner[2], and Hermann Kohlstedt[1] — [1]Nanoelektronik, Technische Fakultät, Christian-Albrechts Universität zu Kiel, Germany — [2]Physikalisches Institut, Experimentalphysik II, Universität Tübingen, Germany

$\pi$ Josephson junctions are promising elements for RSFQ logic [1] and flux qubits [2]. We fabricate and investigate Josephson junctions with barriers made of Si-Fe alloy aiming to achieve high critical current densities $j_c$ in the $\pi$ state. In order to vary parameters like composition and thickness independently in a single wafer run, a combinatorial sputtering technique for alloy and multi layer deposition of Fe and Si is presented. Our approach is based on a common planetary-type sputter system. Both materials were deposited with monotonic thickness gradients which were aligned perpendicular to each other. Alloys are formed by stacking of alternately deposited submonolayers of Fe and Si. Various Nb/Al based Josephson junctions with FeSi alloy interlayers and different combinations of Si|Fe multilayers were prepared. Electrical $I$–$V$ characteristics and $I_c(B)$ look as expected (RSJ-like and Fraunhofer-like), while the critical current density $j_c$ as a function of the Fe content demonstrates non-trivial behavior.

[1] T. Ortlepp, et al., Science **312**, 1495–1497 (2006)
[2] A. K. Feofanov, et. al., Nature Physics **6**, 593–597 (2010)

**15 min. break**

TT 6.8 Mon 11:30 H18

**Fractional Flux Quantization in Loops of Unconventional Superconductors** — •Florian Loder, Arno P. Kampf, and Thilo Kopp — Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

The magnetic flux threading a conventional superconducting ring is typically quantized in units of $\Phi_0 = hc/2e$. The factor 2 in the denominator of $\Phi_0$ originates from the existence of two different types of pairing states with minima of the free energy at even and odd multiples of $\Phi_0$. Here we show that spatially modulated pairing states

exist with energy minima at fractional flux values, in particular at multiples of $\Phi_0/2$. In such states condensates with different center-of-mass momenta of the Cooper pairs coexist. The proposed mechanism for fractional flux quantization is discussed in the context of cuprate superconductors, where $hc/4e$ flux periodicities as well as uniaxially modulated superconducting states were observed.

TT 6.9 Mon 11:45 H18

**Quantum critical temperature of a modulated oscillator** — Lingzhem Guo[1,2], Vittorio Peano[3], •Michael Marthaler[1], Gerd Schön[1], and Mark Dykman[3] — [1]Institut für Theoretische Festkörperphysik — [2]Department of Physics, Beijing Normal University, Beijing 100875, China — [3]Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

We show that the rate of switching between the vibrational states of a modulated nonlinear oscillator is characterized by a quantum critical temperature $T_c \propto \hbar^2$. The rate is independent of $T$ for $T < T_c$. Above $T_c$ there emerges a quantum crossover region where the slope of the logarithm of the distribution over the oscillator states displays a kink and the change of the switching rate with $T$ is independent of the modulation. The results demonstrate the limitations of the conventional instanton theory of switching in systems lacking detailed balance.

TT 6.10 Mon 12:00 H18

**Quantum phase fluctuations in Josephson junction systems** — •Gianluca Rastelli — Universität Konstanz

Coherent Quantum Phase-Slip (CQPS) processes in superconducting systems are an active research topic. They have been studied theoretically [1-3] and experimentally, in 1D Josephson junction chains [4] and in superconducting nanowires [5]. CQPSs are of main interest for the realization of qubits topologically protected against decoherence and for the achievement of a fundamental current standard in quantum metrology [1]. I will discuss CQPSs in Josephson junction rings biased with an external magnetic flux and with an arbitrary (long) range for the electrostatic interaction between the N superconducting islands.I will also present a comparison between the theory and the experimental observations reported by the group of Grenoble.

[1] J. E. Mooij and Y. V. Nazarov, Nat. Physics (2006)
[2] K. A. Matveev et al., PRL (2002)
[3] G. Rastelli et al., arXiv:1201.0539
[4] I. M. Pop et al., Nat. Phys. Lett. (2010)
[5] O. V. Astafiev et al., Nat. Lett. (2012)

TT 6.11 Mon 12:15 H18

**Spin-precession-assisted tunneling in hybrid superconducting point contacts** — •Cecilia Holmqvist[1], Wolfgang Belzig[1], and Mikael Fogelström[2] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Department of Microtechnology and Nanoscience - MC2, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

The charge and spin transport properties of a quantum point contact coupled to a nanomagnet depend strongly on the dynamics of the nanomagnet's spin. We analyze the current-voltage characteristics of a junction coupled to a spin whose dynamics is modeled as Larmor precession brought about by an external magnetic field. The interaction between the spin dynamics and the Josephson effect leads to a rich subgap structure due to spin-precession-assisted multiple Andreev reflections. Additionally, the spin current displays Shapiro-like resonances due to the interplay between the ac Josephson current and the Larmor precession.

TT 6.12 Mon 12:30 H18

**Josephson supercurrent in a graphene-superconductor junction** — •Esmaeel Sarvestani[1] and Seyed Akbar Jafari[2] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of Physics, Sharif University of Technology, Tehran 11155-9161, Iran

Within the tunneling Hamiltonian formulation for the eight-component spinors, the Josephson critical supercurrent has been calculated in a planar superconductor-normal graphene-superconductor junction. Coupling between superconductor regions and graphene is taken into account by a tunneling Hamiltonian which contains two types of tunneling, intravalley and intervalley tunneling. Within the present tunneling approach, we find that the contributions of two kinds of tunneling to the critical supercurrent are completely separable. Therefore, it is possible to consider the effect of the intervalley tunnelings in the critical supercurrent. The incorporation of these type of processes into the tunneling Hamiltonian exposes a special feature of the graphene Josephson junctions. The effect of intervalley tunneling appears in the length dependence plot of critical current in the form of oscillations. We also present the results for temperature dependence of critical supercurrent and compare with experimental results and other theoretical calculations.

TT 6.13 Mon 12:45 H18

**Optical Josephson radiation from a Majorana Josephson junction** — •Christoph Ohm and Fabian Hassler — Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

We consider a voltage-biased Josephson junction between two nanowires hosting Majorana fermions which occur as topological protected zero-energy excitations at the junction. We show that two Majorana fermions localized at the junction, though being neutral excitations, interact with the electromagnetic field and generate coherent radiation similar to the conventional Josephson radiation in a voltage biased Josephson junction. Within a semi-classical analysis of the light field, we find that the optical phase gets locked to the superconducting phase difference and that the radiation is emitted at half of the Josephson frequency. In order to confirm the coherence of the radiation, we study correlations of the light emitted by two spatially-separated junctions in a SQUID geometry taking into account decoherence by spontaneous phase-switchings due to quasi-particle poisoning as well as by thermal effects.

## TT 7: Correlated Electrons: Spin Systems, Itinerant Magnets 1

Time: Monday 9:30–13:00 Location: H19

TT 7.1 Mon 9:30 H19

**Eigenstate thermalization in isolated spin-chain systems** — •Robin Steinigeweg[1,2], Jacek Herbrych[2], and Peter Prelovšek[2] — [1]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig — [2]Department of Theoretical Physics, Jožef Stefan Institute, SI-1000 Ljubljana

The thermalization phenomenon and many-body quantum statistical properties are studied on the example of several observables in isolated spin-chain systems, both integrable and generic non-integrable ones. While diagonal matrix elements for non-integrable models comply with the eigenstate thermalization hypothesis, the integrable systems show evident deviations and similarity to properties of noninteracting many-fermion models. The finite-size scaling reveals that the crossover between two regimes is given by a scale closely related to the scattering length. Low-frequency off-diagonal matrix elements related to d.c. transport quantities also follow in a generic system a behavior analogous to the eigenstate thermalization hypothesis, however unrelated to the one of diagonal elements.

TT 7.2 Mon 9:45 H19

**Emergent critical phase and Ricci flow in a 2D frustrated Heisenberg model** — •Peter Orth[1], Premala Chandra[2], Piers Coleman[2], and Jörg Schmalian[1] — [1]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

We introduce a two-dimensional frustrated Heisenberg antiferromagnet on interpenetrating honeycomb and triangular lattices [1]. Classically the two sublattices decouple, and "order from disorder" drives them into a coplanar state. Applying Friedan's geometric approach to nonlinear sigma models, we obtain the scaling of the spin-stiffnesses governed by the Ricci flow of a 4D metric tensor. At low temperatures, the relative phase between the spins on the two sublattices is

described by a six-state clock model with an emergent critical phase and two Berezinskii-Kosterlitz-Thouless (BKT) phase transitions.

[1] P. P. Orth, P. Chandra, P. Coleman, and J. Schmalian, arXiv:1206.5740v1 (2012) (accepted for Phys. Rev. Lett.)

TT 7.3 Mon 10:00 H19

**Doping effects on Honeycomb lattice iridate $A_2IrO_3$ (A=Na,Li)** — •Soham Manni[1], Yogesh Singh[2], and Philipp Gegenwart[1] — [1]I. Physikalisches Institut, Georg-August-Universitaet Goettingen, Goettingen, Germany — [2]IISER Mohali, Mohali, India

Iridates have recently attracted much attention due to a novel $S_{\text{eff}} = 1/2$ Mott insulating state, driven by the interplay of moderate electronic correlations with strong spin-orbit coupling. We focus on $A_2IrO_3$ (A=Na,Li) which is a layered system with Ir moments sitting on a Honeycomb lattice [1, 2]. Theoretically, this system has been proposed as solid-state realization of the Heisenberg-Kitaev(HK)model. Recently there are many fascinating predictions for doping in $A_2IrO_3$ [3].

The temperature dependence of the susceptibility indicates a dominating antiferromagnetic exchange interaction with $\Theta_W = -125$ K and $-33$ K for the Na- and Li- system, respectively, while $T_N = 15$K for both materials. We discuss the effects of different dopings (iso- and non-isoelectronic) on the A-site and Cu-intercalation by investigation of their structural, electronic and magnetic properties. Different playgrounds like order-disorder effect and chemical pressure effect etc. will be discussed here.

Work supported by the Erasmus Mundus EURINDIA project.

[1] Y. Singh and P. Gegenwart, Phys. Rev. B 82, 064412 (2010)
[2] Y. Singh, S. Manni, P. Gegenwart and others, PRL 108, 127203 (2012)
[3] A. Vishwanath et.al. Phys. Rev. B 86, 085145 (2012).

TT 7.4 Mon 10:15 H19

**Spin-liquid versus spiral-order phases in the anisotropic triangular lattice** — •Luca F. Tocchio[1], Hélène Feldner[1], Federico Becca[2], Roser Valentí[1], and Claudius Gros[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main, Germany — [2]International School for Advanced Studies (SISSA) Trieste, Italy

We study the competition between magnetic and spin-liquid phases in the Hubbard model on the anisotropic triangular lattice, which is described by two hopping parameters $t$ and $t'$ in different spatial directions and is relevant for layered organic charge-transfer salts [1]. By using a variational approach that includes spiral magnetic order, we provide solid evidence that a spin-liquid phase is stabilized in the strongly-correlated regime and close to the isotropic limit $t'/t = 1$. Otherwise, a magnetically ordered spiral state is found, connecting the (collinear) Néel and the (coplanar) 120° phases. The pitch vector of the spiral phase obtained from the unrestricted Hartree-Fock approximation is substantially renormalized in presence of electronic correlations, and the Néel phase is stabilized in a wide regime of the phase diagram, i.e., for $t'/t < 0.75$. We discuss these results in the context of organic charge-transfer salts.

[1] B.J. Powell and R.H. McKenzie, Rep. Prog. Phys. 74, 056501 (2011)
[2] L.F. Tocchio, H. Feldner, F. Becca, R. Valentí, and C. Gros, arXiv:1209.1928

TT 7.5 Mon 10:30 H19

**Lifshitz invariants and $Z_2$-vortex phase in the triangular lattice Kitaev-Heisenberg model** — •Ioannis Rousochatzakis, Ulrich Rössler, Jeroen van den Brink, and Maria Daghofer — IFW Dresden, P.O. Box 27 01 16, D-01171 Dresden, Germany

We present our study on the classical Kitaev-Heisenberg Hamiltonian on a triangular lattice, and discuss the presence of an incommensurate non-coplanar phase, which is identified as a lattice of $Z_2$ vortices. The latter are topological point defects of the SO(3) order parameter in the continuum theory around the nearby Heisenberg antiferromagnet. The defects arise at zero temperature (in contrast to the well known entropic scenario [1]) due to a double-twisting mechanism that is generated by Lifshitz invariants related to spin-orbit coupling. In this respect, this phase is a $Z_2$ analog to the Z-vortex phases of type-II superconductors [2], the twisted grain boundary phases in liquid crystals [3], and to the Skyrmion lattice phases in chiral magnets [4].

[1] H. Kawamura and S. Miyashita, J. Phys. Soc. Jpn. **53**, 4138 (1984)
[2] A. A. Abrikosov, Sov. Phys. JETP **5**, 1174 (1957)
[3] S. R. Renn and T. C. Lubensky, Phys. Rev. A **38**, 2132 (1988)
[4] A. N. Bogdanov and D. A. Yablonskii, Sov. Phys. JETP **68**, 101 (1989); A. N. Bogdanov and A. Hubert, J. Magn. Magn. Mater. **138**, 255 (1994); U. K. Rößler, A. N. Bogdanov, and C. Pfleiderer, Nature **442**, 797 (2006)

TT 7.6 Mon 10:45 H19

**$\mathbb{Z}_2$-vortex phase in a triangular-lattice Kitaev-Heisenberg model: Numerical simulations** — Ioannis Rousochatzakis, Ulrich K. Rössler, Jeroen van den Brink, and •Maria Daghofer — IFW Dresden

We present numerical evidence for a $\mathbb{Z}_2$-vortex phase in the triangular-lattice Kitaev-Heisenberg model. We performed unbiased Monte-Carlo simulations and found at least two incommensurate phases: One of them is dominated by three incommensurate ordering vectors, one for each spin component, $S^x$, $S^y$ and $S^z$. This phase hosts localized defects that are similar to skyrmions, but are here identified as $\mathbb{Z}_2$ vortices. The vortices are seen to form regular lattices that optimize their distance and whose lattice constant is determined by the incommensurate ordering vectors. For very large spin-orbit coupling, a different incommensurate phase emerges, where the symmetry between the three lattice directions (and spin components) is broken. One spin component dominates here and finite temperatures are characterized by nearly decoupled antiferromagnetic Ising chains, as in the square-lattice compass model. Connections to models for iridates will also be discussed.

[1] I. Rousochatzakis, U. K. Rössler, J. van den Brink, M. Daghofer, arXiv:1209.5895

**15 min. break**

TT 7.7 Mon 11:15 H19

**Non-perturbative RG approach to frustrated magnets** — •Nils Hasselmann[1] and Andreas Sinner[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart — [2]Institut für Physik, Theorie II, Universität Augsburg, 86135 Augsburg

Frustrated magnets support in two dimensions topological defects which for Heisenberg models are point-like and of $Z_2$ character. We analyse, using a Ginzburg-Landau-Wilson formulation and a non-local approximation of the interaction, frustrated magnets within the non-perturbative renormalization group approach. At low temperatures we recover the predictions of the usual non-linear sigma-model theory for frustrated magnets. However, in contrast to the usual non-linear sigma-model approach, but in agreement with Monte-Carlo simulations, we find in our approach clear signs of a defect unbinding transition at finite temperatures in frustrated Heisenberg models.

TT 7.8 Mon 11:30 H19

**Strongly Correlated Fermions on a Kagome Lattice: Interplay between Spin and Charge Degrees of Freedom** — •Krishanu Roychowdhury[1], Karlo Penc[2], Chisa Hotta[3], and Frank Pollmann[1] — [1]Max-Planck-Institute fur Physik of Komplexer Systeme, 01187 Dresden, Germany — [2]Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O.B. 49, Hungary — [3]Department of Physics, Faculty of Science, Kyoto Sangyo University, Kyoto 603-8555, Japan

We study strongly correlated electrons on a kagome lattice at 1/3 filling (i.e. two electrons per three sites). The dynamics is described by an extended Hubbard Hamiltonian. We are concerned with the limit $|t| \ll V \ll U$ with hopping amplitude t, nearest-neighbour repulsion V and on-site repulsion U. In this limit, we can neglect double occupancy on the sites as well as states with more than two electrons per triangle. The low energy physics is described by an effective Hamiltonian which includes ring exchange of fermions around hexagons with amplitude g as well as an antiferromagnetic Heisenberg interaction with amplitude J. Using large scale exact-diagonalization, we observe a quantum-phase transition from a resonating plaquette phase at large g/J to a charge ordered phase at low values of g/J. To study the finite temperature physics, we consider a classical version of the problem in which we investigate the effects of a loop tension. This loop tension results from the spin-fluctuations and favours configurations with short loops.

TT 7.9 Mon 11:45 H19

**Quantum phase transitions in coupled-dimer magnets: Sys-**

**tematic expansions and disorder** — •Matthias Vojta — Technische Universität Dresden, Germany

Quantum phase transitions in quantum magnets, with coupled-dimer systems being prominent examples, have been extensively studied both experimentally and theoretically. A standard microscopic approach to coupled-dimer Hamiltonians is the bond-operator technique of Sachdev and Bhatt, which has been widely applied to describe Gaussian magnetic fluctuations. Here we describe extensions of the method in two directions: (i) systematic expansions beyond the Gaussian level, and (ii) the inclusion of quenched disorder. In both cases, we focus on the evolution across the transition using suitable bosonic condensates. Among other things, we address (i) the consistent implementation of Goldstone's theorem, and (ii) the excitation spectrum of quantum Griffiths phases.

TT 7.10 Mon 12:00 H19

**Singular field response and singular screening of vacancies in antiferromagnets** — •Alexander Wollny, Eric C. Andrade, and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden

For isolated vacancies in ordered local-moment antiferromagnets we show that the magnetic-field linear-response limit is generically singular: The magnetic moment associated with a vacancy in zero field is different from that in a finite field $h$ in the limit $h \to 0^+$. The origin is a universal and singular screening cloud, which moreover leads to perfect screening as $h \to 0^+$ for magnets which display spin-flop bulk states in the weak-field limit.

TT 7.11 Mon 12:15 H19

**Electric Field Response of Coulombic Charge Ice** — •Paul McClarty[1], Aroon O'Brien[2], Frank Pollmann[1], and Roderich Moessner[1] — [1]MPI PKS, Noethnitzer Strasse 38, 01187, Dresden, Germany — [2]School of Physics, University of Sydney, Sydney, Australia

Coulomb phases are states of matter which arise in certain geometrically frustrated systems. They are characterized by an emergent low energy gauge freedom which entails the existence of particular anisotropic correlations and fractionalized excitations. The archetypal example of such a state of matter is the spin ice state which appears in some rare earth magnets. Here we consider a manifestation of a Coulomb phase in a model inspired by certain mixed valence ferrites including magnetite. In zero field, we were able to treat this Coulombic charge ice model and the dipolar spin ice model on an equal footing by mapping both to a constrained charge model on the diamond lattice. We found that states of the two ice models are related by a staggering field which is reflected in the energetics of these two models. In this talk, we focus on the screening, within the Coulomb phase, of the long range interaction and the response of charge ice to a static external electric field.

TT 7.12 Mon 12:30 H19

**Anormalous dynamics of electric dipoles on magnetic monopoles in spin ice** — •Christoph Grams, Martin Valldor, and Joachim Hemberger — II. Physikalisches Institut, Universität zu Köln, Cologne, Germany

The coupling of electric dipoles to magnetic monopoles [1] enables us to see magnetic monopoles with dielectric spectroscopy. Therefore we can use our setup in the dilution cryostat to evaluate monopole dynamics in $Dy_2Ti_2O_7$ in a frequency range up to 1 MHz with magnetic and electric field parallel to the [111] direction of the sample down to 100 mK.

Our measurements show an anomaly in the monopole dynamics in a conic area in the (H,T) phase diagram above the critical endpoint (approximately 400 mK and 1 T) of the first order monopole liquid-gas transition [2]. Repeating the measurements with the electric field perpendicular to the magnetic field the abnormal dynamics vanish, indicating an anisotropy of the polarization and thereby promoting the idea of antiferroelectric order in the high field phase.

Work supported by the DFG through SFB 608.

[1] D. I. Khomskii, Nature Commun. 3, 1-13 (2012)
[2] C. Castelnovo et al., Nature 451(7174), 42-5 (2008)

TT 7.13 Mon 12:45 H19

**Anisotropic magnetic Heat Transport in the Spin-Ice Compound $Dy_2Ti_2O_7$** — •Simon Scharffe, Gerhard Kolland, Oliver Breunig, Martin Hiertz, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

The spin-ice compound $Dy_2Ti_2O_7$ is a geometrically frustrated spin system which recently attracted attention due to emerging magnetic monopoles. It consists of corner-sharing $Dy^{3+}$ tetrahedra which form a pyrochlore lattice. Due to strong crystal field effects an Ising anisotropy is present which aligns the $Dy^{3+}$ spins along their local easy-axis in the {111}-directions, pointing into or out of the tetrahedra. The ground state below 1 K is given by the "ice-rule": two spins point into and two out of a tetrahedron. Excited states can be created by flipping one spin, leading to neighboring "1-in/3-out" and "3-in/1-out" configurations. In zero magnetic field, these excitations can deconfine and are discussed as magnetic monopoles. Recently, $\kappa$ has been studied for $\vec{B}||[001]$ and gives evidence for considerable monopole heat transport [1]. Here, we focus on the magnetic field anisotropy of $\kappa_{\mathrm{mag}}$ as for $\vec{B}||[110]$ and $\vec{B}||[111]$ exotic ground states of different degeneracies can be stabilized. In order to separate the phononic and magnetic contribution to $\kappa$, we also investigated $(Dy_{0.5}Y_{0.5})_2Ti_2O_7$ which is a magnetic reference system with suppressed spin-ice features.

This work was supported by the DFG through SFB 608.

[1] Kolland *et. al.* (2012), PRB, **86**(060402)

## TT 8: Transport: Quantum Dots, Wires, Point Contacts 1 (jointly with HL and O)

Time: Monday 9:30–13:00 Location: H20

TT 8.1 Mon 9:30 H20

**Tunneling-induced renormalization in interacting quantum dots** — •Janine Splettstoesser[1], Michele Governale[2], and Jürgen König[3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University — [2]School of Physical and Chemical Sciences, Victoria University of Wellington, New Zealand — [3]Theoretische Physik, Universität Duisburg-Essen, Germany

A single-level quantum dot with arbitrarily strong onsite Coulomb interaction weakly coupled to electronic reservoirs is studied. We here present an analysis of tunneling-induced quantum fluctuations, generating cotunneling processes and renormalizing system parameters. For a perturbative treatment of these quantum fluctuations in the limit of weak tunnel coupling, we remove off-shell parts of the Hamiltonian via a canonical transformation. We find that the tunnel couplings for the transitions connecting empty and single occupation respectively single and double occupation of the dot renormalize with the same magnitude but with *opposite* signs [1]. This has an important impact on the shape of the renormalization extracted for example from the conductance. Finally, we verify the compatibility of our results with a systematic second-order perturbation expansion of the linear conductance performed within a diagrammatic real-time approach.

[1] J. Splettstoesser, M. Governale, J. König, Phys. Rev. B **86**, 035432 (2012).

TT 8.2 Mon 9:45 H20

**Interaction-induced charge and spin pumping through a quantum dot at finite bias** — Hernan L. Calvo[1], •Laura Classen[1], Janine Splettstoesser[1], and Maarten R. Wegewijs[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany and JARA - Fundamentals of Future Information Technology — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

We discuss charge and spin transport through an adiabatically driven, strongly interacting quantum dot weakly coupled to two metallic contacts with finite bias voltage. We identify coefficients of response to the time-dependent external driving and relate these to the concept of emissivity [1]. These coefficients allow for a straightforward analysis of the predicted interaction-induced pumping under periodic modulation of the gate and bias voltage [2]. We extend this adiabatic Coulomb blockade spectroscopy to spin pumping. In the absence of a magnetic field, we show a striking, simple relation between the pumped charge at zero bias and at bias equal to the Coulomb charging energy. At finite

magnetic field, we discuss the possibility to have interaction-induced pure spin pumping. For large-amplitude driving, the magnitude of both the pumped charge and spin saturates at values which are independent of the specific shape of the pumping cycle. Each of these values provides an independent, quantitative measurement of the junction asymmetry.

[1] M. Büttiker, H. Thomas, and A. Prêtre, Z. Phys. B 94, 133 (1994).
[2] F. Reckermann, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. Lett. 104, 226803 (2010).

TT 8.3 Mon 10:00 H20

**Structure and conductance analysis of atomic-sized contacts** — •Manuel Matt[1], Fabian Pauly[1], Juan Carlos Cuevas[2], and Peter Nielaba[1] — [1]University of Konstanz, Department of Physics, 78457 Konstanz, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

We study the conductance histograms of different metals such as Au and Al. Our theoretical approach combines molecular dynamics simulations of the stretching of atomic-sized wires with the non-equilibrium Green's function formalism based on the tight-binding modelling of the electronic system. As compared to pervious work [1,2], we consider substantially larger wires and explore different lattice orientations. The results show good agreement with experiments.

[1] M. Dreher, F. Pauly, J. Heurich, J. C. Cuevas, E. Scheer, and P. Nielaba, Phys. Rev. B 72, 075435 (2005)
[2] F. Pauly, M. Dreher, J. K. Viljas, M. Häfner, J. C. Cuevas, and P. Nielaba Phys. Rev. B 74, 235106 (2006)

TT 8.4 Mon 10:15 H20

**Transport through two interacting resonant levels connected by a Fermi sea** — •Elena Canovi, Alexander Moreno, and Alejandro Muramatsu — Institut für Theoretische Physik III, Universität Stuttgart

We study transport at finite bias, i.e. beyond the linear regime, through two interacting resonant levels connected by a Fermi sea. Our results are obtained by means of time-dependent density matrix renormalization group. We find that at finite size both the current and the occupations of the interacting levels oscillate as a function of time. We determine the amplitude and period of such oscillations as a function of bias and extension of the Fermi sea. In particular, the occupations on the two dots oscillate with a relative phase which depends on the distance between the impurities and on the Fermi momentum of the Fermi sea, as expected for RKKY interactions. The approximant to the steady-state current displays oscillations as a function of the distance between the impurities. In the free case we find that it is affected by resonances. The latter can be understood by considering the transmission coefficient of one particle propagating freely in the system. We discuss finally the incidence of interaction on such a behavior.

TT 8.5 Mon 10:30 H20

**Magnon-driven quantum-dot heat engine** — •Björn Sothmann and Markus Büttiker — Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

Recently, thermoelectric effects have generated a lot of interest. In Ref. [1], transport through two capacitively coupled quantum dots in a three-terminal setup was investigated in the Coulomb-blockade regime. It was shown how such a device can convert a heat current into a directed charge current. This converter is optimal in the sense that it transfers one electron for every quantum of energy delivered by the hot dot and thus allows to reach Carnot efficiency. A generalization to systems with many transport channels was analyzed in Ref. [2].

Here, we discuss a new class of devices where a single-level quantum dot is coupled to two ferromagnetic electrodes as well as to a ferromagnetic insulator at different temperatures [3]. We demonstrate that the system can convert a magnon current into a pure electron spin current or a spin-polarized electron current depending on the magnetic configuration. We analyze the maximal output power as well as the efficiency and show that the tight-coupling limit where heat and charge currents are proportional to each other can be reached.

[1] R. Sánchez and M. Büttiker, Phys. Rev. B **83**, 085428 (2011).
[2] B. Sothmann, R. Sánchez, A. N. Jordan and M. Büttiker, Phys. Rev. B **85**, 205301 (2012).
[3] B. Sothmann and M. Büttiker, EPL **99**, 27001 (2012).

TT 8.6 Mon 10:45 H20

**Iterative summation of path integrals for nonequilibrium molecular quantum transport** — Roland Huetzen[1], •Stephan Weiss[1,2], Michael Thorwart[3], and Reinhold Egger[1] — [1]Heinrich-Heine Universität Düsseldorf, Universitätsstr.1, 40225 Düsseldorf — [2]Universität Duisburg-Essen and CENIDE, 47048 Duisburg — [3]Universität Hamburg, Jungiusstr. 9, 20355 Hamburg

We formulate and apply a nonperturbative numerical approach to the nonequilibrium current, $I(V)$, through a voltage-biased molecular conductor. We focus on a single electronic level coupled to an unequilibrated vibration mode (Anderson-Holstein model), which can be mapped to an effective three-state problem. Performing an iterative summation of real-time path integral (ISPI) expressions, we accurately reproduce known analytical results in three different limits. We then study the crossover regime between those limits and show that the Franck-Condon blockade persists in the quantum-coherent low-temperature limit, with a nonequilibrium smearing of step features in the $IV$ curve.

[1] S. Weiss, J. Eckel, M. Thorwart, and R. Egger, Phys. Rev. B **77**, 195316 (2008).
[2] R. Hützen, S. Weiss, M. Thorwart, and R. Egger, Phys. Rev. B **85**, 121408 (2012).

**15 min. break**

TT 8.7 Mon 11:15 H20

**Spin dynamics in nanoparticles near Stoner instability** — •Philipp Stegmann[1], Björn Sothmann[2], Jürgen König[1], and Yuval Gefen[3] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]Départment de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland — [3]Dept. of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel

We analyse the spin dynamics of a nanoparticle close to the Stoner instability. The nanoparticle is weakly tunnel coupled to two ferromagnetic leads. By mapping to an effective Fokker-Planck description we identify two different types of dynamic behaviour (diffusion vs. drift), which are revealed by characteristic relaxation times and a Fano factor that oscillates as a function of an applied bias voltage. Finally, we propose biasing schemes to generate states with magnetic quadrupole moments that dominate over a negligible dipole moment.

TT 8.8 Mon 11:30 H20

**Nonlinear transport through interacting quantum dots with superconducting leads in the weak coupling regime** — •Sascha Ratz and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We present a nonequilibrium real-time diagrammatic transport theory for the systematic investigation of the quasiparticle and Josephson currents through a hybrid superconductor-quantum dot system in the weak coupling regime. In details, our device consists of an interacting quantum dot coupled to two biased spin-singlet superconducting leads. To describe the transport dynamics, we derive a completely general equation of motion for the reduced density matrix including all the contributions of a perturbation expansion in the tunneling Hamiltonian. Within these investigations, already in fourth order we can identify the contributions of the nonlocal time evolution kernel to the quasiparticle and DC Josephson transport. To clarify the difference between quasiparticle cotunneling and phase-coherent two-particle Andreev tunneling in fourth order, we first choose a single-level Anderson impurity model for the interacting quantum dot. In particular, one can give a clear explanation for subgap features due to proximity effects, which are also important when we finally compare our theoretical results for a carbon nanotube quantum dot with experimental observations.

TT 8.9 Mon 11:45 H20

**Spindephasing and Coherent Control of an Ensemble of Quantum Dots** — •Andre Jovchev and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

We present a numerical treatment of pump-and-probe experiments with an ensemble of singly charged quantum dots in a magnetic field. We examine the excitation of trions, which is part of an effective polarization mechanism for the spin of the residual electrons, precessing around the magnetic field vector. Inhomogeneities in the magnetic g-factor of different electrons lead to dephasing. The effect of the short

pump pulses is described by a unitary operator in the subspace of a spin degenerated electron and trion. For the dynamics between the pulses we apply a Lindblad theory to describe the decoherence due to environmental effects and the hyperfine interaction of the electrons with surrounding nuclei. We study the polarization of the whole ensemble after the application of different pulse protocols, and give an explanation for the polarization of the nuclear spins, which can lead to a remarkably increase of dephasing times which were already seen in experiments.

TT 8.10 Mon 12:00 H20

**Adiabatic pumping in the quasi-one-dimensional triangle lattice** — Michael Schulze[1], •Dario Bercioux[1], and Daniel F. Urban[2,3] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [3]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

We analyze the properties of the quasi-one-dimensional triangle lattice emphasizing the occurrence of flat bands and band touching via the tuning of the lattice hopping parameters and on-site energies [1]. The spectral properties of the infinite system will be compared with the transmission through a finite piece of the lattice with attached semi-infinite leads. Furthermore, we investigate the adiabatic pumping [2] properties of such a system: depending on the transmission through the lattice, this results in nonzero integer charge transfers or transfers that increase linearly with the lattice size.

[1] M. Schulze, D. Bercioux, D. F. Urban, arXiv:1208.6113.
[2] P. W. Brouwer, Phys. Rev. B **58**, 10135(R) (1998).

TT 8.11 Mon 12:15 H20

**Thermoelectric efficiency of a driven double quantum dot** — •Federica Haupt[1], Stefan Juergens[1], Michael Moskalets[2], and Janine Splettstoesser[1] — [1]RWTH Aachen University, Aachen, Germany — [2]Kharkiv Polytechnical Institute, Kharkiv, Ukraine

By applying phase-shifted AC signals to the gates of two quantum dots connected in series, it is possible to transfer charge from one lead to another in a quantized way [1,2], even in the presence of an applied bias voltage or a temperature gradient. In this work we investigate the thermoelectric properties of such a double quantum dot device. We show that not only charge but also heat can be pumped in a quantized way. If the modulation frequency $\Omega$ is sufficiently small, we find regimes in which the unit of heat $2\pi k_B T \ln 2$ is transported during each period, where $T$ is the temperature of the considered lead and the factor $\ln 2$ stems from spin degeneracy. This would open the possibility of using the pumping cycle to transfer heat against a temperature gradient or to extract work from a hot reservoir with Carnot efficiency. However, the performance of a real device is limited by dissipative effects due to leakage currents and finite time operation, which we rigorously take into account by means of a real-time diagrammatic approach in the regime of weak coupling to the leads. We show that despite these dissipative effects, efficiencies up to 70% of the maximal theoretical value can be reached.

[1] H. Pothier, *et al.*, Europhys. Lett **17**, 249 (1992)
[2] S. J. Chorley, *et al.* App. Phys. Lett. **100**, 143104 (2012).

TT 8.12 Mon 12:30 H20

**Controlling entanglement and spin-correlations in double quantum dots in the non-equilibrium regime** — •Carlos Alberto Büsser[1] and Fabian Heidrich-Meisner[2] — [1]Ludwig-Maximilians-Universität, München, München — [2]FAU Erlangen-Nuremberg and LMU München

We study the non-equilibrium dynamics in a parallel double-quantum dot structure induced by a large bias voltage. By applying both a magnetic flux and a voltage, it is possible to generate spin-spin-correlations between the two quantum dots. The sign and absolute value of these correlations can be controlled by changing the bias voltage. Using a canonical transformation we argue that the mechanism that drives the spin-spin correlations can be understood in terms of an effective Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction that is mediated by the current. Our study is based on the Anderson-impurity model and we use time-dependent density matrix renormalization group (tDMRG) simulations to obtain currents and spin-correlations in the steady state of the non-equilibrium regime. We also perform quench in the Hamiltonian to prove the stability of the entangled state.

TT 8.13 Mon 12:45 H20

**Role of coherent state superpositions in the bipolar spin blockade of a triple quantum dot** — Maria Busl[1], Ghislain Granger[2], Louis Gaudreau[2], •Rafael Sánchez[1], Alicia Kam[2], Michel Pioro-Ladrière[3], Sergei Studenikin[2], Piotr Zawadzki[2], Zbigniew Wasilewski[2], Andrew Sachrajda[2], and Gloria Platero[1] — [1]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain — [2]National Research Council Canada, Ottawa, Canada — [3]Université de Sherbrooke, Sherbrooke, Canada

In double quantum dots, Pauli spin blockade manifests as a rectified current: charge flows or is blocked depending on the sign of the applied voltage[1]. We present experimental and theoretical investigations of the equivalent process in triple quantum dots in series. We focus on a configuration where (2,0,2) (2,1,1), (1,1,2) and (2,1,2) states are degenerate. When a bias is applied in a magnetic field beyond 10mT, bipolar spin blockade is observed where current is suppressed independent of the applied bias direction. As the field is reduced to zero, leakage resonances are observed. Of special interest are two very sharp resonances which correspond to triple dot conditions when states in the left and right dot but not the center dot align. One of these resonances is found itself to involve bipolar spin blockade and is found to result from a purely quantum coherent effect: electrons occupy states that involve their transference from one extreme to the other of the triple quantum dot without ever visiting the center[2].

[1] K. Ono et al., Science 297, 1313 (2002).
[2] M. Busl et al., unpublished.

## TT 9: Quantum Liquids, Miscellaneous 1

Time: Monday 9:30–13:00 Location: H21

TT 9.1 Mon 9:30 H21

**Effective interactions and renormalized Bose surface in the normal state of the two-dimensional Bose gas with Rashba spin-orbit coupling** — •Casper Drukier, Kira Riedl, and Peter Kopietz — Institut für Theoretische Physik, J.W.Goethe-Universität Frankfurt, Frankfurt am Main, Germany

The non-interacting energy-dispersion of a two-dimensional system of bosons with Rashba spin-orbit coupling exhibits a continuum of degenerate minima on a circle in momentum space, which is the bosonic analogue of a Fermi surface. Recent theoretical studies [1,2] suggest that this degeneracy is broken by interactions. Using second order perturbation theory for the self-energy, we calculate the renormalization of the Bose surface as well as the damping of the bosonic quasiparticles. We finally discuss different condensation scenarios.

[1] Phys. Rev. A 84, 061604(R) (2011)
[2] Phys. Rev. Lett. 105, 160403 (2010)

TT 9.2 Mon 9:45 H21

**Far-from-equilibrium lattice-transport at high temperatures: breaking Bloch-localization by interactions** — •Stephan Mandt — Princeton Center for Complex Materials, Princeton University, USA

Diffusive transport of energy and mass is typically slower than ballistic transport. However, in some situations, non-interacting particles are localized, but may become delocalized by inter-particle collisions. This is the case for Bloch-oscillating fermions in the Hubbard model in the presence of an additional linear potential. In this talk, we will derive effective coupled diffusion equations for the Hubbard model in a regime governed by Bloch oscillations and rare scattering events. These equations and their solutions are relevant to describe the long-time dynamics of an almost non-interacting cloud of ultracold atoms in an optical lattice, where interactions lead to a breaking of the Bloch periodicity.

TT 9.3 Mon 10:00 H21

**Correlated lattice fermions in a spin-dependent random potential** — •Karol Makuch[1], Jan Skolimowski[1], Prabuddha B. Chakraborty[2], Krzysztof Byczuk[1], and Dieter Vollhardt[3] — [1]Faculty of Physics, Institute of Theoretical Physics, University of Warsaw, Hoza 69, 00-681 Warszawa, Poland — [2]Indian Statistical Institute, Chennai Centre, SETS Campus, MGR Knowledge City, Taramani, Chennai 600113, India — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135, Augsburg, Germany

Motivated by the new possibilities for experiments with ultracold atoms in optical lattices we explore the thermodynamic properties of correlated lattice fermions in the presence of an external spin-dependent random potential. The corresponding Hubbard model with the local on-site spin-dependent disorder is solved within the dynamical mean-field theory. The spin-dependent disorder is found to drive the magnetic polarization of the system when the total number of fermions is fixed. The magnetic response of the system with finite magnetization differs from that of a system with spin-independent disorder. The spin-dependence of the disorder also affects the metal-insulator transition at half filling.

TT 9.4 Mon 10:15 H21

**Long limit of momentum distribution functions in the sudden expansion a spin-imbalanced Fermi gas in one dimension** — •Fabian Heidrich-Meisner[1,2], Carlos Bolech[3], Stephan Langer[1,4], Ian McCulloch[5], Giuliano Orso[6], and Marcos Rigol[7] — [1]LMU Munich — [2]FAU Erlangen-Nuremberg — [3]University of Cinncinati, USA — [4]University of Pittsburgh, USA — [5]University of Queensland, St Lucia, Australia — [6]Universite Paris-Diderot, France — [7]Georgetown University, USA

We study the sudden expansion of a spin-imbalanced Fermi gas with attractive interactions in an optical lattice after quenching the trapping potential to zero [1]. The initial state is of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) type, i.e., a quasi- condensate of fermionic pairs that is modulated in real space. Using time-dependent DMRG, we demonstrate that the momentum distribution functions (MDFs) of majority and minority fermions become stationary after surprisingly short expansion times. This behavior can be understood in terms of a quantum distillation process [2] that leads to a spatial demixing of pairs and excess fermions. As a consequence, the FFLO correlations are rapidly destroyed. The expansion nevertheless yields relevant information on the initial state: we argue that the asymptotic form of the MDFs is directly related to the distribution of the Bethe-ansatz rapidities that characterize the initial conditions for this integrable model.

[1] C. Bolech et al., Phys. Rev. Lett. 109, 110602 (2012)
[2] F. Heidrich-Meisner et al., Phys. Rev. A 80, 041603(R) (2009)

TT 9.5 Mon 10:30 H21

**Dynamical spin correlations in a quantum spin liquid.** — •Johannes Knolle[1], Dima Kovrizhin[1], John Chalker[2], and Roderich Moessner[1] — [1]Max Planck Institut for the Physics of Complex Systems, Dresden, Germany — [2]Theoretical Physics, Oxford University, United Kingdom

We compute the exact time dependence of the spin-spin correlation function for arbitrary times in the gapped and gapless phases of Kitaev's honeycomb model. The resulting dynamical structure factor - observable in a standard inelastic neutron scattering experiment - exhibits signatures of fractional excitations in the spin liquid ground state, namely the gap to creating a pair of emergent static $Z_2$ fluxes, as well as various features of the density of states of the free fermions propagating in its background. Our analysis uncovers rich connections to the field of coherent nonequilibrium quantum dynamics, ranging all the way back to the physics of Andersons orthogonality catastrophe to the physics of Majorana fermions subject to a sequence of local potential quenches.

TT 9.6 Mon 10:45 H21

**Kinetic equations for a system of parametrically excited magnons** — •Andreas Rückriegel and Peter Kopietz — Institut für Theoretische Pysik, Universität Frankfurt

Using the functional integral formulation of the Keldysh technique, we derive kinetic equations for the normal and anomalous momentum distribution functions of a system of parametrically excited magnons with two-body interaction in contact with a thermal phonon bath. We then use the results of self-consistent mean field theory to obtain an effective kinetic equation of the Boltzmann type without particle number conservation. Close to thermal equilibrium, we can use a Kramers-Moyal expansion to replace the integral equation by a differential equation which has the form of a continuity equation with an explicit particle number conservation breaking source term. We use our theory to study the thermalization of magnons in the magnetic insulator yttrium-iron garnet.

**15 min. break**

TT 9.7 Mon 11:15 H21

**Thermalization of magnons in yttrium-iron garnet: nonequilibrium functional renormalization group approach** — •Johannes Hick[1], Andreas Rückriegel[1], Thomas Kloss[2], and Peter Kopietz[1] — [1]Institut für Theoretische Physik, Goethe Universität Frankfurt am Main, Germany — [2]Laboratoire de Physique et Modélisation des Milieux Condensé, CNRS and Université Joseph Fourier, Grenoble, France

Using a nonequilibrium functional renormalization group (FRG) approach we calculate the time evolution of the momentum distribution of a magnon gas in contact with a thermal phonon bath. As a cutoff for the FRG procedure we use a hybridization parameter $\Lambda$ giving rise to an artificial damping of the phonons. Within our truncation of the FRG flow equations the time evolution of the magnon distribution is obtained from a rate equation involving cutoff-dependent nonequilibrium self-energies, which in turn satisfy FRG flow equations depending on cutoff-dependent transition rates. Our approach goes beyond the Born collision approximation and takes the feedback of the magnons on the phonons into account. We use our method to calculate the thermalization of a quasi two-dimensional magnon gas in the magnetic insulator yttrium-iron garnet after a highly excited initial state has been generated by an external microwave field. In this material interactions which do not conserve the magnon particle number are present and are considered in our approach.

TT 9.8 Mon 11:30 H21

**Fractional Chern insulator in the triangular lattice** — •Stefanos Kourtis and Maria Daghofer — Leibniz Institute for Solid-State & Materials Research, Dresden, Germany

The formation of fractional quantum-Hall (FQH) states in lattice systems without externally applied magnetic fields is a recent and promising theoretical proposal that has the potential to render the FQH effect experimentally more accessible. Motivated by the emergence of the relevant physics in 3-orbital Hubbard and Kondo-lattice models on the triangular lattice [1,2], we study numerically an effective interacting spinless-fermion model and show that it yields spontaneously occurring FQH states, recently dubbed fractional Chern insulators (FCI). The Hall conductivity of these states is evaluated and shown to be fractionally quantized. This quantization is found to persist against disorder, demonstrating that the Hall conductivity is characterizing FCI states as a topological invariant. Having thus identified FCI states, we highlight further signatures of their nature in the obtained eigenvalue spectra and discuss the consequences of disorder and competition with conventional ordering.

[1] J.W.F. Venderbos, S. Kourtis, J. van den Brink, and M. Daghofer, Phys. Rev. Lett. 108, 126405
[2] S. Kourtis, J.W.F. Venderbos, and M. Daghofer, arXiv:1208.3481

TT 9.9 Mon 11:45 H21

**Topologically nontrivial and nearly flat bands arising through orbital degrees of freedom** — •Maria Daghofer, Stefanos Kourtis, Jörn W.F. Venderbos, and Jeroen van den Brink — IFW Dresden

We discuss models, where electronic correlations can induce topologically nontrivial electronic states. In particular, we focus on a three-orbital model for $t_{2g}$ orbitals on a triangular lattice [1]. Near half filling, onsite Coulomb repulsion and Hund's rule coupling induce a non-coplanar magnetic phase where electronic bands are topologically nontrivial and can become very flat [2]. Such topologically nontrivial bands with reduced dispersion have been argued [3-5] to support a lattice analog of fractional quantum-Hall states, fractional Chern-insulator (FCI) states, that arise in the absence of a magnetic field. We discuss the competition of FCI states with a charge density wave depending on properties of the nearly flat band [6].

[1] J. W. Venderbos, M. Daghofer, and J. van den Brink, Phys. Rev. Lett. **107**, 116401 (2011)

[2] J.W.F. Venderbos, S. Kourtis, J. van den Brink, and M. Daghofer, Phys. Rev. Lett. **108**, 126405 (2012)
[3] T. Neupert, L. Santos, C. Chamon, and C. Mudry, Phys. Rev. Lett. **106**, 236804 (2010)
[4] K. Sun, Z. Gu, H. Katsura, and S. D. Sarma, Phys. Rev. Lett. **106**, 236803 (2010)
[5] E. Tang, J.-W. Mei, and X.-G. Wen, Phys. Rev. Lett. **106**, 236802 (2010)
[6] S. Kourtis, J.W.F. Venderbos, and M. Daghofer, arXiv:1208.3481

TT 9.10 Mon 12:00 H21

**A New Way to Create Energy Band: Crystal Formed in Phase Space** — •Lingzhen Guo[1,2,3], Michael Marthaler[1,3], and Gerd Schön[1,3] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Department of Physics, Beijing Normal University, Beijing, China — [3]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, Karlsruhe, Germany

We propose a new way to create an energy band structure by properly driving a nonlinear system. In a natural solid, the energy band structure is a result of the periodicity of the Hamiltonian in the real space. For artificial materials, such as photonic crystals and many other quantum metamaterials, the energy band structure comes from artificial periodic structures fabricated in the laboratory. However, it is also possible to create a periodic structure in total phase space. We find that the Duffing oscillator, if driven by an external field via high order coupling, can exhibit such a periodic structure in phase space. We will calculate the resulting quasi-energy bandstructure and the emission spectrum. Compared to the conventional quantum metamaterials, the bandgaps and bandwidths of this phase space crystal can be tuned conveniently by changing the driving field's parameters.

TT 9.11 Mon 12:15 H21

**Dynamical phase transitions and the connections to the nonequilibrium dynamics of local observables** — •Markus Heyl[1], Anatoli Polkovnikov[2], and Stefan Kehrein[3] — [1]Technische Universität Dresden — [2]Boston University — [3]Georg-August-Universität Göttingen

We study general connections between the recently introduced dynamical phase transitions [1] and the dynamics of local observables after a quantum quench. In particular, we show that qualitative changes in the relaxational behavior of equilibrium order parameters occur through dynamical transitions between topologically different ground states. We demonstrate our findings for quantum quenches in the one-dimensional transverse field Ising chain.

[1] M. Heyl, A. Polkovnikov, and S. Kehrein, arXiv:1206.2505

TT 9.12 Mon 12:30 H21

**Time-reversal-invariant Hofstadter-Hubbard model with ultracold fermions** — •Peter Orth[1], Daniel Cocks[2], Stephan Rachel[3], Michael Buchhold[2], Karyn Le Hur[4], and Walter Hofstetter[2] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, — [2]Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt/Main — [3]Institute for Theoretical Physics, Dresden University of Technology, 01062 Dresden — [4]Center for Theoretical Physics, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France

We consider the time-reversal-invariant Hofstadter-Hubbard model which can be realized in cold-atom experiments [1]. In these experiments, an additional staggered potential and an artificial Rashba-type spin-orbit coupling are available. Without interactions, the system exhibits various phases such as topological and normal insulator, metal and semi-metal phases with two or even more Dirac cones. Using a combination of real-space dynamical mean-field theory and analytical techniques, we discuss the effect of on-site interactions and determine the corresponding phase diagram. We study the semi-metal to magnetic insulator transition, and find rich magnetic phases tunable by the spin-orbit coupling terms. We compute spectral functions which allow us to study the edge states of the strongly correlated topological phases.

[1] D. Cocks, P. P. Orth, S. Rachel, M. Buchhold, K. Le Hur, and W. Hofstetter, Phys. Rev. Lett. 109, 205303 (2012).

TT 9.13 Mon 12:45 H21

**Utilizing nonequilibrium effects to probe the Mott-insulator-superfluid transition of a trapped gas of interacting bosons** — •Lev Vidmar[1], Stephan Langer[2], Ian McCulloch[3], Ulrich Schollwöck[1], Ulrich Schneider[1,4], and Fabian Heidrich-Meisner[1,5] — [1]LMU Munich, Germany — [2]University of Pittsburgh, USA — [3]University of Queensland, Australia — [4]MPQ Garching, Germany — [5]FAU Erlangen-Nuremberg, Germany

An increased effort has been lately devoted to explore and establish the possible links between equilibrium and nonequilibrium properties of interacting quantum many-body systems. Recent experiments on optical lattices have shown the possibility of measuring the expansion velocity of an initially trapped system, which after the sudden release of the trap expands in an empty lattice [1]. Recent theoretical studies of interacting fermions indicated that the measurement of expansion velocity may provide information about the initial state [2]. In our work, we show that measuring the expansion velocity of an initially trapped gas of interacting bosons allows one to distinguish between a superfluid and a Mott insulating state in the initial ground state in 1D. We perform time-dependent DMRG calculations of the Bose-Hubbard model in a harmonic trap and a box trap. We derive a state diagram of a trapped system as a function of on-site repulsion and density from the expansion velocity. The resulting diagram is consistent with the state diagram obtained by measuring equilibrium properties such as local density fluctuations and on-site compressibility [3].

[1] Nat. Phys. 8, 213 (2012)
[2] PRA 85, 043618 (2012)
[3] PRA 79, 053605 (2009)

## TT 10: Focused Session: Frontiers of Electronic Structure Theory 1 (jointly with HL and O)

Organizers: R. Drautz (Ruhr-Universität Bochum), N. Marzari (EPFL, Lausanne), Matthias Scheffler (FHI, Berlin)

Time: Monday 10:30–13:15 Location: H36

**Topical Talk** TT 10.1 Mon 10:30 H36

**Fully ab initio determination of free energies: Basis for high-throughput approaches in materials design** — •Joerg Neugebauer, Fritz Kormann, Martin Friak, Blazej Grabowski, and Timann Hickel — MPI für Eisenforschung, Düsseldorf, Germany

A key requirement in developing systematic tools to design novel materials on the computer is the availability of accurate computational tools determining energies not only at T = 0 K but also under realistic conditions, i.e., at finite temperature. Combining accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts allows now to address this issue and to determine free energies and derived thermodynamic quantities such as heat capacity, thermal expansion coefficients, and elastic constants with an accuracy that often rivals available experimental data.

In the talk we will show how novel sampling strategies in configuration space together with highly converged density-functional theory calculations allow an unbiased and accurate determination of all relevant temperature dependent free energy contributions. The flexibility and the predictive power of these approaches and the impact they can have in developing new strategies in materials design will be discussed for modern high strength steels and light weight metallic alloys.

TT 10.2 Mon 11:00 H36

**Fast screening of perovskites' phase stability using AIDA, a materials' informatics platform for materials design and discovery** — •Giovanni Pizzi[1], Andrea Cepellotti[1], Boris Kozinsky[2], Marco Fornari[3], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, EPFL (CH) — [2]Robert Bosch LCC Research and Technology Center, Cambridge (USA) — [3]Dept. of Physics, Central Michigan University (USA)

Many perovskite systems display a high-temperature cubic phase with zero net polarization, whose microscopic nature is still debated. We perform a systematic study of this phase for representative $ABO_3$ perovskites, showing that there is not a unique microscopic model for it. Some systems are consistent with a displacive or an order/disorder model; others can sustain a stable displacement pattern of B-site cations in supercells, preserving zero net polarization. In such high-throughput searches, a key challenge is the need of a "materials' informatics" infrastructure to automatically prepare, execute and monitor workflows of calculations for large classes of materials, and then retrieve, store and analyze the results. To this aim, we are developing an open-source platform for high–throughput (AIDA–"Automated Infrastructure and Database for Ab-initio design"). Using AIDA free-energy workflows, we studied the phase stability of $BaTiO_3$, evaluating the critical temperatures between the cubic, tetragonal, orthorhombic, and rhombohedral phases.

TT 10.3 Mon 11:15 H36

**Fast ab-initio screening of magnetic properties applied to the design of new hard magnetic materials** — •Nedko Drebov[1], Christian Elsässer[1], Lothar Kunz[2], Alberto Martinez[2], Takashi Shigematsu[3], and Thomas Eckl[2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]Robert Bosch GmbH, Stuttgart, Germany — [3]Bosch Corporation, Tokyo, Japan

We present a fast computational ab-initio screening method which we use for the identification of new permanent magnetic materials based on rare-earth (RE) and transition-metal (TM) elements.

The candidates for new hard magnetic phases with specific structures and compositions are selected from ab-initio screening of their magnetic properties by using the TB-LMTO-ASA method. This procedure considers a large variety of possible combinations of RE and TM elements. At rather low computational costs one can get sufficiently accurate magnetic moments and exchange coupling parameters to be subsequently used in the process of virtual material design.

The results for selected candidate phases are further refined with a more accurate ab-initio method without potential-shape approximation. The Curie temperatures of the phases can be estimated from the calculated magnetic moments and exchange coupling by means of Monte Carlo simulations.

Acknowledgement: This work was supported by the Co-Operative Project 'Suche nach neuen hartmagnetischen Phasen mit hoher Energiedichte (REleaMag)' funded by the BMBF.

TT 10.4 Mon 11:30 H36

**Designer Single-Band Hubbard Materials** — •Sinead Griffin and Nicola Spaldin — ETH Zurich, Switzerland

The low-energy physics of the High-Tc superconducting cuprates is believed to be encompassed in a single-band Hubbard model. Much work focuses on the computational solutions of the Hubbard model with a view to understanding the complex nature of metal-insulator transitions, superconductivity and strong-correlations physics in general.

Here we take the opposite approach of designing a real material which has the Hamiltonian of a 'single-band Hubbard model' material using first-principles electronic structure theory. By combining crystal field splitting with chemistry, we engineer a class of candidate materials with a single d-electron band at the Fermi level. We report the results of ab initio calculations of the electronic and magnetic structure of these new designer materials and discuss the possibilities for experimental synthesis.

TT 10.5 Mon 11:45 H36

**The stability of Bi-Sb-Te layered structures: a first-principles study** — •Kirsten Govaerts[1], Marcel H.F. Sluiter[2], Bart Partoens[3], and Dirk Lamoen[1] — [1]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium — [2]Department of Materials Science and Engineering, 3mE, Delft University of Technology, Mekelweg 2, 2628 CD, Delft, The Netherlands — [3]CMT group, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium

Using an effective one-dimensional cluster expansion in combination with first-principles electronic structure calculations we have studied the energetics and electronic properties of Bi-Sb-Te layered systems. Our modified, quintuple based cluster expansion explicitly accounts for the Bi and Sb bilayer formation which is due to a Peierls instability. With this new method, groundstates of Bi-Sb-Te can be found without making the dataset of ab initio calculated structures unreasonably large. Groundstates are found within the binary alloys X-Te, with X corresponding to Bi or Sb, for a Te concentration between 0 and 60 at.%. They form an almost continuous series of (meta)stable structures consisting of consecutive X bilayers next to consecutive $X_2Te_3$ units. Another binary groundstate is the BiSb structure, consisting of alternating Bi and Sb layers, again forming pairs. Groundstates of ternary compounds all consist of consecutive units of $Bi_2Te_3$, $Sb_2Te_3$ and TeSbTeBiTe.

TT 10.6 Mon 12:00 H36

**RPA Correlation Potential in the Adiabatic Connection Fluctuation-Dissipation formalism** — •Stefano de Gironcoli[1], Nicola Colonna[1], and Ngoc Linh Nguyen[1,2] — [1]Scuola Internazionale Superiore di Studi Avanzati (SISSA), via Bonomea 265, I-34136 Trieste, Italy — [2]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH)

Calculations of correlation energies within the formally exact Adiabatic Connection Fluctuation-Dissipation (ACFD) formalism, within the Random Phase Approximation (RPA) for the exchange-correlation kernel, have been recently carried out for a number of isolated and condensed systems. The efficiency of such calculations has been greatly improved by exploiting iterative algorithms to diagonalize RPA dielectric matrices [1]. However for several systems correlation energies may significantly depend about the choice of input single particle wavefunctions [2]. We derive an expression for the RPA self-consistent potential based on Density Functional Perturbation theory and we present self-consistent RPA calculations for weakly bound molecular dimers, including the controversial case of Beryllium dimer. In this case the self-consistent determination of RPA potential is crucial to determine the stability of the system which however results to be unstable toward dissociation in separated fragments.

[1] H.-V. Nguyen and S. de Gironcoli, Phys. Rev. B 79, 205114 (2009); H. F. Wilson, F. Gygi, and G. Galli, Phys. Rev. B 78, 113303 (2008).

[2] Huy-Viet Nguyen and G.Galli, J. Chem.Phys. 132, 044109 (2010).

TT 10.7 Mon 12:15 H36

**The bond-breaking and bond-making puzzle: many-body perturbation versus density-functional theory** — •F. Caruso[1], D. Rohr[2], M. Hellgren[3], X. Ren[1], P. Rinke[1], A. Rubio[4,1], and M. Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Rice University, Houston, USA — [3]SISSA, Trieste, Italy — [4]Universidad del Pais Vasco, Donostia, Spain

Diatomic molecules at dissociation provide a prototypical situation in which the ground-state cannot be described by a single Slater determinant. For the paradigmatic case of $H_2$-dissociation we compare state-of-the-art many-body perturbation theory in the *GW* approximation and density-functional theory (DFT) in the exact-exchange plus random-phase approximation for the correlation energy (RPA). Results from the recently developed renormalized second-order perturbation theory (rPT2) are also reported. For an unbiased comparison and to prevent spurious starting point effects both RPA and *GW* are iterated to *full* self-consistency (i.e. sc-RPA and sc-*GW*). Both include topologically identical diagrams for the exchange and correlation energy but are evaluated with a non-interacting Kohn-Sham and an interacting *GW* Green function, respectively. This has profound consequences for the kinetic and the correlation energy. *GW* and rPT2 are both accurate at equilibrium, but fail at dissociation, in contrast to sc-RPA. This failure demonstrates the need of including higher order correlation diagrams in sc-*GW*. Our results indicate that RPA-based DFT is a strong contender for a universally applicable electronic-structure theory. F. Caruso *et al.* arxiv.org/abs/1210.8300.

TT 10.8 Mon 12:30 H36

**Density-Functional Theory Applied to Rare Earth Metals: Approaches Based on the Random-Phase Approximation** — •Marco Casadei[1], Xinguo Ren[1], Patrick Rinke[1], Angel Rubio[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]University of the Basque Country UPV/EHU, Donostia, Spain

The description of the volume collapse exhibited by some *rare earth* metals poses a great challenge to density-functional theory (DFT) since local/semilocal functionals (LDA/GGA) fail to produce the associated phase transitions. We approach this problem by treating all electrons at the same quantum mechanical level, using both hybrid functionals (e.g. PBE0 and HSE06) and exact-exchange plus correlation in the random-phase approximation (EX+cRPA). We also assess the performance of recently developed beyond RPA schemes (e.g. rPT2 [1]).

The calculations are performed for cerium and praseodymium, that display a volume collapse, and neodymium, in which the volume collapse is absent. The isostructural $\alpha$-$\gamma$ phase transition in cerium is the most studied. The exact exchange contribution in PBE0 and HSE06 is crucial to produce two distinct solutions that can be associated with the $\alpha$ and $\gamma$ phases, but quantitative agreement with the extrapolated phase diagram requires EX+cRPA [2]. [1] Ren *et al.*, J. Mater. Sci. **47**, 7447 (2012). [2] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

TT 10.9 Mon 12:45 H36

**Thermodynamics of the $\alpha \rightleftharpoons \gamma$ transition in cerium from first principles** — •Jordan Bieder and Bernard Amadon — CEA, DAM, DIF, F-91297 Arpajon, France

The Dynamical Mean Field Theory (DMFT) combined with density functional theory has been successful to describe strongly correlated materials [1]. However, the computation of the ground state properties requires a good accuracy from both the DFT and the DMFT side. We use thus a strong coupling Continuous Time Quantum Monte Carlo (CT-QMC) solver, which is fast and able to reach low temperatures, in combination with a projector augmented wave (PAW) DMFT implementation.

Extensive calculations using this implementation allows us to carefully reassess the ground state properties and thermodynamics of the $\alpha \rightleftharpoons \gamma$ phase transition in Cerium at low temperatures. In particular, stochastic noise is small enough to avoid any ambiguity on the interpretation of energy versus volume curves. The DMFT picture is put in perspective with recent DFT calculations [2] and recent experimental investigations [3,4].

[1] G. Kotliar *et al.* Rev. Mod. Phys. 78, 865(2006)
[2] M. Casadei *et al.* Phys. Rev. Lett. 109, 146402(2012)
[3] F. Decremps *et al.* Phys. Rev. Lett. 106, 065701(2011)
[4] M. J. Lipp *et al.* Phys. Rev. Lett. 109, 195705 (2012)

TT 10.10 Mon 13:00 H36

**Exciton dispersion in wide-gap insulators: there and back again** — •Francesco Sottile[1,2] and Matteo Gatti[1,2] — [1]LSI, Ecole Polytechnique, Palaiseau, France — [2]European Theoretical Spectroscopy Facility

We present ab initio calculations of exciton dispersion of wide-gap insulators, like LiF and solid Argon. With the help of the Bethe-Salpeter equation (recently extended to describe full coupling finite momentum excitonic effects) we calculate the momentum dispersion of the first low-lying excitons, both visible and dark. Their particular behaviour (the exciton shows up, lower down, shows up again, to finally disapper) is analized with respect to: direction of the momentum dispersion, the coupling effect, real space exciton distribution and many-body interference effects. The results [1] are finally compared with recent inelastic X-ray scattering experiments [2,3] for what concerns LiF, while they constitutes a completely ab initio prediction for solid Ar.

[1] The Bethe-Salpeter calculation are carried out with the EXC code (http://www.bethe-salpeter.org/) [2] P.Abbamonte et al., PNAS 105, 12159 (2008) [3] C.-C. Lee et al. arXiv:1205.4106v1

## TT 11: Graphene -Spin-Orbit Interaction (jointly with DS,HL,MA,O)

Time: Monday 11:30–13:45 Location: H17

TT 11.1 Mon 11:30 H17

**Impurity-induced spin relaxation time in graphene from first principles** — •Dmitry Fedorov[1], Martin Gradhand[2], Sergey Ostanin[1], Igor Maznichenko[3], Arthur Ernst[1], Jaroslav Fabian[4], and Ingrid Mertig[3,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom — [3]Martin-Luther-Universität Halle, Institut für Physik, 06099 Halle, Germany — [4]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

The spin relaxation time of conduction electrons in graphene caused by carbon and silicon impurities is studied by means of our *ab initio* approach, which was recently developed for bulk systems [1] and adapted now for the film geometry. It is found that both the momentum and spin relaxation times are extremely sensitive to the position of the impurities. We show that adatoms provide spin-flip rates 4 to 5 orders of magnitude larger than in-plane impurities. Our results strongly support the adatom-induced extrinsic mechanism of the experimentally observed spin relaxation in graphene [2].

[1] M. Gradhand et al., PRB 81, 020403(R) (2010)
[2] N. Tombros et al., Nature 448, 571 (2007)

TT 11.2 Mon 11:45 H17

**D'yakonov-Perel' spin dephasing in single and bilayer graphene and the role of contact resistance on the spin dephasing time** — Frank Volmer[1,2], Marc Drögeler[1,2], Eva Maynicke[1,2], •Nils von den Driesch[1,2], Tsung-Yeh Yang[1,2], Gernot Güntherodt[1,2], and Bernd Beschoten[1,2] — [1]II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]JARA: Fundamentals of Future Information Technology, 52074 Aachen, Germany

We investigate spin transport in both single and bilayer graphene nonlocal spin-valve devices. Similar to our previous studies on bilayer graphene [1], we observe an inverse dependence of the spin dephasing time on the carrier mobility in our single layer devices indicating the importance of D'yakonov-Perel' like spin dephasing in exfoliated single and bilayer samples.

This general trend is only observed in devices with large contact resistances (>1 k$\Omega$). In contrast, the spin dephasing time is significantly reduced in samples with low ohmic contacts for both single and bilayer graphene indicating that an additional spin dephasing occurs underneath the spin injection and detection electrodes.

This work has been supported by DFG through FOR 912.

[1] T.-Y. Yang *et al.* Phys. Rev. Lett. **107**, 047206 (2011)

TT 11.3 Mon 12:00 H17

**Intrinsic and substrate induced spin-orbit interaction in chirally stacked trilayer graphene** — •Andor Kormanyos and Guido Burkard — University of Konstanz

We present a combined group-theoretical and tight-binding approach to calculate the intrinsic spin-orbit coupling (SOC) in ABC stacked trilayer graphene. We find that compared to monolayer graphene, a larger set of $d$ orbitals (in particular the $d_{z^2}$ orbital) needs to be taken into account. We also consider the intrinsic SOC in bilayer graphene, because the comparison between our tight-binding bilayer results and the density functional computations allows us to estimate the values of the trilayer SOC parameters as well. We also discuss the situation when a substrate or adatoms induce strong SOC in only one of the layers of bilayer or ABC trilayer graphene. Both for the case of intrinsic and externally induced SOC we derive effective Hamiltonians which describe the low-energy spin-orbit physics. We find that at the $K$ point of the Brillouin zone the effect of Bychkov-Rashba type SOC is suppressed in bilayer and ABC trilayer graphene compared to monolayer graphene.

The the combination of group-theoretical and tight-binding approaches can be used to study the spin-orbit interaction in other quasi-two dimensional materials, such as $MoS_2$, as well.

TT 11.4 Mon 12:15 H17

**Long Electron Spin Lifetimes in Armchair Graphene Nanoribbons** — •Matthias Droth and Guido Burkard — University of Konstanz, 78457 Konstanz

Armchair graphene nanoribbons (aGNR) are promising as a host material for electron spin qubits because of their potential for scalability and long coherence times [1]. The spin lifetime $T_1$ is limited by spin relaxation, where the Zeeman energy is absorbed by lattice vibrations [2], mediated by spin-orbit and electron-phonon coupling. We have calculated $T_1$ by treating all couplings analytically and find that $T_1$ can be in the range of seconds for several reasons: (i) Van Vleck cancellation; (ii) weak spin-orbit coupling; (iii) low phonon density; (iv) vanishing coupling to out-of-plane modes due to the electronic structure of the aGNR. Owing to the vanishing nuclear spin of $^{12}$C , $T_1$ is a good measure for overall coherence. These results and recent advances in the controlled production of graphene nanoribbons [3] make this system interesting for classical and quantum spintronics applications.

[1] B. Trauzettel *et al.*, Nature Phys. **3**, 192-196 (2007).
[2] M. Droth and G. Burkard, Phys. Rev. B **84**, 155404 (2011).
[3] X. Zhang *et al.*, arXiv:1205.3516 (2012).

TT 11.5 Mon 12:30 H17

**Tunneling-induced Spin Anisotropy Barrier in Quantum Dot Spin-Valves** — •Michael Hell[1,2], Maciej Misiorny[1,2], and Maarten Wegewijs[1,2,3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich — [2]JARA - Fundamentals of Future Information Technology — [3]Institut für die Theorie der Statistischen Physik, RWTH Aachen, 52056 Aachen

Spintronics employs the two fundamental properties of a each electron: its charge and its spin-dipole moment. However, recent studies indicate that the interplay of these two degrees of freedom does not exhaust the potential of spintronics when approaching the nano-scale: spin correlations between electrons, partly characterized by the spin-anisotropy, provide an independent resource of spin information, which is stored even in a simple ferromagnet and couples to the spin-dipole moment in quantum dots. The interest in spin anisotropy also emerges from the research on single-molecule magnets (SMMs) and magnetic adatoms, in which the transport is controlled by a large spin anisotropy barrier intrinsically generated by strong spin-orbit coupling. In this talk we show that such a spin-anisotropy barrier can be externally induced by the transport of spin-correlations from ferromagnets into a a spin-isotropic interacting quantum dot with large spin S>1/2 and negligible spin-orbit interaction. This proximity-induced spin-anisotropy has the hallmarks of a spintronic exchange-field of a quadrupolar nature, a generalization of the well-established dipolar exchange field. The barrier increases with the tunnel coupling, achieving values comparable to that of SMMs, but with the flexibility of electric and magnetic tuneability.

TT 11.6 Mon 12:45 H17

**First-principles study of the spin-orbit interaction in graphene induced by hydrogen adatoms** — •Martin Gmitra, Denis Kochan, and Jaroslav Fabian — University of Regensburg

We have performed first principles calculations of the spin-orbit coupling effects in hydrogenated graphene structures, for varying hydrogen coverage densities, using the linearized augmented plane wave method as implemented in the FLEUR code. The covalent bonding between the hydrogen and carbon atoms leads to a local structural puckering of graphene sheets, giving rise to an overlap between the Dirac and sigma electrons and a giant enhancement (from roughly 0.01 to 1 meV) of the local spin-orbit interaction. The calculated effects on the band structure and the emerging spin patterns of the electronic states can be well explained by effective Hamiltonian models derived from group theoretical principles.

This work is supported by the DFG SPP 1285, SFB 689, and GRK 1570.

TT 11.7 Mon 13:00 H17

**Theory of the hydrogen adatoms induced spin-orbit coupling in graphene** — •Denis Kochan, Martin Gmitra, and Jaroslav Fabian — University Regensburg

We have analyzed the first-principles data of the electronic structure of hydrogenation in graphene by means of group theory derived effective Hamiltonians. We propose effective models for semihydrogenated graphene as well as for graphene with a single hydrogen adatom. The chemisorption of hydrogen modifies the structural symmetry of the plane graphene in two essential ways—it breaks the pseudospin (sublattice) symmetry and induces rippling. We show that in addition to the Rashba spin-orbit interaction there emerges another spin-orbit field which is induced by the pseudospin inversion asymmetry due to the adatoms. Our realistic effective Hamiltonians should be useful for spin transport and spin relaxation investigations.

This work is supported by DFG SFB689

TT 11.8 Mon 13:15 H17

**Optical properties of hydrogenated graphene from first principles** — •Sebastian Putz, Martin Gmitra, and Jaroslav Fabian — Universität Regensburg, Universitätsstraße 31, 93053 Regensburg

We investigate the effect of hydrogen coverage on the optical properties of single-side hydrogenated graphene from first principles. To account for different degrees of uniform hydrogen coverage we calculate the complex dielectric function for graphene supercells of various size, each containing a single additional H atom. We use the Linearized Augmented Planewave (LAPW) method, as implemented in WIEN2k, to show that the hydrogen coverage strongly influences the complex dielectric function and thus the optical properties of hydrogenated graphene. The absorption coefficient in the visible range, for example, has different characteristic features depending on the hydrogen coverage. This opens up new possibilities of determining the hydrogen coverage of hydrogenated graphene samples in the experiment by contact-free optical absorption measurements.

This work is supported by the DFG GRK 1570.

TT 11.9 Mon 13:30 H17

**Electron scattering and spin polarization at the graphene/Ni(111) interface** — Aran Garcia-Lekue[1], Timofey Balashov[2], Marc Ollé[2], Gustavo Ceballos[2], Andrés Arnau[1,3], Pietro Gambardella[2], Daniel Sánchez-Portal[1,3], and •Aitor Mugarza[2] — [1]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 San Sebastian, Spain — [2]Catalan Institute of Nanotecnology (ICN), UAB Campus, E-08193 Bellaterra, Spain — [3]Centro de Fisica de Materiales CFM - MPC, Centro Mixto CSIC-UPV, Apdo. 1072, San Sebastian, Spain

The interaction of graphene with a metal often perturbs the unique electronic properties of Dirac electrons in graphene. This interaction can be positively exploited to engineer the Dirac bands and obtained graphene interfaces with different functionalities. In this work we study the electronic properties of graphene nanoislands grown on Ni(111) [1] by combining scanning tunnelling microscopy and ab-initio calculations. We show that the interaction with the Ni surface opens a gap and spin-polarizes the Dirac bands, which results in a spin filtering effect in the transport across the interface [2]. On the other hand, the standing wave pattern created around the nanoislands reveal an asymmetric potential that depends both on the spin and edge type, suggesting a lateral 2D spin-filter effect similar to that occurring across the interface.

[1] M. Olle et al. Nano Lett. 12, 4431 (2012). [2] V. M. Karpan et al. Phys. Rev. Lett. 99, 176602 (2007).

## TT 12: Poster Session Superconductivity

Time: Monday 15:00–19:00 Location: Poster D

TT 12.1 Mon 15:00 Poster D

**Detector development for a neutrino mass determination using the $^{163}$Ho electron capture spectrum** — •P. Ranitzsch, M. Wegner, S. Kempf, L. Gamer, J. Geist, D. Hengstler, M. Krantz, E. Pavlov, C. Pies, S. Schäfer, S. Uhl, T. Wolf, A. Fleischmann, C. Enss, and L. Gastaldo — Kirchhoff-Institute for Physics, Heidelberg University

The absolute scale of the neutrino mass eigenstates is one of the puzzles in modern particle physics and can be directly investigated using electroweak decays. In the context of the ECHO collaboration we are developing metallic magnetic calorimeters (MMCs) to be used with an internal $^{163}$Ho source to measure its electron capture (EC) spectrum.

MMCs are calorimetric particle detectors with paramagnetic temperature sensor operated below 100 mK. The sensor converts the temperature rise of the detector, due to the absorption of an energetic particle, to a change of magnetization which is detected by a SQUID magnetometer. MMCs fulfill the requirements for cryogenic neutrino mass investigations, namely an energy resolution $\Delta E_{\mathrm{FWHM}}$ below 2 eV and pulse formation times of $\tau < 1\,\mu$s, as recently obtained with microfabricated MMCs for soft X-ray detection.

We present the calorimetric measurement of the EC spectrum of $^{163}$Ho obtained with our first detector prototype. We discuss the development of a 64 pixel array readout.

TT 12.2 Mon 15:00 Poster D

**Metallic magnetic calorimeters for high resolution x-ray spectroscopy - Latest results from maXs-20 and maXs-200** — •Mathäus Krantz, Sönke Schäfer, Christian Pies, Daniel Hengstler, Simon Uhl, Sebastian Georgi, Sebastian Heuser,

Thomas Wolf, Sebastian Kempf, Loredana Gastaldo, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Uni Heidelberg, INF 227, 69120 Heidelberg

We are developing metallic magnetic calorimeters (MMC) for high resolution x-ray spectroscopy on highly charged ions in the energy range up to 200keV. MMCs use a paramagnetic temperature sensor, read-out by a SQUID, to measure the energy deposited by single x-ray photons. The recently micro-fabricated and tested prototypes include two linear 8-pixel detector arrays, maXs-20 and maXs-200, optimized for energies up to 20 keV and 200 keV, respectively. We discuss the physics of MMCs, design considerations concerning thermal and electro-magnetic cross talk, and the micro-fabrication. maXs-200 with its $1mm^2$ large and 200 $\mu$m thick absorbers made of electro-deposited gold has high stopping power for hard x-rays and achieves an energy resolution of 40-60 eV (FWHM). maXs-20 with its $250\mu m \times 250$ $\mu$m large and 5 $\mu$m thick absorbers has a stopping power of 98% for 6 keV photons and presently achieves an experimental line width of 3,3 eV (FWHM), with a signal rise time of 90 ns and excellent linearity. We are presently operating maXs-20 at an electron-beam-ion-trap at the MPI-K Heidelberg and will report on first atomic physics measurements as well as the particular challenges to detector operation in the vicinity of the EBIT.

TT 12.3 Mon 15:00 Poster D

**Development of a large-area detector for position and energy resolving detection of molecular fragments** — •L. Gamer, A. Fleischmann, L. Gastaldo, A. Kampkötter, S. Kempf, C. Pies, P. Ranitzsch, S. Schäfer, T. Wolf, and C. Enss — Kirchhoff Institute for Physics, Heidelberg University.

To investigate reactions like the dissociative recombination in laboratory environment, the Max-Planck Institute for Nuclear Physics in Heidelberg is presently building a cryogenic storage ring to prepare molecular ions in their rotational groundstate. The full kinematics of these processes can be resolved by a position and energy sensitive detection of the reaction products/molecule fragments.

We describe the development of a large-area MMC for position sensitive detection of massive particles with kinetic energies of a few keV. The detector encompasses sixteen slice-shaped large-area absorbers to form a circular whole with a diameter of 36 mm. The temperature sensor is positioned on the outer edge of each absorber. Due to the finite thermal diffusivity in the absorber material, the rise-time of the detector-signal depends on the impact location of the particle.

We compare a numerical analysis for the energy and position dependence of the detector signal to results of recent test measurements where energy was deposited at different positions by LED light pulses as well as x-ray photons delivered by an $^{55}$Fe source. For massive particles, potential degradation of instrumental line width as well as energy losses by backscattering, sputtering and lattice damages are discussed using Monte Carlo simulations.

TT 12.4 Mon 15:00 Poster D

**Superconducting nanowire single-photon detectors (SNSPDs) on SOI for near-infrared range** — •Philipp Trojan[1], Konstantin Ilin[1], Dagmar Henrich[1], Matthias Hofherr[1], Steffen Dörner[1], Alexey Semenov[2], Heinz-Wilhelm Huebers[2,3], and Michael Siegel[1] — [1]Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie (KIT) — [2]Institut für Planetenforschung, DLR, Berlin-Adlershof — [3]Institut für Optik und Atomare Physik, Technische Universität Berlin

Superconducting nanowire single-photon detectors are promising devices for photon detectors with high count rates, low dark count rates and low dead times. At wavelengths beyond the visible range, the detection efficiency of today's SNSPDs drops significantly. Moreover, the low absorption in ultra-thin detector films is a limiting factor over the entire spectral range.

Solving this problem requires approaches for an enhancement of the absorption range in feeding the light to the detector element.

A possibility to obtain a better absorption is the use of multilayer substrate materials for photonic waveguide structures.

We present results on development of superconducting nanowire single-photon detectors made from niobium nitride on silicon-on-insulator (SOI) multilayer substrates. Optical and superconducting properties of SNSPDs on SOI will be discussed and compared with the characteristics of detectors on common substrates.

TT 12.5 Mon 15:00 Poster D

**Self-Planarized Process for the Fabrication of Josephson Junction Devices** — •Michael Merker, Johannes Maximilian Meckbach, Simon Buehler, Konstantin Il'in, and Michael Siegel — Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie (KIT), Germany

High performance Josephson junction (JJ) devices require good control of lateral dimensions. Various JJ devices can benefit from sub-$\mu$m feature sizes. In our conventional Nb/Al-$AlO_x$/Nb process, the minimum feature size is however limited by the step height of the layers beneath. In order to overcome this constraint, we refined our process, resulting in almost flat surfaces at intermediate processing steps without the need for time consuming chemical-mechanical polishing (CMP). Sub-$\mu$m feature sizes can be achieved using electron beam lithography (EBL). Due to the application of mix & match lithography, (combination of EBL and photolithography), the turn-around time is not increased significantly compared to our conventional process.

Transport properties of sub-$\mu$m JJs at 4.2 K will be presented. Our JJ process yields excellent quality parameters with sub-$\mu$m feature sizes even in the third metal layer, and is therefore very promising for fabricating sub-$\mu$m JJs for quantum devices such as SQUIDs or receiver devices.

TT 12.6 Mon 15:00 Poster D

**Quasi-optical THz spectroscopy on ultra-thin superconducting films of NbN and TaN.** — •Uwe Santiago Pracht[1], Eric Heintze[1], Marc Scheffler[1], Martin Dressel[1], Konstantin Il'in[2], Dagmar Henrich[2], Qiao Guo[2], and Michael Siegel[2] — [1]1. Physikalisches Institut, University of Stuttgart, Germany — [2]Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie (KIT), Germany

Ultra-thin films of the conventional superconductors niobium nitride (NbN) and tantalum nitride (TaN) have recently attracted attention for devices such as single-photon detectors. Quasi-optical THz spectroscopy is a particularly suited tool with direct access to superconducting properties, such as the superconducting energy gap, which are necessary for a proper understanding of device performance and for future improvements.

With our THz-spectroscopy approach we measure amplitude and phaseshift of coherent radiation (0.09-1.2 THz) passing through thin-film systems. We present the performance and possibilities of our experimental set-up, and we apply it to ultra-thin superconducting films of NbN and TaN. We fit the experimental data to weak-coupling BCS theory, and we obtain frequency- and temperature-dependent superconducting properties such as the complex optical conductivity, the complex dielectric function, the energy gap, the penetration depth, and the superfluid density.

TT 12.7 Mon 15:00 Poster D

**Niobium Nitride Technology for Josephson Junction Devices** — •Johannes Maximilian Meckbach[1], Michael Merker[1], Konstantin Il'in[1], Andreas Häffelin[2], and Michael Siegel[1] — [1]Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie (KIT), Hertzstrasse 16, 76187 Karlsruhe, Germany — [2]Institut für Werkstoffe der Elektrotechnik (IWE), Karlsruher Institut für Technologie(KIT), Adenauerring 20b, 76131 Karlsruhe, Germany

Over the last decades Nb/Al-$AlO_x$/Nb multi-layers have been the primary choice for Josephson junction (JJ) devices such as SIS mixers, SQUIDs and RSFQ. Various applications require high critical-current densities $j_c$ and low sub-gap leakage. Additionally, a large gap-voltage benefits the performance of most devices. Nb/Al-$AlO_x$/Nb technology is limited in $j_c$ due to an increasing transparency of the barrier with increasing $j_c$, and the energy-gap of the Nb electrodes poses an upper frequency limit for SIS mixers.

NbN/AlN/NbN multi-layer technology has emerged as an alternative to Nb/Al-$AlO_x$/Nb. The upper frequency limit of NbN-based SIS mixing element significantly exceeds that of Nb, and AlN-barriers result in higher $j_c$'s at identical thicknesses as compared to $AlO_x$.

We have developed an *in-situ* fabrication technology for NbN/AlN/NbN multi-layers. We found a clear influence of the sputter parameters on the surface morphology of the NbN electrodes, which directly impacts on the quality of the JJs. Transport properties of JJs on different substrates will be presented.

TT 12.8 Mon 15:00 Poster D

**Towards long lived tunable transmon qubit in microstrip geometry** — •Jochen Braumüller, Lucas Radtke, Hannes Rotzinger, Martin Weides, and Alexey V. Ustinov — Karl-

sruhe Institute of Technology (KIT), Physikalisches Institut, 76131 Karlsruhe, Germany

Qubits constitute the main building blocks of a prospective quantum computer. One main challenge is given by short decoherence times. In this work we investigate a transmon qubit based on a superconducting charge qubit with reduced sensitivity to charge noise. This is achieved by operating the qubit at a Josephson to charging energy ratio of about 100. At the same time, a sufficiently large anharmonicity of the energy levels is preserved. The qubit is realized in a 2D geometry based on large capacitor pads being connected by two Josephson junctions in parallel. This split Josephson junction allows the qubit to be tunable in Josephson energy and therefore in resonance frequency. The large area capacitor pads mainly coupled through the substrate and a backside metalization reduce the surface loss contribution. Manipulation and readout of the qubit is mediated by a microstrip resonator coupled to a feedline. We will present resonator and qubit designs together with respective microwave simulations. Preliminary results on circuit fabrication and low temperature measurements will also be discussed.

TT 12.9 Mon 15:00 Poster D

**Quantum behavior of a SQUID qubit manipulated with fast pulses** — •Samuele Spilla[1], Maria Gabriella Castellano[2], Fabio Chiarello[2], Antonino Messina[1], Rosanna Migliore[3], and Anna Napoli[1] — [1]Dipartimento di Fisica dell'Università di Palermo, Via Archirafi 36, 90123 Palermo, Italy — [2]Istituto Fotonica e Nanotecnologie - CNR, Roma, Italy — [3]Institute of Biophysics, National Research Council, via Ugo La Malfa 153, 90146 Palermo, Italy

A SQUID qubit manipulated with fast variation of the energy potential is analyzed. Varying the potential shape from a single to a double-well configuration, quantum behaviors are brought into light and discussed. We show that the presence of quantum coherences in the initial state of the system plays a central role in the appearance of these quantum effects.

TT 12.10 Mon 15:00 Poster D

**Dynamical Coulomb Blockade: From bumpy oscillations to elevator rides** — •Selina Rohrer, Vera Gramich, Björn Kubala, Jürgen T. Stockburger, and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Recently the photonic side of the dynamical coulomb blockade was explored by measuring the emitted radiation of a dc voltage-biased Josephson junction embedded in a microwave resonator [1]. In order to gain a better understanding of the strong coupling case, we investigate the classical (typically chaotic) dynamics of the system. Extending this dynamics to a Langevin-type description, well-defined dynamical steady states are obtained.

In addition to limit cycles with the Josephson frequency $\omega_J$, we observe marginally damped cycles at subharmonics as well as bifurcations. For very strong coupling between resonator and Josephson junction highly structured, asymmetric limit cycles at low frequencies are observed, which can intuitively be interpreted as "elevator-like" dynamics.

[1] M. Hofheinz et al., PRL 106, 217005 (2011)

TT 12.11 Mon 15:00 Poster D

**Observation of Andreev bound states at spin-active interfaces** — •Detlef Beckmann[1], Florian Hübler[1,2], Michael Johannes Wolf[1], and Hilbert von Löhneysen[2,3] — [1]KIT, Institut für Nanotechnologie — [2]KIT, Institut für Festkörperphysik — [3]KIT, Physikalisches Institut

We report on high-resolution differential conductance experiments on nanoscale superconductor/ferromagnet tunnel junctions with ultrathin oxide tunnel barriers. We observe subgap conductance features which are symmetric with respect to bias, and shift according to the Zeeman energy with an applied magnetic field. These features can be explained by resonant transport via Andreev bound states induced by spin-active scattering at the interface. From the energy and the Zeeman shift of the bound states, both the magnitude and sign of the spin-dependent interfacial phase shifts between spin-up and spin-down electrons can be determined. These results contribute to the microscopic insight into the triplet proximity effect at spin-active interfaces.

[1] F. Hübler et al., Phys. Rev. Lett. **109**, 087004 (2012).

TT 12.12 Mon 15:00 Poster D

**Dynamical Coulomb blockade of the nonlocal conductance in normalmetal/superconductor hybrid structures** — •Stefan Kolenda, Michael J. Wolf, and Detlef Beckmann — Institut für Nanotechnologie, KIT, 76021 Karlsruhe, Germany

In normalmetal/superconductor hybrid structures nonlocal conductance is determined by crossed Andreev reflection (CAR) and elastic cotunneling (EC). This was investigated recently both experimentally and theoretically ([1], [2] and references therein). Dynamical Coulomb blockade of EC and CAR was predicted theoretically in [2]. Here we report on experimental investigations of these effects. We found signatures of dynamical Coulomb blockade in local and nonlocal conductance in the normal state. In the superconducting state, we find s-shaped nonlocal differential conductance curves as a function of bias applied on both contacts, as predicted in [2]. These curves were observed for bias voltages both below and above the gap. We compare our results to theory.

[1] J. Brauer et al., Phys. Rev. B **81**, 024515 (2010)
[2] D.S. Golubev and A.D. Zaikin, Phys. Rev. B **82**, 134508 (2010)

TT 12.13 Mon 15:00 Poster D

**Electron entanglement in Cooper pair beam splitter with magnetic fields** — •Stephan Weiss[1], Jürgen König[1], and Yuval Gefen[2] — [1]Universität Duisburg-Essen and CENIDE, 47048 Duisburg — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel

We develop a theory that suggests the efficient manipulation of entangled electrons provided by a Cooper pair beam splitter. The splitting of coherent electrons forming a spin singlet is present if the superconductor is tunnel coupled to a double quantum dot [1]. In order to probe entanglement, we allow for an inhomogeneous and, in general, non-collinear magnetic field. If the DQD-SC system is embedded in a transport setup, non-local current and noise properties are obtained within the real-time diagrammatic method [2]. As a small parameter we use the hybridization between splitter and normal leads. The tunnel coupling to the superconductor is taken into account nonperturbatively. Furthermore, we provide a detailed investigation of the violation of Bell's inequality for various parameter regimes.

[1] J. Eldridge, M. Governale, and J. König, Phys. Rev. B **82** 184507, (2010)
[2] M. Governale, M. Pala, and J. König, Phys. Rev. B **77** 134513, (2008)

TT 12.14 Mon 15:00 Poster D

**Manifestly Non-Gaussian Fluctuations in Superconductor-Normal Metal Tunnel Nanostructures** — •Matti Laakso[1,2], Tero Heikkilä[2], and Yuli Nazarov[3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Aachen, Germany — [2]Low Temperature Laboratory, Aalto University, Espoo, Finland — [3]Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands

Recently, temperature fluctuation statistics has been studied in non-interacting islands [1] and overheated single-electron transistors [2]. We propose [3] a mesoscopic setup which exhibits strong and manifestly non-Gaussian fluctuations of energy and temperature when suitably driven out of equilibrium. The setup consists of a normal metal island (N) coupled by tunnel junctions (I) to two superconducting leads (S), forming a SINIS structure, and is biased near the threshold voltage for quasiparticle tunneling, $eV \approx 2\Delta$. The fluctuations can be measured by monitoring the time-dependent electric current through the system, which makes the setup suitable for the realization of feedback schemes which allow to stabilize the temperature to the desired value.

[1] T.T. Heikkilä and Y.V. Nazarov, Phys. Rev. Lett. **102**, 130605 (2009)
[2] M.A. Laakso, T.T. Heikkilä, Y.V. Nazarov, Phys. Rev. Lett. **104**, 196805 (2010)
[3] M.A. Laakso, T.T. Heikkilä, Y.V. Nazarov, Phys. Rev. Lett. **108**, 067002 (2012)

TT 12.15 Mon 15:00 Poster D

**Resummation approach to interacting quantum dots in contact with superconducting leads** — David Futterer[1], •Jacek Swiebodzinski[1], Michele Governale[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand

The simultaneous occurrence of Coulomb interactions and superconducting correlations combined with a possible non-equilibrium situation makes interacting quantum dots (QD) that are coupled to superconductors a fascinating field of research. To account for all these features in a theoretical description proves however challenging and one has to resort to specific approximations or numerically demanding solving schemes. Here, we consider a QD coupled to one normal and two superconducting leads. We first calculate the transport properties of the system using a perturbative expansion in the dot-normal reservoir coupling. We allow for a finite superconducting gap $\Delta$ by performing a $1/\Delta$ expansion. We then introduce an approach based on partial resummation of diagrams to infinite order in the coupling and calculate the Andreev bound states of the system. The results on the latter show very good agreement with those obtained by the computationly more demanding numerical renormalization group method.

TT 12.16 Mon 15:00 Poster D

**Subgap-anomalies in 3-terminal hybrid superconductor/ normal metal nanostructures** — •Andreas H. Pfeffer[1,2], Hervé Courtois[3], and François Lefloch[1] — [1]CEA/INAC/SPSMS, Grenoble, France — [2]Nanoscience Foundation (RTRA), Grenoble, France — [3]CNRS/Néel Institute and UJF, Grenoble, France

We have studied the electronic transport properties of three terminal superconductor (S) - normal metal (N) - superconductor (S) nanodevices using a new SQUID-based experimental set-up working at very low temperature (30 mK) and dedicated for high sensitive conductance and current noise correlations measurements [1,2]. In a geometry where a T-shaped normal metal (Cu) is connected to three superconducting reservoirs (Al), new subgap anomalies appear in the differential conductance for specific values of the chemical potential applied to the superconductors. The most emphasized line appears when two superconductors (collectors) are biased at opposite voltage with respect to the third superconducting electrode (injector). This anomaly is consistent with the prediction of non-local quartets as the result of double crossed Andreev reflections (dCAR) [3]. In this particular process, a Cooper pair originating from the injector is split in two quasiparticles that recombine into Cooper pairs in each of the two collectors. Additional features appear for other integer voltage ratios and could be attributed to higher order processes of dCAR. The mechanism of non-local quartet opens perspectives toward a new generation of entanglers.

[1] PRL **107**, 077005 (2011)
[2] RSI **83**, 115107 (2012)
[3] PRL **106**, 257005 (2011)

TT 12.17 Mon 15:00 Poster D

**Magnetization-Orientation Dependence of the Superconducting Transition in AF-F/S/F and S/F/F-AF Type Spin Valve Heterostructures** — •Vladimir Zdravkov[1,2], Daniel Lenk[1], Jan Kehrle[1], Günter Obermeier[1], Aladin Ullrich[1], Claus Müller[1], Hans-Albrecht Krug von Nidda[1], Roman Morari[2], Anatoli Sidorenko[2], Lenar Tagirov[3], Siegfried Horn[1], and Reinhard Tidecks[1] — [1]Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany — [2]D. Ghitsu Institute of the Electronic Engineering and Nanotechnologies ASM, MD 2028 Kishiniev, Moldova — [3]Solid State Physics Department, Kazan Federal University, 420008 Kazan, Russia

In F/S/F spin valve core structures, i.e. $Cu_{41}Ni_{59}/Nb/Cu_{41}Ni_{59}$ systems, deposited on an antiferromagnetic CoOx layer, or with such a layer on top, critical temperature oscillations and reentrant superconductivity are observed, which can be well described by the theory. Introducing a Co sub-layer yields exchange bias effects, which influence the magnetic field dependence of the superconducting transition. Aging effects are studied, which especially alter the transparency of the lower F/S interface, resulting in a change of the behavior of the transition temperature as a function of the ferromagnetic layer thickness from extinction, over reentrant, to oscillating.

The results are discussed in comparison to the S/F/F-AF triplet spin valve effect in a $Nb/Cu_{41}Ni_{59}$/nc-Nb/Co/$CoO_x$ system, where nc-Nb acts as a normal conducting spacer to decouple the ferromagnetic layers.

TT 12.18 Mon 15:00 Poster D

**Size dependence of the electric transport properties of thin TiN-films at the superconducting side of the SIT** — •Klaus Kronfeldner[1], Tatyana Baturina[2], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]A. V. Rzhanov Institute of Semiconductor Physics SB RAS, Novosibirsk 630090, Russia

We investigate the electric transport at the superconducting side of the superconductor-insulator transition (SIT) in square-shaped thin TiN-films and its dependence on their lateral size. The resistance at room temperature was tuned by heating up the sample in air, in order to approach the SIT. We revealed a size-dependent magnetoresistance. For the smaller samples a very small magnetic field is sufficient to induce a finite resistance. The larger samples remain superconducting nearly up the nominal critical field ($B \approx 2.8T$) of the TiN-material.

TT 12.19 Mon 15:00 Poster D

**Nonequilibrium Dynamics of Nanoscaled Superconductors** — •Peter Kettmann[1], Thomas Papenkort[1], Mihail Croitoru[2], Vollrath Martin Axt[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10 — [2]Theoretische Physik III, Universität Bayreuth

We theoretically investigate the nonequilibrium dynamics of nanoscaled superconductors. The excitation is achieved by a change of the coupling constant of the electrons. The dynamics are calculated using the Bogoliubov-de Gennes equation for inhomogeneous superconductors. When studying systems that are strongly confined in all three spatial directions we find that the order parameter, the central quantity of the superconductor, oscillates in time. This oscillation consists of many discrete frequencies which mainly correspond to the eigenenergies of the quasiparticles of the system. By increasing the size of the superconductor in one direction we show that the dynamics becomes similar to the one known from the homogeneous case. This is given by a damped oscillation of the order parameter with one collective mode [1]. By using a linear approximation of the equations of motion we show that this behavior can be explained in terms of a sum of independent oscillators dephasing in time.

[1] Papenkort et al., PRB 78, 132505 (2008)

TT 12.20 Mon 15:00 Poster D

**Quasiparticle interference in non-centrosymmetric superconductors** — •Johannes Hofmann[1,2], Raquel Queiroz[1], Andreas P. Schnyder[1], and Dirk Manske[1] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]Julius-Maximilians-Universität Würzburg, Würzburg, Germany

Motivated by recent point contact Andreev reflection measurements on BiPd [1], we study the appearance of topologically protected surface states in non-centrosymmetric superconductors. We determine the signatures of these surface states in quasiparticle interference experiments and show that Fourier transform scanning tunneling spectroscopy (FT-STS) can give direct information about the momentum-space structure of these surface states. In particular, we find that FT-STS allows to distinguish among different types of topological surface states, such as zero-energy flat bands, arc surface states, and helical Majorana modes [2-4]. We investigate non-centrosymmetric superconductors with different point-group symmetries and consider both non-magnetic and magnetic impurity scatterers. In the case of non-magnetic s-wave scatterers, a simple interperation of the quasiparticle interference pattern in terms of the joint density of states is derived.

[1] M. Mondal et al., Phys. Rev. B 86, 094520 (2012).
[2] A. P. Schnyder and S. Ryu, Phys. Rev. B 84, 060504(R) (2011).
[3] P. M. R. Brydon, A. P. Schnyder, and C. Timm, Phys. Rev. B 84, 020501(R) (2011)
[4] A. P. Schnyder, P. M. R. Brydon, and C. Timm, Phys. Rev. B 85, 024522 (2012).

TT 12.21 Mon 15:00 Poster D

**Coulomb interaction in Eliashberg theory of superconductivity.** — •Arkady Davydov and Antonio Sanna — Max-Planck-Institute of Microstructure Physics, Halle (Saale), Germany

The Eliashberg theory [1] of superconductivity allows to describe materials with strong pairing interaction. In the non magnetic case it leads to a system of coupled integral multidimensional equations. Computational costs are usually reduced by an isotropic limit [2], and by restricting the Coulomb interaction to the use of one single parameter, $\mu^*$, often chosen to give the experimental $T_c$. In this work we present the parameter-free approach in which the screened Coulomb interaction fully accounted within the Random Phase Approximation, entering the Eliashberg's equations on the same footing as the phononic interaction. We will compare this approach with Density Functional Theory for Superconductors [3, 4] where the corresponding approxi-

mation leads to a good agreement with experiments.

[1] G.M. Eliashberg, Sov. Phys. JETP 11, 696 (1960)
[2] D.J. Scalapino, Phys. Rev. 148, 263 (1966)
[3] L.N. Oliveira, E.K.U. Gross, Phys. Rev. Lett. 60, 2430 (1988)
[4] M. Lüders, PRB 72, 024545 (2005)

TT 12.22 Mon 15:00 Poster D

**Nematic quantum critical behaviors in high-temperature supreconductors** — •Jing Wang[1,2], Guo-Zhu Liu[1], Jing-Rong Wang[1,3], and Hagen Kleinert[4] — [1]University of Science and Technology of China, Hefei, China — [2]Max Planck Institute, Stuttgart, Germany — [3]Max Planck Institut, Dresden, Germany — [4]Freie Universität Berlin, Berlin, Germany

In the past decade, there have been a number of experimental signatures pointing towards the presence of electronic nematic phase in some high-temperature superconductors [1]. On the basis of these experiments, a nematic quantum phase transition is expectd to exist in the d-wave superconducting dome [2,3]. The critical nematic fluctuation interacts strongly with the gapless nodal quasiparticles, which leads to highly unusual properties. We examine the stability of the nematic quantum critical point against various quenched disorders by means of renormalization group approach [4,5]. We also study the influence of critical nematic fluctuation on some observable quantities, and predict that superconductivity is suppressed at the nematic quantum critical point [4,5].

[1] E. Fradkin et al., Annu. Rev. Condens. Matter Phys. 1, 153 (2010)
[2] E.-A. Kim et al., Phys. Rev. B 77, 184514 (2008)
[3] Y. Huh and S. Sachdev, Phys. Rev. B 78, 064512 (2008)
[4] J. Wang, G.-Z. Liu, and H. Kleinert, Phys. Rev. B 83, 214503 (2011)
[5] G.-Z. Liu, J.-R. Wang, and J. Wang, Phys. Rev. B 85, 174525 (2012)

TT 12.23 Mon 15:00 Poster D

**In-plane upper critical field of d-wave superconductors** — •Wang Jing-Rong[1,2], Liu Guo-Zhu[1], Ribeiro Pedro[2], and Kirchner Stefan[2,3] — [1]Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Determining the full gap symmetry of unconventional superconductors is an important but difficult task. One experimental method to determine the gap symmetry is to measure the angular dependence of the in-plane upper critical field. Due to their large effective mass, heavy fermion superconductors are usually Pauli limited but also orbital coupling contributes to $H_{c2}$. Recent experiments on $CeCu_2Si_2$ indicate that the in-plane upper critical field exhibits a number of interesting behaviors. Motivated by these experiments, we systematically study the angular independence of the upper critical field including both orbital coupling and Zeeman coupling. We compare our theoretical results with the relevant experiments[1].

[1] H. Vieyra et al. PRL **106**, 207001 (2011).

TT 12.24 Mon 15:00 Poster D

**Eight-band model for iron arsenides: Functional renormalization group study** — •Julian Lichtenstein[1], Stefan Maier[1], and Carsten Honerkamp[1,2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]JARA - Fundamentals of Future Information Technology

We analyze an effective two-dimensional eight-band model [1] for LaOFeAs and SmOFeAs within a functional renormalization group (fRG) approach. Upon varying parameters from LaOFeAs to SmOFeAs, we find an increasing critical scale for superconducting instabilities, while the critical scales of spin-density wave ordering change only by a small amount.

[1] O. K. Andersen and L. Boeri, Ann. Phys. (Berlin) **523**, 8 (2011)

TT 12.25 Mon 15:00 Poster D

**Quasiparticle scattering rates in iron pnictides from the functional renormalization group** — •Guido Klingschat[1], Julian Lichtenstein[1], and Carsten Honerkamp[1,2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - Fundamentals of Future Information Technology

We use a function renormalization group approach [1] to compute the quasiparticle scattering rate in eight-band models [2] for iron pnictide superconductors. This way we obtain the anisotropy and temperature dependences of the scattering rates above the critcial scales towards long-range orderings. We study material-specific variations and compare the scattering rate anisotropies with the predicted gap anisotropies in the superconducting state.

[1] C. Honerkamp, Eur. Phys. J. B **21**, 81 (2001)
[2] O. K. Andersen and L. Boeri, Ann. Phys. (Berlin) **523**, 8 (2011)

TT 12.26 Mon 15:00 Poster D

**Evolution of the multiband RKKY interaction: Application to iron pnictides and chalcogenides** — •Alireza Akbari[1], Peter Thalmeier[1], and Ilya Eremin[2] — [1]Max Planck Institute for the Chemical Physics of Solids, 01187 Dresden, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, 44780, Bochum, Germany

The indirect RKKY interaction in iron pnictide and chalcogenide metals is calculated for a simplified four bands Fermi surface (FS) model. We investigate the specific multi-band features and show that distinct length scales of the RKKY oscillations appear. In the paramagnetic state the interaction is spin isotropic however, in the spin density wave (SDW) phases, the RKKY interaction maps into an effective anisotropic XXZ-type Heisenberg exchange model. The anisotropy originates from the breaking of the spin-rotational symmetry induced by the SDW order and its strength depends on the size of the SDW-gap and the structure of the folded Fermi surface. For the regular lattice of the local moments, the generalized RKKY interaction is defined in momentum space. We consider its momentum dependence in paramagnetic and SDW phases, discuss its implications for the possible type of magnetic order and compare it to the results obtained from more realistic tight-binding type Fermi surface model. Our finding can give important clues on the magnetic ordering of the 4f- iron based superconductors.

[1] A. Akbari, I. Eremin, and P. Thalmeier, Phys. Rev. B 84, 134513 (2011)
[2] A. Akbari, P. Thalmeier, and I. Eremin (Preprint)

TT 12.27 Mon 15:00 Poster D

**Nodal spin density wave in iron-based superconductors** — •Felix Ahn and Ilya M. Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

We analyze the competition of SDW and SC orders in the iron-based superconductors, taking into account the orbital matrix elements. We find that the SDW order necessarily possesses the nodal structure as a result of angular dependence of the Fermi-liquid interactions. To obtain the phase diagram we solve the system of coupled mean-field gap equations, which describes the competition between SDW and s++ or s+− superconductivity. We revisit the result, obtained previously, for the constant SDW gap. We further discuss the role played by the spin-orbit coupling.

TT 12.28 Mon 15:00 Poster D

**Experimental setup for magneto-optical measurements on iron pnictides** — •David Neubauer, Sina Zapf, Shuai Jiang, Dan Wu, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Germany

The role of magnetism for high-$T_c$ superconductivity is still under hot debate. $EuFe_2(As_{1-x}P_x)_2$ is a peculiar member of the iron pnictides, as it shows a local ordering of the $Eu^{2+}$ moments at low temperatures ($\approx$20K) besides the $Fe^{2+}$ spin density wave. This leads to exceptional phenomena such as the re-entrance of superconductivity below the Eu magnetic ordering temperature or field induced superconductivity. Magneto-optical measurements on $EuFe_2(As_{1-x}P_x)_2$ will give further insight to the role magnetism plays on the electronic properties of iron pnictides. We are currently setting up an experiment combining the 12T "Spectromag 4000" (Oxford Instruments) with the "IFS 113v " spectrometer (Bruker). The setup will also allow *in situ* gold evaporation in order to account for surface roughness. We present the overall setup and discuss the design of a stage for optical access to the magnet in Voigt- and Faraday-geometry.

TT 12.29 Mon 15:00 Poster D

**Mössbauer and muon spin relaxation investigation of magnetic and superconducting properties of $Ca_{1-x}Na_xFe_2As_2$** — •Philipp Materne[1], Sirko Bubel[1], Hemke Maeter[1], Rajib Sarkar[1], Luminita Harnagea[2], Sabine Wurmehl[2], Bernd Büchner[2], Hubertus Luetkens[3], and Hans-Henning Klauss[1] —

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The antiferromagnetic parent compound, $CaFe_2As_2$, shows a supression of the spin density wave and a subsequent superconducting state upon partial substitution of Ca by Na. Along the substitution series, superconducting transition temperatures up to ≈35 K were found. We studied the electronic phase diagram of $Ca_{1-x}Na_xFe_2As_2$ using Mössbauer spectroscopy and muon spin relaxation experiments. We have analyzed the data in terms of magnetic and superconducting properties and possible coexistence of superconductivity and spin density wave order. We compared our results with recently published data of $Ba_{1-x}Na_xFe_2As_2$ [1].

[1] H. Maeter *et al.*, arXiv:1210.6881

TT 12.30 Mon 15:00 Poster D

**Ultrasonic investigations on the iron-based superconductor $Ba(Fe_{1-x}Co_x)_2As_2$** — •Stephan Knöner[1], Bernd Wolf[1], Pham Thanh Cong[1], Thomas Wolf[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt (M) — [2]Karlsruhe Institute of Technology, D-76131 Karlsruhe

The simultaneous occurrence of a structural transition and long-range magnetic order in the proximity to the superconducting phase in iron-based superconductors raises the question whether the spin or the lattice degrees of freedom manifest the dominant low-energy excitations in the systems which are relevant for the superconductivity. Based on ultrasonic investigations both scenarios have been discussed in the literature. Ultrasonic experiments on $Ba(Fe_{1-x}Co_x)_2As_2$ showed a huge softening of the transverse elastic constant $c_{66}$ related to the structural tetragonal to orthorhombic/antiferromagnetic phase transition at $T_S/T_N$ and a subsequent hardening upon entering the superconducting state at $T_{sc}$. We present measurements of the $c_{33}$ and $1/2(c_{11}+c_{12}+2c_{66})$-mode together with the ultrasonic attenuation on $Ba(Fe_{1-x}Co_x)_2As_2$ single crystals with $x$=0 and $x$=0.06. In the undoped compound, two, slightly separated, step-like anomalies of nearly similar size, corresponding to the structural/magnetic transition at $T_S/T_N$ are clearly visible in the $c_{33}$-mode. According to our characterization measurements by resistivity and susceptibility, our crystal with $x$=0.06 shows neither a structural nor a magnetic transition but is superconducting at $T_{sc}$=24 K. Here the superconducting transition is visible in the $c_{33}$ as well as in the $1/2(c_{11}+c_{12}+2c_{66})$-mode.

TT 12.31 Mon 15:00 Poster D

**Hydrostatic-Pressure Tuning of Magnetic, Nonmagnetic and Superconducting States in Annealed $Ca(Fe_{1-x}Co_x)_2As_2$** — •Sebastian Köhler[1], Elena Gati[1], Daniel Guterding[1], Stephan Knöner[1], Sheng Ran[2], Sergey L. Bud'ko[2], Paul C. Canfield[2], and Michael Lang[1] — [1]Physikalisches Institut, J.W. Goethe-Universität, SPP 1458, 60438 Frankfurt (Main), Germany — [2]Ames Laboratory, Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

Iron-based superconductors exhibit rich phase diagrams including tetragonal, orthorhombic/antiferromagnetic (o/afm) and superconducting (sc) states. For the $AFe_2As_2$ (122) ($A$ = Ba, Sr and Ca) compounds, yet another, nonmagnetic collapsed-tetragonal (cT) phase has been observed at high pressure. It has been shown that for Co-doped Ca 122 single crystals, a postgrowth thermal treatment at an annealing temperature $T_a$ can be used to tune the ground state of the system [1]. Recently we provided evidence that $T_a$ mimics the effect of hydrostatic pressure by demonstrating that for properly heat-treated $Ca(Fe_{1-x}Co_x)_2As_2$ the salient ground states can be accessed all in one sample by applying small, truly hydrostatic pressure [2]. We present results of electrical resistance and magnetic susceptibility under pressure for this compound with different combinations of $x/T_a$. The obtained $p$-$T$ phase diagrams indicate that preserving fluctuations associated with the o/afm transition to low enough temperatures is vital for sc to form here.

[1] S. Ran et al., Phys. Rev. B **83**, 144517 (2011)
[2] E. Gati et al., arXiv:1210.5398 (2012)

TT 12.32 Mon 15:00 Poster D

**Electronic structure of single-crystalline $Sr(Fe_{1-x}Co_x)_2As_2$ probed by x-ray absorption spectroscopy: Evidence for effectively isovalent substitution of $Fe^{2+}$ by $Co^{2+}$** — •Michael Merz[1], Thomas Wolf[1], Peter Nagel[1], Felix Eilers[1], Peter Schweiss[1], Hilbert von Löhneysen[1,2], and Stefan Schuppler[1] — [1]Institut für Festkörperphysik, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

The substitutional dependence of valence and spin-state configurations of $Sr(Fe_{1-x}Co_x)_2As_2$ ($x$ = 0, 0.05, 0.11, 0.17, and 0.38) is investigated with near-edge x-ray absorption fine structure at the $L_{2,3}$ edges of Fe, Co, and As. The present data provide direct spectroscopic evidence for an effectively isovalent substitution of $Fe^{2+}$ by $Co^{2+}$, which is in contrast to the widely assumed Co-induced electron-doping effect. Moreover, the data reveal that not only does the Fe valency remain completely unaffected across the entire doping range, but so do the Co and As valencies as well. The data underline a prominent role of the hybridization between (Fe,Co) $3d_{xy}$, $d_{xz}$, $d_{yz}$ orbitals and As $4s/4p$ states for the band structure in $A(Fe_{1-x}Co_x)_2As_2$ and suggest that the covalency of the (Fe,Co)-As bond is a key parameter for the interplay between magnetism and superconductivity.

TT 12.33 Mon 15:00 Poster D

**Investigation on $KFe_2As_2$ single crystals by means of X-ray spectroscopy** — •Anna Buling[1], Nikolay Skorikov[2], Aswartham Saicharan[3], Sabine Wurmehl[3], Bernd Büchner[3], and Manfred Neumann[1] — [1]Department of Physics, University of Osnabrueck, Barbarastr. 7, D-49069 Osnabrueck, Germany — [2]Institute of Metal Physics, Russian Academy of Sciences-Ural Division, 620219 Yekaterinburg, Russia — [3]IFW Dresden, PF 270116, D-01171 Dresden, Germany

Soon after superconductivity was found in fluorine doped LaOFeAs, the new $AFe_2As_2$ familiy of pnictide superconductors without the LaO spacer layers was discovered.
$KFe_2As_2$ is an endpoint in the $Ba_{1-x}K_xFe_2As_2$ system and takes a special role among the other *122* and *1111* Fe pnictides due to its low $T_c$ around 3.7 K, the lack of the typical orthorhombic structural transition and some other diverse properties. We report on a detailed investigation of the electronic structure of $KFe_2As_2$ *(K122)* single crystals by means of X-ray spectroscopy completed by density functional theory (DFT) calculations. These results will be compared with further already investigated *Ba122* compounds.

TT 12.34 Mon 15:00 Poster D

**Signatures of unconventional superconductivity in dI/dV characteristics** — •Lars Elster and Ewelina Hankiewicz — Institut für Theoretische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg

We study the dI/dV characteristics of superconductors with different order parameters treating normal state - insulator - superconductor (NIS) junctions within the Bogoliubov-de Gennes (BdG) formalism. The dI/dV characteristics are calculated from the coefficients of Andreev and normal reflections at the interface between normal and superconducting phases treating the insulator as a Dirac-delta like potential barrier. In particular, we find that topological superconductors with broken time-reversal symmetry (BTRS) (e.g. d+is order parameter) show a zero bias peak splitting in the nodal direction, which allows to distinguish them from their non-topological counterparts. Therefore the dI/dV characteristic is a powerful tool in probing the pairing potential of unconventional superconductors, and our predictions can be verified by scanning tunneling microscopy.

TT 12.35 Mon 15:00 Poster D

**Josephson currents and resonances observed in STM experiments at milli-Kelvin temperatures** — •Berthold Jäck[1], Matthias Eltschka[1], Maximilian Assig[1], Markus Etzkorn[1], Christian R. Ast[1], and Klaus Kern[1,2] — [1]Max-Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne

Superconducting tunnel junctions allow for the detailed investigation of various tunneling regimes. Besides the superconducting quasi-particle tunneling, new tunneling paths such as the Josephson effect and Andreev reflections open up as the tunneling barrier is decreased. These processes manifest themselves as new structures within the gap of the superconducting quasi-particle density of states. We investigated these sub-gap structures in a Vanadium-Vanadium tunnel junction by using a Scanning Tunneling Microscope (STM) operating at 15 mK. One of the main advantages of using an STM setup is the very precise control of the tunneling resistance and hence the superconductor's coupling, which is a central property of the tunneling processes. We observe harmonic sub-gap features at energies of about 100 $\mu eV$ which do

not originate from Andreev reflections. Their peak positions neither depend on the superconductor's coupling nor on magnetic fields, but change for different Vanadium tips. We will discuss these experimental findings in the framework of low-impedance tunneling junctions and Josephson junctions coupled to an electro-magnetic environment.

TT 12.36 Mon 15:00 Poster D

**STM/STS Study on Co-doped NaFeAs superconductor** — •Pranab Kumar Nag[1], Danny Baumann[1], Ronny Schlegel[1], Rico Pohle[1], Martha Scheffler[1,2], Torben Hänke[1], Robert Beck[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Bernd Büchner[1,2], and Christian Hess[1] — [1]Institut für Festkörperforschung IFW Dresden, — [2]Institut für Festkörperphysik TU Dresden

We have performed scanning tunneling microscopy/spectroscopy measurements on superconducting Co-doped NaFeAs as a function of temperature. After cleaving at low temperature and cryogenic vacuum we were able to investigate the electronic structure of the material by tunneling spectroscopy. The tunneling spectra (dI/dV) reveal several gap-like features near the Fermi level. We compare these result with recent data on LiFeAs.

TT 12.37 Mon 15:00 Poster D

**Specific heat measurements of single-crystalline iron superconductors $K_{1-x}Na_xFe_2As_2$ and of $Li_2ZrCuO_4$ down to 10 mK** — •Patrick Vogt[1], Andreas Reifenberger[1], Mahmoud Abdel-Hafiez[2], Sai Aswartham[2], Sabine Wurmehl[2], Marius Hempel[1], Stefan-Ludwig Drechsler[2], Bernd Büchner[2], Andreas Fleischmann[1], Christian Enss[1], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institute for Physics, University of Heidelberg, D-69120 Heidelberg, Germany — [2]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, D-01171 Dresden, Germany

Specific heat studies down to very low temperatures are applied to study electronic properties in the superconducting phase of $K_{1-x}Na_xFe_2As_2$ and low-energy excitations in the quasi-one-dimensional quantum antiferromagnet $Li_2ZrCuO_4$. A quasi-adiabatical heat-pulse method including the $\tau_2$-effect yields specific heat data on $K_{1-x}Na_xFe_2As_2$ single crystals with different doping levels down to 10 mK. The data show clear evidence for a $T^2$-term in specific heat providing evidence for line nodes in the superconducting order parameter. For insulating $Li_2ZrCuO_4$, a continuous dual-slope method is applied which implies linearly-in-temperature increasing specific heat below 1 K superimposed by an anomaly centered at 60 mK. The anomalously large slope in the linear regime highlights the relevance of quantum fluctuations of presumably magnetic nature.

TT 12.38 Mon 15:00 Poster D

**Optical study of LiFeAs** — •A. V. Pronin[1], R. P. S. M. Lobo[2], G. Chanda[1], J. Wosnitza[1], S. Kasahara[3], T. Shibauchi[3], and Y. Matsuda[3] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]LPEM, ESPCI-ParisTech, CNRS, UPMC, 10 rue Vauquelin, 75231 Paris, Cedex 5, France — [3]Department of Physics, Kyoto University, Kyoto 606-8502, Japan

LiFeAs is unique among the iron-based superconductors in that it is superconducting without carrier doping and the residual resistivity ratio is very high. Thus, the determination of the superconducting gap symmetry is not complicated by the material defects. Various spectroscopic and thermodynamic measurements suggest an isotropic gap without nodes. However, no optical observations of the gap have been reported in LiFeAs. Here, we present a broad-band optical investigation of LiFeAs and discuss the frequency and temperature behavior of its complex conductivity.

TT 12.39 Mon 15:00 Poster D

**Processing of insulation barriers for the development of tunneling junctions based on pnictide superconductors** — •Manuel Monecke, Stefan Schmidt, Sebastian Döring, Martin Feltz, Noor Ali Hasan, David Reifert, Frank Schmidl, and Paul Seidel — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

Josephson junctions are an excellent tool for the investigation on pnictide superconductors, especially for the understanding of the transport mechanisms in such materials. For the preparation of those Josephson junctions it is important to have high resistance insulating tunneling barriers because the measurements are more purposeful than measurements with low resistance conductive barriers. Metal (e.g. gold) as barrier material has a very low resistance even at the maximum layer thickness. Therefore, disturbing effects like Andreev reflection become significant. Because of these issues it is highly important to study these tunnel barrier materials, their electrical properties and deposition processes. We present initial investigations on the deposition of sputtered oxide tunnel barriers and their properties. Furthermore, we discuss interface effects between base electrode, barrier, and cover electrode.

This work was partially supported by DFG under project no. SE 664/15-1, the DAAD, EU project IRON-SEA no. FP7-283141 and the Landesgraduiertenförderung Thüringen.

TT 12.40 Mon 15:00 Poster D

**Josephson junctions based on pnictide superconductors** — •Martin Feltz[1], Stefan Schmidt[1], Sebastian Döring[1], David Reifert[1], Sandra Gottwals[1], Noor Ali Hasan[1], Manuel Monecke[1], Frank Schmidl[1], Kazumasa Iida[2], Fritz Kurth[2], Bernhard Holzapfel[2], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany — [2]IFW Dresden, Institute for Metallic Materials, Helmholtzstrasse 20, 01069 Dresden, Germany

Josephson junctions are a powerful tool for understanding more about the physical behaviour of pnictide superconductors. We built different kinds of Josephson junctions based on pnictide thin films. Planar junctions, edge type junctions, and junctions on bicrystalline substrates were prepared. We present manufacturing techniques and also the electronical properties of the different junctions and compare them. The measurement of $I$-$V$-characteristics show a strong excess current. We have to mind this when calculating the $I_cR_N$ product. The effective $I_cR_N$ values are 6.5$\mu$V for the grain boundary junction, 7.9$\mu$V for the planar structure, and 7.5$\mu$V for the edge junction.

This work was partially supported by the EU within IRON-SEA (project no. FP7-283141), DFG within SPP 1458 (projects SE 664/15-1 and HA 5934/1-1), the DAAD and the Landesgraduiertenförderung Thüringen.

[1] S. Schmidt et al. IEEE-TAS (2012), accepted [arXiv:1211.3879]

TT 12.41 Mon 15:00 Poster D

**Studies on the processing of Ba-122 single crystals for the development of tunnel junctions** — •David Reifert[1], Stefan Schmidt[1], Sebastian Döring[1], Martin Feltz[1], Sandra Gottwals[1], Noor Ali Hasan[1], Manuel Monecke[1], Thomas Wolf[2], Frank Schmidl[1], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany — [2]Karlsruhe Institute of Technology, Institut für Festkörperphysik, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

The investigation of the superconducting properties of iron-based single crystals is important for the understanding of transport mechanisms responsible for superconductivity in those materials. Tunnel junctions are necessary in order to realize phase-sensitive measurement geometries for the investigation of the order parameter symmetry. To fabricate such tunnel junctions on Co-doped $BaFe_2As_2$(Ba-122) single crystals, which were produced with a self-flux method, we had to solve several issues. Using thin film technology requires high quality surfaces, so we show the results of several planarization techniques e.g. chemical mechanical polishing, ion beam smoothing, and crystal cleaving. Finally, we present first electrical measurements on photolithographically patterned Ba-122 single crystals.

This work was partially supported by DFG within SPP 1458 under project no. (SE 664/15-1), the German Academic Exchange Service (DAAD), and the Landesgraduiertenförderung Thüringen.

TT 12.42 Mon 15:00 Poster D

**Conductance spectra investigations of ironarsenide superconductor in planar junctions** — •Sandra Gottwals[1], Sebastian Döring[1], Stefan Schmidt[1], Noor Ali Hasan[1], Frank Schmidl[1], Fritz Kurth[2], Kazumasa Iida[2], Bernhard Holzapfel[2], Ingolf Mönch[3], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena — [2]IFW Dresden, Institut für metallische Werkstoffe, Helmholtzstraße 20, 01069 Dresden — [3]IFW Dresden, Institute for Integrative Nanoscience, Helmholtzstraße 20, 01069 Dresden

To investigate the properties of iron-based superconductor, we used Andreev reflection studies on planar hybrid SNS' junctions, based on Ba-122 (S) thin films with gold layer (N) and a Pb counter electrode (S'). I-V- and differential characteristics were measured at different

temperatures of each electrode as well as the junction itself. It could be noticed that both electrodes significantly effect the junction spectra due to an additional series resistance. This resistance occurs for lead at T>7.2 K and is constant, while for Ba-122 it is strongly nonlinear and suspected to be caused by the underlaying Fe buffer layer. We show how both electrodes influence the junction spectra in the measured temperature range and how to correct this. Thus, we are able to interpret the pure junction spectra within known models.

This work was partially supported by DFG under project no. HA5934/3-1 and SE664/15-1, the EU under project no. FP7-283141 (IRON-SEA), the Deutscher Akademischer Austauschdienst, and the Landesgraduiertenförderung Thüringen.

TT 12.43 Mon 15:00 Poster D

**Isoelectronic substitution of As with Sb in $BaFe_2As_2$** — •Daniel Schmidt and Hans F. Braun — Experimentalphysik V, Universität Bayreuth, D-95440 Bayreuth, Germany

The study of iron based superconductors has lead to the 122 iron pnictide compounds, that allow to investigate the interdependency of chemical doping and physical properties. Hole doping in $BaFe_2As_2$ was successfully achieved and transition temperatures of 38 K were obtained. Other doping procedures are possible, like the electron doping on the iron site and the isoelectronic substitution on the arsenic site. In our work we studied such an isoelectronic substitution of arsenic with the isovalent element Sb which has a larger ionic radius than arsenic. This way we induce chemical pressure in the compound. We tested the substitution level with X-ray powder diffraction measurements. The results of further measurements will be communicated.

TT 12.44 Mon 15:00 Poster D

**Crystal growth of various ruthenates** — •Stefan Kunkemöller[1], Agung Nugroho[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut Teknologi Bandung

Ruthenates of the Ruddlesdon-Popper series exhibit a variety of interesting phenomena ranging from unconventional superconductivity to orbitally polarized Mott insulators. Unfortunately the crystal growth of most of these ruthenates is extremely difficult partially due to the high evaporation of ruthenium; this strongly limits the research on these fascinating materials. We have started to grow single crystals of layered and perovskite ruthenates by the travelling floating-zone method using a Canon SC1-MDH mirror furnace. For the layered $Ca_{2-x}Sr_xRuO_4$ series we focused first on the range of concentration where recent My-SR experiments reveal spin-density wave ordering to occur at relatively high temperature and with a sizeable ordered moment. Good quality crystals of $Ca_{1.5}Sr_{0.5}RuO_4$ can be obtained, when an excess of 15 percent of ruthenium is added to the initial preparation of the rod and when a high growth speed up to 40mm/h is used. Even slight modifications of the growing conditions result in large amounts of $(Sr/Ca)RuO_3$ and $(Sr/Ca)_3Ru_2O_7$ intergrowth phases. First attempts to grow perovskite and double-layered ruthenates will be discussed as well.

TT 12.45 Mon 15:00 Poster D

**Superconductivity in Ge and Si via Ga-ion implantation** — •Richard Skrotzki[1,2], Thomas Herrmannsdörfer[1], Rico Schönemann[1], Viton Heera[1], Jan Fiedler[1], Erik Kampert[1], Frederik Wolff-Fabris[1], Peter Philipp[1], Lothar Bischoff[1], Matthias Voelskow[1], Arndt Mücklich[1], Bernd Schmidt[1], Wolfgang Skorupa[1], Manfred Helm[1], and Joachim Wosnitza[1] — [1]Dresden High Magnetic Field Laboratory (HLD) and Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O. Box 51 01 19, D-01314 Dresden, Germany — [2]Department of Chemistry and Food Chemistry, TU Dresden, 01062 Dresden, Germany

We present current progress of a unique study featuring the origin and use of superconductivity in highly Ga-doped group-IV semiconductors. Thin films have been prepared via ion implantation and subsequent short-term annealing. Germanium offers a high solubility for Ga acceptors (up to 1 at.%). Thus, superconductivity below about 0.5 K has been devoted previously solely to doping. However, recent atom-probe tomography reveals Ga nano-accumulations rendering the possibility of superconductivity in a proximity coupled network. In silicon, we have investigated a 10 nm thin amorphous Ga precipitation layer ($T_c$ = 7 K) that is close to the superconductor to insulator transition. We present high magnetic field measurements up to 40 Tesla and evaluate the critical-field phase diagram. First proof for phase coherence has been detected via magneto-resistance oscillations in lithographically tailored structures. This opens the door for future device fabrication.

TT 12.46 Mon 15:00 Poster D

**Proximity effect induced superconductivity in Cu- nanowires** — •Maksym Kompaniiets[1], Fabrizio Porrati[1], Cornelia Neetzel[2], Wolfgang Ensinger[2], and Michael Huth[1] — [1]Physikalisches Institut, Goethe Universität, Frankfurt a. M — [2]Fachbereich Materialwissenschaften, TU Darmstadt, Darmstadt

Proximity effect induced superconductivity occurs at the interface of a normal metal and a superconductor when Copper pairs leak into the metal. Depending on the microstructure of the normal metal, anomalies just above the temperature of the superconducting phase transition can be observed in the temperature-dependent resistivity. We have studied proximity induced superconductivity in Cu-nanowires in contact with an amorphous superconductor (W-C-Ga-O) prepared by focused ion beam induced deposition (FIBID) employing the precursor $W(CO)_6$; contacts to the $Cu$-nanowires were made by using FIBID of $Pt-C$ leads with the precursor $MeCpPt(Me)_3$ in a dual-beam scanning electron/ion microscope. The nanowires have been prepared by electrochemical deposition in etched heavy-ion-track polycarbonate templates with diameters of 250 to 300 $nm$ and lengths of 30 to 60 $\mu m$.

TT 12.47 Mon 15:00 Poster D

**Superconductivity in Thin La Films** — •Lihui Zhou, Peter Löptien, Alexander Khajetoorians, Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Hamburg, Germany

The issue of how thin superconducting films can get before they lose their superconductivity is of relevance for the fundamental understanding of quantum confined superconductors and for their possible technological applications in nanodevices [1,2]. Here, La islands with different thicknesses in the range of the superconducting coherence length have been grown on the W(110) surface under ultra-high vacuum conditions. Low-temperature scanning tunnelling spectroscopy using non-superconducting and superconducting tips has been applied to determine the superconducting properties, i.e. the energy gap [3] and the lifetime broadening [4] of the quasiparticles. It is found that these parameters decrease linearly with the inverse island thickness, similar to recent experiments with Pb nano-islands on Si(111) [1,2], and in agreement with the theoretical calculation including a surface-energy term in the Ginzburg-Landau free-energy of a superconductor [5].

[1] C. Brun et al., Phys. Rev. Lett. 102, 207002 (2009)
[2] M. M. Özer et al., Nature Phys. 2, 173 (2006)
[3] I. Giaever, K. Megerle, Phys. Rev. 122, 1101 (1961)
[4] R. C. Dynes et al., Phys. Rev. Lett. 41, 1509 (1978)
[5] J. Simonin, Phys. Rev. B 33, 7830 (1986)

TT 12.48 Mon 15:00 Poster D

**Direct measurement of the magnetic anisotropy of thin sputtered $MgB_2$ films** — •Savio Fabretti, Inga-Mareen Imort, and Andy Thomas — Universität Bielefeld, Deutschland

The simple hexagonal crystal structure and large London penetration depth make Magnesium-diboride an excellent candidate for spin polarization measurements using the Meservey-Tedrow method. In a step towards these measurements, we investigated the magnetic anisotropy of thin $MgB_2$ films sputtered onto cubic (001)MgO and R-cut sapphire substrates. We present the high field cooling experiments with an applied magnetic field perpendicular and parallel to the film plane for those samples. These measurements were done in the high field laboratory in Nijmwegen due to the required high upper critical field for thin sputtered films of up to 30 T [1]. Our measurements show an upper critical field of 38.31 T with field parallel to the film plane and 27.7 T with a field perpendicular to the film plane for the samples with 120 nm $MgB_2$. A linear fit shows a good approximation with the data points, although the parallel magnetic field could not destroy the superconductivity. We achieved a magnetic anisotropy ratio of 1.38. Literature values show an anisotropy ratio between 1.25 and 2 for thin films, which was fit with the Ginzburg Landau theory [2]. Therefore our results agrees with the previously estimated anisotropy ratio for thin $MgB_2$ films, where magnetic fields of up to 7 T were used [3].

[1] M.H. Jung et al. Chem. Phys. Lett. 343 (2001) 447
[2] C. Buzea and T. Yamashita, Sci. Technol. 14 (2001) R115
[3] H. Shimakage et al., IEEE Trans. On Appl. Supercond. 15 No2 (2005)

TT 12.49 Mon 15:00 Poster D

**Morphology of superconducting FeSe thin films grown by MBE and RF-sputtering** — •Alexander Kronenberg[1], Eike Venzmer[1], Sebastian ten Haaf[1], Janek Maletz[1,2], and Martin Jourdan[1] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany

Tunneling spectroscopy on planar junctions is the most direct approach for the investigation of superconducting coupling mechanisms [1]. However, it requires smooth interfaces at the tunneling barrier. The morphology of superconducting thin films of FeSe grown by MBE and co-sputtering (RF) from an iron and a selenium target are compared. MBE deposited films show an extreme sensitivity to stoichiometry, deposition temperature and choice of substrate [2]. These films exhibit macroscopic crevices and a pronounced roughness, rendering the preparation of tunneling junctions impossible. However, sputter deposited epitaxial FeSe thin films clearly show a more favorable morphology. Optical microscopy, AFM and SEM demonstrate a smooth surface with segregations which are eliminated by proper choice of the deposition parameters.

[1] M. Jourdan, M. Huth and H. Adrian, Nature *398*, 47 (1999)
[2] M. Jourdan and S. ten Haaf, J Appl. Phys. *108*, 023913 (2010)

TT 12.50 Mon 15:00 Poster D

**Competing instabilities in FeSe/$SrTiO_3$ superlattices** — •Michael Fechner and Nicola Spaldin — ETH Zurich, Department for Material Theory,CH-8093 Zurich, Switzerland

Intercalating FeSe with atomic layers[1] has recently experimentally been shown to lead to an tremendous increase in the superconducting $T_C$. Due to that we discuss here results from first-principle calculations of FeSe/$SrTiO_3$ superlattices. In particular we discuss the competition between lattice instabilities in $SrTiO_3$ and the spin density wave (SDW) in FeSe. It turns out that depending on the interface termination a suppression or enhancement of the SDW is found. Interface doping and hybridization of Fe-oxygen and Ti-Se at the interface explain the results. Finally we discuss the impact of different thicknesses of the two components on the magnetic and electronic properties.

[1] M. Burrard-Luca et al., NatMat 11, 1 (2012).

TT 12.51 Mon 15:00 Poster D

**Transport, magnetic and structural properties of YBCO/LCMO heterostructures grown on STO (110) substrates** — •Luqman Mustafa[1], Soltan Soltan[1,2], Gennady Logvenov[1], Hanns-Ulrich Habermeier[1], and Bernhard Keimer[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]Faculty of science, Helwan University, 11792-Helwan, Cairo, Egypt

YBCO/LCMO bi- and multilayers were grown on STO (110) substrates by Pulsed Laser Deposition (PLD) technique with the goal to study the interface of an oxide ferromagnet and a cuprate superconductor where the CuO2 planes are perpendicular to the film plane. The structure was investigated by X-ray diffractometry, transport and magnetic properties were studied by conventional four-point-probe and SQUID techniques respectively. Depending on the preparation conditions the single layer YBCO as well as bi-layers can be grown in the (110), (103)/(-103), as well as mixed orientations. Large anisotropy of electrical conductivity in these films was observed in case of (110)-oriented YBCO layer and less pronounced anisotropy in case of (103)-oriented one. We present a detailed analysis of the anisotropy of the magnetization of such bi- and multilayers emphasizing its relation to the orientation of the YBCO film.

TT 12.52 Mon 15:00 Poster D

**B-T-phase diagram and Fulde-Ferrell-Larkin-Ovchinnikov State in an Organic Superconductor** — •R. Beyer[1], J. Wosnitza[1], J. A. Schlueter[2], S. Jahns[3], and G. Zwicknagl[3] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA — [3]Institut für Mathematische Physik, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

The low-temperature B-T- phase diagram of the layered organic superconductor $\kappa$-$(ET)_2$ $SF_5CH_2CF_2SO_3$, where ET is bisethylenedithiotetrathiafulvalene, has been studied. The highly precise specific heat measurements show strong variation of the superconducting transition with the orientation of the applied magnetic field. For field directions parallel to the superconducting planes the upper critical field is Pauli-limited exceeding the Chandrasekhar-Clogston limit at low temperatures. The superconducting transition is studied theoretically using realistic Fermi surfaces. Our results suggest that the phase, which separates the homogeneous superconducting state from the normal state is a realization of a Fulde-Ferrell-Larkin-Ovchinnikov state.

TT 12.53 Mon 15:00 Poster D

**Paramagnetic Cooper pair breaking effect in $\alpha$-(BEDT-TTF)$_2$KHg(SCN)$_4$** — •Michael Kunz[1], Sebastian Jakob[1], Werner Biberacher[1], Karl Neumaier[1], Harald Müller[2], and Mark V. Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France

The organic charge transfer salt $\alpha$-$(BEDT\text{-}TTF)_2KHg(SCN)_4$ is a quasi-two-dimensional metal consisting of conducting and insulating layers. At pressures above 2.5 kbar this compound features a low $T_c$ ($\sim$ 0.1 K) superconducting state with an unprecedentedly high anisotropy of the upper critical field depending on whether the magnetic field is oriented parallel or perpendicular to the conducting planes. This is due to a strong suppression of the superconducting shielding currents in the direction perpendicular to the layers. For an exact parallel field orientation the shielding currents become so weak that their effect is replaced by the Pauli paramagnetic effect as the main contribution to the Cooper pair breaking. Clear manifestations of the paramagnetic pair breaking can be seen in the temperature dependence as well as in the angular dependence of the critical field near parallel orientation. At the exact parallel field orientation, the theoretical Chandrasekhar-Clogston paramagnetic limit is exceeded by a factor of 1.3, most likely due to a strong electron-phonon coupling. From the analysis of the temperature dependence of the parallel critical field the Maki parameter can be determined.

TT 12.54 Mon 15:00 Poster D

**de Haas-van Alphen investigations on the filled skutterudite $LaRu_4As_{12}$ superconductor** — •Johannes Klotz[1], Kathrin Götze[1,3], Tomasz Cichorek[2], Zygmunt Henkie[2], and Joachim Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland — [3]TU Dresden, Institut für Festkörperphysik, Germany

$LaRu_4As_{12}$ belongs to the filled skutterudite compounds which show a wide variation in physical properties such as metal-insulator transition, unconventional superconductivity, and quadrupolar or magnetic ordering [1]. It shows enhanced superconducting properties as compared to other skutterudite superconductors ($T_c$ = 10.45 K and $H_{c2} \approx$ 10.2 T) and, more importantly, multiple superconducting gaps have been inferred from the magnetic-field dependence of the specific heat and a positive curvature of $H_{c2}(T)$ close to $T_c$ making $LaRu_4As_{12}$ a rare example of a cubic superconductor displaying multiband effects [2]. We investigated the angular dependence of the dHvA effect using the capacitive torque method at temperatures down to 30 mK and in fields up to 18 T. Effective masses for different bands were determined expecting rather heavy masses due to a high electronic specific-heat coefficient $\gamma$ = 59 mJ/mol $K^2$. In combination with band-structure calculations our results will provide a detailed picture of the Fermi surface and the electronic correlations.

[1] M.B. Maple, E.D. Bauer, *et al.*, Physica B **328** (2003)
[2] L. Bochenek, R. Wawryk, *et al.*, Phys. Rev B **86**, 6 (2012)

TT 12.55 Mon 15:00 Poster D

**High-Field Magnetotransport in the Electron-Doped Cuprate Superconductor $Nd_{2-x}Ce_xCuO_4$** — •Toni Helm[1], M .V. Kartsovnik[1], E. Kampert[2], C. Putzke[2], W. Biberacher[1], P. D. Grigoriev[3], S. Baddoux[4], C. Proust[4], I. Sheikin[4], A. Kiswandhi[5], J. S. Brooks[5], E. S. Choi[5], J. Wosnitza[2], A. Erb[1], and R. Gross[1] — [1]Walther-Meissner-Institute, Garching, Germany — [2]High Magnetic Field Laboratory, Dresden, Germany — [3]L. D. Landau Institute for Theoretical Physics, Chernogolovka, Russia — [4]Laboratoire National des Champs Magnétiques Intenses CNRS, Toulouse-Grenoble, France — [5]National High Magnetic Field Laboratory,Tallahassee, USA

The current status of the high-field magnetotransport studies of the Fermi surface in the electron-doped cuprate superconductor $Nd_{2-x}Ce_xCuO_4$ will be presented. Both the magnetic quantum oscillations and semiclassical angle-dependent magnetoresistance give evidence of a weak ($\pi/a$, $\pi/a$)-superlattice potential existing at the over-

doped regime, $0.15 \leq x \leq 0.17$. The relevant energy gap is very small, $\sim 10 - 2\,\mathrm{eV}$; it is gradually suppressed at increasing the doping level, extrapolating to zero right at the edge of the superconducting dome, $x = 0.175$. On the other hand, decreasing the doping below the optimal level leads to dramatic changes in the behavior of magnetotransport including the Shubnikov-de Haas oscillations, magnetoresistance and Hall effect. Our data suggest a Fermi surface transformation leading to a collapse of the classical closed cyclotron orbits responsible for the conventional galvanomagnetic effects.

TT 12.56 Mon 15:00 Poster D

**Charge-Density-Wave State in the Ladder Compound $Sr_{10}Ca_4Cu_{24}O_{41}$ under High Pressure** — •Armin Huber[1], Rüdiger Klingeler[2], Markus Hücker[3], Bernd Büchner[4], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, D-86159 Augsburg, Germany — [2]Kirchhoff-Institute for Physics, D-69120 Heidelberg, Germany — [3]Brookhaven National Laboratory, Upton, NY 11973-5000, USA — [4]Leibniz-Institut für Festkörper-und Werkstoffforschung Dresden, PF 27 01 16, 01171 Dresden, Germany

Besides the occurrence of superconductivity under pressure in the two-leg ladder compound $Sr_{10}Ca_4Cu_{24}O_{41}$, the existence of a competing charge density wave (CDW) ground state is a highly interesting phenomenon in this material. An earlier study demonstrated how the CDW is suppressed by increasing the calcium content, which was attributed to increased dimensionality and disorder [1].

However, no information is currently available about the evolution of the CDW under pressure. Therefore, we studied the polarization-dependent optical response of $Sr_{10}Ca_4Cu_{24}O_{41}$ in the mid-infrared frequency range as a function of temperature and pressure. Based on these results, we can extend the phase diagram and discuss more quantitatively how holes are transferred from the chains to the ladders under the application of pressure.

Supported by the DFG.

[1] T.Vuletić et al., Phys. Rev. Lett. 90, 257002 (2003)

TT 12.57 Mon 15:00 Poster D

**Phonon line shapes in the vortex state of the phonon-mediated superconductor $YNi_2B_2C$** — •Frank Weber[1], Lothar Pintschovius[1], Klaudia Hradil[2], and Daniel Petitgrand[3] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Physikalische Chemie, Universität Göttingen, Außenstelle FRM-II, Garching, Germany — [3]Laboratoire Léon Brillouin (CEA-CNRS), CEA-Saclay, Gif-sur-Yvette, France

We present an inelastic neutron-scattering study of phonon line shapes in the vortex state of the type II superconductor $YNi_2B_2C$. In a previous study [1] we showed that certain phonons exhibit a clear signature of the superconducting gap $2\Delta$ on entering the superconducting state. Our interest was to find out whether or not the line shape of such phonons reflects the inhomogeneous nature of the vortex state induced by a magnetic field smaller than the upper critical field $\mathbf{B}_{c2}$.We found that this is indeed the case because the observed phonon line shapes can be well described by a model considering the phonon as a local probe of the spatial variation of the superconducting gap.

[1] F. Weber, A. Kreyssig, L. Pintschovius, R. Heid, W. Reichardt, D. Reznik, O. Stockert, and K. Hradil, Phys. Rev. Lett. 101, 237002 (2008)

## TT 13: Multiferroics 2 (jointly with DF, DS, KR, and MA)

Time: Monday 15:00–18:30 Location: H3

TT 13.1 Mon 15:00 H3

**Magnetization control in thin two-phase multiferroic structures via external electric fields** — •Alexander Sukhov[1], Paul P. Horley[2], Chenglong Jia[3], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06120 Halle/Saale, Germany — [2]Centro de Investigation en Materiales Avanzados, S.C. (CIMAV), 31109 Chihuahua, Mexico — [3]Key Laboratory for Magnetism and Magnetic Materials of the Ministry of Education, Lanzhou University, Lanzhou 730000, China

We present a theoretical study of the coupled magnetization and polarization dynamics in a thin multiferroic junction related to a $BaTiO_3$ (rhombohedral phase) layer in contact with Fe-layer. The dynamical properties are discussed in the context of different interfacial magnetoelectric coupling mechanisms. For the magnetoelectric coupling induced by the screening of the spin-polarized electrons in Fe we investigate the minimum strength of the coupling constant which is required for the full switching of the magnetization [1]. In the case of a strain-induced magnetoelectric interaction we show an electric field-induced magnetic switching in the plane perpendicular to the magneto-crystalline easy axis while the total magnetization remains stable [2]. In addition, the response of the multiferroic structure to magnetic radio-frequency fields by means of ferromagnetic resonance and dependent on the applied electric field is studied. [1] P.P. Horley, A. Sukhov, C.-L. Jia, E. Martinez, J. Berakdar, Phys. Rev. B **85**, 054401 (2012). [2] C.-L. Jia, A. Sukhov, P.P. Horley, J. Berakdar, Europhys. Lett. **99**, 17004 (2012).

TT 13.2 Mon 15:15 H3

**Magnetic field induced charge anisotropy in $CoFe_2O_4/BaTiO_3$ nanocomposite** — •Carolin Schmitz-Antoniak[1], Detlef Schmitz[2], Sven Stienen[1], Pavel Borisov[3], Anne Warland[1], Bernhard Krumme[1], Wolfgang Kleemann[1], and Heiko Wende[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, D-47048 Duisburg — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-12489 Berlin — [3]Department of Chemistry, University of Liverpool, Liverpool L69 7ZD

The system of $CoFe_2O_4$ nanopillars in a $BaTiO_3$ matrix represents a multiferroic nanocomposite in which strong ferrimagnetism and strong ferroelectricity coexist at room temperature [1]. The magnetostrictive CFO nanopillars and the piezoelectric BTO matrix are coupled by strain so that it is possible to change the electric properties by a magnetic field and the magnetic properties by an electric field. The charge anisotropy of Ti ions is probed by x-ray linear dichroism (XLD) and the magnetisation of Co ions by x-ray magnetic circular dichroism (XMCD) giving the unique possibility to study the effect of the coupling on a microscopic level as a function of magnetic field strength and direction. The occurrence of significant in-plane components of the electric polarisation is discussed. They are due to shear forces acting on the $BaTiO_3$ matrix while taking into account non-diagonal piezoelectricity components.

Funded by DFG (SFB491) and BMBF (05 ES3XBA/5).

[1] H. Zheng et al., Science 303, 661 (2004)

TT 13.3 Mon 15:30 H3

**Multiferroic CoFe2O4/ BaTiO3 with core shell structure nanoparticles** — •Morad Etier[1], Vladimir V.Shvartsman[1], Yanling Gao[1], Joachim Landers[2], Heiko Wende[2], and Doru C.Lupascu[1] — [1]University of Duisburg-Essen, Institute for Materials Science, Essen, Germany — [2]University of Duisburg-Essen, Faculty of Physics, Duisburg, Germany

Multiferroic materials exhibit ferroelectricity and ferromagnetism simultaneously. Combining piezoelectricity and magnetostriction components in the same composite received more interests in the modern researches. In this work we report synthesis and properties of cobalt iron oxide barium titanate composite with a core shell structure. To synthesize the samples we combine co-precipitation and organosol method. Phases content, microstructure and morphology were studied by x-ray diffraction, SEM and TEM. Multiferroic properties were proved by home-built Sawyer-Tower circuit and SQUID magnetometry. Temperature dependence of magnetic moment was measured in zero field cooling (ZFC) and field cooling (FC) and compared with those cobalt iron oxide nanopowder. The dielectric properties were studied using impedance spectroscopy.

TT 13.4 Mon 15:45 H3

**Strain-induced changes of magnetic anisotropy in epitaxial spinel-type cobalt ferrite films** — •Stefania Florina Rus[1,2], Andreas Herklotz[2,4], Iuliu Grozescu[3], and Kathrin Dörr[4] — [1]Politehnica University of Timişoara, 300006 Timişoara, Romania — [2]IFW Dresden, 01171 Dresden, Germany — [3]Institute for Research and Development in Electrochemistry and Condensed Matter, 300224

Timisoara, Romania — [4]Martin-Luther-Universität Halle-Wittenberg, Institute for Physics, 06099 Halle, Germany

We present results on the effect of biaxial strain on the magnetic anisotropy of thin films of the parent compound CoFe2O4 and films with a partial substitution of Co and Fe by Zr and Pt, respectively. The strain states of the epitaxially grown films are controlled twofold: (i) statically by epitaxial misfit strain via an appropriate choice of substrates and buffer layers and (ii) reversibly by strain transfer from piezoelectric $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ (001) (PMN-PT) substrates. Due to large negative magnetostriction all films show an out-of-plane magnetic easy axis under tensile strain and an in-plane easy axis under compressive strain. Our reversible strain measurements show that the magnetic anisotropy can be efficiently altered by the application of an electric field to the ferroelectric PMN-PT substrates. The effect of substitution with Zr and Pt on the magnetoelectric effect will be discussed. This work is supported by the strategic grant POSDRU ID77265 (2010), co-financed by the European Social Fund, within the Sectoral Operational Programme Human Resources Development 2007-2013. Advising by P. Vlazan is greatly acknowledged.

TT 13.5 Mon 16:00 H3

***Ab initio* study of magneto-phonon interaction in $GaFeO_3$** — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Magnetoelectric (ME) coupling provides a handle for manipulating the magnetization of a material with an electric field, giving a perspective for a new type of non-volatile memory. Unfortunately, materials with ME coupling that is large enough for industrial applications are scarce. Moreover, among the materials which are both ferroelectric and magnetic at room temperature, only $BiFeO_3$ is known. Unfortunately, the ordering of spins in this material is antiferromagnetic (whereas ferro/ferrimagnetic coupling is desired) and the ME coupling is small.

$GaFeO_3$ (GFO) is the first material observed to simultaneously present a strong ME coupling and a resulting magnetization in a single phase. It has the polar structure $Pc2_1n$, which allows disorder in A and B cation sites. By increasing the iron content its Curie temperature can be increased above room temperature [1].

To understand the mechanism of the strong ME coupling in $GaFeO_3$ at the microscopic level, we performed *ab initio* calculations based on density functional theory of the structural properties and magneto-phonon interaction in stoichiometric $GaFeO_3$ compounds in different structures, as well as with different occupancies of the A and B sites.

We acknowledge the support by Helmholtz Young Investigators Group Programme VH-NG-409 and GALIMEO Consortium.

[1] T. Arima *et al.*, Phys. Rev. B **70**, 064426 (2006)

TT 13.6 Mon 16:15 H3

**The effect of ion doping on multiferroic $MnWO_4$** — •safa golrokh bahoosh[1,3], julia m. wesselinowa[2], and steffen trimper[3] — [1]Max Planck Institute of Microstructure Physics,Weinberg 2, 06120 Halle, Germany — [2]University of Sofia, Department of Physics,Blvd. J. Bouchier 5, 1164 Sofia, Bulgaria — [3]Institute of Physics, Martin-Luther-University, 06120 Halle, Germany

We have studied the ion doping effects on different transition temperatures in the multiferroic compound $MnWO_4$ based on a microscopic model and within the framework of Green functions technique. It is shown that the exchange interaction constants can be changed due to the different ion doping radii. This leads to reduction of the magnetic phase transition temperature $T_N$ by doping with non-magnetic ions,such as Zn, Mg, whereas $T_N$ is enhanced by doping withtransition metal ions, such as Fe, Co. The different behavior of the temperature $T_1$ (where up-up-down-down collinear spin structure appears) by Fe and Co doping could be explained taking into account the single-ion anisotropy.

**15 min. break**

TT 13.7 Mon 16:45 H3

**Hybrid improper ferroelectricity in a Multiferroic and Magnetoelectric Metal- Organic Framework** — •Alessandro Stroppa[1], Paolo Barone[1], Prashant Jain[2], Manuel Perez-Mato[3], and Silvia Picozzi[1] — [1]CNR-SPIN Via Vetoio, 67100, L'Aquila (Italy) — [2]Los Alamos National Lab, 30 Bikini Atoll Rd Los Alamos, NM 87545-0001 (505) 664-5265 — [3]Departamento de Fisica de la Materia Condensada, Facultad de Ciencia y Tecnologia, UPV/EHU, Bilbao (Spain)

Metal-organic frameworks (MOFs) show increasing promise as candidates for various applications. Of particular interest are MOFs with the perovskite topology showing hydrogen bonding-related multiferroic phenomena. By using state-of-the-art-ab-initio calculations, we show that in [C(NH2)3]Cr(HCOO)3 MOF, interaction between the cooperative antiferro-distortive Jahn-Teller distortions and the C(NH2)3 cations breaks the inversion symmetry through hydrogen-bonding and induces a ferroelectric polarization. Interestingly, the polar behavior arises due to a trilinear coupling between two unstable modes, namely a Jahn-Teller and a tilting mode, and one stable polar mode. Therefore, this compound represents the first example of hybrid improper ferroelectric in the family of metal-organic compounds. Since rotational modes in perovskite-inorganic compounds usually freeze-in at elevated temperatures (300 K), the trilinear coupling in MOF compounds may provide an interesting route to realize room temperature multiferroic. Last but not least, we show that switching of polarization direction implies the reversal of a large weak ferromagnetic component.

TT 13.8 Mon 17:00 H3

**Ferroelectric properties of $(Ba,Sr)TiO_3/La_{0.7}Sr_{0.3}MnO_3$ multilayered thin films** — •Markus Michelmann[1], Johannes Aprojanz[1,2], Arseni Buryakov[2], Elena Mishina[2], Markus Jungbauer[1], Sebastian Hühn[1], and Vasily Moshnyaga[1] — [1]I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Moscow State Institute of Radioengineering, Electronics and Automation, Prosp. Vernadskogo 78, 119454 Moscow, Russia

$Ba_xSr_{1-x}TiO_3$ (BSTO) epitaxial thin films became feasible for room temperature applications in contrast to the bulk material due to a possibility to enhance the ferroelectric Curie temperature under biaxial compressive strain. Using $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) thin films as metallic electrodes, we have grown highly strained BSTO/LSMO bilayers and LSMO/BSTO/LSMO trilayers on $SrTiO_3$ (100) substrates with BSTO layer thicknesses of 10 - 200 nm by means of metalorganic aerosol deposition. Ferroelectric switching was studied both electrically and by nonlinear optics (second harmonic generation (SHG)). Capacitance-voltage characteristics in a frequency range of $f = 1-10^6$ Hz and PUND measurements prove a ferroelectric hysteretic behavior up to room temperature with a remanent polarization of several $\mu C/cm^2$ and a switching fields in the range of 10−100 kV/cm. This was also supported by the SHG measurements. A detailed study of multiferroic properties will be performed for temperatures, $T = 10-400$ K, and applied magnetic field, $B = 0-9$ T. This work was supported by IFOX of the European Community's 7th Framework Programme.

TT 13.9 Mon 17:15 H3

**Epitaxial thin films of the multiferroic double perovskite $Bi_2FeCrO_6$** — •Vikas Shabadi, Mehran Vafaee, Mehrdad BaghaieYazdi, Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Germany

Co-existence of magnetism and ferroelectricity was theoretically predicted in the ordered double perovskite $Bi_2FeCrO_6$ (BFCO) [1]. We report epitaxial BFCO thin films grown by pulsed laser deposition from a 20% Bi-rich ceramic target on single crystal $SrTiO_3$(100) substrates. The degree of the Fe-Cr cation ordering in the BFCO films was calculated based on the X-ray diffraction patterns. The magnetic moments of the BFCO films were measured with a SQUID magnetometer and analyzed as a function of the Fe-Cr ordering. The discrepancies in the previously reported values of the magnetic moment of BFCO [2,3] are most likely connected to the varying degree of the Fe-Cr cation ordering in the samples. In a recent experiment more than 90% spontaneous B-site ordering in a similar Fe-Cr based double perovskite system has been achieved [4]. Anti-site disorder control is a key challenge to design double perovskite multiferroics.

[1]P. Baettig and N. A. Spaldin, Appl. Phys. Lett. **86**, 012505 (2005)
[2]Kim *et al.*, Appl. Phys. Lett. 89, 102902 (2006)
[3]R. Nechache *et al.*, J. Appl. Phys. **105**, 061621 (2009)
[4]S. Chakraverty *et al.*, Phys. Rev. B **84**, 064436 (2011)
The authors acknowledge support from DAAD.

TT 13.10 Mon 17:30 H3

**Growth of multiferroic heterostructures** — •Sergiu Stratulat, Dietrich Hesse, and Marin Alexe — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Coupling two materials with different order parameters gives great flexibility in engineering multifunctional devices. In achieving the maximum interfacial effects, vertical heterostructures present the maximum potential. Creating well-ordered vertical multiferroic heterostructures is not a trivial task, especially on large areas. We are focusing our attention on the system comprising ferrimagnetic CoFe2O4 and ferroelectric/antiferromagnetic BiFeO3, using pulsed laser deposition as a synthesizing technique. Considering a time-viable process to create the pillar-matrix configuration, we used anodic aluminum oxide masks to pattern the nucleation sites for the cobalt ferrite on previously deposited SrRuO3 bottom electrode on SrTiO3. After removal of the mask, deposition by means of a mixed target leads to ordered arrays of CFO pillars embedded in a BFO matrix. Scanning electron microscopy was employed at every step of the experiments to show the development of the samples, and X-ray diffraction probed the structural parameters. Testing the ferroelectric and magnetic properties locally gives an indication on the coupling influences present in the thin films.

TT 13.11 Mon 17:45 H3

**Self-assembled composite multiferroic films in controlled strain states** — •Mohsin Rafique[1,2,3,4], Andreas Herklotz[3,4], Er-Jia Guo[3,4], Kathrin Doerr[3,4], and Sadia Manzoor[1,2] — [1]Magnetism Laboratory, COMSATS Institute of Information Technology, Park Road 44000, Islamabad, Pakistan — [2]Center for Micro and Nano Devices (CMND), COMSATS Institute of Information Technology, Park Road 44000, Islamabad, Pakistan — [3]IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [4]Institute for Physics, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany

Self-assembled thin-film nanocomposites of piezoelectric and magnetostrictive materials have stimulated increasing research activities because of their potential to exhibit a large magnetoelectric response exploitable in multifunctional devices. Epitaxial thin films of $CoFe_2O_4$ and $BaTiO_3$ (CFO-BTO) composites were grown on $SrTiO_3$ (001) and piezoelectric $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$(001) (PMN-PT) substrates by pulsed laser deposition. Self-assembled nanostructures consisting of spinel nanopillars heteroepitaxially embedded in the ferroelectric perovskite matrix form. X-ray diffraction is utilized to estimate the lattice parameters. The magnetic properties studied by SQUID magnetometry show an out-of-plane easy axis of the CFO nanopillars and a strengthening of the out-of-plane anisotropy with increasing compression along the nanopillar axis. The magnetoelectric coupling in the composite film is revealed at a structural transition of the BTO matrix. Electrically controlled substrate strain of PMN-PT is applied to modify the magnetic anisotropy of the nanopillars.

TT 13.12 Mon 18:00 H3

**Low-lying magnetic excitations in the distorted triangular lattice antiferromagnet $\alpha$-$CaCr_2O_4$** — •Michael Schmidt[1], Zhe Wang[1], Sandor Toth[2], Bella Lake[2], A.T.M.Nazmul Islam[2], Alois Loidl[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany

We will discuss our results on $\alpha$-$CaCr_2O_4$ obtained by FIR and Terahertz spectroscopy. This compound orders below $T_N = 42.6$ K in a proper screw 120° magnetic order, but shows additional low-lying magnetic modes indicative for the vicinity of a more complex magnetic order [1], [2]. Our spectra obtained by FTIR and THz-TD spectroscopy show several optical magnons appearing below the magnetic ordering with anomalous temperature dependence. We will discuss their polarization dependence and a possible magnetoelastic coupling of these modes.

[1] S. Toth *et al.*, Phys. Rev. B 84, 054452 (2011)
[2] S. Toth *et al.*, PRL 109, 127203 (2012)

TT 13.13 Mon 18:15 H3

**Multiferroic $Ni_3V_2O_8$ measured in THz range at low temperatures and in high magnetic fields** — •Malte Langenbach[1], Tobias Hissen[1], Komalavalli Thirunavukkuarasu[1], Holger Schmitz[1], Iván Cámara Mayorga[2], Rolf Güsten[2], Joachim Hemberger[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Köln, Germany; — [2]Max-Planck-Institut für Radioastronomie, Bonn, Germany;

THz spectroscopy in high magnetic fields is an important technique to probe materials with strong magneto-electric coupling. Here, we discuss the Kagomé-staircase compound $Ni_3V_2O_8$. The triangle-based lattice gives rise to a frustration of the short-range antiferromagnetic couplings. This causes a rich variety of magnetic and structural phases at low temperatures.
Below $T_N = 9.8$ K, a incommensurate phase with collinear sinusoidal spin structure is established. This phase is followed by a cycloidal spin structure which is accompanied by the onset of ferroelectricity. Finally, below 3.9 K, the structure changes to a commensurate canted antiferromagnetic phase [1].
We report on elementary excitations in the THz range observed between 2 K and 50 K in fields up to 8 T.

Work supported by the DFG through SFB 608.

[1] G. Lawes et al., Phys. Rev. Lett. **95**, 087205 (2005)

## TT 14: Correlated Electrons: Low-Dimensional Systems - Models 2

Time: Monday 15:00–18:30 Location: H9

TT 14.1 Mon 15:00 H9

**Topological parity invariant in interacting two-dimensional systems from quantum Monte Carlo** — •Stefan Wessel[1], Thomas Lang[1], Victor Gurarie[2], and Andrew Essin[2] — [1]RWTH Aachen, Aachen, Germany — [2]University of Colorado, Boulder, USA

We report results on calculating the parity invariant from imaginary-time Green's functions in quantum Monte Carlo simulations of strongly interacting electron systems. The topological invariant is used to study the trivial- to topological-insulator transitions in the Kane-Mele-Hubbard model with an explicit bond dimerization. We explore the accessibility and behavior of this invariant based on quantum Monte Carlo calculations.

TT 14.2 Mon 15:15 H9

**Series expansions in topologically-ordered systems** — Michael Kamfor[1], Sebastien Dusuel[2], Julien Vidal[3], and •Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany — [2]Lycee Saint-Louis, 44 Boulevard Saint-Michel, 75006 Paris, France — [3]Laboratoire de Physique Théorique de la Matiere Condensee, CNRS UMR 7600, Universite Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris Cedex 05, France

We establish high-order series expansions as a powerful tool to study topologically-ordered quantum systems. In recent years, this has been demonstrated for various magnetic models including the toric code in an external magnetic field. The main focus of these studies were the determination of the zero-temperature phase diagram which demands to pinpoint and to characterize topological phase transitions. To this end the calculation of zero- and one-quasi-particle properties is essential. Here we study for the first time two-quasi-particle properties for the perturbed toric code. We identify bound states, formed by interacting anyons and determine dynamical correlation functions.

TT 14.3 Mon 15:30 H9

**Topological order in classical string-net models** — •Maria Hermanns, Mascha Baedorf, and Simon Trebst — Institute for Theoretical Physics, Cologne, Germany

Topological order has recently attracted a great deal of interest, because it allows for exotic emergent excitations that are robust against local perturbations. It is most commonly thought of as a quantum effect, which is strongly related to an effective low-energy description of the quantum system as a topological field theory. However, topological order can also occur in classical models that have local constraints. Most prominent among these are loop and string-net models. Here, we consider such classical models that are topologically ordered and analyze the relation between the classical topological order and its counter part in the quantum system.

TT 14.4 Mon 15:45 H9

**Topological Phases in gapped edges of fractionalized sys-**

**tems** — •Johannes Motruk[1], Erez Berg[2], Ari M. Turner[3], and Frank Pollmann[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel 76100 — [3]Institute for Theoretical Physics, University of Amsterdam, Science Park 904, P.O. Box 94485, 1090 GL Amsterdam, The Netherlands

We extend the classification scheme for symmetry protected topological phases of fermions in one-dimensional systems to chains of parafermions. We find that parafermionic chains support both topological as well as symmetry-broken phases. The topological phases can be identified by the structure of their entanglement spectrum, while the symmetry broken ones are characterized by a condensation of parafermions. Furthermore, we show that it is not possible to create new topological phases by combining chains. In several recent works, it has been proposed to realize parafermions experimentally at the edge of a fractional topological insulator coupled to superconducting and ferromagnetic domains. The parafermions arise as effective low-energy degrees of freedom. Based on this, we suggest a concrete physical realization at the edge of a $\nu = 1/3$ fractional topological insulator which we can tune into all possible topological phases. We identify the different phases by numerically determining their entanglement spectra.

TT 14.5 Mon 16:00 H9

**Topological phases in ultracold polar-molecule quantum magnets** — •Salvatore R. Manmana[1,2], Miles E. Stoudenmire[3], Kaden R.A. Hazzard[2], Ana Maria Rey[2], and Alexey V. Gorshkov[4] — [1]Institut für Theoretische Physik, Universität Göttingen, Germany — [2]JILA, University of Colorado and NIST, and Department of Physics, CU Boulder, USA — [3]Department of Physics and Astronomy, University of California, Irvine, USA — [4]Institute for Quantum Information & Matter, Caltech, Pasadena (California), USA

We show how to use polar molecules in an optical lattice to engineer quantum spin models with arbitrary spin $S \geq 1/2$ and with interactions featuring a direction-dependent spin anisotropy. This is achieved by encoding the effective spin degrees of freedom in microwave-dressed rotational states of the molecules and by coupling the spins through dipolar interactions. We demonstrate how one of the experimentally most accessible anisotropies stabilizes symmetry protected topological phases in spin ladders. Using the numerically exact density matrix renormalization group method, we find that these interacting phases – previously studied only in the nearest-neighbor case – survive in the presence of long-range dipolar interactions. We also show how to use our approach to realize the bilinear-biquadratic spin-1 and the Kitaev honeycomb models. Experimental detection schemes and imperfections are discussed.

TT 14.6 Mon 16:15 H9

**Topological phase transitions in a perturbed Fibonacci string-net model** — •Marc Daniel Schulz[1,3], Sébastien Dusuel[2], Kai Phillip Schmidt[1], and Julien Vidal[3] — [1]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany — [2]Lycée Saint-Louis, 44 Boulevard Saint-Michel, 75006 Paris, France — [3]Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR 7600, Université Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris Cedex 05, France

Topological order has gained enormous interest during the last years. This is also due to the fact that topologically-ordered systems harbour excitations with exotic exchange statistics, the so-called non-Abelian anyons, which are of interest for the purpose of topological quantum computation. Here, we present a study on the simplest model of Levin-Wen type featuring non-Abelian Fibonacci anyons in the presence of a local perturbation. The phase diagram is obtained by means of high-order series expansions and exact diagonalizations. Most interestingly, evidences for first-order and second-order quantum phase transitions are found.

**15 min. break**

TT 14.7 Mon 16:45 H9

**Formation of Magnetic Moments at Grain Boundaries of High Temperature Superconductors** — •Iris Xhango and Thilo Kopp — Zentrum für Elektronische Korrelationen und Magnetismus, Institut für Physik, 86135 Augsburg, Deutschland

Understanding the physics of grain boundaries in high temperature superconductors is of considerable value for applications of these materials. In this context the investigation of the normal state at the grain boundaries is as important as that of the superconducting state. From various experiments it is known that the normal state resistance at grain boundaries increases for decreasing temperature in contrast to the bulk behavior. A simple theoretical realization of the grain boundary builds on an inhomogeneous one-band Hubbard model. It is shown that local magnetic moments are formed at the grain boundary for finite on-site Coulomb interaction. The impact of the grain boundary and of the magnetic moments on the transport properties of the system are discussed. An increasing resistance for low temperature is obtained.

TT 14.8 Mon 17:00 H9

**Quantum spin models from $\pi$ fluxes in correlated quantum spin hall insulators.** — •Martin Bercx, Martin Hohenadler, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We analyze the signatures of $\pi$ fluxes in quantum spin hall insulators. We have shown in a recent work [1] that in the presence of repulsive electronic interactions each $\pi$ flux gives rise to a Kramers doublet of spinon states. Free spinon states show up in a Curie law behaviour of the magnetic susceptibility. The interaction between spinon states is mediated by a bosonic mode which can be tuned with the electron-electron interaction. This has opened the possibilty to study models of interacting spin 1/2 magnetic moments hosted in the gap of a topological insulator. These effective quantum spin models can be simulated numerically with the quantum Monte Carlo method. In this contribution we present results for spin chains, spin ladders and for various other geometries.

[1] F. F. Assaad, M. Bercx, and M. Hohenadler, arXiv:1204.4728 (2012)

TT 14.9 Mon 17:15 H9

**Flat-band ferromagnetic transition on a Bethe lattice** — •Mykola Maksymenko[1], Kirill Shtengel[2], and Roderich Moessner[1] — [1]MPIPKS, 01187 Dresden, Germany — [2]Department of Physics and Astronomy, University of California, Riverside, California 92521, USA

An exotic example of itinerant-electron magnetism is the so-called "flat-band ferromagnetism", in a wide class of geometrically frustrated lattices. Here electrons become trapped in restricted parts of the lattice and interactions may favor a ferromagnetic state across a range a electronic fillings.

We provide an exact solution for the problem of the para-ferro transition in a Hubbard model on lattices in which trapping cells form a Bethe lattice. This can be studied as a Pauli-correlated percolation transition in which due to spin-rotational degeneracy, different clusterings of electrons obtain different statistical weights [1]. As in the case of recent numerical studies for the 2D case, we show that the paramagnetic phase persists beyond the uncorrelated percolation point and the transition is via a first-order jump to an unsaturated ferromagnetic phase.

[1] M. Maksymenko, A. Honecker, R. Moessner, J. Richter, and O. Derzhko, Phys. Rev. Lett. 109, 096404 (2012)

TT 14.10 Mon 17:30 H9

**Multi-Orbital Effects in Functional Renormalization Group: A Weak-Coupling Study of the Emery model** — •Stefan A. Maier and Carsten Honerkamp — Institut für theoretische Festkörperphysik, RWTH Aachen, Germany and JARA - FIT Fundamentals of Future Information Technology

We perform an instability analysis of the Emery three-band model at hole doping and weak coupling within a channel-decomposed functional renormalization group flow proposed in Phys. Rev. B **79**, 195125 (2009). In our new approach, momentum dependencies are taken into account with less bias than in the truncated formfactor expansions used previously. Around a generic parameter set, we find a strong competition of antiferromagnetic and $d$-wave Cooper instabilities with a smooth behavior under a variation of doping and oxygen-oxygen hopping. For increasingly incommensurate ordering tendencies in the magnetic channel, signatures of $d$-wave Cooper pairing between electrons in non-neighboring unit cells of the direct lattice can be observed. Comparing our results for the Emery model to those obtained for the two-dimensional one-band Hubbard model with effective parameters, we find that, despite considerable qualitative agreement, multi-orbital effects have a significant impact on a quantitative level.

TT 14.11 Mon 17:45 H9

**Magnetic order-by-disorder in a distorted Heisenberg-Kitaev model** — •Max Henner Gerlach[1], Eran Sela[1,2], Hong-Chen Jiang[3], Oliver Wohak[1], and Simon Trebst[1] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Tel Aviv University, Ramat Aviv, Israel — [3]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, USA

Motivated by the recent experimental observation of Mott insulating states for the layered iridates $Na_2IrO_3$ and $Li_2IrO_3$, we discuss possible ordering states of the effective iridium moments in the presence of strong spin-orbit coupling and weak exchange anisotropies induced by lattice distortions. We find that the Heisenberg-Kitaev model – suggested to capture the exchanges of the effective $j = 1/2$ Iridium moments – in the presence of distortions exhibits a rich phase diagram of both conventionally ordered magnetic states as well as exotic topologically ordered and spin liquid states, which we will discuss in detail in this talk. Particular emphasis will be put on the classical counterpart of this model and the order-by-disorder physics that stabilizes certain ordering patterns over wide ranges of its phase diagram.

TT 14.12 Mon 18:00 H9

**Correlations of quantum spin chains from functional equations and su(2) diagrammatics** — •Andreas Klümper — Bergische Universität Wuppertal, Theoretische Physik, Gauss-Strasse 20, 42119 Wuppertal

For integrable quantum spin chains a lattice path integral formulation with finite but arbitrary Trotter number allows to derive a set of discrete functional equations with respect to the spectral parameters appearing in the R-matrices of local interactions. We show that these equations yield a unique characterisation of the density operator and present solutions for the S=1/2 and S=1 Heisenberg chains.

For generic cases, we report on a systematic implementation of su(2) invariance for matrix product states (MPS) with concrete computations cast in a diagrammatic language. As an application we present a variational MPS study of a spin-1/2 quantum chain. For efficient computations, we make systematic use of the su(2) symmetry at all steps of the calculations: (i) the matrix space is set up as a direct sum of irreducible representations, (ii) the local matrices with state-valued entries are set up as superposition of su(2) singlet operators, (iii) products of operators are evaluated algebraically by making use of identities for 3j and 6j symbols.

Results on quantum phase transitions in the considered models are discussed.

TT 14.13 Mon 18:15 H9

**Adiabatic loading of one-dimensional SU($N$) alkaline earth fermions in optical lattices** — •Lars Bonnes[1], Hazzard Kaden[2], Salvatore Manmana[2], Ana Maria Rey[2], and Stefan Wessel[3] — [1]Institute for Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria — [2]JILA, NIST and University of Colorado, and Department of Physics, University of Colorado, Boulder, Colorado 80309-0440, USA — [3]Institute for Theoretical Solid State Physics, JARA-FIT, and JARA-HPC, RWTH Aachen University, Otto-Blumenthal-Str. 26, D-52056 Aachen, Germany

Hubbard models with effective SU(N) symmetry have successfully been implemented in ultra-cold alkaline earth experiments. This paves the way towards the regime of exotic magnetism emerging in the low-energy sector but requiring ultra-cool temperatures below the superexchange scale. Loading N>2 fermions onto optical lattices, however, provides a cooling benefit with respect to conventional SU(2) fermions emerging from the N-scaling of the entropy. Hence the accessible temperature regime is lowered drastically, as already observed in recent experiments by Tanaka et al. We present large-scale quantum Monte Carlo simulations combined with series expansion results to quantitatively study the Pomeranchuk cooling effect for SU(N) fermions loaded onto a one-dimensional optical lattice and find a significant temperature decrease as N is increased. Furthermore, we examine the crossover behavior to the magnetic regime and show that the systems do not only become cooler but also become closer to the magnetic (ground-state) regime with respect to the appearance of magnetic correlations.

## TT 15: Topological Insulators 2 (jointly with DS, HL, O, and MA)

Time: Monday 15:00–18:00 Location: H10

**Invited Talk** TT 15.1 Mon 15:00 H10

**The THz response of topological insulator surface states** — •N. Peter Armitage — The Institute of Quantum Matter, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD 21218, USA

Topological insulators (TIs) are newly discovered states of matter characterized by an *inverted* band structure driven by strong spin-orbit coupling. One of their most touted properties is the existence of robust "topologically protected" surface states. I will discuss what topological protection means for transport experiments and how it can be probed using the technique of time-domain THz spectroscopy applied to thin films of $Bi_2Se_3$. By measuring the low frequency optical response, we can follow their transport lifetimes as we drive these materials through instabilities either by doping through a quantum phase transition into a topologically trivial regime or by reducing the film thickness. I'll also discuss our work on the magnetic field dependence of the Kerr rotation in $Bi_2Se_3$, where we find an unprecedentedly large value of the angle of rotation of reflected light, which is due to the cyclotron resonance of the 2D Dirac fermions.

**15 min. break**

TT 15.2 Mon 15:45 H10

**Peierls dimerization at the edge of 2D topological insulators?** — •Gustav Bihlmayer[1], Hyun-Jung Kim[2], Jun-Hyung Cho[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics and Research Institute for Natural Sciences, Hanyang University, Seoul, Republic of Korea

Edge states of two-dimensional topological insulators (2D-TIs) attracted considerable interest as they support dissipationless spin-currents. Recently, it was proposed that the zigzag-edge of a Bi(111) bilayer, identified as a 2D-TI [1,2], is unstable with respect to a Peierls dimerization [3], a phenomenon that occurs quite general in one-dimensional structures. This proposal was based on an *ab initio* investigation without taking spin-orbit coupling (SOC) into account. We investigate the effect of SOC on the atomic structure of zigzag Bi(111) and Sb(111) nanoribbons. Although we find that edge-reconstructions can influence the number of conductive channels, we conclude that the topological protection of the states in the Bi ribbon actually prevents the Peierls mechanism to get effective, since the opening of a Peierls gap at the zone boundary is forbidden by time-reversal symmetry. We compare the situation to the Sb structure, but also in the topologically trivial case of the Sb(111) bilayer ribbon we find a suppression of the dimerization due to SOC effects.

[1] S. Murakami, Phys. Rev. Lett. 97, 236805 (2006) [2] M. Wada et al., Phys. Rev. B 83, 121310(R) (2011) [3] L. Zhu et al., J. Phys. Chem. C 114, 19289 (2010)

TT 15.3 Mon 16:00 H10

**Engineering quantum anomalous Hall (QAH) phases with orbital and spin degrees of freedom** — •Hongbin Zhang, Frank Freimuth, Gustav Bihlmayer, Marjana Ležaić, Stefan Blügel, and Yuriy Mokrovsov — Peter Grünberg Institut and Institute for Advanced Simulation, FZJ and JARA, 52425 Jülich, Germany

Combining tight-binding models and first-principles calculations, we demonstrate that under external exchange fields, non-zero Chern numbers and nontrivial QAH effects can be induced by on-site spin-orbit coupling (SOC) in buckled honeycomb lattices with *sp* orbitals. In the Haldane model [1], the occurrence of the QAH effect is attributed to complex valued next-nearest-neighbor hopping matrix elements. Detailed analysis of a generic tight binding model reveals that there exist different mechanisms giving rise to complex hoppings, utilising both orbital and spin degrees of freedom of electrons on a lattice. Furthermore, it is shown that in Bi- or Sb(111) bilayers [2], different topological phases exist as function of the magnitude of SOC and external exchange fields. These phases are characterised using Chern and spin Chern numbers [3] in combination with transverse charge

and spin conductivities. At last, we show that introducing ferromagnetic dopants provides a practical way to induce nontrivial topological phases, whereas the physics is altered due to partially filled $d$ states around the Fermi energy. – Support by Helmholtz Young Investigators Group Programmes VH-NG-409 and -513 is acknowledged.

[1] F.D.M. Haldane, PRL **61**, 2015 (1988). [2] H. Zhang, *et al.*, PRB **86**, 035104 (2012). [3] E. Prodan, PRB **83**, 195119 (2011).

TT 15.4 Mon 16:15 H10

**Prediction of weak topological insulators in layered semiconductors** — •Binghai Yan[1,2], Lukas Müchler[1,2], and Claudia Felser[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden — [2]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg University of Mainz, 55099 Mainz

We report the discovery of weak topological insulators by ab initio calculations in a honeycomb lattice. We propose a structure with an odd number of layers in the primitive unit cell as a prerequisite for forming weak topological insulators. Here, the single-layered KHgSb is the most suitable candidate for its large bulk energy gap of 0.24 eV. Its side surface hosts metallic surface states, forming two anisotropic Dirac cones. Although the stacking of even-layered structures leads to trivial insulators, the structures can host a quantum spin Hall layer with a large bulk gap, if an additional single layer exists as a stacking fault in the crystal. The reported honeycomb compounds can serve as prototypes to aid in the finding of new weak topological insulators in layered small-gap semiconductors.

TT 15.5 Mon 16:30 H10

**Dirac States in a Novel Topological Insulator: Epitaxial alpha-Tin Layers on Indium Antimonide** — •J. Schäfer[1], A. Barfuss[1], G. Bihlmayer[2], D. Wortmann[2], L. Dudy[1], P. Höpfner[1], A. Bostwick[3], E. Rotenberg[3], and R. Claessen[1] — [1]Phys. Inst., Universität Würzburg, D — [2]Peter Grünberg Inst. and Inst. Adv. Sim., FZ Jülich, D — [3]Lawrence Berkeley Nat. Lab., USA

This study addresses a new material realization of a topological insulator (TI) thus far only proposed theoretically, which is formed by $\alpha$-Sn in the diamond lattice on InSb substrates. The epitaxial growth opens various pathways to access and manipulate the topological surface state (TSS). This includes the evolution of the Dirac bands as a function of thickness, or surface coating layers which alter the spin-orbit interaction. Interestingly, the TI band properties are closely related to that of strained HgTe, for which the Quantum Spin Hall effect was demonstrated.

Here we report on the electronic structure of $\alpha$-Sn(001) based on angle-resolved photoemission (ARPES), complemented by density functional theory (DFT). We observe the formation of a clearly pronounced Dirac cone. The Fermi level in ARPES is located close to the Dirac point. Its position can be controlled by dopants, which allows to adjust the Fermi level crossings of the TSS. The Dirac cone is discernible down to bulk band energies, and its constant energy surfaces seemingly reflect the lattice symmetry. The experimental findings are consistent with DFT calculations including spin-orbit interaction, which document the formation of a TSS.

TT 15.6 Mon 16:45 H10

**Observation of terahertz photocurrents in the topological insulator $Bi_2Se_3$** — •Lukas Braun[1], Luca Perfetti[2], Martin Wolf[1], and Tobias Kampfrath[1] — [1]Physikalische Chemie, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Laboratoire des Solides Irradiés, Ecole Polytechnique, Palaiseau cedex, France

Recent experiments have indicated that optical excitation of topological insulators (TIs) with circularly polarized light can induce spin-polarized electron currents along the TI surface. The direction of this photocurrent can be controlled by varying the circular polarization of the driving light from right- to left-handed. So far, only DC photocurrents have been detected [J. W. McIver *et al.* Nature Nanotechnology **7**, 96 (2012)]. Since electrons moving through a solid typically undergo scattering on sub-picosecond time scales, it is highly desirable to generate and detect TI photocurrents with femtosecond time resolution.

Here, we drive ultrashort current bursts in n-doped $Bi_2Se_3$ by excitation with a laser pulse (10fs, 800nm, 10nJ). The photocurrent gives rise to the emission of a terahertz (THz) electromagnetic pulse whose transient electric field $E(t)$ is detected by means of electro-optic sampling with a time resolution of 10fs. We observe extremely broadband THz emission covering the range from 10 to 30THz, and the THz intensity is found to depend strongly on the helicity of the pump pulses. A method is presented that allows us to extract the transient current $j(t)$ from the measured $E(t)$. We finally discuss the origin of $j(t)$ and implications for the dynamics of photoexcited TI electrons.

TT 15.7 Mon 17:00 H10

**Static screening properties of topologically protected surface states** — •Daniel Wortmann, Gustav Bihlmayer, Yuriy Mokrousov, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The electrons occupying surface states of topological insulators (TI) provide charges that can screen electric fields applied perpendicular to the surface. Being a very basic phenomenon, its realistic description is rather difficult: model approaches fail to provide quantitative results while DFT calculations of insulating slabs with external electric fields suffer from difficulties arising from the incomplete screening of the field inside the slab.

We demonstrate that the embedded Green function method [1,2] can be utilized to investigate the effects of an applied field on the surface states. Our approach describes the formation of surface states in terms of their scattering properties at the semi-infinite bulk states by means of a generalized logarithmic derivative. Besides discussing the underlying idea of this elegant theoretical tool and its application to prototypical topological insulators, we present a comparison of the expected screening effects seen in a topological insulator with those in a topological material.

[1] see http://www.flapw.de for details of the code

[2] D. Wortmann, H. Ishida, S. Blügel, Phys. Rev. B **65**, 165103 ('02)

TT 15.8 Mon 17:15 H10

**Topological phases of spin chains** — Kasper Duivenvoorden and •Thomas Quella — Universität zu Köln, Institut für Theoretische Physik, Köln, Deutschland

The Haldane phase of one-dimensional $S = 1$ spin chains with $SU(2)$ symmetry is one of the first topological states of matter. In particular, it features a bulk-boundary correspondence, with $S = 1/2$ degrees of freedom emerging at the boundaries of the system. Moreover, it exhibits a diluted anti-ferromagnetic order which can be measured using a non-local string order parameter. With the prospect of being able to simulate spin chains with $SU(N)$ symmetry in the laboratory using ultracold earth-alkaline atoms it is a natural and interesting question whether similar topological phases also exist beyond $N = 2$.

In a recent paper we have shown that this is indeed the case. More precisely, spin chains with $SU(N)$ symmetry allow for up to $N$ different topological phases, $N - 1$ of which are topologically non-trivial. These phases exhibit topological order that is reflected in a specific entanglement pattern resulting from the matrix product state representation of the corresponding ground state wave function. It may be detected using a non-local string order parameter which characterizes each of the $N$ phases unambiguously. Analytical and numerical results confirm that our order parameter may be used to extract a quantized topological invariant.

TT 15.9 Mon 17:30 H10

**Strongly-correlated topological semiconductors** — •Stanislav Chadov[1], Claudia Felser[1], Leon Petit[2], Hubert Ebert[3], and Jan Minár[3] — [1]MPI-CPFS Dresden — [2]STFC Daresbury Laboratory, UK — [3]LMU München

Using the fully-relativistic Green's function formalism we analyze the electronic structure topology in series of the heavy rock-salt type semiconductors PuX, SmX (X=Te, Se, S). Due to the partial filling of their $f$-shells, these materials exhibit strong dynamical correlations which destroy the Bloch-like eigenstates. Thus, the usual analysis based on the symmetry of the eigenstates cannot be applied. Here we recall the adiabatic approach, which allows to analyze the topology based on a purely bulk information disregarding the Bloch or localized character of the electronic states. The dynamical correlations were treated within the DMFT scheme implemented in the framework of the SPR-KKR Green's function method.

TT 15.10 Mon 17:45 H10

**Correlation between linear Magnetoresistance and Mobility of Heusler Topological Insulators** — •C. Shekhar, A. K. Nayak, S. Ouardi, G. H. Fecher, and C. Felser — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Topological insulators (TIs) are a class of quantum materials and belong to a new state of matter with topologically protected gapless Dirac fermionic states. Among the TIs series Heusler compounds are promising candidates for the nanoelectronic devices. If these compounds contain heavy metals (Au, Pb, Pd, Pt, Sb and Bi) and a lanthanide element then they exhibit extraordinary physical properties including *zero band gap*. Generally, gapless compounds show high mobility, where no threshold energy is required to conduct carriers from occupied states to empty states. Very recently, the exciting discovery of graphene is an example of high-mobility compounds due to its linear dispersion of the bands, where charge carriers behave like massless particles. However, the Heusler TIs having *zero band gap* are also expected to show high mobility. The Heusler TIs also exhibit nonsaturating and positive magnetoresistance, that shows systematic variations with temperature. The best fitting of observed MR is found with the combination of linear and quadratic field dependence and may be written in form of a quadratic equation: $MR = a|B| + (b/2)B^2$, where B is applied field. It is clear that this MR originates from the contribution of both linear and parabolic terms. The parabolic term is well known and comes from the Lorentz force, while the origin of the linear MR is intriguing.

## TT 16: Transport: Quantum Dots, Wires, Point Contacts 2 (jointly with HL)

Time: Monday 15:00–17:30 Location: H18

TT 16.1 Mon 15:00 H18

**Bound States in a Carbon Nanotube Quantum Dot Coupled to Superconducting Leads** — •Amit Kumar[1], Martin Gaim[1], Daniel Steininger[1], Andreas K. Hüttel[1], Christoph Strunk[1], Alfredo Levy Yeyati[2], and Alvaro Martín-Rodero[2] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Theoretical Condensed Matter Physics, Universidad Autónoma de Madrid, 28049 Madrid, Spain

We report on tunnelling spectroscopy measurements on a carbon nanotube quantum dot device strongly coupled with niobium superconducting leads at two ends and weakly coupled to a tunnel probe (aluminium) in the middle. Gate dependent differential conductance measurements at low temperature down to 25mK reveal the formation of bound states (Andreev / Yu-Shiba Rusinov) inside the superconducting gap. By virtue of the larger superconducting gap of the niobium, we observe several such states. Odd Coulomb valleys show negative differential conductance features, which are characteristics for bound states with localized spins. These localized spins (odd number of electrons on the quantum dot) are known to generate localized Yu-Shiba Rusinov bound states inside the superconducting gap and are expected to dominate in asymmetrically coupled quantum dot devices. More detailed experimental investigations and theoretical calculations are in progress to understand these experimental findings.

TT 16.2 Mon 15:15 H18

**Kondo Physics in Clean Carbon Nanotubes** — •Daniel Schmid, Alois Dirnaichner, Peter Stiller, Andreas K. Hüttel, and Christoph Strunk — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Clean carbon nanotube quantum dots provide ideal model systems with orbitally degenerate quantum levels to probe novel Kondo physics. Transport measurements on single quantum dots were done down to a base temperature of $T \simeq 20\,\mathrm{mK}$ in the $10 \leq N_{\mathrm{el}} \leq 50$ electron regime, showing the typical signatures of the Kondo effect, as well as co-tunneling features at finite bias.
We focus on a specific charge state with $N_{\mathrm{el}} = 21$ electrons in the intermediate coupling regime $G_{\mathrm{max}} \simeq 0.9(2e^2/h)$. Besides the usual Kondo peak around zero bias voltage ($V_{\mathrm{SD}} = 0$) the differential conductance displays interesting satellites at finite $V_{\mathrm{SD}}$. These satellites depend only weakly on magnetic field and temperature for the range $B < 8\mathrm{T}$ and $T < 1\mathrm{K}$.

TT 16.3 Mon 15:30 H18

**Thermal quasiparticle spectroscopy of a carbon nanotube quantum dot coupled to superconducting leads: part I, experiment** — •Markus Gaass, Andreas K. Hüttel, Tom Geiger, Sebastian Pfaller, Andrea Donarini, Milena Grifoni, and Christoph Strunk — University of Regensburg, 93040 Regensburg, Germany

We present electronic transport measurements of a single wall carbon nanotube quantum dot contacted with Niobium electrodes. At elevated temperatures, within the superconductor energy gap and the Coulomb blockade region additional transport resonances arise, which we attribute to thermally generated quasiparticles in the Nb leads. A detailed comparison of the temperature dependence with model calculations leads to excellent agreement for zero as well as finite applied bias.

TT 16.4 Mon 15:45 H18

**Thermal quasiparticle spectroscopy of a carbon nanotube quantum dot coupled to superconducting leads: part II, theory** — •Sebastian Pfaller, Markus Gaass, Andreas K. Hüttel, Tom Geiger, Andrea Donarini, Christoph Strunk, and Milena Grifoni — University of Regensburg, 93040 Regensburg, Germany

We present in this study a transport theory for a carbon nanotube quantum dot coupled to superconducting leads to lowest order in the tunneling. A generalized master equation is used to model the dynamics. For high enough temperatures, quasiparticles in the superconducting lead get thermally excited across the gap, leading to conductance in the Coulomb blockade including the subgap region. Around zero bias conductance peaks are observed. A comparison of the temperature dependence of these thermally induced conductance peaks with experimental data shows excellent agreement.

TT 16.5 Mon 16:00 H18

**Mapping out the band structure of carbon nanotubes in a magnetic field: part I, experiment** — •Alois Dirnaichner, Daniel Schmid, Magdalena Marganska, Milena Grifoni, Andreas K. Hüttel, and Christoph Strunk — University of Regensburg, 93040 Regensburg, Germany

We report on electronic transport spectroscopy measurements on an ultra-clean carbon nanotube as a quantum dot at low temperature and finite magnetic field. The direction of the magnetic field can be adjusted both parallel and perpendicular to the nanotube axis with flux densities of up to $B = 17\,\mathrm{T}$. Data focusses on the few-electron spectrum, highly regular down to $N_{\mathrm{el}} = 1$, where sharp Coulomb blockade oscillations enable tracing of multiple excited quantum states. We discuss spin-orbit coupling and KK'-mixing in our sample. The data is compared to state-of-the art CNT modeling.

**15 min. break**

TT 16.6 Mon 16:30 H18

**Mapping out the band structure of carbon nanotubes in a magnetic field: part II, theory** — •Magdalena Marganska, Alois Dirnaichner, Daniel Schmid, Andreas K. Hüttel, Christoph Strunk, and Milena Grifoni — University of Regensburg, Germany

We report here an analysis of transport measurements of ultraclean carbon nanotubes in parallel magnetic field. Employing the magnetic field dependence of the energies of ground and excited states of a single excess electron in the CNT-quantum dot we can assign a diameter and chirality to the nanotube present in the device. The data obtained in low fields allow us to extract several of the nanotube parameters, and to refine the minimal Hamiltonian commonly used for CNT quantum dots in parallel magnetic fields. With an additional asymmetry term appearing in the Hamiltonian, we can match the experimental data with high accuracy. Using the results from high magnetic fields we can further refine our analysis and identify the term responsible for electron-hole asymmetry in the spin-orbit splitting.

TT 16.7 Mon 16:45 H18

**Tunable electron-vibron coupling in suspended carbon nanotube quantum dots** — •Christoph Stampfer[1,2], Peter Weber[1,2], Carola Meyer[2], and Stefan Trellenkamp[2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Peter-Grünberg-Institut (PGI-6/8/9), Forschungszentrum Jülich, 52425 Jülich, Germany

Measurements through nano electromechanical systems and single-molecule junctions have shown that electronic transport is strongly influenced by the mechanical motion, leading to transport assisted by emission of vibrons. Furthermore, a strong electron-vibron coupling is expected to lead to a suppression of transport through the vibronic ground state, known as Franck-Condon blockade. Here we report on transport in a quantum dot formed in a partly suspended carbon nanotube devices. The data show Coulomb diamonds with a clear fourfold degeneracy and an experimental confirmation of Franck-Condon blockade mechanism. More interestingly, we show that our four-terminal quantum device allows us to tune the electron-vibron coupling. In particular, we focus on the investigation of spin states and the tunability of electron-phonon coupling in the suspended carbon nanotube quantum dot.

TT 16.8 Mon 17:00 H18

**Spin-dependent coupling to vibrations in suspended carbon nanotube quantum dots** — •Hernán L. Calvo[1,2], Julian Bohle[1,2,3], Christoph Stampfer[2,3,4], and Maarten R. Wegewijs[1,2,3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [2]JARA - Fundamentals of Future Information Technology — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [4]II. Institute of Physics B, RWTH Aachen University, Germany

Recent transport experiments in a semi-suspended carbon nanotube (CNT) quantum dot have shown an electron-vibration coupling that is markedly different for spin singlet and triplet states. In this talk, we show that such an apparent spin-vibration coupling can be understood in terms of a coupling of the electronic valley degree of freedom of the CNT to the observed longitudinal vibration. Strikingly, this Peierls-type coupling in the valley space leads to Franck-Condon sidebands that mostly develop for the triplet excited state. A vibrational modulation of the exchange interaction on the CNT is shown to result in a similar, but weaker effect. The effect can be understood qualitatively from polaronic shifts obtained in the Born-Oppenheimer approximation. In the regimes of interest, however, this approximation breaks down and we present transport calculations accounting for the full pseudo-Jahn-Teller mixing of the vibronic states that show satisfactory agreement with the experiment.

TT 16.9 Mon 17:15 H18

**Graphene quantum dots on hexagonal boron nitride** — •Alexander Epping[1,2], Stephan Engels[1,2], Christian Volk[1,2], Jan Dauber[1,2], Bernat Terres[1,2], Matthias Goldsche[1,2], Kenji Watanbe[3], Takashi Taniguchi[3], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Peter-Grünberg-Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Graphene exhibits unique electronic and mechanical properties making it a promising material for future quantum-electronic applications. However, state of the art graphene quantum dots fabricated on $SiO_2$ substrates suffer from their poor quality due to a large disorder potential. Recently, it has been shown that placing graphene on hexagonal boron nitride (hBN) substantially reduces the disorder potential because of its atomically-flat graphene-like hexagonal structure. Here, we present the fabrication and characterization of single-layer graphene quantum dots on hBN substrates. In particular we show low-temperature transport measurements showing Coulomb diamonds with charging energies between 9 meV and 11 meV.

## TT 17: Correlated Electrons: Spin Systems, Itinerant Magnets 2

Time: Monday 15:00–17:45 Location: H19

TT 17.1 Mon 15:00 H19

**Entanglement Entropy and Quantum Monte Carlo** — •Peter Bröcker — Institut für Theoretische Physik, Universität zu Köln

Entanglement spectra and entanglement entropies have attracted a lot of attention in the last few years. Among other things, they can serve as precise indicators for (quantum) phase transitions as well as for detecting topologically ordered phases. We will report on the calculation of entanglement entropies in Quantum Monte Carlo, in particular in the frameworks of Loop Quantum Monte Carlo and Stochastic Series Expansion. We will also discuss approaches for Auxiliary Field Quantum Monte Carlo, which is of special interest in light of recent advances in simulations of fermionic models in the vicinity of the antiferromagnetic phase transition.

TT 17.2 Mon 15:15 H19

**The phase diagram of the two-orbital Hubbard model by means of the dynamical mean field theory** — •Vlastimil Křápek and Jan Kuneš — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, 162 00 Praha, Czech Republic

The Blume-Emery-Griffiths (BEG) model with repulsive biquadratic coupling exhibits a complex multicritical phase diagram [1]. In our recent work we have shown that the two-orbital Hubbard model can be mapped on BEG model when only certain nearest-neighbor interactions are considered and that this model is relevant for the spin-state transition observed in LaCoO3 [2].

Motivated by this we explore the phase diagram of the two-orbital Hubbard model further, focusing on the following points: (1) By changing the bandwidths we can vary the metallicity of the system while keeping the parameters of the BEG model constant. (2) By changing the temperature and the crystal-field splitting we visit different phases and study the transitions between them. The two-site unit cell is used to allow for the orbital and magnetic ordering. (3) We study the effect of the number of electrons different from the half filling.

[1] W. Hoston and A. N. Berker, Phys. Rev. Lett. 67, 1027 (1991).
[2] J. Kuneš and V. Křápek, Phys. Rev. Lett. 106, 256401 (2011).

TT 17.3 Mon 15:30 H19

**Towards microscopic understanding of skyrmions in $Cu_2OSeO_3$: an effective theory description** — Oleg Janson[1], •Ioannis Rousochatzakis[2], Alexander Tsirlin[3], Ulrich Rössler[2], Jeroen van den Brink[2], and Helge Rosner[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

We present a quantitative physical picture for the spin 1/2 ferrimagnetic helimagnet $Cu_2OSeO_3$ based on a DFT-based microscopic magnetic model. Besides clarifying the relevant low-energy magnetic degrees of freedom, the main successes of the theory are the following: (i) it reveals an intimate connection between $Cu_2OSeO_3$ (an insulating ferrimagnet) and MnSi (a metallic ferromagnet); (ii) it clarifies which Dzyaloshinskii-Moriya terms are responsible for the long-wavelength twisting, and gives a helix period of 58 nm, in very good agreement to the one ($\sim$50 nm) reported by Lorentz transmission electron microscopy by Seki *et al* [1]; (iii) it predicts the presence of a small antiferromagnetic canting which is tied to the long-wavelength twisting; (iv) it reveals the mechanism for the reduction of the Cu moments as observed by Bos *et al* [2].

[1] S. Seki, X. Z. Yu, S. Ishiwata, Y. Tokura, Science **336**, 198 (2012)
[2] J.-W. G. Bos, C. Colin, T. Palstra, Phys. Rev. B **78**, 094416 (2008).

TT 17.4 Mon 15:45 H19

**Towards microscopic understanding of skyrmions in $Cu_2OSeO_3$: a DFT study** — •Oleg Janson[1], Ioannis Rousochatzakis[2], Alexander Tsirlin[1,3], Ulrich Rössler[2], Jeroen van den Brink[2], and Helge Rosner[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

Unlike most undoped cuprates, the $S = 1/2$ Heisenberg magnet $Cu_2OSeO_3$ exhibits a ferrimagnetic ground state and a sizable magnetoelectric coupling. Furthermore, recent experimental studies reported magnetic-field-induced emergence of skyrmions in this insulating ma-

terial. Based on extensive DFT band structure calculations, we evaluate the microscopic magnetic model, including isotropic (Heisenberg) and anisotropic (Dzyaloshinskii-Moriya) terms. We extract five relevant magnetic couplings that form a complex, but non-frustrated spin model which can be described as a pyrochlore lattice of magnetic tetrahedra. The model parameters are justified by quantum Monte-Carlo simulations and subsequent comparison to the experiments.

TT 17.5 Mon 16:00 H19

**Long-wavelength helimanegtic order and skyrmion lattice phase in $Cu_2OSeO_3$** — Alfonso Chacon[1,2], •Tim Adams[1], Michael Wagner[1], Andreas Bauer[1], Georg Brandl[1,2], Bjoern Pedersen[2], Helmuth Berger[3], Peter Lemmens[4], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik-Department E21, D-85748 Garching, Germany — [2]Forschungsneutronenquelle Heinz Maier Leibnitz (FRM II), Lichtenbergstr. 1, 85748 Garching, Germany — [3]Ecole Polytechnique Federale Lausanne, CH-1015 Lausanne, Switzerland — [4]Institute for Condensed Matter Physics, TU Braunschweig, D-38106 Braunschweig, Germany

We report a long-wavelength helimagnetic superstructure in bulk samples of the ferrimagnetic insulator $Cu_2OSeO_3$. The magnetic phase diagram associated with the helimagnetic modulation inferred from small-angle neutron scattering and magnetization measurements includes a skyrmion lattice phase and is strongly reminiscent of MnSi, FeGe, and $Fe_{1-x}Co_xSi$, i.e., binary isostructural siblings of $Cu_2OSeO_3$ that order helimagnetically. The temperature dependence of the specific heat of $Cu_2OSeO_3$ is characteristic of nearly critical spin fluctuations at the helimagnetic transition. This provides putative evidence for effective spin currents as the origin of enhancements of the magnetodielectric response instead of atomic displacements considered so far.

TT 17.6 Mon 16:15 H19

**Mössbauer, NMR und $\mu$SR investigations of microscopic magnetic ordering of $La_2O_2Fe_2OSe_2$** — •Sirko Bubel[1], Marco Günther[1], Rajib Sarkar[1], Hans-Henning Klauss[1], Hubertus Luetkens[2], Gwendolyn Pascua[2], Kwang-Yong Choi[3], and Haidong Zhou[4] — [1]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [3]Institut für Physik der Kondensierten Materie, 38106 Braunschweig, Germany — [4]Experimental Condensed Matter Physics, University of Tennesee

20 years after the first investigations of the antiferromagnetically ordered oxo-chalcogenid $La_2O_2Fe_2OSe_2$ the common picture of microscopic alignment of iron moments in the expanded squarish $Fe_2O$-layers is still controversy discussed [1,2]. Furthermore first superconducting samples of this structural class were succesully synthesized in 2012 [3] linking this oxo-chalcogenid to the pnictide superconductors.

To understand the mechanism of iron magnetism in these systems we investigated a powder sample of $La_2O_2Fe_2OSe_2$ by $^{57}$Fe-Mössbauer spectroscopy, $\mu$SR and $^{139}$La-NMR. These measurements strongly suggest that iron moments are coupled ferromagnetically via selenium and antiferromagnetically via oxygen. We infer a new magnetic structure on the basis of these results, being consistent with Goodenough-Kanamori-rules, and speculate about orbital order in this system.

[1] Y. Fuwa *et al.*, Phys. Rev. B. **84** (2011) 174506
[2] D. J. Free, S. O. Evans, Phys. Rev. B. **81** (2010) 214433
[3] P. Doan *et al.*, J. Am. Chem. Soc. **134**, 16520 (2012)

**15 min. break**

**Topical Talk** TT 17.7 Mon 16:45 H19

**Magnetic Frustration in a Quantum Spin Chain: The Case of Linarite $PbCuSO_4(OH)_2$** — •Anja U.B. Wolter[1], Markus Schäpers[1], Ferdinand Lipps[1], Vladik Kataev[1], Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], Bernd Büchner[1], Rico Beyer[2], Marc Uhlarz[2], Jochen Wosnitza[2], Britta Willenberg[3], Manfred Reehuis[3], Kirrily C. Rule[3], Bachir Ouladdiaf[4], and Stefan Süllow[5] — [1]Leibniz-Institut IFW Dresden, Dresden, Germany — [2]Dresden High Magnetic Field Laboratory, Dresden, Germany — [3]Dresden High Magnetic Field Laboratory, Dresden, Germany — [4]Institute Laue-Langevin, Grenoble, France — [5]IPKM, TU Braunschweig, Braunschweig, Germany

We present a combined neutron diffraction, NMR and bulk thermodynamic study of the natural mineral linarite $PbCuSO_4(OH)_2$. An incommensurate magnetic ordering with a propagation vector k=(0,0.186,1/2) was found below $T_N$=2.8 K in a zero magnetic field. The analysis of the neutron diffraction data yields an elliptical helical structure. From detailed investigations of linarite in magnetic fields up to 12 T, applied along the chain direction, a very rich magnetic phase diagram is established, with multiple field-induced phases, and possibly short-range-order effects occurring in high fields. Our data establish linarite as a model compound of the frustrated one-dimensional spin chain, with ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor interactions. Long-range magnetic order is brought about by interchain coupling one order of magnitude smaller than the intrachain coupling.

TT 17.8 Mon 17:15 H19

**Investigation of Ferromagnetic Copper Oxides** — •Kevin Caslin[1], Reinhard Kremer[1], Mike Whangbo[2], Jia Liu[2], and Franz Pertlik[3] — [1]MPI für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Dept. of Chemistry, North Carolina State Univ., Raleigh, North Carolina 27695-8204, USA — [3]Inst. f. Mineralogie und Kristallographie d. Univ., A-1010 Wien, Österreich

We are investigating low dimensional $S = \frac{1}{2}$ Cu quantum-chain systems. Materials containing Cu $S = \frac{1}{2}$ moments in a distorted oxygen octahedral environment form $CuO_2$ ribbon chains. Such ribbon chains support ferromagnetic (FM) nearest-neighbour (NN) via Cu-O-Cu exchange and antiferromagnetic (AFM) next-nearest-neighbour (NNN) via Cu-O-O-Cu exchange. Often the NNN-AFM interaction is dominant and leads to a low temperature, AFM, long-range ordering. Systems of this type are known to develop unusual structural distortions and incommensurate spiral magnetic structures.[1,2,3] In this study, we search for $S = \frac{1}{2}$ Cu based materials with crystal structures leading to a predominate NN-FM exchange. X-ray diffraction, heat capacity, thermal expansion and magnetic measurements were performed to characterize such materials. DFT and band structure calculations were also carried out for further invesitgation.

[1] B. J. Gibson, R. K. Kremer, A. V. Prokofiev, W. Assmus, and G. J. McIntyre, Physica B **350**, E253 (2004)
[2] C. Lee, Jia Liu, M.-H Whangbo, H.-J. Koo, R. K. Kremer, and A. Simon, Phys. Rev. B **86**, 060407 (2012)
[3] M. G. Banks, R. K. Kremer, C. Hoch, A. Simon, B. Ouladdiaf, J.-M. Broto, H. Rakoto, C. Lee, and M.-H. Whangbo, Phys. Rev. B **80**, 024404 (2009)

TT 17.9 Mon 17:30 H19

**Quantum helimagnets: detriments and new chances for multipolar phases** — Satoshi Nishimoto[1], •Stefan-Ludwig Drechsler[1], Roman Kuzian[2], Johannes Richter[3], and Jeroen van den Brink[1] — [1]Institut für Theoretische Festkörperphysik am IFW-Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Institute for Materials Science, Kiiv, Ukraine — [3]Universiät Magdeburg, Institut für Theoretische Physik, Germany

Arbitrarily strong coupled frustrated spin-1/2 chains in high magnetic fields described within the ferro- antiferromagnetic $J_1$-$J_2$ Heisenberg model and various types of interchain coupling are studied by DMRG, hard-core boson, and spin-wave theory approaches. Multipolar phases related to multimagnon bound states are destroyed (supported) by weak antiferromagnetic (ferromagnetic) interchain couplings $J_{\rm ic}$. We show that quantum spin nematics (quadrupolar phase) might be found for $LiVCuO_4$ whereas for $Li(Na)Cu_2O_2$ it is prevented by a sizeable antiferromagnetic $J_{\rm ic}$. Instead $PbCuSO_4(OH)_2$ (linarite) with sizable easy-axis anisotropy for ferromagnetic nearest neighbor inchain coupling $J_1$ of about 12% might be a good candidate for a triatic (octupolar) phase.

# TT 18: Focused Session: Correlations in Topological Bands (jointly with DS, HL, MA, and O)

Topological ideas have been among the most profound recent additions to the field of condensed matter physics, and they have provided some of the most unexpected new developments, most recently through the proposed existence of fractional Chern insulators: these are lattice systems in which fractional quantum Hall physics occurs in partially filled non-dispersive topological "Chern" bands. Our ability to create such environments is central to advancing the understanding of correlated electron physics.

This session focuses on the twin aspects of the new physics that can be found in such settings on one hand, and recent progress towards realizing such settings on the other. It contains theoretical and experimental contributions, from nano-, semiconductor and cold atomic physics.

Organizer: Roderich Moessner (MPI PKS, Dresden)

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

**Invited Talk** TT 18.1 Mon 15:00 H20

**Designer Dirac Fermions, Topological Phases, and Gauge Fields in Molecular Graphene** — •Hari C. Manoharan — Dept. of Physics, Stanford University, Stanford, California 94305, USA

Using low-temperature scanning tunneling microscopy and spectroscopy, we show the emergence of Dirac fermions in a fully tunable condensed-matter system—molecular graphene—assembled via atomic manipulation of a conventional two-dimensional electron system in a surface state. We embed, image, and tune the symmetries underlying the two-dimensional Dirac equation into these electrons by sculpting the surface potential with manipulated molecules. By distorting the effective electron hopping parameters into a Kekulé pattern, we find that these natively massless Dirac particles can be endowed with a tunable mass engendered by the associated scalar gauge field, in analogy to the Higgs field. With altered symmetry and texturing of the assembled lattices, the Dirac fermions can be dressed with gauge electric or magnetic fields such that the carriers believe they are in real fields and condense into the corresponding ground state, as confirmed by tunneling spectroscopy. Using these techniques we ultimately fabricate a quantum Hall state without breaking time-reversal symmetry, in which electrons quantize in a gauge magnetic field ramped to 60 Tesla with zero applied laboratory field. We show that these and other chiral states now possible to realize have direct analogues in topological insulators, and can be used to guide or confine charge in nontrivial ways [1].

[1] Gomes et al., Nature **483**, 306–310 (2012).

**Invited Talk** TT 18.2 Mon 15:30 H20

**Fractional Topological Insulators** — •Claudio Chamon[1], Christopher Mudry[2], Titus Neupert[2], and Luiz Santos[3] — [1]Boston University — [2]Paul Scherrer Institute — [3]Perimeter Institute

The prediction and experimental discovery of topological band insulators and topological superconductors are recent examples of how topology can characterize phases of matter. In these examples, electronic interactions do not play a fundamental role. In this talk we shall discuss cases where interactions lead to new phases of matter of topological character. Specifically, we shall discuss fractional topological states in lattice models which occur when interacting electrons propagate on flattened Bloch bands with non-zero Chern number. Topologically ordered many-particle states can emerge when these bands are partially filled, including a possible realization of the fractional quantum Hall effect without external magnetic fields. We also discuss the importance of geometric band attributes to stabilize certain fractional states, highlighting the importance of geometry and not just topology for reaching fractional states of matter.

**Topical Talk** TT 18.3 Mon 16:00 H20

**Hierarchy of Fractional Chern Insulators and Competing Compressible States** — •Andreas Läuchli — Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Österreich

The recent engineering of simple tight binding models harboring flat bands with non-zero Chern number calls for a detailed study of the possible many-body phases occurring in partially filled Chern bands and their analogies and differences compared to the continuum Landau level problem. We first report the numerical phase diagram for a flat Chern band with $C = 1$ on the checkerboard lattice, where we find hierarchy multiplets of incompressible states at various fillings $\nu$ These are accounted for by an analogy to Haldane pseudopotentials extracted from an analysis of the two-particle problem. Important distinctions to standard fractional quantum Hall physics are striking: absent particle-hole symmetry in a single band, an interaction-induced single-hole dispersion appears, which perturbs and eventually destabilizes incompressible states as $\nu$ increases [1]. In second study we investigate the occurrence of fractional Chern insulating phases in a series of bands with higher Chern numbers $C = N > 1$. We find compelling evidence for a series of stable states at $\nu = 1/(2N + 1)$ for fermions as well as bosonic states at $\nu = 1/(N + 1)$. By examining the topological ground state degeneracies and the excitation structure as well as the entanglement spectrum, we conclude that these states are Abelian [2].

[1] A. M. Läuchli, Z. Liu, E.J . Bergholtz, and R. Moessner, arxiv:1207.6094 (2012)
[2] Z. Liu, E. J. Bergholtz, H. Fan, and A. M. Läuchli, Phys. Rev. Lett. **109**, 186805 (2012)

**15 min. break**

**Topical Talk** TT 18.4 Mon 16:45 H20

**Designing Topological Bands for Ultracold Atomic Gases** — •Nigel Cooper — Cavendish Laboratory, University of Cambridge, UK

One of the most important techniques in the ultracold atom toolbox is the optical lattice: a periodic scalar potential formed from standing waves of light. Optical lattices are central to the use of atomic gases as quantum simulators, and allow the exploration of strong-correlation phenomena related to condensed matter systems. I shall describe how to design new forms of optical lattice - so-called "optical flux lattices" - in which optically dressed atoms experience a periodic effective magnetic flux with high mean density. Optical flux lattices have narrow energy bands with nonzero Chern numbers, analogous to the Landau levels of a charged particle in a uniform magnetic field. These lattices will greatly facilitate the achievement of the quantum Hall regime for ultracold atomic gases.

**Topical Talk** TT 18.5 Mon 17:15 H20

**Probing Topological Bloch Bands Using Ultracold Quantum Gases** — •Immanuel Bloch — Max-Planck Institut für Quantenoptik, Garching, Germany — Ludwig-Maximilians Universität, München, Germany

Over the past years, ultracold quantum gases have emerged as highly controllable testbeds for probing fundamental condensed matter phenomena. In my talk, I will show how strong effective magnetic fields can be realized for neutral atoms held in an especially engineered optical lattice potential. The effective field strengths that can be reached, are 10-100 times larger than what can be achieved even with the strongest magnets in real material systems, allowing one to take the artificial quantum matter into a new parameter regime. Furthermore, I will show how by carrying out matter wave interferometry within the Bloch bands, we have been able to measure the Zak phase - the Berry phase in one dimension - and to directly determine topological invariants. As an example, I will present results for the celebrated Su-Schrieffer-Heeger model of polyacetylene that can be modelled by using optical superlattice potentials.

# TT 19: Quantum Liquids, Miscellaneous 2

Time: Monday 15:00–16:30 Location: H21

TT 19.1 Mon 15:00 H21

**Structures forming out of quantum seeds in Bose condensates with time-dependent tunnel coupling** — Clemens Neuenhahn[1], Anatoli Polkovnikov[2], and •Florian Marquardt[1] — [1]Universität Erlangen-Nürnberg, Germany — [2]Boston University, USA

Quantum fluctuations can be amplified into macroscopic structures in the course of time. This can happen in quench scenarious, where some parameter is time-dependent, and it has wide-ranging implications, from condensed matter physics to cosmology.

Here, we investigate the behaviour of a model system of two 1D clouds of bosonic atoms. Specifically, we track the time-evolution of the quantum field that describes the relative phase between the quasi-condensates as a function of position. When suddenly switching on the tunnel-coupling, the subsequent dynamics is first governed by parametric amplification of the initial quantum fluctuations. At a later stage, nonlinear dynamics takes over, and localized phase structures form. These structures, which we term 'quasi-breathers', then stochastically form and decay, and we characterize their features using numerical simulations of the underlying sine-Gordon equation based on the truncated Wigner approximation. We then turn to a scenario where the tunnel coupling is changed smoothly over time. It turns out this can be mapped to the evolution of the quantum sine-Gordon field in an expanding 1+1 dimensional toy universe, giving insight into nonlinear structure formation in cosmology.

TT 19.2 Mon 15:15 H21

**Interference effects in Fock space in Bose-Hubbard systems** — •Thomas Engl[1], Juan Diego Urbina[1], Arturo Argüelles Parra[2], Julien Dujardin[2], Peter Schlagheck[2], and Klaus Richter[1] — [1]Universität Regensburg — [2]Universite de Liege

Semiclassical techniques have so far been applied mainly to single particle systems. For these systems they provide a powerful toolbox to study interference effects and allow analytical calculations even in the presence of classical chaos.

On the other hand there have been attempts to apply the semiclassical approximation to the Feynman path integral for bosonic quantum fields in coherent state representation. The resulting coherent state path integral however leads to complex actions which does not give clear insight in interference effects.

We have succeeded in finding a representation in which the semiclassical approximation leads to a van-Vleck propagator with real action and therefore shows interference in Fock space explicitly. We use this propagator to predict various interference effects for Bose-Hubbard systems in three different regimes of the ratio of interaction and hopping strength, and we show that the probability of return is enhanced due to interference.

TT 19.3 Mon 15:30 H21

**Fractional charge separation in the hard-core Bose Hubbard Model on the Kagome Lattice** — •Xuefeng Zhang and Sebastian Eggert — Department of the Physics,Univ. Kaiserslautern, Kaiserslautern, Germany

We consider the hard core Bose Hubbard Model on a Kagome lattice with fixed (open) boundary conditions on two edges. We find that the fixed boundary conditions lift the degeneracy and freeze the system at 1/3 and 2/3 filling at small hopping. At larger hopping strengths, fractional charges spontaneously separate and are free to move to the edges of the system, which leads to a novel compressible phase with solid order. The compressibility is due to excitations on the edge which display a chiral symmetry breaking that is reminiscent of the quantum Hall effect. Large scale Monte Carlo simulations confirm the analytical calculations.

TT 19.4 Mon 15:45 H21

**Propagation of lines of excitations in the two-species Bose Hubbard model** — •Carlo Krimphoff[1], Masud Haque[2], and Andreas M. Läuchli[1] — [1]Institut für Theoretische Physik, Universität Innsbruck, Österreich — [2]Max-Planck-Institut für Physik komlexer Systeme, Dresden, Deutschland

We investigate numerically and analytically the time evolution of lines of overturned spins in the one and two-dimensional spin-1/2 Heisenberg XXZ model after a local quench of the magnetic field. In one dimension a rich sequence of bound states has already been observed, and these states propagate at different velocities. We investigate here how this picture changes and enriches as we move from decoupled one-dimensional chains towards the two-dimensional plane.

As the spin-1/2 Heisenberg model is the strong coupling limit of the two-species Bose Hubbard model at unit filling, our results will shed light on the expected dynamics of lines of mobile spin impurities in two-species bosonic atoms confined to a two-dimensional optical lattice.

TT 19.5 Mon 16:00 H21

**Exotic Ising dynamics in a Bose-Hubbard model** — •Luis Seabra and Frank Pollmann — Max-Planck-Institut fur Physik komplexer Systeme, 01187 Dresden, Germany

We explore the dynamical properties of a one-dimensional Bose-Hubbard model, where two different bosonic species interact via Feshbach resonance. We focus on the region in the phase diagram which is described by an effective, low-energy ferromagnetic Ising model in both transverse and longitudinal fields. In this regime, we numerically calculate the Ising dynamical structure factor of the Bose-Hubbard model using the Time-Evolving Block Decimation method. In the ferromagnet phase, we observe both the continuum of excitations and the bound states for different values of the longitudinal field. Near the Ising critical point, we observe the celebrated $E_8$ mass spectrum in the excited states. We also discuss possible measurements which could be used to detect these excitations in an optical lattice experiment.

TT 19.6 Mon 16:15 H21

**Damping of phase fluctuations in superfluid Bose gases** — •Philipp Lange[1], Peter Kopietz[1], and Andreas Kreisel[2] — [1]Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany — [2]Department of Physics, University of Florida, 32611 Gainesville, FL, USA

Using Popov's hydrodynamic approach we derive an effective Euclidean action for the long-wavelength phase fluctuations of superfluid Bose gases in $D$ dimensions. We then use this action to calculate the damping of phase fluctuations at zero temperature as a function of $D$. For $D > 1$ and small wavevectors $k = |\mathbf{k}|$ we find that, to leading order, the damping $\gamma_k$ is proportional to $A_D k^{2D-1}$, where $A_D$ is a constant prefactor that depends on the dimensionality. However, for $D = 1$ the coefficient $A_D$ vanishes and one has to go beyond perturbation theory. Within a self-consistent calculation we find that in $D = 1$ the damping acquires an additional power of $k$, leading to the long wavelength behavior $\gamma_k \propto k^2$. In one dimension, we also calculate the entire spectral function of phase fluctuations.

# TT 20: Transport: Spincaloric Transport (jointly with MA)

Results -partially also obtained in DFG Priority Program "Spin Caloric Transport" SPP1538 (www.spincat.info)- on spin-dependent transport phenomena initiated and controlled by thermal effects in magnetic nanostructures are discussed.

Time: Monday 15:00–18:45 Location: H22

TT 20.1 Mon 15:00 H22

**Transverse magneto-thermoelectric effects in Permalloy films.** — •Sasmita Srichandan, Maximilian Schmid, Michael Vogel, Christoph Strunk, and Christian Back — Institute of

experimental and applied Physics, University of Regensburg, 93040 Regensburg, Germany

Thermally induced transversal magneto transport phenomena have been studied on 20 nm Py films deposited on MgO and GaAs substrates as well as on 100 nm thick SiN membranes. With an in plane thermal gradient $\nabla$T, the transverse voltage $V_T$ is measured on 10nm thick patterned Pt stripes on top of the Py films with respect to applied external magnetic field B at an angle $\theta$ where $\theta$ is the the angle between B and $\nabla$T. The observed $\sin\theta\cos\theta$ dependence of $V_T$ indicates the planar Nernst effect (PNE). Additionally we observe an asymmetry in the signal between the positive and negative B directions which is proportional to $\cos\theta$. This can be attributed to the anomalous Nernst effect (ANE) caused by a temperature gradient normal to the plane of the sample resulting from thermal radiation. The contribution of the transverse spin Seebeck effect (TSSE) which shares the same $\cos\theta$ symmetry as the ANE, has been separated and it turns out to be one order smaller than reported in the literature [1]. The above measurements have also been performed on SiN membranes and they result in Nernst signals being an order higher than for bulk samples owing to the large local T gradient.

[1] K. Uchida et.al, Observation of spin Seebeck effect. Nature **455**,778-781(2008).

TT 20.2 Mon 15:15 H22

**Tunnel magneto-Seebeck effect in high temperature gradients** — •Marvin Walter[1], J. C. Leutenantsmeyer[1], V. Zbarsky[1], T. Eggebrecht[1], M. Münzenberg[1], K. Rott[2], A. Böhnke[2], G. Reiss[2], A. Thomas[2], M. Czerner[3], and C. Heiliger[3] — [1]I. Phys. Inst., Universität Göttingen, Germany — [2]Dept. of Physics, Bielefeld University, Germany — [3]I. Phys. Inst., Universität Giessen, Germany

CoFeB/MgO/CoFeB devices showing a giant TMR effect are possible candidates for the generation of spin-currents by thermal heating and the tunnel magneto-Seebeck effect was already observed. It is theoretically predicted that for a 3 monolayer MgO barrier the torque of the spin-polarized tunneling electrons might be sufficient to observe thermal spin transfer torque (T-STT).

The samples presented in this work consist of a minimal pseudo-spin-valve stack with sputtered Ta and CoFeB layers and an e-beam evaporated MgO barrier with thicknesses down to 3 monolayers. The MTJs are heated by a Ti:Sa femtosecond laser to achieve high temperature gradients. The heating of the MTJ by a femtosecond laser is simulated using finite element methods. Using the parameters observed in the experimental setup, the simulations show temperature differences across the MgO barrier of more than 10K for a duration in the order of picoseconds. This temperature difference should be sufficient to achieve T-STT. Furthermore, the thermomagnetoelectric properties in high temperature gradients of MTJs with perpendicular magnetic anisotropy and switching current densities of $2 \cdot 10^5$ A/cm$^2$ are investigated.

TT 20.3 Mon 15:30 H22

**Spin-filtering efficiency of ferrimagnetic spinels $CoFe_2O_4$ and $NiFe_2O_4$** — Nuala Caffrey[1], Daniel Fritsch[2], Tom Archer[1], Stefano Sanvito[1], and •Claude Ederer[3] — [1]School of Physics and CRANN, Trinity College Dublin, Ireland — [2]H. H. Wells Physics Laboratory, University of Bristol, United Kingdom — [3]Materials Theory, ETH Zurich, Switzerland

We assess the potential of the ferrimagnetic spinel ferrites $CoFe_2O_4$ and $NiFe_2O_4$ to act as spin-filtering barriers in magnetic tunnel junctions. Our study is based on the electronic structure calculated by means of first-principles approaches within different approximations for the exchange correlation energy. We show that, in agreement with previous calculations, the densities of states suggest a lower tunneling barrier for minority spin electrons, and thus a negative spin-filter effect. However, a more detailed analysis based on the complex band-structure reveals that both signs for the spin-filtering efficiency are possible, depending on the band alignment between the electrode and the barrier material.

TT 20.4 Mon 15:45 H22

**Longitudinal spin Seebeck effect and anomalous Nernst effect in thin $NiFe_2O_4$/Pt films** — •Daniel Meier[1], Timo Kuschel[1], Liming Shen[2], Arunava Gupta[2], Takashi Kikkawa[3], Ken-ichi Uchida[3], Eiji Saitoh[3], Jan-Michael Schmalhorst[1], and Günter Reiss[1] — [1]University of Bielefeld, Germany — [2]University of Alabama, Tuscaloosa, USA — [3]Tohoku University of Sendai, Japan

When a temperature gradient is applied along a ferromagnet/Pt system a spin current parallel to this temperature gradient is generated, which can be converted into an electromotive force ($V_{Pt}$) via the inverse spin Hall effect in the Pt. One can measure a voltage between the ends of the Pt film in a range of a few $\mu$V. In a ferromagnetic insulator/Pt system no regions are expected which are conductive and spin-polarized simultaneously. That is the reason why thermomagnetic effects like the anomalous Nernst effect could be neglected.
In this work we present data for the conductivity of the $NiFe_2O_4$ films and for $V_{Pt}$ taken for $NiFe_2O_4$ films with a thin Pt film on top obtained in a setup for measurements at room temperature and in another one for investigations in a low temperature range. The $NiFe_2O_4$ films show semiconductive characteristics. Therefore, a detailed temperature dependence is studied as well as the influence of direction of an external magnetic field. The origin of the measured effects is discussed on the base of temperature dependent conductivity measurements in order to correlate the longitudinal spin Seebeck effect and the anomalous Nernst effect.

TT 20.5 Mon 16:00 H22

**Dynamics of domains in thermal gradients** — •Frank Schlickeiser, Denise Hinzke, and Ulrich Nowak — Universität Konstanz, 78457 Konstanz, Germany

Many of the recently proposed future magnetic storage devices are based on laser-pulse or current-induced writing schemes, as for example opto-magnetic writing [1]. An unavoidable by-product of these writing schemes are thermal gradients, so that the understanding of their interaction with magnetic structure becomes important. We investigate the dynamics of domains in thin ferromagnetic CoPd films triggered by thermal gradients by means of computer simulations, based on the Landau-Lifshitz-Bloch-equation. The latter describes the dynamics of a thermally averaged spin polarization on micro-magnetic length scales [2]. We show that in a Gaussian temperature profile the magnetic structure is modified towards a radial orientation of the domains. Our numerical results are compared with recently performed measurements. We acknowledge financial support by the DFG through SFB 767. [1] K. Vahaplar et al.,Phys. Rev. Lett. 103, 117201 (2009), [2] D. Hinzke and U. Nowak, Phys. Rev. Lett. 107, 027205 (2011).

TT 20.6 Mon 16:15 H22

**Thermally excited magnonic spin currents probed by the longitudinal spin-Seebeck effect in YIG** — •Andreas Kehlberger[1], René Röser[1], Gerhard Jakob[1], Benjamin Jungfleisch[2], Burkard Hillebrands[2], Ulrike Ritzmann[3], Denise Hinzke[3], Dong Hun Kim[4], Caroline Ross[4], Ulrich Nowak[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany — [2]Department of Physics, Institute of Technology Kaiserslautern, 67663 Kaiserslautern, Germany — [3]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [4]Department of Materials Science and Engineering, MIT , Cambridge, MA 02139, USA

In the research field of spin caloric transport one of most the prominent and still not understood effects is the spin-Seebeck effect (SSE) in magnetic insulators [1]. Many explanations consider thermally excited magnons as the underling mechanism, for which direct evidence is missing so far. We present a systematic study of the SSE in Yttrium Iron Garnet (YIG) films of different thicknesses. From the thickness dependence of the measured inverse spin Hall effect we can unambiguously identify the SSE effect . Corresponding simulations on atomistic length scales allow us to deduce the propagation length of the thermally excited magnons, which could be used to manipulate domain walls [2]. [1] K. Uchida et al., Nature Mater. 9, 894 (2010) [2] D. Hinzke et al., Phys. Rev. Lett. 107, 027205 (2011)

TT 20.7 Mon 16:30 H22

**Laser induced magneto-Seebeck effect on different substrate materials** — •Alexander Böhnke[1], Marvin Walter[2], Karsten Rott[1], Andy Thomas[1], Markus Münzenberg[2], and Günter Reiss[1] — [1]Thin Films and Physics of Nanostructures, Bielefeld University, Germany — [2]I. Physikalische Institut, Georg-August-Universität Göttingen, Germany

Since the discovery of the magneto-Seebeck effect [1,2,3] (TMS, *tunnel magneto-Seebeck*) a proper interpretation of the time-resolved voltage traces has been missing [1]. Improvements in the time resolution of the TMS setup now give access to the investigation of the origin of the Seebeck voltage.

Further, we investigated magnetic tunnel junctions (MTJs) on two

different substrate materials: Insulating MgO and semiconducting p-doped Si covered by 50 nm of $SiO_2$. TMS measurements on both sample types lead to same results. However, the time-resolved voltage traces in the case of silicon substrate showed a sharp peak when the laser is turned on. On MgO substrate this peak is not found. SPICE simulations of comparable MTJs on both substrates were performed and can give a first glance on thermal voltages occurring in the layer stacks and the substrates due to laser heating and capacitive coupling.

[1] M. Walter et al., Nat. Mater. 10 (2011), 742.
[2] C. Heiliger et al., Phys. Rev. B 83 (2011), 1.
[3] N. Liebing et al., Phys. Rev. Lett. 107 (2011), 177201.

**15 min. break**

TT 20.8 Mon 17:00 H22

**Ab initio investigations on the magnetothermopower of thin Co/Cu multiple spin-valves** — •Voicu Popescu and Peter Kratzer — Faculty of Physics, University Duisburg-Essen, Duisburg, Germany

We have modelled multiple spin-valve configurations by stacking Co and Cu layers of various thickness and number of repetitions. Theoretical investigations on their magneto-thermoelectric properties were performed by calculating the conventional and magnetic Seebeck coefficient using a spin-polarized relativistic implementation of the Landauer-Büttiker conductance formula within the framework of Korringa-Kohn-Rostoker method.

In line with experimental expectations, we find that the anti-parallel (AP) alignment of the adjacent Co layers is characterized by a much larger Seebeck coefficient than the parallel (P) configuration: from $1-2\ \mu$V/K in the P-case, the AP Seebeck coefficient can reach as much as 10 $\mu$V/K at room temperature. A correspondence between these values and the giant magneto-resistance characteristic to the Co/Cu spin valves could thus be established.

We show that an increase in the thickness of the Co layer further enhances the magnetothermopower whereas the Cu layer thickness variation has a negligible effect. In addition, we investigate the magnetic anisotropy in the Seebeck coefficient for these systems, by changing the magnetization orientation from parallel to perpendicular to the current. Our results suggest that a strong Seebeck magnetic anisotropy could be detected in typical GMR elements.

TT 20.9 Mon 17:15 H22

**Altering the thermopower by magnetic fields** — •Steven Achilles[1], Volodymyr V. Maslyuk[2], and Ingrid Mertig[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, D-06120 Halle, Germany — [2]Institute of Electron Physics, National Academy of Sciences of Ukraine, 88017 Uzhgorod, Ukraine

Transport properties of nanocontacts are unusual and determined by quantum effects as soon as the characteristic diameter decreases towards the nanometer scale. Besides the investigation of transport properties under low temperature conditions, temperature induced transport becomes more and more important [1].

In this work, we present an ab-initio study of both conductance and thermopower in a non-collinear magnetic system. We focus on an organometallic vanadium-benzene ($V_4Bz_5$) molecule attached to two Co electrodes oriented in fcc (001) direction with non-collinear magnetic order. Such vanadium-benzene complexes were synthesized and remain stable up to room temperature [2].

We show that, besides the formation of a non-collinear magnetization through the molecule, the sign and magnitude of the thermopower can be addressed directly altering the orientation of the leads magnetization. Furthermore, a non-monotonous behavior of the thermopower as a function of angle between the lead magnetization directions is found [3].

[1] Reddy et al., Science **315 (5818)**, 1568 (2007).
[2] K. Miyajima et al., Eur. Phys. J. D **34**, 177-182 (2005).
[3] V. V. Maslyuk et al., submitted.

TT 20.10 Mon 17:30 H22

**Thermal spin-transfer torques in magnetic tunnel junctions** — Michael Czerner, Christian Franz, and •Christian Heiliger — I.Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

The emerging research field of spin caloritronics combines the spin-dependent charge transport with energy or heat transport. In comparison to thermoelectrics the spin degree of freedom is considered as well. We present ab initio calculations based on density functional theory using a Green's function KKR method. We compute the non-equilibrium density in a non-collinear regime, which allows us to calculate the spin-transfer torque. In our investigation we focus on the material dependence of the thermal spin-transfer torque in MgO based tunnel junctions. In particular, we investigate Fe, Co, and FeCo alloys as lead materials. The FeCo alloy is described by the coherent potential approximation (CPA) including vertex corrections for the non-equilibrium density. The thermal spin-transfer torque is calculated for several barrier thicknesses. It turns out that the size of the thermal spin-transfer torque is orders of magnitude smaller than spin-transfer torque at an applied bias voltage. Consequently, the thermal spin-transfer torque can be utilized only for very thin barrier thicknesses.

TT 20.11 Mon 17:45 H22

**Quantum Isobaric Process and Thermodynamic Diesel Cycle in $Ni_2$** — •Chuanding Dong, Georgios Lefkidis, and Wolfgang Hübner — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Box 3049, 67653 Kaiserslautern, Germany

Building thermodynamic cycles with magnetic molecules extends quantum thermodynamics to real systems [1,2] and provides a unique opportunity to explore the thermodynamic properties of the spin degree of freedom. Here we propose a quantum isobaric process in the $Ni_2$ dimer, and build a quantum Diesel engine [3]. The level scheme of $Ni_2$ is obtained using *ab-initio* calculation and the perturbative inclusion of an external magnetic field. Our isobaric process is realized by adjusting the bath temperature in dependence on the interatomic distance. The boundary condition of keeping the pressure constant imposes a limitation on the allowed bond lengths, which we call isobaric range.

In the quantum Diesel cycle, since the preceding adiabatic process brings the $Ni_2$ dimer to a nonequilibrium state, the isobaric process is realized through a modified Boltzmann distribution. Due to its strong effect on the distribution profile, novel features, such as the crossing of the two adiabatic strokes, can appear on the projection on the two-dimensional $P-V$ diagram.

[1] H. T. Quan, Phys. Rev. E **79**, 041129 (2009).
[2] T. D. Kieu, Phys. Rev. Lett. **93**, 140403 (2004).
[3] C. D. Dong, G. Lefkidis, and W. Hübner, J. Supercond. Nov. Magn (in press).

TT 20.12 Mon 18:00 H22

**Ab-initio study of the temperature dependent electron transport through magnetic nanostructures** — •Roman Kováčik, Phivos Mavropoulos, Daniel Wortmann, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recent developments in the field of the spin caloritronics have triggered many questions about the origin and character of the observed phenomena (e.g., spin-dependent Seebeck versus spin Seebeck effect [1]). To contribute to the understanding of the underlying mechanisms at the microscopic level, we investigate spin-dependent electron transport through various magnetic nanostructures between non-magnetic leads as a function of the temperature. The electronic structure of the studied systems is calculated within the multiple scattering screened Korringa-Kohn-Rostoker (KKR) Green function framework [2]. The Monte-Carlo methodology is then used to simulate the effect of temperature on the magnetic configurations with the exchange coupling parameters calculated according to [3]. Finally, the Landauer-Büttiker approach for the ballistic transport within the KKR framework [4] is extended to account for the non-collinear magnetic effects. Support from the DFG (SPP 1538) is gratefully acknowledged.

[1] G.E.W. Bauer *et al.*, Nature Mater. 11, 391 (2012).
[2] N. Papanikolaou *et al.*, J. Phys. Condens. Matter 14, 2799 (2002), also see: www.kkr-gf.org.
[3] A.I. Liechtenstein *et al.*, J. Magn. Magn. Mater. 67, 65 (1987).
[4] Ph. Mavropoulos *et al.*, Phys. Rev. B 69, 125104 (2004).

TT 20.13 Mon 18:15 H22

**Origin of the spin Seebeck effect in thin films** — •Michael Schreier[1], Akashdeep Kamra[2], Mathias Weiler[1], Rudolf Gross[1], and Sebastian T.B. Goennenwein[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands

The spin Seebeck effect (SSE) originates from a finite temperature difference $\Delta T$ between the magnons in a ferromagnet (FM) and

the electrons in a normal metal (NM) which supposedly stems from weak magnon-phonon interaction and different boundary conditions on phonon and magnon mediated heat currents. Also, recent experiments [1] suggest that the magnon-phonon interaction is much stronger than originally assumed, which again reduces the expected SSE [2]. Hence the established theory can not account quantitatively for the longitudinal SSE signals in thin films. A factor that has, however, been neglected so far is the Kapitza resistance which leads to an additional contribution to $\Delta T$ by introducing a discontinuity in the phonon temperature distribution at the FM/NM interface. This has been modelled using an analytical model and 3D finite elements simulations which show that, for thin layers, the contribution to $\Delta T$ originating from the Kapitza resistance is indeed of the same order of magnitude as the one from the original model. Hence the acoustic properties of the FM and NM play an important role in the origin of the SSE. This work is supported by the DFG via SPP1538.

[1] M. Agrawal et al., arXiv (2012)
[2] M. Weiler et al., Phys. Rev. Lett. 108, 106602 (2012)

TT 20.14 Mon 18:30 H22

**Scattering-Independent Contribution to the Anomalous Nernst Effect** — •Jürgen Weischenberg, Frank Freimuth, Stefan Blügel, and and Yuriy Mokrousov — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In analogy to the electric conductivity tensor [1], the thermoelectric- or Peltier conductivity tensor may be decomposed into a scattering-dependent and a scattering-independent term. Using the full-potential linearized augmented plane-wave method within the density functional theory, we compute all the contributions to the scattering-independent term, namely the intrinsic contribution and the side-jump contribution, and show that in ferromagnetic materials they are both of equal importance. In particular, the comparison of our theoretical values with experiments suggests that the anomalous Nernst effect in Fe, Co, Ni, FePd and FePt is largely caused by the scattering-independent term [2]. Moreover, the consequences of magnetic disorder on thermoelectric transport phenomena are also discussed. Financial support by the HGF-YIG Programme VH-NG-513 is gratefully acknowledged. J. W. was supported under grant SPP 1538 SpinCaT by the German Science Foundation.

[1] J. Weischenberg, F. Freimuth, J. Sinova, S. Blügel and Y. Mokrousov, PRL **107**, 106601 (2011)
[2] J. Weischenberg, F. Freimuth, S. Blügel and Y. Mokrousov, arXiv:1210.8283 [cond-mat.mtrl-sci]

## TT 21: Graphene - Electronic Properties and Transport 1 (jointly with DS, HL, MA, and O)

Time: Monday 16:00–19:00 Location: H17

TT 21.1 Mon 16:00 H17

**Epitaxial silicene - tunable hybridization with the substrate and weak interactions with epitaxial organic overlayers** — •Rainer Friedlein[1], Antoine Fleurence[1], Fabio Bussolotti[1,2], and Yukiko Yamada-Takamura[1] — [1]School of Materials Science, Japan Advanced Institute of Science and Technology (JAIST), Nomi, Ishikawa 923-1292, Japan — [2]present address: Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan

The electronic and structural properties of epitaxial silicene formed on $ZrB_2$(0001) thin films grown on Si(111) wafers upon adsorption of either potassium atoms and anthracene molecules have been studied using photoelectron spectroscopy and electron diffraction. For pristine silicene, a particular, atomic-scale buckling leads to the opening of a direct band gap at the Γ point, while $ZrB_2$-related surface states are not affected. This is consistent with only a minor degree of hybridization beween Si- and Zr-derived states. The electronic interactions at the interface can be tuned by electron donation from adsorbed potassium atoms, upon which hybridization is progressively switched on.
At 140 K, anthracene molecules are found to grow as epitaxial multilayers that exhibit a point-on-line commensurate relationship with silicene. The results indicate that the charge-density modulation associated with the buckling of silicene render the interactions with organic adsorbates as compared to graphene, which allows for specific epitaxial conditions. On the other hand, the results also confirm that silicene is strikingly different from other Si surfaces for which the presence of dangling bonds leads to chemisorption of organic adsorbates.

TT 21.2 Mon 16:15 H17

***Ab initio* study of graphene nano domes on Ir(111) surface** — •Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, in a combined experimental and theoretical work we have unveiled the bonding mechanism of graphene on Ir(111) surface as physisorption with a local chemical modulation [1]. In this contribution we extend our previous density functional theory (DFT) study to analyse the bonding of graphene nano domes on a clean and an oxygen pre-covered Ir(111) substrate.

As previously shown [1], the inclusion of the long-range van der Waals interactions is mandatory and in our *ab initio* study these dispersion interactions were considered at a semi-empirical [2] or first-principle [3] level, the latter as implemented in our real-space JuNoLo code [4]. In particular, the non-local correlation vdW-DF functional [3] provides an unique visual insight on the origin of a different graphene bonding on Ir(111) due to a non-local and a semi-local description of the correlation effects in DFT.

[1] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).
[2] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).
[3] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).
[4] P. Lazić *et al.*, Comp. Phys. Commun. **181**, 371 (2010).

TT 21.3 Mon 16:30 H17

**Effects of strain on the excitonic Fano resonance in the optical spectrum of graphene** — •Daniela Ullrich[1,2], Patrick Herlinger[1], Harald Giessen[2], Jurgen Smet[1], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]4th Physics Institute, University of Stuttgart

Using transmission and reflection spectroscopy we examine the optical response of graphene from the visible to the UV regime. The absorbance spectrum of free-standing graphene is dominated by an asymmetric peak in the UV at about 4.7 eV. We show that this resonance can be described by a simple Fano model which includes an excitonic state beneath the saddle point of graphene's band structure [1]. When strain is applied to a graphene sheet, the symmetry of the lattice and thus also of the band structure is broken. As predicted recently [2], this should result in a splitting of the absorbance peak in the optical spectrum as well as a strong dependence on polarization and lattice orientation. Here, we present our findings on the effects of strain on the Raman and reflectivity spectra of graphene on flexible substrates.

[1] Chae et al., Nano Lett. 11, 1379 (2011)
[2] Liang et al., J. Mater. Res. 27, 403 (2012)

TT 21.4 Mon 16:45 H17

**Probing Hot Electron Distributions in Graphene on Ni(111) with High Harmonic Radiation** — •Carsten Winter[1], Thorben Haarlammert[1], Luca Bignardi[2], Petra Rudolf[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster — [2]Zernike Institute for Advanced Materials, University of Groningen

Theoretical calculations and experimental observations of hot electron distributions in graphene show an initial ultrafast carrier relaxation accompanied by a population of optical phonons, which decay on a picosecond time scale. In this talk we present an experimental set-up suited to measure the lifetime of excited electrons and their relaxation dynamics via time-resolved 2PPE. Through frequency conversion by High Harmonic Generation coherent radiation at 39 eV photon energy is generated and subsequently used as the probe pulse in two-photon photoemssion.

A graphene sheet was produced by decomposition of ethylene on a Ni(111) substrate. Hot electron distributions were generated in graphene on Ni(111) by applying 800nm pulses. The energy dependent lifetimes of these distributions have been measured. The lifetimes have been determined to 20-50 fs in the lower energy parts of

the distribution (E-$E_F$ < 1eV) and show a strong Ni-like behavior. In the upper energy parts lifetimes of 10-20 fs have been measured and a graphite-like behavior dominates.

TT 21.5 Mon 17:00 H17

**Reversible Photooxidation of Graphene** — •Stefan Böttcher, Hendrik Vita, and Karsten Horn — Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany

Graphene oxide is often discussed in the context of a technical usage of graphene in future electronic devices. The necessity to obtain a tunable band gap in possible electronic applications makes graphene oxide a promising covalent modification of graphene. However, the homogeneous preparation of graphene oxide has so far been a challenging task, using mainly an aggressive chemical or complex physical treatment of graphene. Here we present a method to selectively produce graphene oxide from epitaxially grown graphene on transition metal surfaces such as Ir(111). Using $NO_2$ as an adsorbate we transform graphene into graphene oxide by irradiation with UV light at low temperatures, leading to specific signatures in the core and valence level photoemission and -absorption spectra. The graphene oxide thus prepared is stable up to room temperature, but its formation is thermally completely reversible to graphene at higher temperatures.

TT 21.6 Mon 17:15 H17

**Edge charge disorder in graphene** — •Cornelie Koop, Manuel Schmidt, and Carsten Honerkamp — Institut für Theoretische Festkörperphysik, RWTH Aachen University, Deutschland

We study the interplay of edge roughness and electron-electron interaction in graphene nanoribbons. Our focus is the charge response of a rough edge to (possibly random) potentials induced by adatoms. While the bulk density response in graphene is rather small due to the vanishing density of states at the charge neutrality point, it turns out that edges show a strongly increased response - a fact that may be traced back to the presence of localized states at rough edges. The existence of these localized states depends on the structural properties of the edge. They are the disordered analogs to the well known edge states in clean zigzag ribbons and lead to a random sequence of peaks in the local density of states along the rough edge. As a consequence there may be strongly localized charges randomly distributed along the edge. We discuss the conditions for this effect, which we call edge charge disorder, its strength, and its consequences on the bulk electrons in a graphene nanoribbon.

TT 21.7 Mon 17:30 H17

**Electronic and magnetic properties of zigzag graphene nanoribbons on the (111) surface of Cu, Ag and Au** — •Yan Li[1], Wei Zhang[1], Markus Morgenstern[2], and Riccardo Mazzarello[1] — [1]Institute for Theoretical Solid State Physics and JARA, RWTH Aachen University, D-52074 Aachen, Germany — [2]II. Physikalisches Institut B and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany

We have carried out an *ab initio* study of the structural, electronic and magnetic properties of zigzag graphene nanoribbons (GNRs) on Cu(111), Ag(111) and Au(111). Both H-free and H-terminated GNRs are considered revealing that the nanoribbons invariably possess edge states when deposited on these surfaces. In spite of this, they do not exhibit magnetism at the edge, with the exception of H-terminated GNRs on Au(111), whose zero-temperature magnetic properties are comparable to those of free-standing GNRs. The absence of edge magnetism is due to the hybridization between the $2pz$ orbitals of the carbon atoms and the $d$ states of the metal and, for some models, to the charge transfer between the GNR and the surface, which shifts the edge state away from the Fermi level. Only in the case of H-terminated GNRs on Au(111) is the interaction between the substrate and the GNR sufficiently weak so as not to affect the magnetic properties of the edge state significantly.

TT 21.8 Mon 17:45 H17

**The atomic and electronic structure of well-defined graphene nanoribbons studied by scanning probe microscopy** — •Joost van der Lit[1], Mark Boneschanscher[1], Mari Iljas[2], Ari Harju[2], Andreas Uppstu[2], Daniel Vanmaekelbergh[1], Peter Liljeroth[2], and Ingmar Swart[1] — [1]Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands — [2]Department of Applied Physics, Aalto University, Finland

Recently, graphene nanostructures have gained a lot of interest since they introduce a bandgap in graphene, which is important for (opto-) electronics applications. Graphene nanoribbons can have a bandgap as large as 3 eV[1,2], which can be tuned by varying its width. By using a chemical bottom-up approach, we have synthesized graphene nanoribbons (GNR) on an Au(111) substrate[3]. By combining scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with reactive and non-reactive tips, we can relate the electronic properties of the GNRs with their atomic structure. Furthermore, we can use the STM tip to (i) deliberately create well-defined atomic scale defects and (ii) control the interaction with the substrate. Hence, we are able to directly study the robustness of the properties of the graphene nanostructures. [1] P. Ruffieux, et al. , ACS Nano 6 (2012) 6930. [2]M. Koch, F. Ample, C. Joachim, L. Grill, Nat. Nanotechnol. 7 (2012)713. [3] J. Cai et al., Nature, 446 (2010) 470-473.

TT 21.9 Mon 18:00 H17

**Intact Dirac cones at broken sublattice symmetry: photoemission study of graphene on Ni and Co** — •Dmitry Marchenko[1], Andrei Varykhalov[1], Jaime Sánchez-Barriga[1], Markus R. Scholz[1], Bart Verberck[2], Björn Trauzettel[3], Tim O. Wehling[4,5], Carlo Carbone[6], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Universiteit Antwerpen — [3]Universität Würzburg — [4]Universität Bremen — [5]Bremen Center for Computational Materials Science — [6]Consiglio Nazionale delle Ricerche Trieste

A band gap at the Dirac point of graphene can be created by breaking of the sublattice symmetry through epitaxial growth on a substrate crystal. One of the strongest sublattice-symmetry-breaking interactions with predicted and measured band gaps ranging from 400 meV to more than 3 eV has been attributed to the interfaces of graphene with Ni and Co, which are also promising spin filter interfaces. We apply angle-resolved photoemission to epitaxial graphene on Ni(111) and Co(0001) to show the presence of intact Dirac cones in a strongly n-doped system. Our results challenge the common belief that breaking of sublattice symmetry by a substrate and opening of the band gap at the Dirac energy are in a straightforward relation. A simple effective model of a biased bilayer structure composed of graphene and a sublattice symmetry broken layer, corroborated by density functional theory calculations, demonstrates the general validity of our conclusions.

TT 21.10 Mon 18:15 H17

**$sp^2$ carbon hybrid junctions** — Pablo Robert[1,2], Renjun Du[1], Fan Wu[1], Kristina Hönes[1], Jens Mohrmann[1], Frank Hennrich[1], Manfred Kappes[1,3,4], Hilbert von Löhneysen[1,2,4,5], and •Romain Danneau[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, — [2]Institute of Physics, Karlsruhe Institute of Technology, Germany — [3]Institute of Physical Chemistry, Karlsruhe Institute of Technology, Germany — [4]DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology, Germany — [5]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Germany

Lowering the contact resistance is a key issue to improve graphene field effect device performance. The connection between a metal and graphene depends on many parameters such as the work function mismatch between the two connected material, the adsorption of the metal on graphene, the quality of the deposited material as well as the strain induced on the graphene sheet. We have studied electronic transport through carbon nanotube (CNT)-graphene and graphene-graphene junctions produced by nano-manipulation and transfer. For the CNT-graphene junctions, we first demonstrate that the influence of the CNT on the charge distribution of the graphene sheet is limited to few nanometers. Our experiments show that the junction transparency is strongly gate dependent due to the variation of the CNT-graphene distance, and the charge carrier injection occurs via a single point. For the graphene-graphene junctions, our measurements show low resistance and prove that graphene makes a good connection to graphene.

TT 21.11 Mon 18:30 H17

**Graphene on boron nitride microwave transistors driven by graphene nanoribbon back-gates** — Christian Benz[1,2], •Maximilian Thürmer[1], Fan Wu[1], Zeineb Ben Aziza[1], Jens Mohrmann[1], Hilbert von Löhneysen[1,2,3,4], Kenji Watanabe[5], Takashi Taniguchi[5], and Romain Danneau[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]Institute of Physics, Karlsruhe Institute of Technology, Germany — [3]DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology,

Germany — [4]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Germany — [5]Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan

We have designed ultra-thin graphene microwave transistors by using pre-patterned metal or graphene nanoribbon back-gates and hexagonal boron nitride (h-BN) as a dielectric substrate. Despite the inhomogeneities induced by the graphene transfer process, we show that it is possible to operate these types of devices across a broad range of microwave frequencies. For the graphene nanoribbon gates, we observe a deviation of the current gain from the usual 1/f trend that can be attributed to the large gate resistance of these systems as we demonstrate with our small-signal model. The scattering parameter analysis shows a very limited back-action from the channel onto the graphene nanoribbon gates. Our work thus proves that graphene microwave transistors could be driven by graphene nanoribbon gates.

TT 21.12 Mon 18:45 H17

**Strong gate hysteresis in graphene on mica field effect devices** — •Jens Mohrmann[1], Kenji Watanabe[2], Takashi Taniguchi[2], and Romain Danneau[1,3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [2]Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan — [3]Institute of Physics, Karlsruhe Institute of Technology, Germany

One of the outstanding properties of graphene is the unbeatable ratio of surface to volume. As a membrane of only one atomic layer of carbon, graphene is extremely sensitive to external influences. The large area contact with the substrate thus causes a large influence of the used substrate on the electronic properties of graphene. Therefore, a lot of effort is being made in order to understand the interaction between graphene and its substrate, and to find new and possibly better materials. One material under investigation is muscovite mica. The layered structure allows perfect basal (001) cleavage with atomically flat terraces, and using mechanical exfoliation, very thin crystals can be created and used as a substrate and gate dielectric. Transport measurements of graphene on mica show a very high hysteresis with respect to the gate voltage. Here, we investigate this effect using dual gated devices, with both mica and hexagonal boron-nitride dielectrics.

## TT 22: Focused Session: Frontiers of Electronic Structure Theory 2 (jointly with HL and O)

Time: Monday 16:00–19:15 Location: H36

TT 22.1 Mon 16:00 H36

**Excited States of the divacancy in SiC** — •Michel Bockstedte[1], Thomas Garratt[1], and Adam Gali[2] — [1]Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudstr. 7B2, D-91058 Erlangen — [2]Wigner Research Centre for Physics, Hungarian Academy of Sciences, PO Box 49, Budapest 1525, Hungary

The negatively charged nitrogen-vacancy center in diamond has emerged as a candidate for the implementation of a qbit in quantum computing. Silicon Carbide also fullfils necessary conditions[1] which makes it a suitable material for this purpose. With the neutral divacancy it possess a defect center with a high spin ground state, which can be manipulated by spin-resonance techniques.[2] Optical excitation of the triplet ground state and subsequent spin-selective recombination via yet unknown intermediate spin-singlet states enables spin-initialization with $M_z$=0, which is requisit for a qbit. Here we investigate the excitation spectrum of the divacancy based *ab initio* methods. DFT and TD-DFT calculations[3] reveal a Jahn-Teller effect for the first excited triplet state that is absent for the NV-complex. TD-DFT and an *ab initio* many body hamiltonian nicely reproduce the prominent photoluminescence transitions. The latter method also describes the spin-singlet states. We discuss the defect excitation spectrum in the light of the Jahn-Teller distortion.

[1] J. R. Weber *et al.*, PNAS **107**, 8513 (2010).
[2] F. Koehl *et al.*, Nature **479**, 84 (2011).
[3] A. Gali, phys. status solidi (b) **248**, 1337 (2011).

TT 22.2 Mon 16:15 H36

**Extending the random phase approximation for electronic correlation energies: The renormalized adiabatic local density approximation** — •Thomas Olsen — Technical University of Denmark

The adiabatic connection fluctuation-dissipation theorem with the random phase approximation (RPA) has recently been applied with success to obtain correlation energies of a variety of chemical and solid state systems. The main merit of this approach is the improved description of dispersive forces while chemical bond strengths and absolute correlation energies are systematically underestimated. In this work we extend the RPA by including a parameter-free renormalized version of the adiabatic local density (ALDA) exchange-correlation kernel. The renormalization consists of a (local) truncation of the ALDA kernel for wave vectors $q > 2k_F$, which is found to yield excellent results for the homogeneous electron gas. In addition, the kernel significantly improves both the absolute correlation energies and atomization energies of small molecules over RPA and ALDA. The renormalization can be straightforwardly applied to other adiabatic local kernels.

TT 22.3 Mon 16:30 H36

**First-principles IXS spectra for $TiO_2$ and $HfO_2$** — •Linda Hung and Francesco Sottile — Ecole Polytechnique, Palaiseau, France

Using time-dependent DFT and many-body perturbation theory, we determine the inelastic x-ray scattering (IXS) spectra for bulk $TiO_2$ and $HfO_2$. Excitations from valence and semi-core states are modeled, corresponding to transition energies up to 60 eV. By varying momentum transfer, plasmon dispersion can be observed. We characterize differences in the spectra for the rutile, anatase, and brookite polymorphs of $TiO_2$, as well as the cubic, tetragonal, and orthogonal polymorphs of $HfO_2$. These spectra are also Fourier transformed, allowing us to image the real-time and real-space electron density response to external perturbations.

TT 22.4 Mon 16:45 H36

**Linear-scaling time dependent density-functional theory in the linear response formalism** — •Tim J. Zuehlsdorff, Nicholas D. M. Hine, James S. Spencer, Nicholas M. Harrison, and Peter D. Haynes — Imperial College London, UK

In recent years, linear-scaling approaches to density-functional theory have enabled the computation of ground-state properties of large nanostructures and biomolecules. While these methods are now well established, the linear-scaling computation of excited state properties via time-dependent density-functional theory (TDDFT) in the linear response regime is less developed.

In this talk we will present an implementation of TDDFT in the linear response formalism, enabling the computation of low-energy optical absorbtion spectra for large molecules and nanostructures. The method avoids any explicit reference to canonical representations of either occupied and unoccupied Kohn-Sham states and thus achieves linear-scaling computational effort with system size. In contrast to conventional localised orbital formulations where a single basis set is used to represent the occupied and unoccupied Kohn-Sham states, we make use of two sets of in-situ optimised localised orbitals, one for the occupied and one for the unoccupied Kohn-Sham space. The double basis set approach avoids known problems of representing the unoccupied space with localised orbitals optimised for the occupied space, while the in-situ optimisation procedure allows for efficient calculations with a minimal set of basis functions. The method is applied to a number of large-scale test systems in order to demonstrate its validity.

TT 22.5 Mon 17:00 H36

**Dynamical spin and charge excitations with spin–orbit coupling in 3d adatoms on Cu(111) and Pt(111)** — •Manuel dos Santos Dias, Benedikt Schweflinghaus, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The presence of spin–orbit coupling has a fundamental impact on the magnetic excitation spectrum: there is a finite gap at zero frequency and spin and charge excitations become coupled. The excitation spectrum is derived from the dynamical magnetic susceptibility of the electronic system, for which we developed a formalism based on Time–Dependent Density Functional Theory, as implemented in the

Korringa–Kohn–Rostoker Green function method [1,2]. As an application, we present first–principles calculations of the charge, longitudinal and transverse magnetic excitations of 3d adatoms deposited on the Cu(111) and Pt(111) surfaces. Focus is on the expected spin–charge coupling induced by the the spin–orbit interaction, and on the dynamical anisotropic effects that generalize the familiar magnetic anisotropy.

Work supported by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).
[1] S. Lounis, A. T. Costa, R. B. Muniz and D. L. Mills, Phys. Rev. Lett. **105**, 187205 (2010)
[2] S. Lounis, A. T. Costa, R. B. Muniz and D. L. Mills, Phys. Rev. B **83**, 035109 (2011)

TT 22.6 Mon 17:15 H36

**Beyond the *GW* approximation: a second-order screened exchange correction** — •Patrick Rinke[1], Xinguo Ren[1], Noa Marom[2], Fabio Caruso[1], and Matthias Scheffler[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Texas, Austin, USA

Despite the success of the *GW* method in describing the photoemission spectra of solids, molecules and clusters, challenges remain. For aromatic molecules for example absolute as well as relative positions of ionisation energies and affinities are not well reproduced in perturbative $G_0W_0$ schemes with different starting points as well as in self-consistent *GW* [1], sometimes even giving the wrong orbital order. Motivated by renormalized second-order perturbation theory [2] for the ground-state energy, we propose a second-order screened exchange correction (SOSEX) to the *GW* self-energy. This correction follows the spirit of the SOSEX correction to the random-phase approximation for the electron correlation energy and reduces the self-correlation error. The performance of the *GW*+SOSEX scheme has been benchmarked for a set of molecular systems, including the G2 set, commonly used acceptor molecules, benzene and the azabenzene molecules. We find that the SOSEX correction improves the description of the spectral properties including the orbital order with respect to the different *GW* schemes, highlighting the importance of reducing the self-correlation error. [1] N. Marom *et al.*, arXiv:1211.0416 [2] X. Ren *et al.*, J. Mater. Sci. **47**, 7447 (2012)

TT 22.7 Mon 17:30 H36

**A strategy for finding a reliable starting point for $G_0W_0$ demonstrated for molecules** — •Thomas Körzdörfer[1] and Noa Marom[2] — [1]Institut für Chemie, Universität Potsdam, D-14476 Potsdam — [2]Center for Computational Materials, Institute of Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX 78712, USA

Many-body perturbation theory in the $G_0W_0$ approximation is an increasingly popular tool for calculating electron removal energies and fundamental gaps for molecules and solids. However, the predictive power of $G_0W_0$ for molecules is limited by its sensitivity to the density functional theory (DFT) starting point. In this contribution, the starting point dependence of $G_0W_0$ is demonstrated for several organic molecules. Analysis of the starting point dependence leads to the development of a non-empirical scheme that allows to find a consistent and reliable DFT starting point for $G_0W_0$ calculations by adapting the amount of Hartree-Fock-exchange in a hybrid DFT functional. The $G_0W_0$ spectra resulting from this *consistent starting point (CSP) scheme* [1] reliably predict experimental photoelectron spectra over the full energy range. This is demonstrated for a test set of various typical organic semiconductor molecules.

[1] T. Körzdörfer and Noa Marom, Phys. Rev. B Rapid Communications **86**, 041110 (2012).

TT 22.8 Mon 17:45 H36

**Electronic properties of isolated and supported organic dyes modeled through the GW method** — •Paolo Umari[1], Filippo De Angelis[2], Luigi Giacomazzi[3], Mariachiara Pastore[2], and Stefano Baroni[3] — [1]Dipartimento di Fisica e Astronomia, Università di Padova, Italy — [2]Istituto CNR di Scienze e Tecnologie Molecolari, Perugia, Italy — [3]Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy

The first-principles GW method is used for investigating the electronic levels of isolated and supported dyes for electrochemical solar cells. We consider a set of all-organic dyes, (L0,L2,L3,L4) exhibiting the same donor and anchor groups. First, we calculate the energy levels in the limit of isolated molecules obtaining nice agreement with available experimental photoelectron spectra. Then, we consider the L0 and the L2 dyes while adsorbed on the anatase $TiO_2$ (101) surface. Also in this case we find good agreement when comparing with available experimental photoelectron spectra. We find that the HOMO -LUMO gap of the dye is reduced with respect to the isolated molecule and that the HOMO level is slightly shifted towards higher energies due to image charge effects. This permits us to derive a simple model for obtaining approximate GW energy levels for the HOMO and the LUMO of the adsorbed molecule and for the valence band maximum and the conduction band minimum of the substrate performing just one complete GW calculation of the isolated molecule and one of the bulk $TiO_2$ combined with a calculation at the DFT level of the adsorbed molecule complex. In this way, we can investigate larger, more realistic, model structures.

TT 22.9 Mon 18:00 H36

**Ab-initio description of satellites in semiconductors** — •Matteo Guzzo[1,2], Josh J. Kas[3], Lorenzo Sponza[1,2], Christine Giorgetti[1,2], Francesco Sottile[1,2], Debora Pierucci[4], Mathieu G. Silly[4], Fausto Sirotti[4], John J. Rehr[3], and Lucia Reining[1,2] — [1]LSI, Ecole Polytechnique, Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]UW, Seattle, USA — [4]Synchrotron Soleil, Gif-sur-Yvette, France

The GW method from Many-Body Perturbation Theory has been very successful in describing photoemission spectra in a variety of systems. In particular, GW is known to give good quasiparticle properties like band gaps, but it has shown some limitations in the description of complex correlation effects like satellites. Satellite peaks in photoemission come from higher-order excitations and are still poorly studied in the valence bands. In perturbative GW the spectral function can describe additional features beside the quasiparticle peaks, but these satellites are known to be too weak and too low in energy, as it appears from calculations on the Homogeneous Electron Gas and some real materials. Including additional diagrams in the Green's function we obtain an excellent description of satellites series in the test case of bulk silicon, where GW is unable to cope [1]. This approach can be extended to more complex system, i.e. graphite. Using our newly measured XPS valence data, we investigate the effects of anisotropies on satellites and give a prediction on the spectral changes following the transition towards true freestanding graphene. [1] M. Guzzo et al., Phys. Rev. Lett. 107, 166401 (2011)

TT 22.10 Mon 18:15 H36

**Optical spectra of alkali-metal fluorides** — •Christoph Sommer, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany

We have studied the virtue of different approximations for quasiparticle energies in the calculation of optical spectra including excitonic effects by solving the Bethe-Salpeter equation (BSE). To this end, we have computed exemplarily optical spectra of the three alkali-metal fluorides LiF, NaF, and KF using quasiparticle energies resulting from two different approximations of the self-energy operator in Hedin's *GW* approach as well as electronic energies and wave functions obtained by employing self-interaction corrected pseudopotentials. The energetic positions of characteristic peaks in the calculated and measured spectra are in very good agreement when quasiparticle energies are used that result after an update of the screened interaction $W$ on the basis of a preceding $G_0W_0$ calculation. Additionally, two simple further approximations for one-particle energies that use input either from experiment or from quasiparticle calculations for a small set of wave vectors are included into this investigation.

TT 22.11 Mon 18:30 H36

**Bethe-Salpeter Equation from many-body perturbation theory** — •Tobias Sander, Ronald Starke, and Georg Kresse — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The Green function formalism is a powerful tool to calculate not only electronic structure within the quasi-particle (QP) picture, but it also gives access to optical absorption spectra. Starting from QP energies within the GW method, the polarizability, as central quantity, is calculated from the solution of a Bethe-Salpeter-like equation (BSE). It is usually solved within the Tamm-Dancoff Approximation (TDA) which neglects the coupling of resonant (positive frequency branch) and anti-resonant (negative frequency branch) excitations. In this work we

solve the full BSE [1] (beyond TDA) based on self-consistently calculated QP orbitals and energies [2] for typical systems. The dielectric function is averaged over many low dimensional shifted **k**-meshes to obtain **k**-point converged results. We compare the results to recently introduced approximation to the BSE kernel [3]. Additionally, the time-evolution ansatz [4] is employed to calculate the polarizability, which avoids the direct solution of the BSE.

[1] S. Albrecht, L. Reining, R. Del Sole, G. Onida, PRL 80, 4510 (1998)
[2] M. Shishkin, M. Marsman, G. Kresse, PRL 99, 246403 (2007)
[3] L. Reining, PRL 88, 66404 (2002)
[4] W. G. Schmidt, S. Glutsch, P. H. Hahn, F. Bechstedt, PRB 67, 085307 (2003)

TT 22.12 Mon 18:45 H36

**Acceleration of the response function convergence using the effective energy techniques within the ultrasoft pseudopotential and PAW methods** — •Jiří Klimeš and Georg Kresse — Faculty of Physics, University of Vienna, A-1090 Vienna, Austria

Calculations of quasiparticle spectra based on the GW approximation or evaluation of total energies using the RPA method are of a wide interest in the computational materials community. However, their applicability is to a large extent limited by the cost of evaluating the response function or the selfenergy where a large number of unoccupied bands needs to be included. A promising way to speed-up the convergence is to use the resolution of identity and replace the sum over an infinite number of unoccupied states by an effective correction [1,2]. However, the available schemes have been only formulated for norm-conserving pseudopotentials and when applied directly within the ultrasoft pseudopotentials (USPPs) or the PAW method they introduce an error since the correction term doesn't vanish when the number of included bands is increased. Here we present an implementation of the schemes within the formalism of USPPs or the PAW method which gives the proper behaviour of the correction term. We also show how the convergence of the scheme given in [2] can be further improved and discuss the efficiency of the methods for RPA total energy calculations.

[1] F. Bruneval and X. Gonze, PRB **78**, 085125 (2008)
[2] J. A. Berger, L. Reining, and F. Sottile, PRB **82**, 041103(R) (2010); PRB **85**, 085126 (2012)

TT 22.13 Mon 19:00 H36

**SnO: GW band gap of a van der Waals bonded system** — •Kirsten Govaerts[1], Rolando Saniz[2], Bart Partoens[2], and Dirk Lamoen[1] — [1]EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium — [2]CMT group, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerpen, Belgium

In this work we have investigated the structural and electronic properties of SnO, which is built up by layers kept together by van der Waals (vdW) forces. The combination of a vdW functional (within DFT) and GW calculations leads to accurate values for the c/a ratio and the fundamental band gap. A comparison is made between three starting points for the GW calculation: a regular PBE calculation, one with the vdW effect included, and a hybrid functional calculation. The difference between different levels of self-consistency is also investigated.

## TT 23: Superconductivity: Fe-based Superconductors - 1111

Time: Monday 16:45–17:45 Location: H21

TT 23.1 Mon 16:45 H21

**Anisotropy of normal state and superconducting properties of oxypnictides** — •Silvia Haindl[1], Martin Kidszun[1], Alexander Kauffmann[1], Nadja Kozlova[1], Kazumasa Iida[1], Thomas Thersleff[1,2], Takahiko Kawaguchi[3], Hiroshi Ikuta[3], Erik Kampert[4], Jochen Wosnitza[4], Oleksii Vakaliuk[1], Nadezda Panarina[1], Christian Hess[1], and Bernd Büchner[1] — [1]IFW Dresden, P.O.Box 270116, 01171 Dresden, Germany — [2]The Ångström Laboratory, Department of Engineering Sciences, Division of Applied Materials Science, Uppsala University, 752 37 Uppsala, Sweden — [3]Department of Crystalline Materials Science, Nagoya University, Nagoya 464-8603, Japan — [4]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany

The very large upper critical fields of the oxypnictides complicate the experimental determination of their anisotropy, $\gamma_{Hc2}$, especially at low temperatures. In Kidszun et al., PRL 106, 137001 (2011), we have applied the anisotropic Ginzburg-Landau scaling on angular-dependent critical-current densities measured for an epitaxially grown $La(O_{1-x}F_x)FeAs$ thin film (see review by Haindl et al., Int. J. Mod. Phys. B). The obtained scaling parameter matches $\gamma_{Hc2}$ as can be demonstrated by recent magnetotransport measurements in pulsed magnetic fields up to 70 T and down to 2 K. Using the method of critical current scaling $H_{c2}^{ab}$ for $Nd(O_{1-x}F_x)FeAs$ is extrapolated. In addition we discuss normal state electrical transport properties of $La(O_{1-x}F_x)FeAs$ and $Nd(O_{1-x}F_x)FeAs$ thin films.

Work supported by DFG: projects HA5934/1-1, HA5934/4-1 and partially HA5934/3-1.

TT 23.2 Mon 17:00 H21

**Phase diagram of F- and Co-doped CeFeAsO** — •Oleksii Vakaliuk, Sabine Wurmehl, Christine Malbrich, Eva Brüning, Hans-Joachim Grafe, Christian Hess, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstr. 20, 01069 Dresden Germany

We carried out an experimental systematic electronic resistivity investigation of CeFeAsO system in a wide Co-doping range (0 - 0.12) and compare it to F-doped (0 - 0.10) CeFeAsO. The resistivity of the pristine compound: i) exhibits a pronounced peak at approximately 150 K, followed by a steep decrease and ii) an inflection point which are clear signatures of the tetragonal to orthorhombic structural transition, and the antiferromagnetic spin density wave transition, respectively. iii) At low temperature the resistivity shows a kink-like anomaly due to ordering of Ce magnetic moments. Upon doping these anomalies shifts to lower temperature, and become suppressed and broadened. From these observations we construct the magnetic/superconducting phase diagrams for both compounds. Furthermore, NMR/NQR studies reveal a new type of microscopic order in the underdoped normal state regime.

TT 23.3 Mon 17:15 H21

**Spin Fluctuations in Iron Based Superconducters Probed by NMR Relaxation Rate** — •Uwe Gräfe[1], Franziska Hammerath[1,2], Tim Kühne[1], Sabine Wurmehl[1], Guillaume Lang[3], Bernd Büchner[1], and Hans-Joachim Grafe[1] — [1]IFW Dresden, Institute for Solid State Research, PF 270116, 01171 Dresden, Germany — [2]Department of Physics "A. Volta", University of Pavia-CNISM, I-27100 Pavia, Italy — [3]3LPEM-UPR5, CNRS, ESPCI Paris Tech, 10 Rue Vauquelin, 75005 Paris, France

We present $^{75}$As nuclear magnetic resonance (NMR) results in F doped LaOFeAs iron pnictides. In the underdoped superconducting samples, pronounced spin fluctuations lead to a peak in the NMR spin lattice relaxation rate, $(T_1T)^{-1}$. The peak shows a typical field dependence that indicates a critical slowing of spin fluctuations: it is reduced in height and shifted to higher temperatures. In contrast, a similar peak in the underdoped magnetic samples at the ordering temperature of the spin density wave does not show such a field dependence. Furthermore, the peak is absent in optimally and overdoped samples, suggesting the absence of strong spin fluctuations. Our results indicate a glassy magnetic ordering in the underdoped samples that is in contrast to the often reported Curie Weiss like increase of spin fluctuations towards $T_c$. Additional measurements of the linewidth and the spin spin relaxation rate are in agreement with such a glassy magnetic ordering that is most likely competing with superconductivity. Our results will be compared to Co doped $BaFe_2As_2$, where a similar peak in $(T_1T)^{-1}$ has been observed [Ning, JPSJ 2009].

TT 23.4 Mon 17:30 H21

**Carrier doping by current injection into LaOFFeAs** — •Irina Lazareva[1], Yury Koval[1], Christian Steiner[1], Sabine Wurmehl[2], Bernd Büchner[2], Tobias Stürzer[3], Dirk Johrendt[3], and Paul Müller[1] — [1]Department of Physics, Universität Erlangen, Detschland — [2]IFW Dresden, Deutschland — [3]Department Chemie, LMU München, Detschland

Recently, we were able to change the carrier concentration of hole-doped high-$T_c$ superconductors by injection of large currents along the c-axis. We extend this type of experiments to electron-doped pnictides. From our earlier interpretation we should expect that trapping of electrons caused by current injection would decrease the available carrier concentration. Indeed, by various experiments with superconductors from the $LaO_{1-x}F_xFeAs$ family we are able to show that trapped electrons caused by current injection perpendicular to the FeAs planes decrease the carrier concentration. We present a spectacular confirmation of this interpretation by the $T_c$ increase by more than 15 K in heavily overdoped $La_{O.74}F_{0.26}FeAs$. We performed similar experiments with the recently discovered 1048 layered pnictides of the composition $Ca_{10}(FeAs)_{10}(Pt_4As_8)$ [1]. The general tendency of carrier doping by trapped electrons was confirmed. A rather interesting discovery was the evolution of hysteretic c-axis IV-characteristics. This is a strong indication of intrinsic Josephson effects. We discuss these results in terms of a change of anisotropy by carrier doping.

[1] T. Stürzer, G. Derondeau, D. Johrendt, Phys. Rev. B 86, 060516(R) (2012).

## TT 24: Focused Session: Dirac Fermions in Solid-State Systems (jointly with HL)

The observation of massless Dirac fermions in monolayer graphene has initiated a new area of research exploring charge carriers that behave relativistically within solid-state systems. Both massless and massive Dirac fermions are studied in a growing range of materials that include most prominently few-layer graphene and topological insulators. The symposium will highlight some of the recent developments in this quickly advancing field. (Organizers: Roland Winkler, Northern Illinois University, and Ewelina Hankiewicz, Universität Würzburg)

Time: Tuesday 9:30–12:15 Location: H2

**Topical Talk** TT 24.1 Tue 9:30 H2

**Localization at graphene system and topological insulator edges** — •Markus Buttiker — University of Geneva, Dept. of Theoretical Phys., 24 Quai E. Ansermet, 1211 Geneva, Switzerland

Graphene systems share a number of features with topological insulators. We investigate localization phenomena at the edges of these two systems [1,2]. In bilayer graphene subject to a strong perpendicular electric field we have found that in the presence of a strongly disordered edge a sequence of localized states appears. Interestingly the localization length depends only on the size of the bulk gap but is otherwise universal, i.e. independent of the type and strength of the disorder [1]. The appearance of these localized states reflects the marginal topological properties of bilayer graphene, a bipartite square lattice with similarly disordered edges does not show edge states localized at the edge.

In two-dimensional topological insulators such as HgTe/CdTe there exists a pair of helical edge states which are protected against non-magnetic disorder. However, if time-reversal symmetry is removed by the application of a magnetic field the protection is removed and these states localize. We investigate the divergence of the localization length as the magnetic field tends to zero and find that the localization length saturates at higher fields [2].

[1] Jian Li, Ivar Martin, Markus Buttiker, Alberto F. Morpurgo, Nat. Phys. 7, 38-42 (2011); Phys. Scr. Physica Scripta T146, 014021 (2012).

[2] Pierre Delplace, Jian Li, Markus Büttiker , Phys. Rev. Lett. 109. 246803 (2012).

**Topical Talk** TT 24.2 Tue 10:00 H2

**Controlling Quantized Edge Transport in Two-dimensional Topological Insulators** — Viktor Krueckl, Sven Essert, and •Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Robustness of edge channels against disorder scattering is an outstanding feature of two-dimensional topological insulators (TIs). Here we consider quantized transport and mesoscopic interference phenomena in HgTe-based TIs, systems where the quantum spin Hall state has first been experimentally observed [1]. On the one hand, we discuss mechanisms to steer the spin orientation, and thereby the charge flow between different edges in TI constrictions that turn out to provide rather robust spin transistor functionality [2]. On the other hand, we study the combined effect of a time-reversal symmetry breaking magnetic field and disorder on transport to explore the limits of topological protection and the competition between reflectionless modes, metallic behavior and Anderson localization. In particular, transport in hybrids composed of normal conducting and TI regions shows peculiar quantization phenomena.

[1] M. König et al., Science **318**, 766 (2007);

[2] V. Krueckl, K. Richter, Phys Rev. Lett. **107**, 086803 (2011).

**Topical Talk** TT 24.3 Tue 10:30 H2

**First-principles studies of Dirac-cones in graphene and 3D topological insulators** — •Gustav Bihlmayer — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany

The unique properties of graphene, in particular the two Dirac-cones determining the transport phenomena in this material, led the way to the first theoretical proposal of the quantum spin Hall effect at the edges of a graphene ribbon by Kane and Mele in 2005. Since spin-orbit coupling (SOC) effects are extremely weak at the Dirac points, this phenomenon is hard to observe experimentally. I discuss several theoretical proposals and experiments that have been made to enhance intrinsic SOC effects. Here, density functional theory (DFT) provides a quantitative tool to predict the properties of these two-dimensional topological insulator phases.

In three-dimensional topological insulators topologically protected edge states form Dirac-cones with chiral spin texture (in contrast to the spin-degenerate Dirac-cone of graphene). We discuss the spin-polarization and -orientations in this state for Bi and Se chalcogenides and its interaction and modification with magnetic adatoms. Also here DFT results will be compared to experiments where available.

**Coffee break**

**Topical Talk** TT 24.4 Tue 11:15 H2

**Lifetime broadening of topological surface states with and without magnetic moments** — •Oliver Rader[1], Markus Scholz[1], Jaime Sánchez-Barriga[1], Andrei Varykhalov[1], Dmitry Marchenko[1], Emile Rienks[1], Andrey Volykhov[2], and Lada Yashina[2] — [1]Helmholtz-Zentrum Berlin — [2]Moscow State University

The lifetime broadening of the angle-resolved photoemission signal from the surface states of $Bi_2Se_3$ and $Bi_2Te_3$ is studied. It is revealed that hexagonal warping in $Bi_2Te_3$ introduces an anisotropy for electrons propagating along $\overline{\Gamma}$-$\overline{K}$ and $\overline{\Gamma}$-$\overline{M}$. Moreover, we show that the electron-phonon coupling strength is substantial and in good agreement with theoretical predictions. The small Fermi surface is believed to limit the number of phonon modes for electron scattering. In line with this, the imaginary part of the self-energy from the surface state electrons declines with higher binding energies. In addition, we find that Fe surface impurities have a much stronger influence on the lifetimes as compared to Ag. This is independent of the sign of the doping which is p-type when Fe is deposited at low temperature.

**Topical Talk** TT 24.5 Tue 11:45 H2

**Transport in topological insulators - experiments** — •Christoph Brüne — Experimentelle Physik 3, Physikalisches Institut, Universität Würzburg

The prediction and discovery of topological insulators (TIs) has attracted wide interest in the physics community during the past years. The first topological insulator state was predicted and discovered in 2 dimensional systems. I will present our results concerning the quan-

tum spin Hall effect in HgTe quantum wells. The quantum spin Hall effect is the signature state of a 2-dimensional topological insulator.

In 3 dimensions this new state of mater is characterized by conducting Dirac type surface states while the bulk of the material remains insulating. Such surface states have been observed in e.g. Bi2Te3, Bi2Se3 and Sb2Te3. These materials do, however, exhibit large defect densities paired with low carrier mobilities. So far this prevented transport studies in the quantum Hall regime of 3D TIs. Recently, however, we succeeded in using strained bulk HgTe as 3D TI. This enabled us to measure the quantum Hall effect from the 3D TI surface state in transport experiments.

## TT 25: Correlated Electrons: Low-Dimensional Systems - Models 3

Time: Tuesday 9:30–13:15 Location: H9

TT 25.1 Tue 9:30 H9

**Interacting Fröhlich and Holstein bipolarons** — •Monodeep Chakraborty[1], Masaki Tezuka[2], and Byung Il Min[1] — [1]Department of Physics, POSTECH, Pohang, 790-784, Korea — [2]Department of Physics, Kyoto University, Kyoto 606-8502, Japan

Polarons and bipolarons have been long-term subjects of interest in many areas of condensed matter. We have investigated the bipolaron-bipolaron interaction for the Holstein-Hubbard (HH) and the Fröhlich-Hubbard(FH) model on a discrete one-dimensional (1D) lattice. We have generated a variational space by repeated application of our chosen Hamiltonian on a initial state and then used conjugate-gradient technique to obtain the ground state energy as well as the wavefunction for a few electron (two, four and six) and phonon system. The HH model has also been studied with density-matrix renormalization group (DMRG). Both methods lead to the same conclusion that there exists no bipolaron-bipolaron attraction in the HH model. However, we obtain clear cut bipolaron-bipolaron attraction within the Fröhlich paradigm above a critical electron-phonon coupling forming the bipolaron cluster. The bipolaron cluster can survive in spite of the Hubbard-$U$ effect up to a finite $U$ and then separates into individual bipolarons or polarons. The bipolaron-bipolaron attraction could be a possible mechanism of the phase separation in many condensed matter systems with the strong electron-phonon interaction.

TT 25.2 Tue 9:45 H9

**Non-equilibrium dynamics of the Kondo cloud following quenches in the Resonant Level Model** — •Shreyoshi Ghosh, Pedro Ribeiro, and Masud Haque — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We study the non-equilibrium dynamics of lattice realizations of the Resonant Level Model. In equilibrium, the conduction electrons form a screening cloud around the impurity site. This impurity screening cloud has been the subject of longstanding fascination, especially in the Kondo model, from which the resonant level model emerges in the Toulouse limit. We present results on the time evolution of the spatial structure of the impurity screening cloud, after local and global quenches of system parameters.

TT 25.3 Tue 10:00 H9

**Breakdown of flat bands in highly-frustrated spin systems** — •Michael Powalski[1], Kris Coester[1], Roderich Moessner[2], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

In several highly-frustrated spin systems the low-energy excitation band is known to be exactly flat up to a certain perturbative order. One important example is the fully-frustrated transverse field Ising model on the kagome lattice. Its lowest one-particle band is extremely flat becoming dispersive only in order eight perturbation theory in the high-field limit. This behaviour can be traced back to the existence of a local mode being an exact eigenstate up to seventh order.
Here we use high-order series expansions to investigate the occurrence and the breakdown of flat bands in geometrically frustrated systems. It is shown that the breakdown of such flat bands is connected to quantum fluctuations which do not interfere destructively. This can be understood intuitively via the used linked cluster expansion.

TT 25.4 Tue 10:15 H9

**Renyi entropies of classical loop gases and string nets** — •Mascha Baedorf, Maria Hermanns, and Simon Trebst — Universitaet zu Koeln, Germany

Since the seminal work of Shannon the concept of entropy is closely connected to the information content of a many-body state. This link has been widely employed in recent years to characterize quantum many-body states whose defining characteristic eludes a description in terms of correlation functions and a local order parameter. Probably the most prominent example of the latter are topologically ordered states, for which the so-called topological entanglement entropy provides an unambiguous identification and partial characterization of the non-local topological order. Here we discuss the classical analog of the Renyi entropy and via extensive numerical simulations demonstrate its ability to positively identify topological order in classical loop gas and possibly string net states.

TT 25.5 Tue 10:30 H9

**Tunable Superconductivity with Ultracold Polar Molecules and Enhanced Superconducting Phases in dipolar $t-J_\perp$ chains** — •Salvatore R. Manmana[1,2], Kaden R.A. Hazzard[2], Gang Chen[2], Alexey V. Gorshkov[3], and Ana Maria Rey[2] — [1]Institut für Theoretische Physik, Universität Göttingen, Germany — [2]JILA, University of Colorado and NIST, and Department of Physics, CU Boulder, USA — [3]Institute for Quantum Information & Matter, Caltech, Pasadena, California, USA

By selecting two dressed rotational states of ultracold polar molecules in an optical lattice, we obtain a highly tunable generalization of the t-J model, which we refer to as the t-J-V-W model. In addition to XXZ spin exchange, the model features density-density interactions and density-spin interactions, all of them $\sim 1/r^3$. Full control of all interaction parameters in both magnitude and sign can be achieved independently of each other and of the tunneling. We apply the density matrix renormalization group method to obtain the 1D phase diagram in the case of nearest neighbor hopping and long-range transverse spin-exchange $J_\perp$. The anisotropy in the spin-exchange and the long-range nature of the interactions lead to an enhanced superconducting phase. We discuss that the long-range interactions despite the presence of a gap lead to an algebraically decaying contribution to correlation functions.

TT 25.6 Tue 10:45 H9

**Bosonic Fractional Quantum Hall States in Rotating Optical Lattices: Projective Symmetry Group Analysis** — •Tanja Duric and Achilleas Lazarides — Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

We study incompressible ground states of bosons in a two-dimensional rotating square optical lattice. The system can be described by the Bose-Hubbard model in an effective uniform magnetic field present due to the lattice rotation. To study ground states of the system, we map it to a frustrated spin model, followed by Schwinger boson mean field theory and projective symmetry group analysis. Using symmetry analysis we identify bosonic fractional quantum Hall states, predicted for bosonic atoms in rotating optical lattices, with possible stable gapped spin liquid states within the Schwinger boson formalism. In particular, our results indicate that previously obtained fractional quantum Hall states induced by the lattice potential, and with no counterpart in the continuum, correspond to pi-flux spin liquid states of the frustrated spin model.

**15 min. break**

**Topical Talk** TT 25.7 Tue 11:15 H9

**One-dimensional fermion systems beyond the Luttinger Liquid paradigm** — •Thomas L. Schmidt[1,2], Adilet Imambekov[3], and Leonid I. Glazman[1] — [1]Department of Physics, Yale University, New Haven, Connecticut 06520, USA — [2]Department of Physics, University of Basel, CH-4056 Basel, Switzerland — [3]Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA

For many years, Luttinger liquid theory has served as a useful paradigm for the description of 1D quantum fluids in the limit of low energies. This theory is based on a linearization of the dispersion relation of the particles constituting the fluid. In this talk, I will review recent progress in understanding 1D fermion systems beyond the low-energy limit, where the nonlinearity of the dispersion relation becomes essential. I will present results for the dynamic correlation functions of spinless and spinful fermion systems, and discuss the fate of spin-charge separation, one of the hallmarks of the linear Luttinger liquid theory, beyond the low-energy limit.

TT 25.8 Tue 11:45 H9

**Impurity effects in frustrated magnets with subextensive degeneracies** — •Stefan Bittihn and Simon Trebst — Universität zu Köln, Germany

We consider the effects of local impurities in frustrated honeycomb-lattice antiferromagnets, which exhibit large but nonextensive ground-state degeneracies. In the absence of impurities magnetic order is induced via a thermal order-by-disorder mechanism. In the presence of impurities this entropic selection of states is put into competition with an energetic selection of states favored by the impurities, a more conventional order by quenched disorder mechanism. We characterize the latter via extensive numerical simulations on large-scale lattices.

TT 25.9 Tue 12:00 H9

**Expansion dynamics of interacting bosons in homogeneous lattices** — •Jens Philipp Ronzheimer[1,2], Michael Schreiber[1,2], Simon Braun[1,2], Sean S. Hodgman[1,2], Stephan Langer[2,3], Ian P. McCulloch[4], Fabian Heidrich-Meisner[5,2], Immanuel Bloch[1,2], and Ulrich Schneider[1,2] — [1]LMU München — [2]MPQ Garching — [3]University of Pittsburgh, USA — [4]University of Queensland, Brisbane, Australia — [5]Universität Erlangen-Nürnberg, Erlangen

We study out-of-equilibrium dynamics and transport properties of interacting many-body systems using ultracold atoms in optical lattices. Specifically, we experimentally and numerically investigate the expansion dynamics of initially localized bosons in homogeneous 1D and 2D Hubbard systems. We find that the fastest, ballistic expansions occur in the integrable limits of the system. In 1D, these are both the non-interacting and the strongly-interacting limits where the system enters into the hard-core boson regime. Any deviation from these limits, either through finite interactions or the admixture of double occupancies in the initial state, significantly slows down the expansion. In 2D, the strongly interacting limit is fundamentally different. The system expands ballistically only in the non-interacting case, while all interactions lead to strongly diffusive behavior. This is in full analogy to previous experiments with interacting fermions. By controlling the tunneling along individual lattice axes, we can gradually change the dimensionality of the system from 1D to 2D. In the strongly interacting case, we observe how the initially ballistic dynamics in a 1D system turn diffusive when additional degrees of freedom become available.

TT 25.10 Tue 12:15 H9

**The Role of Local and Non-Local Conserved Quantities in the Thermalization of Closed Quantum Systems** — •Nikolaos P. Konstantinidis and Jesko Sirker — Fachbereich Physik und Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany

We investigate thermalization after a sudden quench for antiferromagnetic Heisenberg models on finite rings, with extrapolation of the results to the thermodynamic limit. We show that in the non-integrable case, which results from the inclusion of next-nearest neighbor interactions, only local conservation laws are important for the thermalization of local quantities, while the contribution of non-local operators vanishes exponentially with system size. The equilibrated system in the thermodynamic limit is thus described by a canonical ensemble. We also examine how in the integrable case the additional local but longer-range conserved quantities affect thermalization.

TT 25.11 Tue 12:30 H9

**The eigenstate thermalization hypothesis near integrable points** — •Wouter Beugeling, Masud Haque, and Roderich Moessner — Max Planck Institute for the Physics of Complex Systems (MPI-PKS), Dresden, Germany

In the field of nonequilibrium quantum dynamics, the issue of thermalization in isolated systems has been the topic of intense recent interest. The eigenstate thermalization hypothesis (ETH) has been proposed as a mechanism for the thermalization of nonintegrable systems. According to the ETH, the expectation values of typical physical observables in eigenstates vary smoothly as a function of the corresponding eigenenergies.

We discuss systems that can be tuned towards and away from integrability by the variation of parameters in the Hamiltonian. We present results on whether and how the ETH progressively breaks down as we approach an integrable point. We also address the role played by the choice of physical observable.

TT 25.12 Tue 12:45 H9

**Exact description of the magnetoelectric effect in the spin-1/2 XXZ-chain with Dzyaloshinskii-Moriya interaction** — •Vadim Ohanyan[1], Andreas Kluemper[2], and Michael Brockmann[2,3] — [1]Yerevan State University, 1 Alex Manoogian 0025 Yerevan, Armenia — [2]Bergische Universitaet Wuppertal, Gauss str.20, D-42119, Wuppertal, Germany — [3]University of Amsterdam, Science Park 904, 1098 XH Amsterdam, Netherlands

We considered the S=1/2 XXZ-chain with DM-term in the context of magnetoelectric effect realized by means of Katsura-Nagaosa-Baladsky(KNB) mechanism, which connects the local polarization with the cross product of two neighboring spin. Considering, thus, the DM-term as an interaction between local polarization and external electric field, we apply the quantum transfer matrix(QTM) and non-linear integral equation(NLIE) technique for exact description of the mutual influence of magnetic and dielectric properties at finite temperatures, known as the magnetoelectric effect. We obtain the exact plots of polarization(magnetization) dependence on magnetic(electric) filed as well as temperature dependence of the magnetoelectric tensor. The results, particularly, show several possible regimes of polarization, linear, square-root, quadratic and some combination of them. The switching between different regimes can be easily performed by adjusting the magnetic field.

TT 25.13 Tue 13:00 H9

**Quantum state renormalization group approach to symmetry-protected topological phases** — •Ching-Yu Huang[1], Frank Pollmann[1], Feng-Li Lin[2], and Xie Chen[3] — [1]MPIPKS, Dresden,Germany — [2]NTNU, Taipei, Taiwan — [3]UC Berkeley,Berkeley, USA

Topologically phases do not break symmetries and can thus not be characterized by local order parameters. A particular kind of topological phases are the so-called symmetry-protected topological phases (SPTP) which are only distinct from a trivial phase as long as certain symmetries are preserved. The first example of a SPTP is the Haldane phase in S=1 spin chains. We use a symmetry preserving quantum state renormalization group (QSRG) method to characterize SPTP. The QSRG removes short range entanglement and yields a fixed point state which is then used to characterize the phase. For this, we first apply the infinite time-evolving block decimation (iTEBD) method to numerically find the ground state wave function which is then used as initial state for the QSRG procedure. As a simple example we study the one-dimensional Haldane phase. We then extend the method to two dimensions, and study the SU(2) symmetric, two-dimensional quantum spin-3/2 systems on the honeycomb lattice as well as a recently introduced model which realizes a SPTP.

# TT 26: Graphene - Electronic Properties and Transport 2 (jointly with DS, HL, MA, and O)

Time: Tuesday 9:30–12:45 Location: H17

TT 26.1 Tue 9:30 H17

**Transport properties of high-quality reduced graphene oxide** — •Michael Enzelberger[1], Siegfried Eigler[2], Philipp Hofmann[1], Stefan Grimm[2], Andreas Hirsch[2], and Paul Müller[1] — [1]Department of Physics and Interdisciplinary Center for Molecular Materials, Universität Erlangen-Nürnberg — [2]Department of Chemistry and Pharmacy, and Institute of Advanced Materials and Processes (ZMP), Universität Erlangen-Nürnberg

Chemical production of graphene, especially reducing graphene oxide has gained a lot of interest in recent years. Yet the transport properties of such materials are usually not compatible to those of graphene.

We have found a way to overcome this problem using a modification of the standard Hummer's method. Single flakes of reduced graphene oxide have been investigated. The graphene oxide was deposited onto a $SiO_2$/Si substrate and subsequently reduced using hydrogen iodine. The resulting reduced graphene oxide samples were patterned by electron beam lithography. We have characterized the quality of the samples by combining Raman spectroscopy and Hall mobility measurements in magnetic fields up to $14\,T$ and temperatures down to $0.3\,K$.

High-quality samples had a Raman D/G ratio of better than 1 and showed Hall mobilities exceeding 1000 $cm^2/Vs$. This is nearly two orders of magnitude higher than what is known for standard reduced graphene oxide. The best samples even show Shubnikov-de Haas oscillations and Hall plateaus.

TT 26.2 Tue 9:45 H17

**Magnetoresistance of Nanocrystalline Graphene** — •Daniel Steininger[1], Paul Linsmaier[1], Ina Schneider[1], Christoph Strunk[1], Matthias Büenfeld[2], Nils-Eike Weber[2], Andrey Turchanin[2], Miriam Grothe[3], and Thomas Weimann[3] — [1]Institute for Experimental and Applied Physics, University of Regensburg, Universitätsstr. 31, D-93053 Regensburg, Germany — [2]Faculty of Physics, University of Bielefeld,Universitätsstr.25, D-33615 Bielefeld, Germany — [3]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

We report on the magnetotransport in Hall bar structures of nanocrystalline graphene. The graphene sheets were prepared by electron-beam-induced cross-linking and subsequent pyrolysis of aromatic self-assembled monolayers [1]. The I-V characteristics show considerably non-linear behaviour at low temperatures. One low resistive sample (≈ 200 kOhm/sq at T = 4 K) shows positive magnetoresistance values up to + 20 % in the perpendicular magnetic field for temperatures below 6 K, while above this temperature the magnetoresistance becomes negative. Measurements of the transversal voltage in the linear regime exhibit anomalous behaviour which cannot be explained by the conventional Hall effect. If the magnetic field is aligned parallel to the graphene sheet the magnetorestance exhibits large positive values up to + 300 %. Measurements on a highly resistive sample (≈ 30 MOhm/sq at T = 4 K) reveal a non-monotonic behaviour of the magnetoresistance in a perpendicular magnetic field.

[1] A. Turchanin et al., ACS Nano 5 (2011) 3896-3904.

TT 26.3 Tue 10:00 H17

**Quantum Monte Carlo Study of Edge-State Magnetism on Chiral Graphene Nanoribbons** — Michael Golor[1], Thomas C. Lang[1,2], and •Stefan Wessel[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen — [2]Department of Physics, Boston University

We investigate the edge-state magnetism of chiral graphene nanoribbons using projective Quantum Monte Carlo (QMC) simulations and a self-consistent mean-field approximation of the Hubbard model. Previous QMC simulations support edge-state ferromagnetism in sufficiently wide zigzag terminated ribbons. We extended these calculations to include the class of chiral graphene nanoribbons and investigate the influence of chirality and ribbon width on spin-spin correlations. The static magnetic correlations are found to rapidly increase with the width of the ribbons for all chiralities, such that already for ribbons of moderate widths we observe a strong trend towards mean-field-type ferromagnetic correlations along the edges. We extract dynamical edge state signatures which can be used to detect edge-state magnetism by scanning tunneling microscopy.

TT 26.4 Tue 10:15 H17

**Even-odd effects in NSN scattering problems: Application to graphene nanoribbons** — •Francois Crepin[1], Hans Hettmansperger[1], Patrik Recher[2], and Bjoern Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Wuerzburg, 97074 Wuerzburg, Germany — [2]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

We study crossed Andreev reflection (CAR) of electrons or holes in normal metal-superconductor-normal metal junctions and highlight some very strong effects of the underlying lattice. In particular, we demonstrate that for sharp interfaces and under certain, albeit generic, symmetry conditions, the CAR probability exactly vanishes for an even number of atoms in the superconducting region. This even-odd effect applies notably to NSN junctions made of graphene nano-ribbons with armchair edges and for zigzag edges with somewhat more restrictive conditions. We analyze its robustness towards smoothing of the boundaries or doping of the sample.

TT 26.5 Tue 10:30 H17

**Efficient quantum transport simulation for bulk graphene heterojunctions: Klein backscattering revisited** — •Ming-Hao Liu and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

The quantum transport formalism based on tight-binding models is known to be powerful in dealing with a wide range of open physical systems subject to external driving forces but is, at the same time, limited by the memory requirement's increasing with the number of atomic sites in the scattering region. Here we demonstrate how to achieve an accurate simulation of quantum transport feasible for experimentally sized bulk graphene heterojunctions at a strongly reduced computational cost [1]. Without free tuning parameters, we show excellent agreement with recent experiments on Klein backscattering [2,3].

[1] M.-H. Liu and K. Richter, Phys. Rev. B **86**, 115455 (2012).
[2] A. F. Young and P. Kim, Nat. Phys. **5**, 222 (2009).
[3] S.-G. Nam, D.-K. Ki, J. W. Park, Y. Kim, J. S. Kim, and H.-J. Lee, Nanotechnology **22**, 415203 (2011).

TT 26.6 Tue 10:45 H17

**Combined effect of vacancies and strain on the conductance of graphene nanoribbons** — •Thomas Lehmann, Dmitry A. Ryndyk, and Gianaurelio Cuniberti — Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany

The understanding and engineering of electron properties of carbon-based nanostructures, in particular graphene nanoribbons, is an important challenge for modern theory of nanoscale systems. We investigate the influence of vacancy defects and uniaxial strain on the electronic transport properties of intermediate-scale graphene nanoribbons using the numerical approach based on the semi-empirical or ab initio based tight-binding model, the Landauer-Büttiker formalism and the recursion method for Green functions. We calculate the transmission of graphene nanoribbons in the quantum coherent regime with different types and concentration of defects. Further, we apply uniform planar tension to non-ideal graphene ribbons with randomly distributed and oriented single and double vacancies and Stone-Wales defects. Since transport characteristics of graphene are found to be very sensitive to edge termination and aspect ratio and it has been shown that energy gaps can emerge under critical strain, the interplay of both effects needs to be studied.

**15 min. break**

TT 26.7 Tue 11:15 H17

**Spin conductance of diffusive graphene nanoribbons** — •Jan Bundesmann[1], Ming-Hao Liu[1], Inanc Adagideli[2], and Klaus Richter[1] — [1]University of Regensburg, Regensburg, Germany — [2]Sabanci University, Istanbul, Turkey

Graphene, when cut along a zigzag edge, shows a strongly increased density of states at energies close to the charge neutrality point. The electron states that are the source of this increased DOS are pseudospin-polarized, i.e. they occupy mainly one sublattice, while their wavefunction decays exponentially from the zigzag edge.

In such systems one expects magnetic ordering which anifests as an antiferromagnetic alignment of the two sublattices. Due to the pseudospin polarization of the states finite local magnetic moments appear along the edges.

We investigate how the formation of these local magnetic moments influences charge and spin transport in graphene. It will be shown how this can lead to a finite spin conductance of a single graphene nanoribbon and that within the localized transport regime the spin conductance fluctuations exhibit universal behaviour in the sense that they don't depend on the exact modelling of the magnetization and even a large amount of edge roughness does not lead to deviations from this universal behaviour.

TT 26.8 Tue 11:30 H17

**Superlattice Effects on Electronic- and Transport Properties of Nanomaterials** — •Fedor Tkatschenko, Viktor Krueckl, and Klaus Richter — Universität Regensbug, Germany

As recently discoverded by various groups [1,2] the electronic properties of two dimensional systems such as graphene show interesting characteristics in presence of superlattices including the emergence of extra Dirac points accompanied by an anisotropic velocity renormalization. Other interesting effects are Bloch-oscillations in presence of resonant Zener tunneling [3] giving rise to a negative differential conductance in the current voltage characteristics.

We focus on a scalar superlattice system extended by a constant mass term which opens a gap between the valance and conduction band in the minibandstructure. Analytical calculations within the effective Dirac model show that it is possible to tune the energy gap by variation of the superlattice amplitude. By additional numerical calculations based on the tight-binding model we confirm the analytical results.

[1] L. Brey and H. Fertig, Phys. Rev. Lett. **103**, 046809 (2009)
[2] M. Barbier, P. Vasilopoulos, and F. Peeters, Phys. Rev. B **81**, 075438 (2010)
[3] V. Krueckl and K. Richter, Phys. Rev. B **85**, 115433 (2012)

TT 26.9 Tue 11:45 H17

**Hot Spots and Boundary Conditions in the Quantum Hall Effect** — •Tobias Kramer — Universitaet Regensburg, Inst. Theor. Physik, Germany

I discuss the influence of metallic boundary conditions due to the device contacts on the observation and current distribution in the quantum Hall effects. The current density differs in the presence of hot-spots completely from the often assumed edge-state transport picture. A model for transport in graphene [1] based on the self-consistent solution of the classical Hall effect [2] is put forward.

[1] T. Kramer, C. Kreisbeck, V. Krueckl, E. Heller, R. Parrott, and C.-T. Liang, Phys. Rev. B **81**, 081410(R) (2010)
[2] T. Kramer, V. Krueckl, E. Heller, and R. Parrott, Phys. Rev. B **81**, 205306 (2010)

TT 26.10 Tue 12:00 H17

**Current resonances in graphene with time dependent potential barriers** — Sergey E. Savel'ev[1], •Wolfgang Häusler[2], and Peter Hänggi[2] — [1]Department of Physics, Loughborough University, United Kingdom — [2]Universität Augsburg, Germany

A method is derived to solve the massless Dirac-Weyl equation describing electron transport in a mono-layer of graphene with a scalar potential barrier $U(x,t)$, homogeneous in the $y$-direction, of arbitrary $x$- and time dependence. Resonant enhancement of both electron backscattering and currents, across and along the barrier, is predicted when the modulation frequencies satisfy certain resonance conditions. These conditions resemble those for Shapiro-steps of driven Josephson junctions. Surprisingly, we find a non-zero $y$-component of the current for carriers of zero momentum along the $y$-axis.

[1] Sergey E. Savel'ev, Wolfgang Häusler, Peter Hänggi, Phys. Rev. Lett. **109**, 226602 (2012).

TT 26.11 Tue 12:15 H17

**Mie scattering analogon in graphene: particle confinement, scattering resonances, and Fano effect** — •Rafael Leslie Heinisch, Christian Schulz, Franz Xaver Bronold, and Holger Fehske — Institut für Physik, Universität Greifswald

We study the scattering of an incident electron by a circular step in a graphene monolayer in analogy to Mie scattering of light by a sphere. Klein tunnelling results in the absence of backscattering and often entails enhanced forward scattering. For low electron energies we identify sharp resonances originating from quasi-bound states at the dot. The energy and dot radius dependent temporary electron trapping significantly increases the electron density in the dot and induces a vortex pattern in the current field. The angle-resolved scattering exhibits Fano resonances which - counter-intuitive for Klein tunnelling - dramatically suppress forward scattering.

This work is supported by the DFG through SPP 1459.

TT 26.12 Tue 12:30 H17

**Mechanical strain on graphene nanoribbons in contact with metal electrodes** — •Arezoo Dianat, Dmitry A. Ryndyk, and Gianaurelio Cuniberti — Institute for Materials Science, Dresden University of Technology, 01062 Dresden, Germany

Carbon-based materials are recently of great interest for electronic devices. One of the important issues in graphene based nanoelectronics is to control its electronic and transport properties. The manipulation of electronic properties of graphene nanoribbons (GNR) has been suggested via mechanical strain, vacancies and chemical doping. From modeling point of view, few studies have been reported to investigate the electronic properties of mechanically stretched GNR in a contact with metal electrodes. In this work, we aim to elucidate the combined effects of mechanical strain and the role of metal contact area on the electronic and transport properties of GNR.

The structural and electronical properties of stretched GNR on Nickel and Palladium surfaces with different contact area and suspended strained graphene junction between metal electrodes are investigated by means of density functional theory using Vienna Ab initio Simulation Package (VASP). The structure stability as well as stress-strain curve are analyzed for several strain coefficients.

## TT 27: Superconductivity: Fe-based Superconductors - 122

Time: Tuesday 9:30–13:15 Location: H18

**Topical Talk** TT 27.1 Tue 9:30 H18

**Hydrostatic-Pressure Tuning of Magnetic, Nonmagnetic and Superconducting States in Annealed $Ca(Fe_{1-x}Co_x)_2As_2$** — •Elena Gati[1], Sebastian Köhler[1], Daniel Guterding[1], Bernd Wolf[1], Stephan Knöner[1], Sheng Ran[2], Sergey L. Bud'ko[2], Paul C. Canfield[2], and Michael Lang[1] — [1]Physikalisches Institut, J.W. Goethe-Universität, SPP 1458, D-60438 Frankfurt (Main), Germany — [2]Ames Laboratory, Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

Iron-based superconductors manifest rich phase diagrams where antiferromagnetic (afm), tetragonal (t), orthorhombic (o) and superconducting (sc) phases are observed in close proximity. We report on measurements of the magnetic susceptibility and electrical resistance under $^4$He-gas pressure on single crystals of $Ca(Fe_{1-x}Co_x)_2As_2$. We demonstrate that for accurately heat-treated crystals with modest Co-concentration the salient ground states associated with iron-arsenide superconductors, i.e., o/afm, sc, and nonmagnetic collapsed-t states can be accessed all in one sample with reasonably small and truly hydrostatic pressure. Systematic investigations of the various phase transitions and ground states through pressure tuning revealed no coexistence of bulk superconductivity with the o/afm phase which we relate to the strongly first-order character of the o/afm transition in the present compound. Our results [1], together with literature results, indicate that preserving fluctuations associated with the o/afm transition to low enough temperatures is essential for superconductivity to form.

[1] E. Gati et al., arXiv:1210.5398 (2012)

TT 27.2 Tue 10:00 H18

**Electronic structure, magnetic and superconducting properties of co-doped iron-arsenide superconductors** — •Helge Rosner[1], Walter Schnelle[1], Franziska Weikert[2,3], Michael

Nicklas[1], Jochen Wosnitza[3], and Andreas Leithe-Jasper[1] — [1]MPI CPfS Dresden — [2]Los Alamos National Laboratory, New Mexico, US — [3]HLD Dresden Rossendorf

We present a joint experimental and theoretical study of co-doped iron-arsenide superconductors of the 122 family $A_{1-x}K_xFe_{2-y}T_yAs_2$ ($A$=Ba,Sr,Eu; $T$=Co,Ru,Rh). In these systems, the co-doping enables the separation of different parameters - like electron count, disorder or the specific geometry of the FeAs layer - with respect to the position of the respective compounds in the general 122 phase diagram. For a series of compounds, we investigate the relevance of the different parameters for the magnetic, thermodynamic and superconducting properties. Our experimental investigations are supported by density functional electronic structure calculations applying different approximations for doping and disorder.

TT 27.3 Tue 10:15 H18

**Crystal growth and physical properties of Na-doped $BaFe_2As_2$ superconducting single crystals** — •S. Aswartham[1], M. Abdel-Hafiez[1], D. Bombor[1], A. U. B. Wolter[1], M. Kumar[1], C. Hess[1], D. V. Evtushinsky[1], V. B. Zabolotnyy[1], A. A. Kordyuk[1], T. K. Kim[1,2], S. V. Borisenko[1], S. Wurmehl[1], and B. Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, D 01069 Dresden, Germany — [2]Diamond Light Source Ltd., Didcot OX11 0DE, United Kingdom

Single crystals of $Ba_{1-x}Na_xFe_2As_2$ with $x$ = 0, 0.25, 0.35, 0.4 were grown using a self-flux high temperature solution growth technique. The superconducting and normal state properties were studied by temperature dependent magnetic susceptibility, electrical resistivity and specific heat revealing that the magnetic and structural transition is rapidly suppressed upon Na-substitution at the Ba-site in $BaFe_2As_2$, giving rise to superconductivity. A superconducting transition as high as 34 K is reached for a Na-content of $x$=0.4. The positive Hall coefficient confirms that the substitution of Ba by Na results in hole-doping similarly to the substitution of Ba by K. Angle resolved photoemission spectroscopy was performed on all $Ba_{1-x}Na_xFe_2As_2$ crystals. The Fermi surface of hole-doped $Ba_{1-x}Na_xFe_2As_2$ is to high extent the same as the Fermi surface found for the K-doped sister compounds, suggesting a similar impact of the substitution of Ba by either K or Na on the electronic band dispersion at the Fermi level.

TT 27.4 Tue 10:30 H18

**Raman active phonons in twin-free $BaFe_2As_2$** — •Andreas Baum[1], Bernhard Muschler[1], Florian Kretzschmar[1], Jiun-Haw Chu[2,3], James G. Analytis[2,3], Ian R. Fisher[2,3], and Rudi Hackl[1] — [1]Walther-Meissner-Institut, 85748 Garching, Germany — [2]SIMES, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [3]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. The main focus is placed on the anomalies of the lattice dynamics upon entering the spin density wave (SDW) phase. Since the related lattice distortion is very small the crystals are twinned, and in the existing experiments the properties of the phonons could only partially be clarified. To overcome the problem of twinning uniaxial stress was applied before cool down. In the twin-free crystals the symmetry properties of the phonons could be pinned down. The $E_g$ vibration of the Fe and As atoms at 135 $cm^{-1}$ splits into a $B_{2g}$ and a $B_{3g}$ mode at 138 and 128 $cm^{-1}$, respectively, below the SDW transition. The unexpected leakage of the As $A_{1g}$ phonon observed in the tetragonal $B_{2g}$ symmetry can be traced back to a resonance effect occuring only when the incoming and outgoing photon polarizations are oriented parallel to the new orthorhombic $b$ axis along which the Fe spins order ferromagnetically.

TT 27.5 Tue 10:45 H18

**Thermopower as sensitive probe of electronic nematicity in iron pnictides** — Shuai Jiang[1,2], H.S. Jeevan[1], Jinkui Dong[1], and •Philipp Gegenwart[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]1.Physikalisches Institut, Universität Stuttgart, Germany

We study the in-plane anisotropy of the thermoelectric power and electrical resistivity on detwinned single crystals of isovalent substituted $EuFe_2(As_{1-x}P_x)_2$. Compared to the resistivity anisotropy the thermopower anisotropy is more pronounced and clearly visible already at temperatures much above the structural and magnetic phase transitions. Most remarkably, the thermopower anisotropy changes sign below the structural transition. This is associated with the interplay of two contributions due to anisotropic scattering and orbital polarization, which dominate at high- and low-temperatures, respectively.

[1] S. Jiang, H. S. Jeevan, J. Dong, P. Gegenwart, arXiv:1210.2634

**15 min. break**

TT 27.6 Tue 11:15 H18

**Softening of the elastic shear mode $C_{66}$ in iron-based superconductors** — •Anna Böhmer[1,2], Philipp Burger[1,2], Frédéric Hardy[1], Peter Schweiss[1], Rainer Fromknecht[1], Thomas Wolf[1], Christoph Meingast[1], Marius Reinecker[3], and Wilfried Schranz[3] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, D-76021 Karlsruhe — [2]Karlsruher Institut für Technologie, Fakultät für Physik, D-76128 Karlsruhe — [3]Universität Wien, Fakultät für Physik, A-1090 Wien

The structural phase transition of underdoped iron-based superconductors is accompanied by a large softening of the elastic shear mode $C_{66}$, which has attracted considerable attention. This softening has been discussed both in terms of orbital and spin-nematic fluctuations which would be responsible for the structural phase transition and, possibly, superconductivity. However, sample requirements have so far restricted experimental investigations of $C_{66}$ (via measurements of the ultrasound velocity) to the $Ba(Fe,Co)_2As_2$ system.

Here, we report on a new technique, based on a three-point bending setup, to probe the Young's modulus of a sample with a capacitance dilatometer. For certain orientations, the Young's modulus is related to the elastic constant $C_{66}$ whose effective temperature dependence can be obtained. Platelet-like samples, as frequently encountered for iron-based systems, are easily studied with our setup. Data on several systems will be presented and discussed.

TT 27.7 Tue 11:30 H18

**Paramagnetic limiting of the upper critical field of $KFe_2As_2$ studied by low temperature thermal expansion and magnetostriction** — •Diego A. Zocco[1], Kai Grube[1], Sebastian Zaum[1], Felix Eilers[1], Roland Schäfer[1], Thomas Wolf[1], Philipp Burger[1], Frédéric Hardy[1], Anna Böhmer[1], Christoph Meingast[1], and Hilbert von Löhneysen[1,2] — [1]Institut für Festkörperphysik, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany — [2]Physikalisches Institut, Karlsruhe Institute of Technology, D-76031 Karlsruhe, Germany.

We present low-temperature thermal expansion and magnetostriction measurements of single crystals of $KFe_2As_2$ ($T_c \sim 3.4$ K) in magnetic fields up to 14 T applied parallel and perpendicular to the $c$-axis of the samples ($B_{c2}^c \sim 1.5$ T and $B_{c2}^{ab} \sim 4.8$ T). In the normal state, quantum oscillations of the sample length were observed for $B \parallel c$ and $B \perp c$, giving estimated mean-free-path values of 177 and 52 nm, respectively, indicating that the superconducting state can be described as being in the clean limit ($\xi_0^{ab} \sim 10$ nm). While the superconducting state is limited by orbital pair-breaking effects when magnetic fields are applied parallel to the $c$-axis, our measurements confirm strong paramagnetic effects on $B_{c2}(T)$ along the $ab$ direction, as it was similarly found in other Fe-based materials such as LiFeAs and $FeSe_{1-x}Te_x$.

TT 27.8 Tue 11:45 H18

**Pressure dependencies and first-order transition in $KFe_2As_2$** — •Philipp Burger[1,2], Anna Böhmer[1,2], Frédéric Hardy[1], Thomas Wolf[1], Peter Schweiss[1], Rainer Fromknecht[1], and Christoph Meingast[1] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [2]Fakultät für Physik, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany

Here we present a thermodynamic study on $KFe_2As_2$ single crystals ($T_c$=3.4 K) using high-resolution thermal-expansion, specific heat, magnetostriction and magnetization measurements. From these measurements we extract the uniaxial pressure dependencies of the Sommerfeld coefficient $\gamma$, the critical temperature $T_c$, the upper critical field $H_{c2}$, the magnetic susceptibility $\chi$ and the thermodynamical critical field $H_c$. Interestingly, the normalized pressure derivatives of $T_c$ and $H_c$ are about a factor of 10 larger than the pressure dependence of gamma, clearly showing that $T_c$ is not closely correlated with $\gamma$. In particular the pressure dependencies of $T_c$ show a very anisotropic behavior for the two different directions. Similar anisotropic behavior is also observed for $H_{c2}$ and $H_c$ indicating that they are strongly coupled to each other.

In addition, magnetostriction and magnetization data for H parallel $a$-axis show that the superconducting transition is changing from second-order to first-order around 2 K. These results support that the upper critical field $H_{c2}$ is strongly suppressed via Pauli paramagnetism.

TT 27.9 Tue 12:00 H18

**Effect of uniaxial stress and doping on structural and electronic properties of $BaFe_2As_2$ and $CaFe_2As_2$** — •Milan Tomic, Roser Valenti, and Harald O. Jeschke — Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany

We investigate the effects of the uniaxial tensile and compressive stresses applied along **a**, **b** and **a**+**b** directions in $BaFe_2As_2$ and $CaFe_2As_2$ in the framework of ab initio density functional theory calculations. While the systems remain in the orthorhombic phase at moderate pressures, we observe an inversion of magnetism at a critical strain happening when the **a** and **b** axes approach the tetragonal condition. Furthermore, the doping-temperature-pressure phase diagrams of the 122 family of superconductors have been discussed intensively due to electronic nematicity above the structural and superconducting transition and the complex coupling between electronic and lattice degrees of freedom. We employ density functional theory to predict the structure of supercells of $Ca_{1-x}Sr_xFe_2As_2$ and $CaFe_2(As_{1-x}P_x)_2$. We then predict structural transitions of the doped compounds under pressure and compare to the parent compound. We carefully analyze the changes in the electronic structure caused by doping and stress.

TT 27.10 Tue 12:15 H18

**Coherent phonon oscillations in 122 FeAs compounds** — •L. Rettig[1], R. Cortes[2], T. Rohwer[3], P. Gegenwart[4], H.S. Jevaan[4], T. Wolf[5], B. Kamble[6], I. Eremin[6], L. Kipp[3], K. Rossnagel[3], M. Bauer[3], J. Fink[7], M. Wolf[2], and U. Bovensiepen[1] — [1]Universität Duisburg-Essen, D-47048 Duisburg — [2]Fritz-Haber-Institut d. MPG, D-14195 Berlin — [3]Christian-Albrechts-Universität Kiel, D-24118 Kiel — [4]Georg-August-Universität Göttingen, D-37077 Göttingen — [5]Karlsruhe Institute of Technology, D-76021 Karlsruhe — [6]Ruhr-Universität Bochum, D-44801 Bochum — [7]Leibniz-Institute for Solid State and Materials Research Dresden, D-01171 Dresden

We present time- and angle-resolved photoemission spectroscopy results on various 122 FeAs compounds employing fs UV and XUV pulses. We observe coherent oscillations of the spectral weight near $E_F$ and identify three coherent modes - the most prominent Raman active $A_{1g}$ mode and two weaker modes. The analysis of the transient electron distribution allow us to separate the oscillating chemical potential from the relaxation dynamics of the excited electronic distribution.

Similar experiments using a high-harmonics light source enable the analysis of the electron dynamics at the Γ-point and at the X-point, which shows an in-phase oscillation of the chemical potential at the two Fermi surface sheets. This indicates a substantial modification of the electronic density of states by the coherent oscillations, which is corroborated by theoretical investigations of the influence of the $A_{1g}$ mode on the electronic structure in 122 FeAs compounds.

TT 27.11 Tue 12:30 H18

**Strain induced bulk superconductivity in $BaFe_2As_2$ thin films** — •Jan Engelmann[1,2], Paul Chekhonin[2], Werner Skrotzki[2], Ruben Hühne[1], Fritz Kurth[1,2], Silvia Haindl[1], Kazumasa Iida[1], Ludwig Schultz[1,2], Holzapfel Bernhard[1,3], and Grinenko Vadim[1] — [1]IFW Dresden, P. O. Box 270116, 01171 Dresden, Germany — [2]Dresden University of Technology, Department of Physics, 01062 Dresden, Germany — [3]TU Bergakademie Freiberg, 09596 Freiberg, Germany

We report superconductivity in non-doped $BaFe_2As_2$ (Ba122) thin films grown on Fe buffered Spinel single crystalline substrates. Superconductivity was achieved in our thin films by varying the thickness of the Ba122. Increasing the thickness to a critical value of approximately 10 nm results in an increase of the superconducting critical temperature to $T_c$=28 K whereas films with a thickness of >100 nm do not show any superconductivity. We connect this appearance of superconductivity with the inclusion of strain in our samples. Very thin samples are fixed to the Fe buffer layer and substrate lattice constant (increased a-axis lattice constant and shortened c-axis lattice constant) whereas with increasing thickness the Ba122 layer relaxes to its bulk values. We will present via X-ray analysis the relaxation of the c-axis lattice constant coming along with structural changes showed via transmission electron microscopy (TEM) and atomic force microscopy (AFM). The bulk nature of superconductivity was determined by measurements of the critical current density and via magnetic measurements using a SQUID.

TT 27.12 Tue 12:45 H18

**Intrinsic ab-Plane Pinning in Epitaxial Pnictide Thin Films** — •Jens Haenisch[1], Kazumasa Iida[1], Fritz Kurth[1], Michael Schulze[1], Sabine Wurmehl[1], Shinya Ueda[2], Michio Naito[2], Chiara Tarantini[3], Jan Jaroszynski[3], Ludwig Schultz[1], and Bernhard Holzapfel[1] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Tokyo University A & T, Koganei, Tokyo 184-8588, Japan — [3]NHMFL, 1800 E. Paul Dirac Drive, Tallahassee, FL 32310, USA

In type II superconductors with short coherence lengths $\xi$ and large uniaxial crystallographic anisotropy, the order parameter may be modulated along the $c$-axis or even be restricted to superconducting planes. In such a case, flux lines may be pinned intrinsically by this modulation. This is well known for the high-$T_c$ cuprates. The pnictides as well full-fill the conditions for intrinsic pinning. However, up to now it has not been reported. $FeSe_{0.5}Te_{0.5}$ thin films have been grown by PLD in a temperature series between 350 °C and 550 °C. For the film deposited at 450 °C we found clear signature of intrinsic pinning for $B > 7$ T and $T < 4$ K. $J_c(B)$ is constant in this region and the $V(I)$ exponent $n$ shows a strong dip in its angular dependence for field orientations near $ab$. For the lowest $T$, $n$ is rising again. This behavior is explained by trapping and lock-in of flux lines and the presence of double-kink excitations. An MBE-grown SmFeAs(O,F) thin film with very clean microstructure and a $T_c$ of 55.7 K has been investigated in high static magnetic fields. This compound shows the same intrinsic-pinning behaviour for $B > 35$ T: constant $J_c$ and a change of $n(B, \theta)$.

TT 27.13 Tue 13:00 H18

**Investigations of pnictide superconductors - three Josephson junction aproaches** — •Stefan Schmidt[1], Sebastian Döring[1], Martin Feltz[1], Noor Ali Hasan[1], Sandra Gottwals[1], Frank Schmidl[1], Silvia Haindl[2], Kazumasa Iida[3], Fritz Kurth[3], Bernhard Holzapfel[3], and Paul Seidel[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]IFW Dresden, Institute for Solid State Research, Helmholtzstrasse 20, 01069 Dresden, Germany — [3]IFW Dresden, Institute for Metallic Materials, Helmholtzstrasse 20, 01069 Dresden, Germany

The investigation of fundamental electrical properties in iron pnictide superconductors has to be pursued in order to realize devices and applications in the future. Particularly, Josephson junctions are a very important tool to examine device-oriented interface effects in hybrid and all-pnictide contacts. We present results on different junction geometries based on thin film technology using Co-doped Ba-122 as base electrode. Planar SNS' junctions that favor transport along the c-axis are compared to edge-type (hybrid) and grain boundary junctions (all-pnictide) where charge carriers are transported within the ab-plane of the superconductor.

This work was partially supported by the EU within IRON-SEA (project no. FP7-283141), DFG within SPP 1458 (projects SE 664/15-1 and HA 5934/1-1), the DAAD, and the Landesgraduiertenförderung Thüringen.

S. Schmidt et al., IEEE-TAS (accepted, 2012), arXiv.org: 1211.3879

# TT 28: Correlated Electrons: Spin Systems, Itinerant Magnets 3

Time: Tuesday 9:30–12:45 Location: H19

TT 28.1 Tue 9:30 H19

**Structure and Phase Transitions of the Spiral Antiferromagnet $Ba_2CuGe_2O_7$** — •Sebastian Mühlbauer[1], Markus Garst[2], Ekaterina Pomjakushina[3], Severian Gvasaliya[4], Eric Ressouche[5], Charles Dewhurst[5], Joachim Kohlbrecher[3], and Andrey Zheludev[4] — [1]Forschungsneutronenquelle Heinz Maier-Leibnitz, Garching, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Germany — [3]Paul Scherrer Institut, Villigen, Switzerland — [4]Neutron Scattering and Magnetism, ETH Zürich, Switzerland — [5]Institut Laue Langevin, Grenoble, France

Neutron diffraction and small angle neutron scattering (SANS) in combination with measurements of susceptibility and specific heat have been used to systematically study the different magnetic structures of the non-centrosymmetric tetragonal antiferromagnet (AF) $Ba_2CuGe_2O_7$, that evolve for different orientation of the magnetic field. A complete description of the magnetic phase diagram could be achieved [1,2]: For magnetic field close to the tetragonal $c$-axis, a phase transition from the soliton lattice to a recently reported incommesurate double-$k$-phase is confirmed. In contrast, for large angles enclosed by the magnetic field and the $c$-axis, a complexly distorted non-sinusoidal structure is observed. For magnetic field in the basal $a$,$b$-plane, a incommensurate/commensurate transition is observed at 9 T. The staggered component of the Dzyaloshinsky-Moriya vector is identified as key element for the understanding of $Ba_2CuGe_2O_7$.

[1] S. Mühlbauer et al., Phys. Rev. B **84**, 180406 (2011).
[2] S. Mühlbauer at al., Phys. Rev. B **86** 02217 (2012).

TT 28.2 Tue 9:45 H19

**Spin-charge-lattice coupling in the semimetallic ferromagnet $EuB_6$** — •F. Schnelle[1], R. S. Manna[1], P. Das[1], J. Müller[1], Z. Fisk[2], and M. Lang[1] — [1]Institute of Physics, Goethe-University Frankfurt, 60438 Frankfurt (M), Germany — [2]Department of Physics, University of California, Irvine, California 92697, USA

The semimetallic $EuB_6$ exhibits a complex sequence of electronic and magnetic phase transitions at ∼15.5 K ($T_{c1}$) and ∼12.5 K ($T_{c2}$). In the paramagnetic regime below ∼35 K, magnetic polarons (MPs) are expected to form since it is energetically favorable for the charge carriers to localize and thereby spin polarize the local $Eu^{2+}$ moments over a finite distance. Thermal expansion measurements show pronounced lattice effects at the phase transition temperatures, the one occurring at $T_{c2}$ being much larger than that at $T_{c1}$. By applying a small magnetic field of less than 50 mT, the anomaly at $T_{c1}$ is fully suppressed, while the one at $T_{c2}$ shifts to higher temperature and broadens as the field is increased and finally fades out at a field $B > 5$ T. The complementary magnetostriction measurements for a set of temperatures from below $T_{c2}$ to above $T_{c1}$ highlight the extraordinarily large magnetoelastic effects in this material. This supports the notion that charge localization, due to the formation of isolated MPs at temperatures corresponding to the paramagnetic regime, gives rise to lattice expansion. By cooling or applying external magnetic fields, the MPs merge and percolation sets in, resulting in lattice contraction. We discuss the relation of this mechanism to the observed large negative magnetoresistance in this material.

TT 28.3 Tue 10:00 H19

**Studying the local magnetic induction of $EuB_6$ by high-resolution micro-Hall magnetometry** — •Merlin Pohlit[1], Adham Amyan[1], Jens Müller[1], and Zachary Fisk[2] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — [2]University of California, Irvine, USA

In the ferromagnetic semimetal $EuB_6$ two consecutive transitions occur at $T_{c1}$=15.5 K and $T_{c2}$=12.6 K. They are related to electronic and magnetic phase separation, and bulk magnetic ordering, but the details are not yet fully understood. Recently, there has been experimental evidence for the CMR effect observed at $T_{c1}$ beeing caused by percolation of magnetic polarons [1]. Local magnetic measurements, however, have not been performed so far. In this talk we discuss local magnetic induction measurements on a high-quality single crystal using micro-Hall magnetometers based on a high-mobility 2DEG in GaAs/AlGaAs. The sample is positioned on top of the Hall device where a series of adjacent lithographically defined crosses allow for spatially-resolved measurements with micron-size resolution. Strayfield measurements close to the sample give evidence for a spontaneous magnetisation at $T_{c1}$ and allow further insights in the field and temperature dependence of the magnetic transitions. Simultanously performed measurements below the sample give evidence for magnetic domains/inhomogeneities which seem to exist even below the second magnetic transition but vanish by application of a small external field.

[1] Das et al., Phys. Rev. B 86, 184425 (2012)

TT 28.4 Tue 10:15 H19

**Analysis of chemical and external pressures in ReCoPO (Re = La, Pr) and LaCoAsO by means of $\mu^+$ spin spectroscopy** — •Giacomo Prando[1], Pietro Bonfà[2], Gianni Profeta[3], Rustem Khasanov[4], Fabio Bernardini[5], Marcello Mazzani[2], Eva Maria Bruening[1], Anand Pal[6], Veer Awana[6], Hans-Joachim Grafe[1], Bernd Buechner[1], Roberto De Renzi[2], Pietro Carretta[7], and Samuele Sanna[7] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, Germany — [2]Dipartimento di Fisica, Universitá di Parma and CNISM, Italy — [3]SPIN-CNR and Dipartimento di Fisica, Universitá dell'Aquila, Italy — [4]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, Switzerland — [5]Dipartimento di Fisica, Universitá di Cagliari, Italy — [6]National Physical Laboratory (CSIR), New Delhi, India — [7]Dipartimento di Fisica,, Universitá di Pavia and CNISM, Italy

In this contribution we will discuss the local magnetic properties of ReCoPO (Re = La, Pr) as investigated by means of muon spin spectroscopy. Electrons localized on the $Pr^{3+}$ ions do not play any role in the overall magnetic features of the compounds. The increase of the chemical pressure triggered by the different ionic radii of $La^{3+}$ and $Pr^{3+}$ plays a crucial role in enhancing the value of the critical temperature to the magnetic phase and can be mimicked by the application of external hydrostatic pressure. A sharp discontinuity in the local magnetic field at the muon site in LaCoPO suggests a sizeable modification in the band structure of the material upon increasing $P$. This scenario is qualitatively supported by *ab-initio* DFT calculations.

TT 28.5 Tue 10:30 H19

**Heisenberg like critical properties, Magnetocaloric effect and Scaling in Lead doped $NdMnO_3$ Single Crystal** — •Nilotpal Ghosh — School of Advanced Sciences, VIT University, Vellore-632014, Tamilnadu

Magnetic isotherms for single crystals of $Nd_{0.7}Pb_{0.3}MnO_3$ have been measured around the ferromagnetic(FM) to paramagnetic(PM) transition temperature $T_C$. Critical exponents have been obtained by modified Arrott plots and the Kouvel Fisher method. The values of exponents are consistent with those expected for 3D Heisenberg universality class. Magnetocaloric effect (MCE) has been also studied from the magnetic isotherms. Relative cooling power (RCP) is estimated as 56.725, 66.252 and 77.163 J/Kg for 1.2, 2.2 and 4.8 T fields respectively. Universal scaling behaviour in the relative change of magnetic entropy $\Delta S_M$ has been observed. The rescaled magnetic entropy change curves for different applied fields are noticed to collapse onto a single curve. It has been found that the peak entropy change, $\Delta S_M$ peak at $T_C$ and RCP follow a scaling power law in magnetic field H with the exponents which are reduced in comparison to their theoretically estimated value.

[1] N. Ghosh, Journal of Superconductivity and Novel Magnetism, accepted (2012)
[2] N. Ghosh, S. Roessler, U.K. Roessler, K. Nenkov, S. Elizabeth, H.L. Bhat, K. Doerr, and K.H. Mueller, J. Phys.: Condens. Matter **18**, 557-567 (2006)

TT 28.6 Tue 10:45 H19

**From Skyrmions to Helices: Changing the Topology in Chiral Magnets** — •Stefan Buhrandt and Achim Rosch — Universität Köln

In chiral magnets, a small magnetic field stabilizes a lattice of magnetic whirls, so called skyrmions. They are characterized by a topologically quantized winding number. Using classical Monte Carlso simulations, we investigate the first order phase transition from the skyrmion phase to a helical phase when the magnetic field is reduced. As the topology of the magnetic texture changes, the phase transition is driven by singular magnetic configuration, which we identify as hedgehog point

defect. These hedgehogs are responsible for the merging of skyrmions and changes of the winding number.

**15 min. break**

TT 28.7 Tue 11:15 H19

**Thermal transport properties of single-crystal MnSi** — •Marlies Gangl, Anna Kusmartseva, Andreas Bauer, and Christian Pfleiderer — Technische Universität München, Physik Department E21, Garching, Germany

The B20 transition metal compound MnSi has long been recognised as a model system for studies of weak itinerant ferromagnetism [1], when ignoring the formation of a well-understood helical modulation that may be suppressed in small magnetic fields. We report the thermal conductivity and thermopower of high-quality single crystals of MnSi over a wide range of temperatures from 2 to 300 K under magnetic fields up to 14 T. We discuss our findings in the framework of the spin fluctuation theory of weakly ferromagnetic compounds as recently advertised in the context of related studies of $ZrZn_2$ [2,3].

[1] G. Lonzarich and L. Tailefer, J. Phys. C: Solid State Phys. **18**, 4339 (1985)
[2] R.P. Smith et al., Nature **455**, 1220-1223 (2008)
[3] M. Sutherland et al., Phys. Rev. B **85**, 035118 (2012)

TT 28.8 Tue 11:30 H19

**Neutron polarimetry of the fluctuation-induced first order helimagnetic transition in MnSi** — •Jonas Kindervater[1], Wolfgang Häussler[1,2], Markus Garst[3], Marc Janoschek[4], Christian Pfleiderer[1], and Peter Böni[1] — [1]Physik Department E21, TU München — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz, TU München — [3]Institute for Theoretical Physics, Universiät zu Köln — [4]Los Alamos National Laboratory

Chiral magnets, like the B20 compound MnSi, have recently attracted much scientific interest because a new spin structure representing a skyrmion lattice has been identified under moderate magnetic fields [1]. Besides these topological spin textures the phase transition from heli- to paramagnetism in MnSi has been under active investigation. Different scenarios on the mechanism of the transition have been proposed, ranging from a topological skyrmion liquid phase [2] over a second order mean field transition [3] to a fluctuation induced first order Brazovskii phase transition [4] that was recently confirmed experimentally in small angle neutron diffraction [5]. We report a comprehensive study of the so-called chiral fraction in MnSi using a newly developed miniature spherical neutron polarimetry device "MiniMuPAD". The temperature dependence and the isotropic decay of the measured chiral fraction are in excellent agreement with the Brazovskii scenario.

[1] S. Mühlbauer *et al.*, Science **323**, 915 (2009)
[2] C. Pappas *et al.*, PRL **102**, (2009)
[3] S. V. Grigoriev *et al.*, PRB **72**, 13 (2005)
[4] S. A. Brazovskii, Sov. Phys. JETP **41**, 85 (1975)
[5] M. Janoschek *et al.*, arXiv:1205.4780 (2012)

TT 28.9 Tue 11:45 H19

**Thermodynamic signatures of the skyrmion lattice phase in MnSi and $Mn_{1-x}Fe_xSi$** — •Andreas Bauer and Christian Pfleiderer — Physik Department E21, Technische Universität München, D-85747 Garching, Germany

The recent discovery of skyrmion lattices in cubic helimagnets like MnSi, $Fe_{1-x}Co_xSi$, and $Cu_2OSeO_3$ lead to a large number of studies in this class of compounds. We report detailed measurements of the specific heat across the magnetic phase diagram of single-crystal MnSi and $Mn_{1-x}Fe_xSi$. Our data is fully consistent with earlier reports, e.g., in Ref. [1,2], showing a narrow peak ontop of a broad shoulder at the helimagnetic phase transition. However, a quasi-adiabatic large heat pulse technique enabled us to resolve distinct signatures of the skyrmion lattice phase for the first time. A peak upon entering the skyrmion lattice phase from low temperatures is observed in MnSi for all magnetic field directions studied as well as in $Mn_{1-x}Fe_xSi$ up to $x = 0.08$. This peak is a key signature of the first order phase transition where the topological winding number of the magnetic structure jumps from 0 to -1.

[1] S. M. Stishov *et al.*, PRL **105**, 236403 (2010)
[2] A. Bauer *et al.*, PRB **82**, 064404 (2010)

TT 28.10 Tue 12:00 H19

**Magnetic properties of $Mn_{1-x}Fe_xGe$** — •Sven-Arne Siegfried[1], Nadezhda Potapova[2], Evgeny Moskvin[2], Vadim Dyadkin[3], Dirk Menzel[4], Charles D. Dewhurst[5], Anatoly V. Tsvyashchenko[6], Dieter Lott[1], Andreas Schreyer[1], and Sergey Grigoriev[2] — [1]Helmholtz-Zentrum Geesthacht, Geesthacht, Germany. — [2]Petersburg Nuclear Physics Institute, Gatchina, Russia. — [3]Swiss-Norwegian Beamlines at ESRF, Grenoble, France — [4]TU Braunschweig, Braunschweig, Germany — [5]Institut Laue-Langevin, Grenoble, France — [6]Institute for High Pressure Physics, Troitsk, Russia

The cubic B20 type transition-metal monogermanides belong to the $P2_13$ space group. B20 systems order in a helical spin structure which can be transformed by a magnetic field into a conical and even a parallel ferromagnetic configuration. Close to the ordering temperature the so called A-phase exists. Polycrystalline $Mn_{1-x}Fe_xGe$ samples have been synthesized by high pressure method and investigated by SQUID magnetization measurements and small angle neutron scattering. For this compounds the variation of the helical period from 18 nm for MnGe up to 70 nm for FeGe comes along with a change in the ordering temperatures from 170 K up to 280 K. For concentrations below x = 0.5 our SANS patterns at zero field show a temperature dependent decrease of the helical wavelength with increasing temperature. For field dependent measurements different characteristic patterns appears indicating a complex H-T magnetic phase diagram for this compounds.

TT 28.11 Tue 12:15 H19

**Signature of gap closure in the phonon spectra of FeSi** — •Sven Krannich[1], Daniel Lamago[2], Rolf Heid[1], Klaus-Peter Bohnen[1], Yvan Sidis[2], Jean-Michel Mignot[2], Paul Steffens[3], Alexander Ivanov[3], and Frank Weber[1] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, 76021 Karlsruhe — [2]Laboratoire Léon Brillouin, CEA - Saclay, F - 91191 Gif sur Yvette Cedex, France — [3]Institut Laue Langevin, F-38042 Grenoble Cedex, France

We report an inelastic neutron scattering study of the lattice degrees of freedom in the narrow gap semiconductor FeSi over a large temperature range 10 K $\leq$ T $\leq$ 790 K. In our measurements we observe an unusually strong softening of various phonon modes with some notable exceptions. Calculations based on density-functional-perturbation theory (DFPT) show that only the softening between T = 100 K and room temperature is anomalous, i.e. cannot be explained by normal thermal expansion. Further calculations simulating a vanishing electronic gap at elevated temperatures can account for this anomalous softening and need not involve strong anharmonic lattice effects. Our results support a band-like approach to FeSi where electron-electron correlations are responsible for the gap closure.

TT 28.12 Tue 12:30 H19

**Highly Dispersive Scattering From Defects In Non-Collinear Magnets** — •Wolfram Brenig[1,2] and Alexander L. Chernyshev[3] — [1]Institute for Theoretical Physics, Technical University Braunschweig, Germany — [2]Technical University of Lower Saxony, NTH, Germany — [3]Department of Physics, University of California, Irvine, USA

We demonstrate that point-like defects in non-collinear magnets give rise to a highly dispersive structure in the magnon scattering, violating a standard paradigm of its momentum independence. For a single impurity spin coupled to a prototypical non-collinear antiferromagnet, we find that the resolvent is dominated by a distinct dispersive structure with its momentum-dependence set by the magnon dispersion and shifted by the ordering vector. This feature is a consequence of umklapp scattering off the impurity-induced *spin texture*, which arises due to the non-collinear ground state of the host system. Detailed results for the staggered and uniform magnetization of this texture as well as the $T$-matrix from numerical linear spin-wave theory are presented.

# TT 29: Transport: Quantum Dots, Wires, Point Contacts 3 (jointly with HL)

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

TT 29.1 Tue 9:30 H20

**Theory of Spin Relaxation in Two-Electron Laterally Coupled GaAs and Si Quantum Dots** — •Martin Raith[1], Peter Stano[2,3], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland — [3]Institute of Physics, Slovak Academy of Sciences, 845 11 Bratislava, Slovakia

We present quantitative results of the phonon-induced spin relaxation in two-electron lateral double quantum dots. Both spin-orbit coupling and hyperfine coupling are taken into account. Our analysis of GaAs [1] and silicon [2] based dots includes the variation of the electric field (detuning), the exchange coupling, and the magnetic field strength and orientation. We find that even in strong magnetic fields, the hyperfine coupling can dominate the relaxation rate of the unpolarized triplet in a detuned GaAs double dot. This feature is absent in silicon (we assume a $^{29}$Si abundance of 4.7%). Where the spin-orbit coupling dominates, the rate is strongly anisotropic and its maxima and minima are generated by an in-plane magnetic field either parallel or perpendicular to the dots' alignment dependent on specifics, such as spectral (anti-) crossings (spin hot spots), or the detuning strength. We emphasize the differences between GaAs and Si based dots. This work marks a crucial step toward the realization of two-electron semiconductor qubits.

This work is supported by the DFG under grant SPP 1285.

[1] M. Raith et. al., PRL 108, 246602 (2012)
[2] M. Raith et. al., arXiv:1206.6906

TT 29.2 Tue 9:45 H20

**Nonequilibrium effect in a NISIN turnstile** — •Andreas Heimes[1], Ville Maisi[2,3], Jukka Pekola[2], Michael Marthaler[1], Dmitry Golubev[1], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, Wolfgang-Gaede-Str. 1, D-76128 Karlsruhe, Germany — [2]Low Temperature Laboratory (OVLL), Aalto University School of Science, P.O. Box 13500, 00076 Aalto, Finland — [3]Centre for Metrology and Accreditation (MIKES), P.O. Box 9, 02151 Espoo, Finland

A single electron transistor consisting of a superconducting island coupled to two normal leads is investigated. By periodically changing the gate voltage this setup works as a single electron pump. However during the turnstile operation quasiparticles are injected onto the superconductor, which relax via inelastic electron-phonon scattering and effectively heat up the island. We theoretically model the time evolution of the charge transport and the quasiparticle distribution during the pumping process. By analyzing the dependence on pumping frequency we discuss the experimental ability to measure the relaxation dynamics of quasiparticles in the superconducting island.

TT 29.3 Tue 10:00 H20

**Keldysh effective action theory for universal physics in spin-1/2 Kondo dots** — •Sergey Smirnov and Milena Grifoni — Institut I - Theoretische Physik, Universität Regensburg, Universitätsstraße 31, D-93040 Regensburg, Deutschland

We present a theory for the Kondo spin-1/2 effect in strongly correlated quantum dots. The theory is applicable at any temperature and voltage. It is based on a quadratic Keldysh effective action parameterized by a universal function. We provide a general analytical form for the tunneling density of states through this universal function for which we propose a simple microscopic model [1]. We apply our theory to the highly asymmetric Anderson model and describe its strong coupling limit, weak coupling limit and crossover region within a single analytical expression.

We further extend our theory to describe the Kondo regime when the quantum dot is placed in an external magnetic field. The modern experimental issues of the critical magnetic field, at which the zero bias maximum of the differential conductance starts to split into two maxima, as well as the distance between these maxima as a function of the magnetic field are also addressed.

[1] S. Smirnov and M. Grifoni, arXiv:1203.4360 (2012)

TT 29.4 Tue 10:15 H20

**Superfermions in Liouville space as a powerful tool for investigating quantum transport out of equilibrium: new insights into the Anderson model** — •Roman Saptsov[1,2] and Maarten 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

Recently, we introduced a new formalism of superfermions in Liouville space for a renormalization group study of the non-linear transport through an Anderson quantum dot (QD) at zero temperature [1]. This formalism turns out to be a very useful tool to study other aspects of non-equilibrium phenomena, as well. In the wide band limit for a strongly interacting QD it allows one to sum up exactly temperature-independent contributions and obtain a general form of the QD effective Liouvillian as well as some exact relations for its eigenvalues. In the non-interacting case, U=0, our approach describes time evolution of the QD in the most simple way: we show that a "Pauli super-exclusion principle" for the superfermions leads to the exact truncation of the time-dependent perturbation series at the second order in a coupling constant. Using our approach we are able also to explore the time-evolution of the initial dot-reservoir correlations. We discuss the extension of this U=0 result to the case of finite U. Finally, we discuss other useful applications of our formalism, such as: path integrals in Liouville space and "super- mean-field theory".

[1] R.B. Saptsov, M.R. Wegewijs, arXiv:1207.3207

**Invited Talk** TT 29.5 Tue 10:30 H20

**Nano-Conductors as Measurement Devices and Driving Sources** — •Sigmund Kohler — Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain

The capacitive coupling between electrically isolated nano-circuits bears a wealth of novel transport effects. One prominent realization is the coupling of a quantum dot to a quantum point contact, where the latter acts as charge monitor. Most interesting is the backaction of the point contact to quantum superpositions in the measured system and the decoherence induced in this way. For example, it has been predicted that, despite decoherence, a charge monitor may be used for qubit phase readout with good fidelity [1]. Moreover, a point contact may act upon a double or triple quantum dot not only as detector or decoherence source, but may also impose useful non-equilibrium driving and thereby, e.g., induce a pump current. This effect leaves its fingerprints in the charging diagram of double quantum dots [2] and in the full-counting statistics [3]. If the point contact is replaced by a double quantum dot, coherent tunnel oscillations in the latter may induce phenomena known from ac-driven transport.

[1] C. Kreisbeck and S. Kohler, PRB **81**, 125404 (2010)
[2] M. Stark and S. Kohler, EPL **91**, 20007 (2010)
[3] R. Hussein and S. Kohler, PRB **86**, 115452 (2012)

**15 min. break**

TT 29.6 Tue 11:15 H20

**Electronic structure and the Aharonov-Bohm effect in inhomogeneous Möbius rings** — •V. M. Fomin[1], S. Kiravittaya[1,2], and O. G. Schmidt[1,3] — [1]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany — [2]Department of Electrical and Computer Engineering, Naresuan University, Phitsanulok 65000, Thailand — [3]Material Systems for Nanoelectronics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Nanostructure fabrication techniques can be exploited to generate non-trivially shaped objects with man-designed topological space metrics. A symbiosis of the geometric potential and an inhomogeneous twist renders an observation of the topology effect on the electron ground-state energy in microscale Möbius rings into the realm of experimental verification. We predict a 'delocalization-to-localization' transition for the electron ground state as the Möbius ring is made more inhomogeneous [1]. This transition can be quantified through the Aharonov-Bohm quantum-interference effect on the ground-state persistent current as a function of the magnetic flux threading the Möbius ring. Our theoretical considerations may receive practical relevance in view of the emerging experimental realizations of topologically nontrivial manifolds at the nanoscale.

[1] V. M. Fomin, S. Kiravittaya, and O. G. Schmidt, Phys. Rev. B 86, 195421 (2012).

TT 29.7 Tue 11:30 H20

**Transport across an Anderson quantum dot in the intermediate coupling regime** — •Johannes Kern and Milena Grifoni — Universität Regensburg, Institut für Theoretische Physik, 93040 Regensburg

We describe transport across a quantum dot coupled to leads at different chemical potentials. For this we use the master equation approach. The current is determined via the reduced density matrix by "kernels", the contributions to those are visualized by diagrams. Because of the huge variety and complexity of the diagrams, we take into account only the diagrams within a selection which we call the "dressed second order" (DSO)[1]. We apply this to the case of the single impurity Anderson model and show that the DSO allows the description of various effects: the transition from thermally broadened to tunnel broadened peaks of the linear conductance as well as of the differential conductance as function of the bias; the shift of the conductance peaks with temperature; a zero bias anomaly in the differential conductance; the splitting of this anomaly in case a magnetic field is applied. To conclude, we see the strength of the DSO in its simplicity as well as in its applicability to various problems including the transport across more complicated quantum dots.

[1] J. Kern and M. Grifoni, arXiv:1209.4995.

TT 29.8 Tue 11:45 H20

**Helical nuclear spin order and conduction reduction in two subband quantum wires** — •Tobias Meng and Daniel Loss — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

In quantum wires, the hyperfine coupling between conduction electrons and nuclear spins can lead to an ordering of the latter at low temperatures. This order acts back onto the electrons and gaps out part of their spectrum. In the presence of two subbands with distinct Fermi momenta $k_{F1}$ and $k_{F2}$, we discuss how the nuclear spins order in a superposition of two helices with pitches $\pi/k_{F1}$ and $\pi/k_{F2}$, thus exhibiting a beating patter. This ordering results in a reduction of the electronic conductance in two steps of $e^2/h$ upon lowering the temperature.

TT 29.9 Tue 12:00 H20

**Electron Waiting Times in Non-Markovian Quantum Transport** — •Konrad Thomas and Christian Flindt — Département de Physique Théorique, Université de Genève, 1211 Genève, Switzerland

We formulate a quantum theory of electron waiting time distributions for charge transport in nano-structures described by non-Markovian generalized master equations. We illustrate our method by calculating the waiting time distribution of electron transport through a dissipative double quantum dot, where memory effects are present due to a strongly coupled heat bath. We consider the influence of non-Markovian dephasing on the distribution of electron waiting times and discuss how spectral properties of the heat bath may be detected through measurements of the electron waiting time.

TT 29.10 Tue 12:15 H20

**Coherence and indistinguishability of single electron wavepackets emitted by independent sources** — Erwann Bocquillon[1], Vincent Freulon[1], Jean-Marc Berroir[1], Pascal Degiovanni[2], Bernard Plaçais[1], Antonella Cavanna[3], Yong Jin[3], and •Gwendal Feve[1] — [1]Laboratoire Pierre Aigrain, Ecole Normale Supérieure, Paris, France — [2]Laboratoire de Physique de l Ecole Normale Supérieure de Lyon, Lyon, France — [3]Laboratoire de Photonique et Nanostructures, Marcoussis, France

Using two independent on-demand electron sources [1], two single-electron wavepackets are emitted on one-dimensional chiral edge channel located at at different inputs of an electronic beamsplitter. Whereas classical particles would be randomly partitioned by the splitter, we observe two-particle interferences resulting from quantum exchange in this electronic analog [2,3] of the optical Hong-Ou-Mandel [4] experiment. Both electrons, emitted in indistinguishable wavepackets with synchronized arrival time on the splitter, exit in different outputs as recorded by the low frequency current noise. Full random partitioning is recovered when the arrival of one electron is delayed with respect to the other. This two-electron interference experiment demonstrates the possibility to generate on-demand coherent and indistinguishable single-electron wavepackets in a quantum conductor.

[1] G. Fève et al., Science 316, 1169 (2007)
[2] Ol'khovskaya et al., Phys. Rev. Lett. 101, 166802 (2008)
[3] T. Jonckheere et al., Phys. Rev. B 86, 125425 (2012)
[4] C. K. Hong et al., Phys. Rev. Lett. 59, 2044 (1987)

## TT 30: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Tuesday 9:30–13:00 Location: H21

TT 30.1 Tue 9:30 H21

**Kondo effect on the surface of 3D topological insulators: Signatures in scanning tunneling spectroscopy** — •Lars Fritz[1], Andrew Mitchell[1,2], Dirk Schuricht[3], and Matthias Vojta[4] — [1]Universität zu Köln, Institut für Theoretische Physik — [2]Department of Chemistry, Physical and Theoretical Chemistry, Oxford University, UK — [3]Institute for Theory of Statistical Physics and JARA-Fundamentals of Future Information Technology, RWTH Aachen University — [4]nstitut für Theoretische Physik, Technische Universität Dresden

We investigate the scattering off dilute magnetic impurities placed on the surface of three- dimensional topological insulators. In the low-temperature limit, the impurity moments are Kondo- screened by the surface-state electrons, despite their exotic locking of spin and momentum. We determine signatures of the Kondo effect appearing in quasiparticle interference (QPI) patterns as recorded by scanning tunneling spectroscopy, taking into account the full energy dependence of the T matrix as well as the hexagonal warping of the surface Dirac cones. We identify a universal energy dependence of the QPI signal at low scanning energies as fingerprint of Kondo physics, markedly different from the signal due to non-magnetic or static magnetic impurities. Finally, we discuss our results in the context of recent experimental data.

TT 30.2 Tue 9:45 H21

**Solution of the Anderson impurity model via the functional renormalization group** — Simon Streib, •Aldo Isidori, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany

We show that the functional renormalization group is a numerically cheap method to obtain the low-energy behavior of the Anderson impurity model describing a localized interacting electron coupled to a bath of conduction electrons. Our approach uses an external magnetic field as flow parameter, partial bosonization of the transverse spin fluctuations, and frequency-independent interaction vertices which are fixed by Ward identities. We calculate the quasi-particle residue and the spin susceptibility in the particle-hole symmetric case and obtain excellent agreement with the Bethe ansatz results for arbitrary strengths of the interaction.

TT 30.3 Tue 10:00 H21

**Kondo effect and magnetic frustration in a system of magnetic trimer on a metal surface** — •Hoa Nghiem — Forschungszentrum Jülich, PGI-2/IAS-3, Jülich, Germany

We use quantum Monte Carlo simulation to clarify the competition between Kondo screening and magnetic frustration in a system of three magnetic adatoms on a metal surface [1]. We observe the feature of spectral density depending on the geometric configuration of three magnetic adatoms on the surface [2, 3]. In the isosceles configuration, the spectral density exhibits a significant peak near the Fermi level, which we attribute to the Yosida-Kondo resonance. In the equilateral configuration, no peak is observed near the Fermi level. This observation suggests the two separate regimes; the Yosida-Kondo dominant regime with the singlet ground state, and the magnetic frustration

dominant regime with the degenerate ground state, - changing from one regime to another is realized as we gradually switch the geometric configuration from the isosceles triangle to equilateral one. By calculating the spectral density and the magnetic susceptibility in a wide range of temperatures, we prove the existence of the two separate regimes and suggest the critical crossover between them.

[1] N. T. M. Hoa, W. A. Diño, and H. Kasai: J. Phys. Soc. Jpn. 81 (2012) 023706
[2] T . Jamneala, V. Madhavan, and M. F. Crommie: Phys. Rev. Lett 87 (2001) 256804
[3] N. T. M. Hoa, W. A. Diño, and H. Kasai: J. Phys. Soc. Jpn. 79 (2010) 113706

TT 30.4 Tue 10:15 H21

**Magnetic exchange coupling mediated by Kondo singlets** — •Andrej Schwabe, Irakli Titvinidze, and Michael Potthoff — University Hamburg, Hamburg, Germany

When a magnetic impurity is antiferromagnetically exchange coupled to a metallic bath its spin degree of freedom may be quenched due to the Kondo effect. For several impurities, this competes with the RKKY indirect magnetic exchange. In a finite quantum box and for a weak coupling, this competition may encounter drastic modifications due to the presence of a finite size gap [1,2].
Here we extend our previous studies to the strong-coupling regime where almost local Kondo singlets are formed. In the ideal situation of a one-dimensional nano chain and large coupling, the bath is effectively cut into several pieces, which are magnetically coupled by a new type of indirect exchange that is mediated by virtual excitations of the local Kondo singlets. We derive an effective low-energy Hamiltonian for this strong-coupling regime. Its main contributions stem from an "inverse indirect magnetic exchange" between substrate pieces connected by local Kondo singlets. Different magnetic states depending on the number and the position of the impurities are analysed and compared with numerical calculations performed with a variational matrix-product states code. These can be understood by the adiabatic connection between the weak and the strong-coupling regime.

[1] A. Schwabe, D. Gütersloh, M. Potthoff, arXiv:1208.2209 (2012)
[2] W. B. Timm, J. Kroha, J. von Delft, PRL **82**, 2143 (1999)

TT 30.5 Tue 10:30 H21

**Identifying Kondo orbitals through spatially resolved STS** — •Andrey Antipov[1,2], Pedro Ribeiro[2], Johann Kroha[3], and Stefan Kirchner[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [3]Physikalisches Institut and Bethe Center for Theoretical Physics, Universitat Bonn, Nussallee 12, 53115 Bonn, Germany

In this contribution we study the influence of angular degrees of freedom of magnetic adatoms on metallic surfaces onto scanning tunneling spectra. Kondo scattering of conduction electrons off the adatom changes the local density of states near the Fermi level. The spatial dependence of this correction is set by the orbital structure of the local moment localized on the adatom. By considering a multilevel Anderson model with non-degenerate orbitals of differing orbital structure, using the multi orbital extension of the slave-boson mean field theory [1] we demonstrate that the spatial dependence of the scanning tunneling spectrum contains sufficient information to infer the orbital degrees of freedom of the magnetic adatom [2].

[1] P. Coleman, Phys. Rev. B 29, 3035-3044 (1984); J. Kroha et al., Physica E 18, 69 (2003)
[2] A. E. Antipov, P. Ribeiro, J. Kroha, S. Kirchner, to be published

TT 30.6 Tue 10:45 H21

**Hydrogen-induced Kondo effect for single Co atoms adsorbed on Pt(111)** — Quentin Dubout, Fabian Calleja, Markus Etzkorn, •Fabio Donati, Laurent Claude, Anne Lehnert, Pietro Gambardella, and Harald Brune — Institute of Condensed Matter Physics (ICMP),Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.

We report on 0.4 K STM measurements revealing the H-induced Kondo effect for single Co atoms on a Pt(111) surface. Clean Co/Pt(111) has $S = 1$ and out-of-plane anisotropy [1], its ground state is $m = \pm 1$ and therefore cannot exhibit a first order Kondo effect [2]. Upon $H_2$ adsorption, or upon exposing the sample to the residual gas of the UHV chamber, we find two hydrogenated species, CoH and $CoH_2$. Both complexes show a number of differential conductance steps, some shift upon isotope substitution, revealing their vibrational origin. The most interesting feature is that $CoH_2$ presents a large conductance peak at the Fermi level. It shows the thermal broadening and magnetic field splitting identifying its origin as the Kondo effect. The $CoH_2$ complex has $S = 3/2$ and in-plane hard axis. To our knowledge, this is the first observation of adsorbate induced Kondo effect. In our case, the adsorbate changes the spin and the magnetic anisotropy energy.

[1] P. Gambardella et al., Science **300**, 1130 (2003).
[2] A. F. Otte et al., Nat. Phys. **4**, 847 (2008).

**15 min. break**

TT 30.7 Tue 11:15 H21

**Single magnetic impurities in the Kane-Mele model** — •Florian Goth, David J. Luitz, and Fakher F. Assaad — Institut für theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The realization of the spin-Hall effect in quantum wells has led to a plethora of studies regarding the properties of the edge states of a 2D topological insulator. These edge states constitute a class of one-dimensional liquids, called the helical liquid, where an electron's spin direction is coupled to its direction of movement. In contrast to one dimensional conductors, magnetic impurities — below the Kondo temperature — cannot block transport and one expects the current to circumvent the impurity. To study this phenomenon, we consider the single impurity Anderson model embedded into an edge of a Kane-Mele ribbon with up to $512 \times 80$ sites and use numerically exact continuous time QMC methods to study the Kondo effect. We present results on the temperature dependence of the spectral properties of the impurity and the bulk system that show the behaviour of the system in the various regimes of the Anderson model. Furthermore we show results on the spatial behaviour of the spin-spin correlation functions.

TT 30.8 Tue 11:30 H21

**2-channel Kondo fixed point without fine tuning in a 3-level SU(3) quantum impurity: NRG results** — •Evaristus Fuh Chuo, Katinka Ballmann, Laszlo Borda, and Johann Kroha — Physikalisches Institut, Universität Bonn

The 2-channel Kondo (2CK) effect with its exotic ground state properties has remained difficult to realize in physical systems. At low energies, a quantum impurity with orbital degree of freedom, like a proton bound in an interstitial lattice space, comprises a 3-level system with a unique ground state and (at least) doubly degenerate rotational excitations with excitation energy $\Delta$. When immersed in a metal, electronic angular momentum scattering induces transitions between any two of these levels (couplings $J$), while the electron spin is conserved. We show by extensive NRG calculations that without fine-tuning of parameters this system exhibits a 2CK fixed point, due to Kondo correlations in the excited-state doublet whose degeneracy is stabilized by the the host lattice parity, while the channel symmetry (electron spin) is guaranteed by time reversal symmetry. We find a pronounced plateau in the entropy at $S(T_K < T < \Delta) = k_B \ln 2$ between the high-$T$ value, $S(T \gg \Delta) = k_B \ln 3$, and the 2CK ground state value, $S(0) = k_B \ln \sqrt{2}$. This indicates a down-renormalization of the doublet *below* the non-interacting ground state, thus realizing the 2CK fixed point, in agreement with earlier conjectures [1]. We map out the phase diagram in the $J$–$\Delta$ plane and compare with analytical results. $T_K$ shows non-monotonic $J$-dependence, characteristic for 2CK systems.

[1] M. Arnold, T. Langenbruch, J. Kroha, PRL **99**, 186601 (2007)

TT 30.9 Tue 11:45 H21

**Out-of-equilibrium steady-states near quantum critical points - A dynamical large-N study of the Bose-Fermi Kondo model** — •Pedro Ribeiro[1] and Stefan Kirchner[1,2] — [1]Max Planck Institute for the Physics of Complex Systems - Nothnitzer Str. 38, , D-01187 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids - Nothnitzer Str. 40, D-01187 Dresden, Germany

We study the out-of-equilibrium steady state properties of the Bose-Fermi-Kondo model, describing a local magnetic moment coupled to two ferromagnetic leads that support bosonic (magnons) and fermionic (Stoner continuum electrons) low energy excitations. In equilibrium, this model describes the destruction of the Kondo effect as the coupling to the bosons is increased, its phase diagram comprises three non-trivial fixed points. Using a dynamical large-N approach on the Keldysh contour, we study two different non-equilibrium setups: (a)

a finite bias voltage and (b) a finite temperature gradient, imposed across the leads. The scaling behavior of the charge and energy currents is identified and characterized for the different fixed points. We report the existence of an effective temperature, defined based on the fluctuation dissipation relations of the local spin-susceptibility, that permits to recover the equilibrium scaling behavior of both dynamical and static spin susceptibilities in all the studied cases.

TT 30.10 Tue 12:00 H21

**Inverse indirect magnetic exchange in one and higher dimensions** — •Irakli Titvinidze, Andrej Schwabe, Anke Braun, and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Deutschland

It is well known that magnetic adatoms on a metallic substrate surface experience the Ruderman-Kittel-Kasuya-Yosida (RKKY) indirect magnetic exchange. Here we consider the limit of a strong antiferromagnetic Kondo coupling $J$ which for certain geometries can lead to a quantum confinement of conduction electrons and the formation of local magnetic moments at substrate sites. It is argued that these local moments may couple magnetically via almost completely localized Kondo singlets that are formed for strong $J$. This novel inverse indirect magnetic exchange (IIME) is investigated numerically by means of the density-matrix renormalization group for one-dimensional multi-impurity Kondo models and for diluted Kondo lattices with "adatoms" present at every second "substrate" site. For the latter, our calculations show that as a function of $J$ there is a crossover from ferromagnetic order driven by the RKKY interaction at weak $J$ to ferromagnetism induced by the IIME interaction for strong $J$. We find excellent agreement with the results of corresponding calculations obtained by real-space dynamical mean-field theory (R-DMFT). R-DMFT is then used to study different adatom nanostructures on top of a two-dimensional substrate. We analyze the conditions under which the IIME interaction and ferromagnetic order induced by IIME also persists in two- and higher-dimensional systems.

TT 30.11 Tue 12:15 H21

**Correlations outside the light cone** — •Mariya Medvedyeva and Stephan Kehrein — Goerg-August University, Goettingen

We consider a Kondo impurity which couples to the conduction band electrons at some moment t=0. The commutator of the spin of the impurity and the spin of the conduction band electron vanishes outside the light cone determined by the speed of the propagation of the quasiparticles from the conduction band, as a consequence of the relativistic nature of the latter. While the correlation of the spin of the impurity and the spin of the conduction is non-zero outside the effective lightcone and follows a power law/exponential decay at zero/non-zero temperature. Non-zero correlation reveals the initial entanglement of the ground state of the conduction band electrons.

TT 30.12 Tue 12:30 H21

**Possible non-Fermi liquid behavior in transport through Co doped Au chains** — •Andreas Weichselbaum[1], Solange Di Napoli[2], Pablo Roura-Bas[2], Armando A. Aligia[3], Yuriy Mokrousov[4], and Stefan Blügel[4] — [1]Ludwig-Maximilians-Universität, München, Germany — [2]Departamento de Física de la Materia Condensada, Buenos Aires, Argentina — [3]Centro Atómico Bariloche and Instituto Balseiro, Bariloche, Argentina — [4]Institut für Festkörperforschung, Forschungszentrum Jülich, Germany

We calculate the conductance as a function of temperature G(T) through monoatomic Au chains, which contain one Co atom as a magnetic impurity and are connected to two conducting leads with a 4-fold symmetry axis. Using the information derived from ab initio calculations, we construct an effective model Hamiltonian $H_{\text{eff}}$ that hybridizes a $3d^7$ quadruplet at the Co site with two $3d^8$ triplets through the hopping of $5d_{xz}$ and $5d_{yz}$ electrons of Au. The quadruplet is split by a term $DS^2_{z,\text{Co}}$ due to spin-orbit coupling at the Co site. Solving $H_{\text{eff}}$ with the numerical renormalization group (NRG), we find at low temperatures $G(T) = a - b\sqrt{T}$ together with a ground state impurity entropy of $\ln(2)/2$, a behavior similar to the two-channel Kondo model. Stretching the chain one expects a quantum phase transition to a non-Kondo phase, with the physics of the underscreened Kondo model at the quantum critical point.

TT 30.13 Tue 12:45 H21

**Interaction-driven transition between topological states in a Kondo insulator** — •Jan Werner and Fakher Assaad — Theoretische Physik 1, Universität Würzburg, Deutschland

Heavy fermion materials naturally combine strong spin-orbit interactions and electronic correlations. When there is precisely one conduction electron per impurity spin, the coherent heavy fermion state is insulating. This Kondo insulating state has recently been argued to belong to the class of quantum spin Hall states [1]. Motivated by this conjecture and a very recent experimental realisation of this state[2], we investigate a model for Kondo insulators with spin-orbit coupling. Using DMFT, we observe an interaction-driven transition between two distinct topological states, indicated by a closing of the bulk gap and a simultaneous change of the $Z_2$ topological invariant. Upon reopening of the bulk gap the system remains a topological insulator, however with a zero energy edge mode now at the X-point instead of the Gamma-point.

[1] M. Dzero, K. Sun, P. Coleman, and V. Galitski, Phys. Rev. B 85, 045130 (2012)
[2] S. Wolgast et. al., arXiv:1211.5104 (2012)

## TT 31: Correlated Electrons: Low-Dimensional Systems -Materials 1

Time: Tuesday 9:30–12:15 Location: H41

TT 31.1 Tue 9:30 H41

**Charge density waves and lattice dynamics in 1T-$TaS_2$** — •Tobias Ritschel[1,5], Jan Trinckauf[1], Gaston Garbarino[2], Alexei Bosak[2], Martin von Zimmermann[3], Helmuth Berger[4], Bernd Büchner[1,5], and Jochen Geck[1] — [1]IFW Dresden — [2]ESRF, Grenoble — [3]HASYLAB, Hamburg — [4]Ecole polytechnique Federale de Lausanne — [5]TU Dresden

The layered compound 1T-$TaS_2$ shows an interesting interplay of charge density wave (CDW) order and superconductivity. We studied the static CDW order by means of elastic X-ray diffraction as a function of temperature and external pressure, in order to shed light on the relation between these two collective electronic states. In addition, we investigated the pressure dependency of the lattice dynamics using inelastic X-ray scattering. The phonon dispersion around the CDW wave vector is strongly pressure dependent and a Kohn anomaly is observed well above the nearly commensurate to incommensurate phase transition temperature. We present the experimental data along with model calculations and discuss the results in relation to the pressure-induced superconductivity.

TT 31.2 Tue 9:45 H41

**Phonon Softening in the CDW Systems $NbSe_2$ and $TiSe_2$** — •Roland Hott[1], Rolf Heid[1], Klaus-Peter Bohnen[1], Frank Weber[1,2], Stephan Rosenkranz[2], John-Paul Castellan[1,2], Raymond Osborn[2], Takeshi Egami[3], Ayman Said[4], and Dmitry Reznik[1,5] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, P. B. 3640, D-76021 Karlsruhe, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, Illinois, 60439, USA — [3]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee, 37996, USA — [4]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, 60439, USA — [5]Department of Physics, University of Colorado at Boulder, Boulder, Colorado, 80309, USA

We present new results on the soft-mode behaviour of phonons in the Charge Density Wave (CDW) systems $NbSe_2$ and $TiSe_2$. Our theoretical predictions from Density Functional Theory (DFT) based on ab-initio phonon calculations coincide with the CDW instability behaviour that we observed experimentally by means of high resolution Inelastic X-ray Scattering (IXS). While $TiSe_2$ shows a rather sharp phonon anomaly at T = 190 K, the anomaly in $NbSe_2$ at T = 33 K is much broader than expected for a Fermi surface nesting driven CDW instability. For $NbSe_2$, we exclude Fermi surface nesting as main origin of the phonon softening. For $TiSe_2$, the phonon softening seems to be well described within the framwork of DFT.

TT 31.3 Tue 10:00 H41

**Charge Density Wave Transport Properties of the (DCNQI-$d_6$)$_2$Cu radical anion salt** — •Florian Hüwe[1], Matthias Schmiddunser[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius-Maximilians University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The class of organic metals provides intriguing examples of how the physical properties depend on the respective dimensionality of the underlying material system. The organic radical anion salt (DCNQI-$d_6$)$_2$Cu undergoes a pronounced first-order phase transition upon cooling from a highly conducting quasi-3D metallic state with a conductivity of $\sigma_{RT} \approx 10^3 \frac{S}{cm}$ into a quasi-1D semiconducting, commensurate charge density wave (CDW) state.

Our contribution reports on the transport properties of electrocrystallized (DCNQI)$_2$Cu single crystals in this CDW regime. Below the phase transition temperature of $T_c = 75K$ the resistance of the about $2cm$ long needle-like samples increases more than five orders of magnitude along the [001]-direction of preferred conductivity. In addition, features of non-linear conduction occur above threshold fields of $E_{th} \approx 10 - 100 \frac{V}{cm}$ which we examined with respect to heating and interference effects by (pulsed) current-voltage and noise measurements. Small $\mu m$-sized samples grown by microelectrolysis on a substrate with evaporated gold contacts allow for the investigation of electrical transport in the high-field limit. Finally, a connection between transport characteristics and charge carrier density is drawn.

Financial support by the DFG (project PF385/6-1) is gratefully acknowledged.

TT 31.4 Tue 10:15 H41

**The Luttinger liquid theory of molybdenum purple bronze $Li_{0.9}Mo_6O_{19}$** — •Piotr Chudzinski[1,2], Thomas Jarlborg[1], and Thierry Giamarchi[1] — [1]DPMC-MaNEP, Universite de Geneve — [2]University of Regensburg

We study a quasi-1D material, the purple bronze $Li_{0.9}Mo_6O_{19}$ which becomes superconductor at 1.9K. Firstly, the band structure is calculated by use of ab-initio DFT-LMTO method. The unusual, very 1-dimensional band dispersion obtained in previous band calculations is confirmed and the overall band structure agrees reasonably with existing photoemission data. Dispersion perpendicular to the main dispersive direction is obtained and investigated in detail. Temperature and disorder effects are evaluated, in particular we check their influence on the band broadening. Based on this, in the second part of our work we derive an effective low energy theory within the Luttinger liquid framework. We estimate the strength of possible instabilities and values of charge modes compressibilities. Our aim is to understand experimental findings, in particular the ones which are certainly lying within 1D regime. We discuss the validity of our approach and further perspectives for the lower energy phases.

TT 31.5 Tue 10:30 H41

**Competing soft phonon modes in $TbTe_3$** — •Michael Maschek[1], Rolf Heid[1], Stefan Rosenkranz[2], Ayman Said[2], Bogdan Leu[2], Paula Giraldo-Gallo[3], and Ian Fisher[3] — [1]Institute of Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Material Science Division, Argonne National Laboratory, Argonne, USA — [3]Geballe Laboratory for Advanced Materials, Stanford University, Stanford, USA

We report high energy resolution inelastic x-ray measurements of competing soft phonon modes in the vicinity of the charge-density-wave (CDW) phase transition in $TbTe_3$. We investigated two phonon modes having each a transverse polarization within the basal plane of the nearly tetragonal unit cell (a=4.308, b=25.57, c=4.314) but are dispersing along the reciprocal (100) and the (001) directions. Only the latter one is expected to go soft at $q_{\mathrm{CDW}} = (0, 0, 0.296)$ and $T_{\mathrm{CDW}} = 332K$. We found that both phonon modes go soft approaching $T_{\mathrm{CDW}}$ from high temperatures. The softenings are identical down to $T = 350K$, and only for $T < 350K$ we see a significantly stronger softening of the mode at $q_{\mathrm{CDW}}$. Our results are corroborated by lattice dynamical calculations demonstrating the degeneracy between the two crystallographic axes with respect to the formation of CDW order.

**15 min. break**

TT 31.6 Tue 11:00 H41

**High-mobility two-dimensional electron gas at a new oxide heterointerface** — •Romain Giraud[1], Joseph Dufouleur[1], Yunzhong Chen[2], Nini Pryds[2], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany — [2]Department of Energy Conversion and Storage, Technical University of Denmark, Ris⌀ Campus, 4000 Roskilde, Denmark

In oxides heterostructures, it is generally accepted that the formation of a two-dimensional electron gas (2DEG) occurs at the interface between two insulators with different band gaps, due to band bending. However, there is still an ongoing debate about the mechanisms that drive charge transfer at the interface.

In this work, we evidence the formation of a 2DEG at a new oxide heterointerface, which will be presented in detail. The universality of the overlayer critical thickness for the onset of metallicity will be discussed, as well as the origin of charge transfer. A thorough analysis of the Shubnikov-de Haas oscillations observed above 1 T at T = 22 mK will be presented. These reveal the enhanced mobility of electrons and the influence of magnetic interactions on the 2DEG band structure. Due to a long a phase coherence length, this heterointerface offers a unique opportunity to study quantum coherent transport in strongly-correlated d-electron systems.

TT 31.7 Tue 11:15 H41

**High mobility of the strongly confined hole gas in $AgTaO_3$/$SrTiO_3$** — •Udo Schwingenschlögl, Safdar Nazir, and Mousumi Upadhyay-Kahaly — KAUST, PSE Division, Thuwal, Saudi Arabia

A theoretical study of the two-dimensional hole gas at the $(AgO)^-$/$(TiO_2)^0$ p-type interface in the $AgTaO_3/SrTiO_3$ (001) heterostructure is presented. The Ag 4d states strongly hybridize with the O 2p states and contribute to the hole gas. It is demonstrated that the holes are confined to an ultra thin layer ($\sim$ 4.9 Å) with a considerable carrier density of $\sim 10^{14}$ cm$^{-2}$. We estimate a hole mobility of 18.6 cm$^2$V$^{-1}$s$^{-1}$, which is high enough to enable device applications.

[1] Appl. Phys. Lett. **100**, 201607 (2012)

TT 31.8 Tue 11:30 H41

**Electronic Reconstruction in (001) and (111) oriented $LaAlO_3/SrTiO_3$ interfaces** — •David Doennig and Rossitza Pentcheva — Department of Earth and Environmental Sciences, Section Crystallography and Center of Nanoscience, University of Munich, Theresienstr. 41, DE-80333 Munich, Germany

The observation of a quasi two-dimensional electron gas (q2DEG), superconductivity and magnetism at the (001) interface between the band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) has opened possibilities for novel electronics applications. Based on density functional calculations, we explore if these multifunctional properties can be extended by changing the crystal orientation from (001) to (111). Despite the difference in stacking with AO and $BO_2$ planes of the perovskite $ABO_3$ structure in (001) oriented superlattices versus $AO_3$ and B layers in the (111) direction, analogous effects such as polar discontinuity arise when the A and B cations are varied across the interface. A further intriguing feature in (111) oriented interfaces is the formation of a buckled honeycomb lattice of the B-site cations. This lattice geometry, well known from graphene, promises to host even more exotic topological phases. The effect of interface termination, thickness of the substrate and strain will be discussed.

We acknowledge funding by the DFG, SFB/TR80.

TT 31.9 Tue 11:45 H41

**Modelling random oxygen defects and magnetism at titanate interfaces** — •Natalia Pavlenko[1,2], Thilo Kopp[1], G.A. Sawatzky[3], and J. Mannhart[2] — [1]EKM und Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada V6T1Z1

We analyze the magnetic state at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface within density unctional theory and provide evidence that it depends strongly on the oxidation state of the interfaces. We show that oxygen defects at titanate interfaces induce a complex multiorbital reconstruction which involves a lowering of the local symmetry and an inversion of $t_{2g}$ and $e_g$ orbitals resulting in the occupation of the eg orbitals of Ti atoms neighboring the O-defects. In contrast to stoichiometric nonmagnetic interfaces of $LaAlO_3$ and $SrTiO_3$, the defect-induced orbital reconstruction at LAO/STO interfaces generates a two-dimensional interface magnetic state not observed in bulk $SrTiO_3$. Using an effective two-band Hubbard model with disorder,

we analyze the stability of the 2d-magnetic states at titanate interface for different concentrations of random defects.

TT 31.10 Tue 12:00 H41

**Gating a two-dimensional electron gas using a multiferroic** — •Christian Mix[1,2], Mathias Kläui[1], and Gerhard Jakob[1] — [1]Institute of Physics, Universität Mainz, Germany — [2]Graduate school of excellence MAINZ, Mainz, Germany

Recently, research on oxide interfaces has exposed a unexpected conducting state at the interface of lanthanum aluminate (LAO) and strontium titanate (STO), two bulk insulators [1]. Laser ablation enables to the deposition of a wide range of oxide multilayer systems with thickness control at atomic level. Many interesting applications can be introduced by the use of multilayered, epitaxial perovskite structures [2,3]. The sheet resistivity of the 2DEG at the STO/LAO interface possesses a strong dependence on an out-of-plane electrical field. Thus the use of a ferroelectric layer on top of the STO/LAO interface system can lead to a remanent control of the conductivity of the 2DEG. Here, results on the growth and characterization of the multiferroic $BiFeO_3$ on the STO/LAO interface system containing a 2DEG are shown. On the other hand, piezo force microscopy (PFM) is utilized as a tool to observe the ferroelectric domain structure of the BFO thin film with the 2DEG as a back electrode.

[1] J. Mannhart, D.H.A. Blank, H.Y. Hwang, A.J. Millis, J.-M. Triscone, MRS Bullentin **33** (2008) 1027
[2] N.A. Spaldin, M. Fiebig, Science **309** (2005) 391
[3] C. Chen, S. Thiel, J. Mannhart, J. Levy, Science **323** (2009) 1026

## TT 32: Focused Session: Frontiers of Electronic Structure Theory 3 (jointly with HL and O)

Time: Tuesday 10:30–13:15 Location: H36

**Topical Talk** TT 32.1 Tue 10:30 H36

**Materials for Alternative Energies: Computational Materials Discovery and Crystal Structure Prediction** — •Chris Wolverton — Northwestern University, Evanston, IL, USA

Many of the key technological problems associated with alternative energies may be traced back to the lack of suitable materials. The materials discovery process may be greatly aided by the use of computational methods, particular those atomistic methods based on density functional theory. In this talk, we present an overview of recent work on energy-related materials from density-functional based approaches. We have developed novel computational tools which enable accurate prediction of crystal structures for new materials (using both Monte Carlo and Genetic Algorithm based approaches), materials discovery via high-throughput, data mining techniques, and automated phase diagram calculations. We highlight applications in the area of Li battery materials and hydrogen storage materials.

TT 32.2 Tue 11:00 H36

**Doping at the Si-SiO2 interface** — Fabiano Corsetti[1] and •Arash Mostofi[2] — [1]CIC nanoGUNE Consolider, Donostia-San Sebastian, Spain — [2]Dept. of Materials & the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, UK

The Si-SiO2 interface is a common feature in modern silicon-based CMOS technology for the fabrication of integrated circuits. The ongoing miniaturisation drive for such devices makes it increasingly important to understand the effect of the interface on the dopant distribution and properties. Indeed, in some cases channel lengths can be a few tens of nanometres, with the device properties being determined by only about 100 dopant atoms.

We have investigated the properties of arsenic dopants at the Si-SiO2 interface. We use a large supercell to simulate both ordered ($\alpha$-cristobalite) and disordered silica interfaces with crystalline Si. The disordered interface is generated using a multiscale approach in which a Monte Carlo method, parametrised with density-functional theory (DFT) calculations, is used to access the long time scales required for amorphising the oxide. The segregation of arsenic dopants in silicon at the interface is then studied using DFT.

We are able to accurately characterise the long-range quantum confinement effect due to the interface, which is found to result in a small energy barrier for segregation. We also investigate the effect of the local stress at the defect site on its segregation energy, and show that a simple 'particle in a box' model can be used to explain the calculated segregation energies at all substitutional silicon sites.

TT 32.3 Tue 11:15 H36

**Pressure-induced structural transformations in nanomaterials: a linear-scaling DFT investigation** — •Niccolo Corsini[1], Peter Haynes[1], Carla Molteni[2], and Nicholas Hine[1] — [1]Imperial College, London, UK — [2]King's College, London, UK

Semiconductor nanomaterials, including nanocrystals, nanorods and tetrapods, display a number of peculiar and tunable properties that distinguish them from their bulk counterparts and make them versatile materials for use as e.g. effective optical probes in medical diagnostics or photovoltaic devices. Of particular interest is their response to applied pressure, as they transform from one crystalline or amorphous structure to another. Accurate simulations are important for understanding finite size effects in the atomistic mechanisms of phase transformations (difficult to observe clearly in macroscopic experiments), for the opportunity to uncover novel metastable phases stabilized in finite systems, and for potentially innovative applications of nanomaterials. First-principles methods are essential to accurately describe the bond breaking/making in phase transformations and the realistic description of surfaces (often covered by complex surfactants). However the computational cost limits both the length- and time-scales attainable. We have combined an order-N density functional theory code for large systems and an electronic-enthalpy method to apply pressure to finite systems to model with quantum mechanical precision processes induced by pressure in nanomaterials (including their surfaces) under realistic conditions. The focus is on Si, CdSe and CdS nanocrystals that are currently favoured for technological applications.

TT 32.4 Tue 11:30 H36

**Density functional / molecular dynamics simulations of nucleus-driven crystallization of amorphous Ge2Sb2Te5** — •Jaakko Akola[1,2,3], Janne Kalikka[4], Julen Larrucea[4], and Robert O. Jones[3] — [1]Department of Physics, Tampere University of Technology, Finland — [2]COMP Centre of Excellence, Department of Applied Physics, Aalto University, Finland — [3]GRSS and PGI-1, Forschungszentrum Jülich, Germany — [4]Nanoscience Center, Department of Physics, University of Jyväskylä, Finland

Early stages of nucleus-driven crystallization of the prototype phase change material Ge2Sb2Te5 have been studied by massively-parallel density functional/molecular dynamics simulations for amorphous samples (460 and 648 atoms) at 500, 600, and 700 K [1]. All systems assumed a fixed cubic seed of 58 atoms and 6 vacancies in order to achieve sub-nanosecond phase transition. Crystallization occurs within 600 ps for the 460-atom system at 600 and 700 K, and signs of crystallization (nucleus growth, percolation) are present in the others. Crystallization is accompanied by an increase in the number of ABAB squares (A: Ge, Sb, B: Te) [2,3], and atoms of all elements move significantly. The evolution of cavities/vacancies is closely monitored. The existence of Te-Te, Ge-Ge, Ge-Sb, and Sb-Sb (wrong) bonds is an inevitable consequence of rapid crystallization.

[1] J. Kalikka, J. Akola, J. Larrucea, and R. O. Jones, Physical Review B 86, 144113 (2012). [2] J. Akola and R. O. Jones, Phys. Rev. B 76, 235201 (2007). [3] J. Akola and R. O. Jones, Phys. Rev. Lett. 100, 205502 (2008).

TT 32.5 Tue 11:45 H36

**Large-Scale Moiré Patterns of hexagonal Boron Nitride on Cu(111): DFT Studies of Structural and Electronic Properties** — •Ralph Koitz, Ari P Seitsonen, Marcella Iannuzzi, and Jürg Hutter — Institute of Physical Chemistry, University of Zurich, Switzerland

Hexagonal boron nitride ($h$-BN) adsorbed on metal surfaces shows great promise for applications in nanoscience. Interesting structural and electronic properties have been found, e.g. for $h$-BN on Rh(111) and Ru(0001), where the overlayer is strongly corrugated. Recent experiments with $h$-BN on Cu(111) indicate that the difference in lattice constants and a rotation of the monolayer lead to moiré patterns with periodicities greater than 5 nm. To thoroughly understand this system,

however, further insight is needed at the atomic level.

In this contribution we present an in-depth DFT study of a moiré pattern of a rotated 24×24 *h*-BN sheet on a 23×23 Cu(111) slab. The periodic pattern extends over 6 nm, making this simulation the largest of its kind so far reported. We study the gradual change of adsorption registry of the monolayer, and its influence on the electronic structure. Both B and N occupy the entire range of *top, hcp, fcc*, and bridging positions. This modulation over the unit cell is reflected in the projected DOS, the electrostatic potential, and the contrast in simulated STM images. Contrary to other *h*-BN/metal systems, only minute structural changes occur upon adsorption. Our results show that the observed corrugation is chiefly electronic in nature and strongly related to the lateral variation of adsorption registries.

TT 32.6 Tue 12:00 H36

**A computational perspective for the development of electronic excited-states calculations** — •Xavier Andrade — Department of Chemistry and Chemical Biology, Harvard University, Cambridge, United States

In this talk I present different aspects of my work, focused on improving electronic structure theory for excited states with the aim of making it suitable for current computer architectures.

First, I will present an approach to approximate the exchange and correlation (XC) term in density functional theory. In this approach the XC potential is considered as an electrostatic potential. Based on this representation we develop a scheme that fixes the asymptotic behavior of an approximated XC potential. Additionally, from the procedure it is possible to extract the derivative discontinuity of the XC potential to directly obtain the gap of atoms and molecules.

Real-time methods like molecular dynamics and real-time time-dependent density functional theory are a good alternative for computing response properties. However, long propagation times are needed to obtain resolved properties. As a second topic of this talk, we address this problem by using a state-of-the-art signal-analysis technique: compressed sensing. By using this method instead of a Fourier transform, we find that the total propagation time required for resolved spectra can be reduced by a factor of five.

Finally, I will discuss my work on electronic structure calculations on graphical processing units (GPU) and the strategies to profit from the data parallelism available in the density functional formalism.

TT 32.7 Tue 12:15 H36

**Nuclear quantum effects in first principles molecular dynamics by colored-noise thermostats** — •Michele Ceriotti — University of Oxford, United Kingdom

Oftentimes atomistic computer simulations treat atomic nuclei as purely classical particles, even when the electronic structure problem is treated quantum mechanically. This is a very good approximation when the system contains only heavy atoms. However, lighter nuclei such as hydrogen exhibit a strong quantum behavior, which manifests itself as sizable zero-point energy, tunnelling, isotope effects, etc.

Path integral methods are the state-of-the-art technique to model quantum nuclei, but they are computationally very demanding. Here I will discuss how a correlated-noise Langevin dynamics can be used to approximate nuclear quantum effects inexpensively, and how it can reduce by an order of magnitude the cost of quantitatively accurate path integral molecular dynamics. I will also present applications to the simulation of nuclear quantum effects in hydrogen-bonded materials by ab initio molecular dynamics.

TT 32.8 Tue 12:30 H36

**Semiconductor and Metal-Oxide Nanocrystal Simulations with Linear-Scaling PAW DFT** — •Nicholas Hine — Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom — Cavendish Laboratory, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Nanocrystals enable tuning of material properties by varying attributes not available in bulk crystals, such as size, shape and surface termination, and such systems have innumerable applications in the field of energy materials, particularly in photovoltaics and photocatalysis. While whole nanocrystals are too large to be studied with traditional cubic-scaling first-principles methods, linear-scaling formulations of density functional theory (LS-DFT) enable the study of systems of many thousands of atoms. This allows nanocrystal simulations to make contact with the realistic size regime of 5-10nm, thus overlapping with the feasible scale of experimental characterisation and control. I will discuss recent developments in the ONETEP LS-DFT code that enable these large-scale, high-accuracy simulations, including the Projector Augmented Wave method, and recent applications to TiO2 nanocrystals, pressure-induced phase transformations in II-VI semiconductor nanocrystals, and wurtzite-structure III-V semiconductor nanorods. I will discuss the origin of the large dipole moments which can be observed in such structures, and show how an effect akin to Fermi-level pinning can have a determining influence on the overall polarisation, explaining its variation with size, shape, surface chemistry and composition.

TT 32.9 Tue 12:45 H36

**Many-body effects on the carrier dynamics of graphene** — •Cheol Hwan Park — Department of Physics and Astronomy, Seoul National University, Seoul, Korea

It is very important to understand how a charge carrier in real materials interacts with other charge carriers or with the lattice vibration. In this presentation, I will explain that the measured carrier scattering rate versus energy behavior in graphene can be quantitatively described from first-principles calculations considering electron-electron interactions within the GW approximation and electron-phonon interactions within the Migdal approximation [1]. Then, I will show that our calculation can also explain (i) the mismatch between the extrapolations of the upper and lower Dirac cones in heavily doped graphene [2] and (ii) the significant deviation from linear energy dispersion in extremely low-doped graphene [3]. Last, I will show that first-principles calculations on the intrinsic electrical resistivity of graphene arising from electron-phonon interactions [4] can quantitatively explain the transport experiments on heavily doped graphene [5].

[1] C.-H. Park, F. Giustino, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. 99, 086804 (2007).

[2] C.-H. Park, F. Giustino, C. D. Spataru, M. L. Cohen, and S. G. Louie, Nano Lett. 9, 4234 (2009).

[3] D. A. Siegel, C.-H. Park, C. Hwang, J. Deslippe, A. V. Fedorov, S. G. Louie, and A. Lanzara, Proc. Nat. Acad. Sci. 108, 11365 (2011).

[4] C.-H. Park et al., in preparation.

[5] D. K. Efetov and P. Kim, Phys. Rev. Lett. 105, 256805 (2010).

TT 32.10 Tue 13:00 H36

**Theory of nanomagnetic and graphene hybrid systems: adatoms and multiorbital Kondo physics** — •Tim Wehling — Institute for Theoretical Physics and BCCMS, University of Bremen, D-28359 Bremen, Germany

Graphene combines chemical inertness with a distinctly symmetric low energy electronic structure. Here, we show based on first-principles calculations that these two characteristics largely determine its interaction with adatoms. We find that covalent bonds to first row elements cause midgap states which can control electron transport [1] and the dielectric properties [2] of graphene based systems. The special nature of the Dirac electrons furthermore governs the coupling of magnetic adatoms to graphene by orbital selection rules and leads to peculiar multiorbital Kondo physics [3,4]. Finally, it is shown how multiorbital effects control the physics of magnetic transition metal atoms coupled to normal metals [5] and topological insulators [6].

[1] T. O. Wehling et al., Phys. Rev. Lett. 105, 056802 (2010).
[2] S. Yuan et al., Phys. Rev. Lett. 109, 156601 (2012).
[3] T. O. Wehling et al., Phys. Rev. B 84, 235110 (2011).
[4] T. O. Wehling et al., Phys. Rev. B 81, 115427 (2010).
[5] B. Surer et al., Phys. Rev. B 85, 085114 (2012).
[6] J. Honolka et al., Phys. Rev. Lett. 108, 256811 (2012).

# TT 33: Topological Insulators 3 (jointly with HL, MA, and O)

Time: Wednesday 9:15–13:00 Location: H16

TT 33.1 Wed 9:15 H16

**Topological Excitonic Superfluids in Three Dimensions** — •Ewelina M. Hankiewicz[1], Youngseok Kim[2], and Matthew Gilbert[2] — [1]Wuerzburg University — [2]University of Illinois, Urbana

We study the equilibrium and non-equilibrium properties of topological dipolar intersurface exciton condensates within time-reversal invariant topological insulators in three spatial dimensions without a magnetic field. We elucidate that, in order to correctly identify the proper pairing symmetry within the condensate order parameter, the full three-dimensional Hamiltonian must be considered. As a corollary, we demonstrate that only particles with similar chirality play a significant role in condensate formation. Furthermore, we find that the intersurface exciton condensation is not suppressed by the interconnection of surfaces in three-dimensional topological insulators as the intersurface polarizability vanishes in the condensed phase. This eliminates the surface current flow leaving only intersurface current flow through the bulk. We conclude by illustrating how the excitonic superfluidity may be identified through an examination of the terminal currents above and below the condensate critical current. Reference: Phys. Rev. B 86, 184504 (2012).

TT 33.2 Wed 9:30 H16

**$Bi_2Te_3$: A dual topological insulator** — •Tomáš Rauch[1], Markus Flieger[1], Arthur Ernst[2], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The class of $\mathcal{Z}_2$ topological insulators requires time reversal symmetry, while topological crystalline insulators require a mirror symmetry (an example is SnTe [1]).

We show that the well-known $\mathcal{Z}_2$ topological insulator $Bi_2Te_3$ with $\mathcal{Z}_2$ invariant $(1;0\,0\,0)$ is also a topological crystalline insulator with mirror Chern number $-1$. This dual topological character allows to dope $Bi_2Te_3$ magnetically, thereby breaking time-reversal symmetry, while keeping the topological crystalline character. As a consequence, magnetized $Bi_2Te_3$ shows a Dirac state at its (111) surface shifted off the time-reversal invariant momentum $\overline{\Gamma}$, provided the magnetization is perpendicular to a mirror plane.

These fundamental features are elaborated by means of tight-binding calculations of both the bulk and the surface electronic structure as well as of the topological invariants. $\vec{k}\cdot\vec{p}$ model calculations and *ab initio* KKR calculations complement and support these results.

Our findings open a new path toward device applications that rely on topological insulators with magnetically controllable topological character.

[1] L. Fu, Phys. Rev. Lett. **106** (2011) 106802; T. Hsieh *et alii*, Nature Comms. **3** (2012) 982.

TT 33.3 Wed 9:45 H16

**Three-dimensional Models of Topological Insulator Films: Dirac Cone Engineering and Spin Texture Robustness** — David Soriano[1], •Frank Ortmann[1], and Stephan Roche[1,2] — [1]Catalan Institute of Nanotechnology, Barcelona (Spain) — [2]ICREA, Barcelona (Spain)

Topological insulators feature surface states which exhibit certain robustness to disorder and which can be gapped due to inter-surface tunneling. By designing three-dimensional models of topological insulator thin films, we demonstrate a tunability of surface states and the odd number of Dirac cones on opposite surfaces by modifications of the atomic-scale geometry at the boundaries. [1,2] This enables the creation of a single Dirac cone at the $\Gamma$ point as well as possible suppression of quantum tunneling between Dirac states at opposite surfaces. We further analyze the robustness of the spin texture to bulk disorder which may help in quantifying bulk disorder in materials with ultraclean surfaces. [2]

[1] L. Fu, C.L. Kane, and E.J. Mele, Phys. Rev. Lett. 98, 106803 (2007)

[2] D. Soriano, F. Ortmann, and S. Roche, Phys. Rev. Lett. (in press)

TT 33.4 Wed 10:00 H16

**Transport properties of point contacts between helical edge states** — •Christoph P. Orth and Thomas L. Schmidt — University of Basel, Switzerland

We study a 2D topological insulator with helical edges that are connected by local electron tunneling. The edges are in contact with four reservoirs held at different chemical potentials. In contrast to existing theories, we treat the tunneling exactly but apply perturbation theory for the electron-electron interactions to calculate the current. Furthermore, we allow for a slow momentum dependent spin-rotation of the helical fields which can be created, e.g., by Rashba spin-orbit coupling. This allows inelastic spin-flip tunneling processes between the edges. Our results help to understand the interplay between electron-electron and spin-orbit interactions in topological insulators.

TT 33.5 Wed 10:15 H16

**Exotic magnetic properties of diluted magnetic binary chalcogenides** — •Maia G. Vergniory[1], Xabier Zubizarreta[1], Mikhail M. Otrokov[2], Igor V. Maznichenko[3], Juergen Henk[3], Evgueni V. Chulkov[4], and Arthur Ernst[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Tomsk State University, Tomsk, Russia — [3]Martin-Luther-University, Halle-Wittenberg, Germany — [4]Donostia International Physics Center, Donostia-San Sebastian, Spain

Using first-principles Green function approach we studied electronic and magnetic properties of diluted magnetic binary chalcogenides $A_2B_3$, doped with transition metals substituing the A element. The electronic structure of the impurities in the chalcogenides is mainly featured by the crystal field splitting. We found that two main mechanisms are responsible for long-range magnetic order in these materials: hole mediated magnetism within the layer of A atoms and indirect interaction between magnetic moments via a B atom. We also estimated Curie temperature of these systems, which was found in good agreement with the available experimental data. Our results shed light on the understanding of magnetic interaction and control in toplogical insulators.

TT 33.6 Wed 10:30 H16

**Quasiparticle study of the bulk topological insulators $Bi_2Se_3$, $Bi_2Te_3$, and $Sb_2Te_3$ including spin-orbit coupling.** — •Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We present $GW$ calculations of the topological insulators $Bi_2Se_3$ and $Bi_2Te_3$ within the all-electron FLAPW formalism and compare them with previous calculations. We extend the study to the topological insulator $Sb_2Te_3$, which poses additional problems when studied with $GW$ based on non-relativistic density functional theory (DFT) as it exhibits a negative DFT band gap. In contrast to the previous $GW$ calculations, we fully take into account spin-orbit coupling (SOC) allowing spin-off-diagonal elements in the Green function and the self-energy, and we discuss the differences to a simpler perturbative approach (*i.e.*, treating SOC on DFT level *a posteriori*). Additionally, we show that the inclusion of SOC induces fundamental changes in the Green function $G$, whereas changes in the screened interaction $W$ are negligible. We also discuss the influence of off-diagonal elements of the self-energy matrix.

After inclusion of quasiparticle effects, we observe a direct band gap at the $\Gamma$ point for $Bi_2Se_3$, in disagreement with predictions from DFT but in accordance with experiment. For all compounds, in the most critical case of the band-inversion region around the $\Gamma$ point, we show that the $GW$ effective masses are significantly different from DFT ones.

Funding was provided by the Alexander von Humboldt Foundation.

TT 33.7 Wed 10:45 H16

**Controllable magnetic doping of the surface state of a topological insulator** — •A. Eich[1], T. Schlenk[1], M. Bianchi[2], M. Koleini[3], O. Pietzsch[1], T.O. Wehling[3], T. Frauenheim[3], A. Balatsky[4], J.-L. Mi[5], B. B. Iversen[5], J. Wiebe[1], A.A. Khajetoorians[1], Ph. Hofmann[2], and R. Wiesendanger[1] — [1]Institute for Applied Physics, Universität Hamburg, Germany — [2]iNano, Aarhus University, Denmark — [3]Bremen Center for Computational Materials Science, Universitiy of Bremen, Germany — [4]NORDITA, Stockholm, Sweden — [5]Center for Materials Crystallog-

raphy, iNano, Aarhus University, Denmark

A combined experimental and theoretical study of doping individual Fe atoms into $Bi_2Se_3$ is presented. It is shown through a scanning tunneling microscopy study that single Fe atoms initially located at hollow sites on top of the surface (adatoms) can be incorporated into subsurface layers by thermally-activated diffusion. Angle-resolved photoemission spectroscopy in combination with ab-initio calculations within density functional theory suggest that the doping behavior changes from electron donation for the Fe adatom to neutral or electron acceptance for Fe incorporated into substitutional Bi sites. According to the calculations, these Fe substitutional impurities retain a large magnetic moment thus presenting an alternative scheme for magnetically doping the topological surface state. For both types of Fe doping, we see no indication of a gap at the Dirac point.

T. Schlenk et al., arXiv: 1211.2142v1 (2012) [cond-mat.mtrl-sci]
J. Honolka et al., PRL **108**, 256811 (2012)

**Coffee break**

TT 33.8 Wed 11:15 H16

**Induced superconductivity in the topological surface state of mercury telluride (HgTe)** — •Luis Maier, Manuel Grimm, Peter Schüffelgen, Daniel Knott, Christopher Ames, Christoph Brüne, Philipp Leubner, Jeroen Oostinga, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, 97074 Würzburg

It has been recently demonstrated, that a strained grown layer of of HgTe is a 3D topological insulator (TI) exhibiting a single family of Dirac cone states at its surface. Since the bulk has nearly no carriers left, the transport through these structures is strongly dominated by the surface states [1].

Because of the prediction of creation of Majorana bound states [2] we are looking at a superconductor-TI interface. This talk presents our results on highly transparent S-TI-S junctions where we observe unusual behaviour in the Josephson current.

Preliminary results of this project are published in [3].

[1] C. Brüne et al., Phys. Rev. Lett. 106, 126803 (2011)
[2] L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008)
[3] L. Maier et al., Phys. Rev. Lett. 109, 186806 (2012)

TT 33.9 Wed 11:30 H16

**Strained bulk HgTe as a 3D topological insulator** — •Cornelius Thienel, Christopher Ames, Philipp Leubner, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Universität Würzburg, Lehrstuhl für experimentelle Physik III

HgTe is a semimetal that has an inverted band structure. We show that strained on CdTe the HgTe opens a bandgap and becomes a 3D topological insulator (TI). By magnetotransport measurements we confirm the existence of a 2D topological state and observe QHE from the surface. An analysis of SdH oszillations allows us to distinguish between two TI surfaces perpendicular to the magnetic field that have different charge carrier densities due to different electrostatic environments. When structuring a top gate on the sample, we are able to match the carrier densities of the surface states and therefore see a sequence of odd integer Hall plateaus, as predicted by Dirac physics.

TT 33.10 Wed 11:45 H16

**Comparing scattering processes in topological insulators and giant Rashba semiconductors** — •Peter Lemmens[1], Vladimir Gnezdilov[2], Dirk Wulferding[1], Patrik Recher[3], Helmuth Berger[4], Yoichi Ando[5], Angela Möller[6], R. Sankar[7], and Fang-Cheng Chou[7] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE, Kharkov, Ukraine — [3]IMAPH, TU-BS, Braunschweig — [4]EPFL, Lausanne, Switzerland — [5]ISIR, Osaka, Japan — [6]Dept. of Chemistry, Univ. Houston, USA — [7]CCMS, National Taiwan Univ., Taipei, Taiwan

Using Raman scattering experiments we probe scattering processes in BiTeI and topological insulators. In the former systems the surface termination, either by Iodine - Bi or Tellur - Bi determines the low energy scattering properties. A comparison of these surface induced signals with effects seen in topological insulators leads to a considerable gain of understanding of scattering mechanisms and the respective role of symmetry. Work supported by DFG, B-IGSM and NTH School for Contacts in Nanosystems.

TT 33.11 Wed 12:00 H16

**Local photocurrent generation in thin films of the topological insulator $Bi_2Se_3$** — •Christoph Kastl[1], Tong Guan[2], Xiaoyue He[2], Kehui Wu[2], Yongqing Li[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching, Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

We report on the optoelectronic properties of thin films of the three-dimensional topological insulator $Bi_2Se_3$ grown by molecular beam epitaxy. In spatially resolved scanning photocurrent experiments, we observe submicron photocurrent patterns with positive and negative amplitude [1]. The patterns are independent of the applied bias voltage, but they depend on the width of the circuits. We interpret the patterns to originate from a local photocurrent generation [2] due to potential fluctuations [3]. Furthermore, we verify and discuss the impact of the circular photogalvanic effect in optoelectronic $Bi_2Se_3$-based circuits [4].

[1] C. Kastl et al., arxiv: 1210.4743 (2012).
[2] J. C. W. Song and L. S. Levitov, arxiv:1112.5654 (2011).
[3] H. Beidenkopf et al., Nat. Phys. 7, 939 (2011).
[4] C. Kastl et al. (2013).

TT 33.12 Wed 12:15 H16

**$Bi_{1-x}Sb_x$(110): A non-closed packed surface of a topological insulator** — Lucas Barreto, Wendell Simoes da Silva, Malthe Stensgaard, Søren Ulstrup, Marco Bianchi, •Xie-Gang Zhu, Matteo Michiardi, Maciej Dendzik, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center Århus University, 8000 Århus C, Denmark

Topological insulators are characterised by an insulating bulk band structure, but topological considerations require their surfaces to support gap-less, metallic states. Meanwhile, many examples of such materials have been predicted and found experimentally, but work has concentrated on the closed-packed (111) surface of the topological insulators. Thus, the theoretical picture of an insulating bulk embedded in a metallic surface from all sides of a crystal still needs to be confirmed. Here we present angle-resolved photoemission spectroscopy results from the (110) surface of the topological insulator $Bi_{1-x}Sb_x$ ($x \approx 0.15$). The observed band structure and Fermi contour is in excellent agreement with theoretical predictions and slightly different from the electronic structure of the parent surface Bi(110), in particular around the $X_1$ time-reversal invariant momentum. We argue that the preparation of surfaces different from (111) opens the possibility to tailor the detailed electronic structure and properties of the topological surface states.

TT 33.13 Wed 12:30 H16

**Charge screening at the surface of a topological insulator: Rb on $Bi_2Se_3$** — •Peter Löptien, Lihui Zhou, Jens Wiebe, Alexander A. Khajetoorians, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Germany

Adsorption of Rb atoms on $Bi_2Se_3$ leads to the formation of a two-dimensional electron gas (2DEG) in the conduction band at the surface of the topological insulator [1]. We investigated the coverage dependent distribution of the singly charged Rb atoms by low temperature STM. By a statistical analysis of the interatomic distances between the adatoms we quantitatively derived the pair interaction [2], which fits a screened Coulomb potential. Interestingly, screening length and dielectric constant turn out to be rather small, due to the contribution of the 2DEG and topological surface state.

[1] M. Bianchi, R. C. Hatch, Z. Li, P. Hofmann, F. Song, J. Mi, B. B. Iversen, Z. M. Abd El-Fattah, P. Löptien, L. Zhou, A. A. Khajetoorians, J. Wiebe, R. Wiesendanger, and J. W. Wells, ACS Nano 6, 7009 (2012)
[2] J. Trost, T. Zambelli, J. Wintterlin, and G. Ertl, Phys. Rev. B 54, 17 850 (1996)

TT 33.14 Wed 12:45 H16

**Fabrication and characterization of thin $Bi_2Se_3$ topological insulators** — •Srujana Dusari[1], Philipp Meixner[1], Anna Mogilatenko[2], Saskia F. Fischer[1], Jaime Sanchez-Barriga[3], Lada V. Yashina[4], Florian Kronast[3], Sergio Valencia[3], Akin Ünal[3], and Oliver Rader[3] — [1]Novel Materials, Humboldt Universität zu Berlin, D-12489 Berlin — [2]Ferdinand Braun Institut, D-12489 Berlin — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, D-

12489 Berlin — [4]Dep. Chemistry, Moscow State University, Russia

Topological insulators (TIs) have electrically insulating states in the bulk and robust conducting states along the edges [1, 2]. The real-life TI samples available today contain residual bulk charge carriers that hinder exploiting their surface properties in device form. The aim of our work is to investigate the controlled combination of dimensionality and designed impurity and metallic defect structures on the quantum transport properties of well known $Bi_2Se_3$ TIs, in particular with respect to the implications for devices. Here we report preparation and characterization of exfoliated $Bi_2Se_3$ flakes. The samples are characterized using atomic force microscopy, transmission electron microscopy, and energy-dispersive X-ray spectroscopy. Surface stability and composition are determined using photoemission electron microscopy. Low temperature transport measurements are presented.

[1] C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).
[2] M. Z. Hasan and J. E. Moore, Annu. Rev. Condens. Matter. Phys. 2: 55-78 (2011).

## TT 34: Transport: Molecular Electronics (jointly with CPP, HL, MA)

Time: Wednesday 9:30–12:45 Location: H2

TT 34.1 Wed 9:30 H2

**Inelastic scattering effects and electronic shot noise** — •Amin Karimi, Markus Herz, and Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

The study of shot noise for junctions formed by single molecules offers interesting new information that cannot be easily obtained by other means. At low bias it allows determining the transmission probability and the number of current carrying conductance channels [1]. We investigate the effects of phonon scattering on the electronic current noise through nano junctions with mechanically controllable break junction (MCBJ). Equivalent measurements have recently been reported to be able to reveal inelastic transport contributions to the current through gold atomic contacts [2]. We developed a new and versatile measurement system enabling measurements of the noise in a rather broad range of conductance values from 0.01 $G_0$ to 1 $G_0$ without the necessity of double wiring. First results on gold atomic contacts and benzendithiol will be presented.

[1] D. Djukic and J. M. van Ruitenbeek, Nano Lett. 6, 789-793 (2006)
[2] M. Kumar, R. Avriller and J. M. van Ruitenbeek, Phys. Rev. Lett. 108, 146602 (2012)

TT 34.2 Wed 9:45 H2

**Electrical Characterization of Single Molecules via MCBJ** — •Matthias Wieser[1], Torsten Sendler[1], Shou-Peng Liu[2], Samuel Weisbrod[2], Zhuo Tang[2], Andreas Marx[2], Jannic Wolf[2], Elke Scheer[2], Francesca Moresco[3], Grebing Jochen[1], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., D-01328 Dresden — [2]Universität Konstanz, D-78457 Konstanz — [3]Max Bergmann Center of Biomaterials, D-01069 Dresden

For future molecular electronics applications the detailed knowledge about the electrical transport properties of single molecules is very important. To achieve this goal we are using the mechanical controllable break junction technique in liquid environments in combination with insulating substrates. We characterize the electrical conductance and I-V characteristics of single molecules which consist of three phenyl rings connected by triple carbon bonds with two oxygen sidegroups binding to the central ring. The I-V characteristics are further investigated by creating 2D histograms for hundreds of I-V curves and by fitting a single level model which provides us the metal-molecule junction coupling constants and the molecular energy level.

TT 34.3 Wed 10:00 H2

**Charge transmission through a molecular junction driven by a time–dependent voltage** — •Yaroslav Zelinskyy[1,2], Yoram Selzer[3], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]Bogolubov Institute for Theoretical Physics, National Academy of Science of Ukraine, 14-b Metrologichna str., UA-03683, Kiev, Ukraine — [3]School of Chemistry, Tel Aviv University, Ramat Aviv, 69978 Tel Aviv, Israel

Time-dependent electron transport through a molecular junction driven by voltage pulses with a duration even in the sub-ps region is investigated theoretically. The transient behavior of the current is analyzed in focusing on the sequential transport regime and in utilizing a density matrix approach. As a quantity detectable in the experiment the averaged dc-current resulting from a sequence of voltage pulses is also calculated. The obtained data are analyzed with respect to their dependence on the voltage pulse shape, the magnitude and asymmetry of the lead-molecule coupling, and the mechanism and strength of intramolecular relaxation. All the findings are confronted with recent computations on transient currents due to optical excitation of the junction [1,2].

[1] L. Wang and V. May, Phys.Chem.Chem.Phys. 13, 8755 (2011)
[2] Y. Zelinskyy and V. May, Nano Lett. 12, 446 (2012)).

TT 34.4 Wed 10:15 H2

**Surface Plasmon Enhanced Electroluminescence of a Molecular Junction** — •Yuan Zhang[1,2], Yaroslav Zhelinskyy[1], and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany — [2]University of Science and Technology Beijing, XueYuan Road 30, 100083 Beijing, P. R. China

There are some first experiments indicating surface plasmon enhanced emission of a molecular junction. We present a coherent theory for this phenomenon, which is based on our previous work on molecule metal nanoparticle complexes [1,2,3,4]. Ultilizing a density matrix description our theory accounts for electron transfer in junction, photon emission and energy exchange coupling between the molecule and spherical leads. As a central result, we report on a three order of magnitude enhanced molecular photon emission, which dependence on molecular and junction parameters are also discussed.

[1] Y. Zelinskyi, Y. Zhang, and V. May, J. Phys. Chem. A, DOI: 10.1021/jp305505c
[2] Y. Zhang, Y. Zelinskyy, and V. May, J. Phys. Chem. C, accepted
[3] Y. Zhang, Y. Zelinskyy, and V. May, J. Nanophot., in press
[4] Y. Zelinskyy and V. May, Nano Lett. **12**, 446 (2012)

TT 34.5 Wed 10:30 H2

**Dynamics of a nano-scale rotor driven by single-electron tunneling** — Alexander Croy[2] and •Alexander Eisfeld[1] — [1]MPIPKS Dresden — [2]Chalmers University of Technology S-412 96 Göteborg, Sweden

We investigate theoretically the dynamics and the charge transport properties of a rod-shaped nano-scale rotor, which is driven by a similar mechanism as the *nanomechanical single-electron transistor (NEMSET)*. We show that a static electric potential gradient can lead to self-excitation of oscillatory or continuous rotational motion. We identify the relevant parameters of the device and study the dependence of the dynamics on these parameters. We discuss how the dynamics are related to the measured current through the device. Notably, in the oscillatory regime we find a negative differential conductance. The current-voltage characteristics can be used to infer details of the surrounding environment which is responsible for damping.

[1] A. Croy and A. Eisfeld, *EPL (Europhys Lett)* **98**, 68004

TT 34.6 Wed 10:45 H2

**First-principles investigation of electron transport through molecular junctions in an STM configuration** — •Shigeru Tsukamoto, Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

Molecular electronics is exciting by the perspective that various types of functionalities are potentially realized only by single molecules with unique electronic structures. A number of interesting experiments on the transport properties have been performed in an STM configuration, in which a probing tip approaches a molecule on a metal surface.

By means of first-principles methods, we report about a systematic series of calculations on electron transport through molecules in the STM configuration. The molecules to be investigated are a Terephthalic acid molecule and its derivatives, which chemisorb on Cu(110)

surfaces.

Electron transmissions are investigated by varying the tip–molecule distance in an STM configuration, as well as by tuning molecular electronic structures. As approaching the tip toward the molecule, some of the transmission peaks originating from unoccupied states move to lower energy due to the hybridization of tip and molecular states. This peak-shift contributes to increasing the electron transmission around the Fermi energy, which is an essential property in molecular devices. This exhibits that in molecular electronics, not only the molecule itself but also the geometrical configuration between a molecule and the electrodes is an important parameter to determine the functionality.

**15 min. break**

TT 34.7 Wed 11:15 H2

**STM theory for $\pi$-conjugated molecules on thin insulating films** — •Benjamin Siegert, Andrea Donarini, Sandra Sobczyk, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg

We present a microscopic STM theory, based on the reduced density matrix formalism, which is able to describe transport and topographical properties of interacting $\pi$-conjugated molecules on thin insulating films. Simulated current-voltage characteristics and constant height and constant current STM images for a Cu-Phthalocyanine (CuPc) molecule are presented as experimentally relevant examples. We predict negative differential conductance resulting from interference between degenerate many-body states of CuPc [1]. Criteria are given to find and identify the interference blocking scenario in experimental measurements.

[1] A. Donarini, B. Siegert, S. Sobczyk, and M. Grifoni, PRB **86**, 155451 (2012).

TT 34.8 Wed 11:30 H2

**Influence of Electronic Properties of Graphene on Current-Voltage Characteristics of Molecule-Graphene Nanojunctions** — •Ivan A. Pshenichnyuk, Pedro B. Coto, André Erpenbeck, and Michael Thoss — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

Graphene, thanks to its peculiar mechanical and electronic properties, is today considered as a perspective material in future electronics. Its well-known band structure with "zero band-gap" as well as the existence of so-called edge states leads to a non-trivial density of states distribution in graphene-based devices. This causes, in particular, distinctive current-voltage characteristics of molecule-graphene nanojunctions, where a single molecule is connected to two graphene nanosized contacts. We study the transport characteristics of graphene-based nanojunctions using tight-binding models and first-principles DFT calculations combined with the Landauer transport formalism.

TT 34.9 Wed 11:45 H2

**Electron Transport properties of metallic carbon nanotubes with metal contacts** — •Andreas Zienert[1], Jörg Schuster[2], and Thomas Gessner[1,2] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Metallic carbon nanotubes (CNTs) are quasi ballistic one-dimensional conductors capable to carry large current densities. This makes them ideal candidates for applications in future microelectronic devices, partially replacing state-of-the-art copper interconnect lines. The performance of such a system not only depends on intrinsic properties of the CNTs but is also strongly affected by its size and the contact.

We investigate the transport properties of metal–CNT–metal devices theoretically, applying semiempirical (extended Hückel theory) and ab initio (density functional theory) electronic structure methods, combined with a Green's function formalism for ballistic transport at low bias. The study focuses on $(6, 0)$ CNTs of different length comparing the metal contacts Al, Cu, Pd, Pt, Ag, Au in a highly symmetric end-to-end configuration.

It turns out that Al forms the most transparent contacts, followed by Pd, Pt and Cu. The noble metals Au and Ag perform worse. Results are visualized and discussed in terms of the local density of states of the combined metal–nanotube systems and its isolated parts, as well as their contact distances, binding energies, and work functions.

TT 34.10 Wed 12:00 H2

**First principles study of charge and heat transport through $\pi$-stacked molecules** — •Thomas Hellmuth[1], Marius Bürkle[2], Fabian Pauly[3], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Nanosystem Research Istitute, National Institute of Advanced Industrial Science and Technology, Japan — [3]Theorie der Nanostrukturen, Universität Konstanz, 78457 Konstanz, Germany

We analyze charge and heat transport properties of $\pi$-stacked, multilayered paracyclophane molecules using density functional theory combined with non-equilibrium Green's function techniques. The conductance of that class of molecules was measured in Ref. 1. Beside the elastic conductance we investigate the not yet measured thermopower and inelastic electron tunneling spectra (IETS). The transmission eigenchannels show that the current is mainly carried by the $\pi$ system of the paracyclophane molecules and by taking into account different contact geometries, we find that this is independent of the binding motif. While the conductance decays exponentially with increasing molecular length, the thermopower increases linearly and may change its sign. Similarly, we analyze how the IETS and the heat transport depend on the molecular length and vibrational modes in the specific junction geometries.

[1] S. T. Schneebeli *et al.* J. Am. Chem. Soc. **133**, 2136 (2011)

TT 34.11 Wed 12:15 H2

**Spin selective transport in chiral systems** — •Rafael Gutierrez, Thomas Brumme, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

Recent experiments have demonstrated that the transmission of electrons through layers of chiral molecules can be strongly spin-dependent [1,2]. Here, we extend a previous model [3] to discuss the interrelation between the observed effect and the presence of a spin-orbit coupling interaction induced by helical electrostatic fields. Hereby, we present a minimal model Hamiltonian based on a representation of the Schroedinger equation on a helical pathway and discuss the influence of several parameters on the spin polarization. Complementary to it, full 3D wave packet propagation is discussed in the presence of spin-orbit coupling. Our results suggest that a spin polarization can be induced as a result of the symmetry of the system. However, it appears that a full 3D description of the problem may be necessary.

[1] B. Goehler, V. Hamelbeck, T. Z. Markus, M. Kettner, G. F. Hanne, Z. Vager, R. Naaman, H. Zacharias, Science **331**, 894 (2011)
[2] Z. Xie, T. Z. Markus, S. R. Cohen, Z. Vager, R. Gutierrez, R. Naaman, Nano Letters **11**, 4652 (2011)
[3] R. Gutierrez, E. Diaz, R. Naaman, G. Cuniberti, Phys. Rev. B **85**, 081404(R) (2012)

TT 34.12 Wed 12:30 H2

**Full ab initio description of strong electronic correlations in molecular devices** — •David Jacob — Max-Planck-Institut für Mikrostrukturphysik, Halle

In order to obtain a *full* first-principles description of the correlated electronic structure and transport properties of nanoscopic devices we combine the so-called Coulomb-Hole-Screened-Exchange (COHSEX) approximation with more sophisticated many-body techniques such as the Dynamical Mean-Field Theory (DMFT). While the former yields an effective mean-field description of the weakly correlated conduction electrons, the latter describes the dynamic correlations of the strongly interacting electrons in the $3d$- or $4f$-shells of transition metal atoms. The combination of DMFT with COHSEX instead of Density Functional Theory (DFT) improves upon our recently developed "Molecular DMFT" approach [1,2] in two important aspects: First, the COHSEX yields the effective Coulomb interaction U for the strongly interacting electrons. Second, unlike in DFT+DMFT calculations the double-counting correction for COHSEX+DMFT is exactly known and straight-forward to calculate. With this approach it is now possible to actually predict e.g. the occurance of the Kondo effect in magnetic atoms and molecules on metal surfaces and attached to metallic leads, and to investigate the complex nature of the Kondo effect in these sytems.

[1] D. Jacob *et al.*, PRL **103**, 016803 (2009); PRB **82**, 195115 (2010)
[2] M. Karolak *et al.*, PRL **107**, 146604 (2011)

# TT 35: Graphene - Characterization and Devices (jointly with DS, HL, MA, and O)

Time: Wednesday 9:30–13:00 Location: H17

TT 35.1 Wed 9:30 H17

**Polarization dependence of phonon modes in graphene nanoribbons** — •Felix Kampmann[1], Nils Scheuschner[1], Bernat Terrés[2,3], Christoph Stampfer[2,3], and Janina Maultzsch[1] — [1]Institut für Festkörperphysik, TU Berlin, Hardenbergstraße 36, 10623 Berlin, Germany, EU — [2]JARA-FIT and II. Institute of Physics B, RWTH Aachen University, Aachen, Germany, EU — [3]Peter Grünberg Institute (PGI-6/8/9), Forschungszentrum Jülich, Jülich, Germany, EU

Polarization dependent Raman spectroscopy has lately been used to investigate the edge states of few layer graphene revealing insight into the selection rules of their Raman modes.

Here we report polarization dependent Raman measurements on single-layer graphene nanoribbons with varying width down to 30 nm.

We show that the $\cos^2(\theta)$ behavior of the intensity ratio I(D)/I(G) can be reproduced as it has already been known for the graphene edge states. Furthermore we found a similar behavior for I(D′)/I(G) and discuss the dependence on the nanoribbon width.

TT 35.2 Wed 9:45 H17

**Manifestation of charged and strained graphene layers in the Raman response of graphite intercalation compounds** — Julio Chacon-Torres[1], •Ludger Wirtz[2], and Thomas Pichler[1] — [1]Faculty of Physics, University of Vienna, Austria — [2]Physics and Material Sciences Unit, University of Luxembourg, Luxembourg

We present recent Raman measurements together with a detailed analysis of potassium graphite intercalation compounds (GICs): stage II to stage VI (where stage n means one intercalant layer after every nth graphene layer). By ab-initio calculations of the charge densities and the electronic band dispersions, we demonstrate that most (but not all) of the charge donated by the K atoms remains on the outer graphene layers, i.e., the once adjacent to the intercalant layer. This leads to an electronic decoupling of the inner (uncharged) from the outer (charged) layers and consequently also to a decoupling of the corresponding Raman spectra: The G-line splits into two peaks and the 2D line is entirely due to the uncharged inner layers while the 2D line of the outer layers is suppressed due to the strong charging. The quantitative interpretation of the peak positions requires that the internal strain of the graphene layers is taken into account. This allows to unambiguously identify the Raman response of strained charged and uncharged graphene layers and to correlate it to the in-plane lattice constant. Raman spectroscopy is thus a very powerful tool to identify internal strain in single and few-layer graphene as well as to to identify the strain in nanoelectronic and optoelectronic devices or the local interfacial strain in other graphene composites.

TT 35.3 Wed 10:00 H17

**C–axis transport in graphite and few–layered–graphene** — •Ole Pfoch, Yuri Koval, Michael Enzelberger, and Paul Müller — Department of Physics and Interdisciplinary Center for Molecular Materials, Universität Erlangen

Electrical transport in single or few layered graphene was intensively investigated during the last decade. However, most experiments were performed with electronic transport in the plane. Measurements in perpendicular direction are rare and the results are rather sensitive to materials properties. For instance, the literature data for the anisotropy of the electrical conductivity in plane and along the c–axis varies between 100 and 10 000. One of the reasons for the wide spread of anisotropy data might be a significant influence of structural defects. We reduce the influence of these defects by decreasing the cross section of the measured structures down to $2 \times 2\,\mu\mathrm{m}^2$. Mesa type structures were prepared by e–beam lithography and $O_2$–plasma etching. The influence of the mesa size on the c–axis conductivity and its temperature dependence were investigated. We have found that the c–axis conductivity is rather sensitive to the prehistory of the sample and to the origin of the graphite material. We present our recent results and discuss the mechanism of c–axis electrical transport.

TT 35.4 Wed 10:15 H17

**Electronic transport of metallic thin films and islands on graphene with scanning tunneling spectroscopy** — •Anne Holtsch, Hussein Shanak, Haibin Gao, and Uwe Hartmann — Institute for Experimental Physics, Saarland University, P.O. Box 151150, 66041 Saarbrücken

Electronic properties of graphene without and with metallic thin films and islands on top are investigated. The graphene layers are epitaxially grown on rhodium using a chemical vapor deposition (CVD) method. In a second step, metallic thin films and islands (Au) are deposited onto the surface of the graphene layer. Investigations are performed by using scanning tunneling spectroscopy (STS). An introduction to a method for an automated comparison and characterization of different spectroscopic curves is the focus of this presentation. This method will be used to clarify which impact the metallic thin films and islands have on the electronic properties of graphene. Therefore a comparison between the results obtained from graphene samples without and with metalic thin films and islands is presented.

TT 35.5 Wed 10:30 H17

**Fano-Profiles in HOPG and graphene flakes.** — •Matthias Städter, Matthias Richter, and Dieter Schmeisser — Brandenburg University of Technology, Cottbus, Germany

We investigated the electronic structure of the valence and conduction band of HOPG by 2D resonant photoemission spectroscopy. Our aim is to understand the electronic structure of defects and inhomogeneities in graphene and related materials in more detail. From our measurements we find that the transition from the $\sigma$-band to the $\pi^*$-band at the M-point shows a characteristic Fano-Profile. A Fano-Profile occurs as the result of the interference of the band to band transition and a parallel transition to a discrete energy level within the band gap.The theory of Fano enables us to determine the energetic location of these discrete level. It is found to be several meV above the Fermi-Energy. Additional measurements on graphene flakes lead to similar results for the $\sigma$- to $\pi^*$-band transition and the location of the discrete energy state. With this we not only can determine the energetic states of defects but also get a better understanding of the origin of the Fano profile which is a particular detail of the resonant absorption process.

TT 35.6 Wed 10:45 H17

**Multiple Auger Decay at resonant photo-excitation In carbon thin films** — •Matthias Richter, Matthias Städter, Ioanna Paloumpa, and Dieter Schmeisser — Brandenburg University of Technology Cottbus, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

We use resonant photoemission at the C1s edge to study the electronic structure of HOPG, graphene flakes and monolayer graphene. We find remarkable differences in the profile of the Auger decay channels, which we attribute to an additional multiple-Auger with a three-hole final state. A prerequisite for the appearance of this decay mechanism is the existence of localized excitonic states, which cause the appearance of the multiple Auger decay. Defects (pits, holes, steps and kinks) can act as localized excitonic states. We use those effects to identify the existence and the quantity of such defect states within the $\pi^*$-band regime in carbon thin films, because the intensity of the three-hole Auger decay is varying with the defect density of the carbon films. The defect-excitonic states can be either localized in the band-gap at the M-point or in case of surface defects like steps, kinks or pits even at the K-point by losing the pure $sp^2$ character of the films. We find that the appearance of the multiple Auger decay is different for multilayer and monolayer graphene. In particular the interaction of impurities leads to broadening of the C1s core levels. The three-hole Auger decay spectroscopy is a new method to detect such contaminations with a high sensitivity.

TT 35.7 Wed 11:00 H17

**Characterization of large-scale graphene CVD with far-infrared radiation** — •Christian Cervetti[1], Boris Gorshunov[1,4,5], Elena Zhukova[1,4,5], Martin Dressel[1], Klaus Kern[2,3], Marko Burghard[2], and Lapo Bogani[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Max Planck Institut für Festkörperforschung — [3]Institute de Physique de la Matière Condensée, Ecole Polytechnique de Lausanne, Switzerland — [4]A.M.Prokhorov General Physics Institute, Russian Academy of Sciences, Russia — [5]Moscow Institute of Physics and Technology (State University), Russia

We use monochromatic terahertz (THz) spectrometer and standard Fourier-transform spectrometer to measure the conductance of large scale single layer graphene obtained by chemical vapor deposition. We demonstrate the extreme sensitivity of the THz conductance to copper particles produced on graphene during the transfer process, making THz spectroscopy a powerful tool for monitoring the removal of unwanted leftovers during the production of large scale graphene samples.

**Coffee break**

TT 35.8 Wed 11:30 H17

**Terahertz generation in freely suspended graphene** — •Andreas Brenneis[1], Leonhard Prechtel[1], Helmut Karl[2], Dieter Schuh[3], Werner Wegscheider[4], Li Song[5], Pulickel Ajayan[6], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, TU München, Germany — [2]Institute of Physics, University of Augsburg, Germany — [3]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [4]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland — [5]University of Science and Technology of China — [6]Rice University, Houston, Texas, USA

We report on THz generation and picosecond photocurrents in freely suspended bilayers of graphene [1]. The graphene layers are connected to coplanar strip lines which serve as source and drain contacts. A pump laser pulse excites charge carrier in the graphene. The resulting charge carrier dynamics couple to the strip line circuit and propagate along the strip line. With a probe laser pulse focused onto an on-chip photo switch, the propagating signal is read out via a third contact with a picosecond time resolution. By varying the delay of the probe pulse relative to the pump pulse, the optoelectronic signal can be measured time-resolved. We discuss the generation of THz radiation, ultrafast displacement currents, and thermoelectric currents within the optically excited graphene. Financial support by the ERC-grant NanoREAL is acknowledged.

References: [1] L. Prechtel, L. Song, D. Schuh, P. Ajayan, W. Wegscheider, A.W. Holleitner, Nature Comm. 3, 646 (2012).

TT 35.9 Wed 11:45 H17

**Broadband THz detection with graphene flakes** — •Martin Mittendorff[1,2], Stephan Winnerl[1], Josef Kamann[3], Jonathan Eroms[3], Harald Schneider[1], and Manfred Helm[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Universität Dresden, Germany — [3]Universität Regensburg, Germany

We demonstrate a broadband THz detector based on graphene flakes, which are produced by scotch-tape method on $SiO_2/Si$, combined with a logarithmic periodic antenna. The antenna is coupled to the graphene flake with an interdigitated comb-like structure in the center. The detectors were characterized at roomtemperature using the free-electron laser FELBE at the Helmholtz-Zentrum Dresden-Rossendorf. The responsivity is above 1 nA/W for wavelengths from $30\mu m$ to $220\mu m$. The rise time of the measured signals is below 100 ps and their length is in the range of 200 ps, while the pulse duration of the FEL pulses is around 20ps. The effect of the antenna coupling could be confirmed via polarization dependent measurements. Due to the spectral bandwidth combined with high temporal resolution and simple handling these detectors can be very useful for timing purposes of short laser pulses.

TT 35.10 Wed 12:00 H17

**Electrostatic force and Raman spectroscopy measurements on graphene replicating water layers on mica** — •Vitalij Scenev, Philipp Lange, Nikolai Severin, and Jürgen P. Rabe — Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Deutschland

Recently it has been argued that graphenes exfoliated onto mica become hole-doped by the substrate and that the doping level can be blocked by molecular water interlayers confined during sample preparation [1]. We use Scanning Probe Microscopy (SPM), Electrostatic Force Microscopy (EFM) and Raman Spectroscopy to investigate both the structure and the electronic properties of graphene conforming to molecular water layers on the mica surface. The layers are fluid, since variation of ambient humidity allows to control in-situ the layer thicknesses in the range of a monolayer [2]. Our data imply that graphene is hole-doped by the water layers with the doping level increasing with the water layer thickness.

1. Shim, J., et al., Water-Gated Charge Doping of Graphene Induced by Mica Substrates. Nano letters, 2012. 12(2): p. 648-654.

2. Severin, N., et al., Reversible dewetting of a molecularly thin fluid water film in a soft graphene-mica slit pore. Nano letters, 2012. 12(2): p. 774-779.

TT 35.11 Wed 12:15 H17

**Tailoring the graphene/silicon carbide interface for monolithic wafer-scale electronics** — •Stefan Hertel[1], Daniel Waldmann[1], Johannes Jobst[1], Andreas Albert[1], Matthäus Albrecht[1], Sergey Reshanov[2], Adolf Schöner[2], Michael Krieger[1], and Heiko B. Weber[1] — [1]Chair for Applied Physics, Erlangen, Germany — [2]ACREO AB, Kista, Sweden

The vision of graphene as future material for electronic devices is derived from impressive material parameters. However, it is evident that graphene will not readily take over the role of a semiconductor. In particular, an efficient switch is lacking due to graphene's missing bandgap.

By focusing not only on the graphene layer, but considering the silicon carbide (SiC) substrate as an essential part of the system, we developed an easy scheme to fabricate transistors with high ON/OFF ratio - suited for logic - by tailoring the interface between SiC and the graphene layer [1]. Therefore we currently work with two graphene materials on SiC: as grown monolayer graphene (MLG) and hydrogen intercalated quasi-freestanding bilayer graphene (QFBLG). We proved the high-quality ohmic contact of MLG to n-type SiC and also characterized the Schottky-like behavior of QFBLG.

Using these components we are currently able to demonstrate transistors with ON/OFF ratios exceeding 104 at room temperature in normally-on and normally-off operation mode. We present a concept for inverters using a resistor-transistor logic scheme.

[1] S. Hertel *et al.*, Nature Communications **3**, 957 (2012)

TT 35.12 Wed 12:30 H17

**Electrical interfacing of cells with graphene field effect transistors** — •Felix Rolf, Lucas H. Hess, Tobias Schneider, Benno Blaschke, Moritz Hauf, and Jose A. Garrido — Walter Schottky Institut, TU München

The next generation of neuroprosthetic devices will need novel solid-state sensors with improved performance. Increased signal detection capability, better mechanical and physiological compatibility with living tissue, and in general a higher stability in biological environments are among the main requirements. Due to its electronic and electrochemical characteristics, as well as its physico-chemical properties, graphene is one of the most suitable candidates to meet these demanding requirements.

In this talk, we will report on arrays of graphene solution-gated field effect transistors (G-SGFETs) which are able to detect the electrical activity of electrogenic cells. It will be discussed how the combination of high carrier mobilities in graphene and the large interfacial capacitance at the graphene/electrolyte interface results in such high signal sensitivities. Thereby it is possible for instance, to show the generation and propagation of action potentials in cardiomyocyte-like HL-1 cell cultures. Another application is the single cell-transistor coupling using Human Embryonic Kidney (HEK293) cells. In the latter case the response of the G-SGFETs to electrical activity as well as the cell chemical activity will be discussed. Our results confirm that G-SGFETs are able to outperform state-of-the-art devices, suggesting that G-SGFETs can play an important role in future bioelectronic systems.

TT 35.13 Wed 12:45 H17

**Exploring the electronic performance of graphene FETs for bio-sensing** — •Lucas Hess, Benno Blaschke, Max Seifert, and Jose Garrido — Walter Schottky Institut, TU München

For medical applications such as neuroprostheses and for fundamental research on neuronal communication, it is of utmost importance to develop a new generation of electronic devices which can effectively detect the electrical activity of nerve cells. The outstanding electronic and electrochemical performance of graphene hold great promise for bioelectronic applications. For instance, we have reported on arrays of CVD-grown graphene solution-gated FETs (SGFETs) for cell interfacing, demonstrating their ability to transduce with high resolution the electrical activity of individual electrogenic cells.

In this contribution, we will present a detailed discussion on the suitability of CVD-grown graphene SGFETs for in-electrolyte operation, together with a study of the effect of electrolyte composition on the device performance. The sensitivity of SGFETs is dominated by two characteristic parameters: transconductance and electronic noise,

which will be analyzed in this talk by in-electrolyte Hall-effect experiments and low-frequency noise characterization. Finally, we will briefly report on the pH and ion sensitivity of graphene devices, highlighting the influence of the chosen substrate for the device fabrication, as well as the effect of surface contamination from the fabrication technology.

This work demonstrates the potential of graphene to outperform state-of-the-art Si-based devices for biosensor and bioelectronic applications.

## TT 36: Superconductivity: Fe-based Superconductors - Fe(Se,Te), LiFeAs, and other Materials

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

TT 36.1 Wed 9:30 H18

**Interplay between lattice and spin degrees of freedom in FeSe superconductors** — Vladimir Gnezdilov[1], •Peter Lemmens[2], Yurii Pashkevich[3], Tatiana Shevtsova[3], Alexander Gusev[3], Dirk Wulferding[2], Dmitriy Chareev[4], and Alexander Vasiliev[5] — [1]ILTPE, Kharkov, Ukraine — [2]IPKM, TU-BS, Braunschweig — [3]DonFTI, Donetsk, Ukraine — [4]IEM, RAS, Moscow, Russia — [5]Moscow State Univ., Moscow, Russia

Recently grown high quality FeSe single crystals show pronounced anomalies in the temperature dependent Raman spectra. An anomalous hardening of one phonon mode upon decreasing temperature is related to local fluctuations of the Fe orbital occupation, described by the Fe spin state. The enhancement of the low-frequency spectral weight above the structural phase transition temperature $T_S$ and its change below $T_S$ is discussed in connection with the opening of a spin state gap which results in the absence of magnetic order in FeSe. Work supported by DFG, B-IGSM and NTH School for Contacts in Nanosystems.

TT 36.2 Wed 9:45 H18

**Phonon driven phase transition in FeSe** — •Michael Fechner and Nicola Spaldin — ETH Zurich, Department for Material Theory,CH-8093 Zurich, Switzerland

One of the chemically simplest, but physically complex, iron based superconductors is FeSe. Here we present results from first-principle calculations of its competing magnetic phases. In particular we compare calculated electronic properties of coherent FeSe films under different tensile strains, corresponding to $SrTiO_3$ and MgO substrates, and electron/hole doping with experimental findings. The main result is that for moderate applied strain the spin density wave (SDW) in FeSe is suppressed, whereas there is a sudden strong enhancement for larger strain. Given that superconductivity disappears in highly strained FeSe on MgO, our results thus give an interesting insight in which energy ranges the SDW still compete with superconductivity. The results are finally discussed with respect to the possibility of phonon driven superconductivity in FeSe.

TT 36.3 Wed 10:00 H18

**Preparation and characterization of thin films of the superconductor FeSe** — Eike Venzmer[1], •Alexander Kronenberg[1], Sebastian ten Haaf[1], Janek Maletz[2], and Martin Jourdan[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55128 Mainz, Germany — [2]IFW-Dresden, Institute for Solid State Research, PO Box 270116, D-01171 Dresden, Germany

The recently discovered class of iron pnictide compounds features a presumably unconventional mechanism of superconductivity. We investigate the iron chalcogenide FeSe, which is the structurally simplest representative of this class of materials. Epitaxial thin films are prepared by rf-sputtering from a stoichiometric FeSe target and alternatively by co-sputtering from separate Fe and Se targets. Both methods yield superconducting epitaxial thin films on MgO(100) as well as on $YAlO_3$(010) substrates. The influence of deposition rates and substrate temperature on phase formation, sample homogeneity, morphology and electronic transport properties are discussed. A comparison with the properties of previously prepared by MBE [1] will be presented. The main advantage of the sputter deposited samples is an improved morphology which is promising for the future integration in planar tunneling junctions for spectroscopic investigations.

[1] M. Jourdan, S. ten Haaf, J. Appl. Phys. 108, 023913 (2010)

TT 36.4 Wed 10:15 H18

**Terahertz spectroscopy on $Rb_{1-x}Fe_{2-y}Se_2$** — •Zhe Wang, Jonas Fisher, Michael Schmidt, Vladimir Tsurkan, Alois Loidl, and Joachim Deisenhofer — Experimentalphysics V, EKM, Institute of Physics, University of Augsburg, Germany

Single crystals of superconducting and non-superconducting $Rb_{1-x}Fe_{2-y}Se_2$ [1] have been investigated by terahertz time-domain transmission spectroscopy as a function of temperature. In the superconducting samples, we observe the signatures of the superconducting transition [2] and an isosbestic point in the temperature dependence of optical conductivity in the vicinity of 100 K, which could be related to the reported phase separation in these compounds. In the non-superconducting samples, the optical conductivity exhibits features which can be interpreted in terms of spin wave excitations in agreement with neutron experiments [3].

[1] V. Tsurkan et al. Phys. Rev. B 84, 144520 (2011)
[2] A. Charnukha et al. Phys. Rev. B 85, 100504 (2012)
[3] M. Wang et al. Nature Communications 2, 580 (2011)

TT 36.5 Wed 10:30 H18

**Terahertz spectroscopy of superconducting Fe(Se,Te)** — •G. Chanda[1], A. V. Pronin[1], J. Wosnitza[1], S. Molatta[2], R. Hühne[2], B. Holzapfel[2], and K. Iida[2] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]IFW Dresden, Institute of Metallic Materials , 01171 Dresden, Germany

Among the iron-based superconductors, Fe(Se,Te) has received special attention due to its simple crystal structure, which is formed by Fe(Se,Te) layers only. Studies of the optical conductivity at terahertz and far-infrared frequencies may bring information about the superconducting energy gap size and symmetry. Here, we present a terahertz investigation of superconducting Fe(Se,Te) thin films at temperatures from 2 to 300 K. The measurements have been performed with a backward-wave-oscillator spectrometer, which allows phase-sensitive measurements of transmission at terahertz frequencies. Thus, both components of the complex dynamical conductivity can be directly obtained from these measurements. In this talk, we will discuss the frequency and temperature dependence of complex conductivity in Fe(Se,Te).

TT 36.6 Wed 10:45 H18

**Incommensurate magnetism and structural phase transition in $Fe_{1+y}Te$** — •Oliver Stockert[1], Sahana Rössler[1], Enrico Faulhaber[2], Astrid Schneidewind[2], Cevriye Koz[1], Dona Cherian[3], Suja Elizabeth[3], Ulrich Schwarz[1], and Steffen Wirth[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany — [2]Gemeinsame Forschergruppe, Helmholtz-Zentrum Berlin - TU Dresden, Lichtenbergstraße 1, 85474 Garching — [3]Department of Physics, Indian Institute of Science, Bangalore 560012, India

The superconductivity with transiton temperature $T_c = 8$ K found in $Fe_{1.01}Se$ ignited interest due to its simple crystal structure. The bulk $Fe_{1+y}Te$ is non-superconducting, but exhibits an antiferromagnetic order that is not driven by the Fermi suface nesting and relatively large ordered moment on the Fe-sublattices. $Fe_{1+y}Te$ also undergoes a structural distortion at low temperatures, and both magnetic and structral transitions can be strongly influenced by tunig parameters such as excess Fe ($y$) or external pressure [1, 2]. The themodynamic measurements revealed a single first-order transition for $Fe_{1.11}Te$, whereas two distinct phase transitions have been found for $Fe_{1.13}Te$. Here we present the results of neutron diffraction experiments on single crystalline $Fe_{1.11}Te$ and $Fe_{1.13}Te$ samples and show that $Fe_{1+y}Te$ display unique interplay of incommensurate magnetism and structural phase transition in comparison to the other parent Fe-superconductors.

[1] S. Rößler et al., Phys. Rev. B 84, 174506 (2011)
[2] C. Koz et al., Phys. Rev. B 86, 094505 (2012)

**15 min. break**

TT 36.7 Wed 11:15 H18

**Structural phase transitions in the vicinity of putative tricritical point in $Fe_{1+y}Te$** — Cevriye Koz, •Sahana Rössler, Alexander A. Tsirlin, Steffen Wirth, and Ulrich Schwarz — Max Planck Institute for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany

$Fe_{1+y}Te$, the parent compound to the chalcogenide superconductors displays a complex phase diagram with several structural and magnetic phase transitions within the homogeneity range $0.06 \leq y \leq 0.15$. The control parameters such as external pressure and excess Fe content ($y$) have similar influence on the phase transitions [1, 2]. Upon increasing $y$, the first-order transition temperature systematically decreases from 70 K to 58 K. For y $\geq$ 0.12, two transitions occur: first a continuous magnetic transition followed by a first-order structural transition at a lower temperature. This behavior suggests the presence of a tricritical point close to this composition. We present low-temperature synchrotron powder x-ray diffraction studies on $Fe_{1+y}Te$ in the vicinity of this putative tricritical point. From a careful analysis of the powder diffraction patterns and the temperature dependence of the peak-width, we conclude that for y $\geq$ 0.12 the phase transitions are sluggish due to a strong competition between different phases. We present a revised temperature-composition phase diagram for $Fe_{1+y}Te$ based on the temperature dependence of the crystal structure, specific heat, and magnetization measurements.

[1] Rößler *et al*. Phys. Rev. B, 84, 174506 (2011)
[2] Koz *et al*. Phys. Rev. B, 86, 094505 (2012)

TT 36.8 Wed 11:30 H18

**Mössbauer and muon spin rotation investigations of magnetic and structural phase transitions in $Fe_{1+y}Te$** — •Philipp Materne[1], Til Goltz[1], Sirko Bubel[1], Rajib Sarkar[1], Mathias Doerr[1], Cevriye Koz[2], Sahana Rössler[2], Steffen Wirth[2], Ulrich Schwarz[2], Ulrich K. Rössler[3], Hubertus Luetkens[4], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, TU Dresden, 01062 Dresden, Germany — [2]MPI for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany — [3]IFW Dresden, 01171 Dresden, Germany — [4]PSI, 5232 Villigen, Switzerland

$Fe_{1+y}Te$, the antiferromagnetic parent compound of the Fe-chalcogenide superconductors displays separated magnetic ($T_N$) and structural ($T_s$) transitions with $T_N > T_s$ for $y > 0.12$ [1]. Such behavior is uncommon for the parent systems of pnictide superconductors. We performed Mössbauer spectroscopy and muon-spin relaxation experiments on two representative levels of iron excess: i) $Fe_{1.06}Te$ with $T_N = T_s = 69$ K and ii) $Fe_{1.13}Te$ with well separated transitions at $T_N = 57$ K followed by $T_s = 46$ K. Both Mössbauer and muon-spin relaxation results clearly display a precursor magnetic state which is only present in $Fe_{1.13}Te$. Further, in $Fe_{1.13}Te$ a complex magnetic phase has been observed in the temperature range 40 K $\lesssim T \lesssim$ 75 K. We discuss our experimental results in the context of recently published thermodynamic and neutron scattering data on $Fe_{1+y}Te$[1], [2].

[1] S. Rößler et al., Phys. Rev. B **84** (2011) 174506
[2] E. E. Rodriguez et al., Phys. Rev. B. **84** (2011) 064403

TT 36.9 Wed 11:45 H18

**Iron Chalcogenides: Correlated Materials far from Mott** — •Markus Aichhorn[1], Gianluca Giovannetti[2], Massimo Capone[2], and Christoph Heil[1] — [1]Institut für theoretische Physik - Computational Physics, TU Graz, Austria — [2]SISSA, Trieste, Italy

Combining density-functional theory and dynamical mean-field theory we investigate the ground-state of iron-chalcogenide materials, focusing on the materials $KFe_2Se_2$ and $K_2Fe_4Se_5$. We show that, although having large substantial mass enhancements and scattering rates, these materials are not close to a Mott Metal-To-Insulator transition. However, increasing interaction parameters in a physically reasonable range does lead to enhanced orbital differentiation. From RPA susceptibility calculations we get further evidence that also superconducting pairing is mediated by local spin-fluctuations, and not by Fermi-nesting mechanisms.

TT 36.10 Wed 12:00 H18

**Resolving the quasiparticle scattering paradox in superconducting LiFeAs** — •Christian Hess[1], Steffen Sykora[1], Torben Hänke[1], Ronny Schlegel[1], Danny Baumann[1], Volodymyr Zabolotnyy[1], Luminita Harnagea[1], Sabine Wurmehl[1], Jeroen van den Brink[1,2], and Bernd Büchner[1,2] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]Department of Physics, TU Dresden, D-01069 Dresden, Germany

Several angle resolved photoemission spectroscopy (ARPES) studies reveal a poorly nested Fermi surface of LiFeAs, far away from a spin density wave instability, and clear-cut superconducting gap anisotropies. On the other hand a very different, more nested Fermi surface and dissimilar gap anisotropies have been obtained from quasiparticle interference (QPI) data, which were interpreted as arising from intraband scattering within hole-like bands. Here we show that this ARPES-QPI paradox is completely resolved by interband scattering between the hole-like bands. The resolution follows from an excellent agreement between experimental quasiparticle scattering data and $T$-matrix QPI calculations (based on experimental band structure data), which allows disentangling interband and intraband scattering processes.

TT 36.11 Wed 12:15 H18

**The electronic phase diagram for $Na_{1-\delta}FeAs$ with partial substitution of Co, Rh, Ni, Ru, Pd, Cr and Mn** — •Robert Beck[1], Maria Roslova[2], Igor Morozov[2], Saicharan Aswartham[1], Christian G. F. Blum[1], Mahmoud Abdel-Hafiez[1], Dirk Bombor[1], Frank Steckel[1], Jürgen Eckert[1], Anja U. B. Wolter-Giraud[1], Christian Hess[1], Sabine Wurmehl[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, D-01171 Dresden, Germany — [2]Moscow State University, Moscow, 119991 Russia

Single-crystals of $Na_{1-\delta}FeAs$ with partial substitution of Fe by Co, Rh, Ni, Ru, Pd, Cr and Mn were grown by a self-flux technique. A systematic investigation of the structure by powder X-ray diffraction, temperature dependence of magnetic susceptibility, electronic transport and specific heat were carried out. We map out the corresponding electronic phase diagram for the Co substituted $Na_{1-\delta}FeAs$, compared with Literature [1, 2] and map out the corresponding electronic phase diagram for the Rh substituted $Na_{1-\delta}FeAs$.

[1] Parker, D. R. et al., Chem. Commun. 16, 2189 (2009)
[2] Wang, A.F. et al., Phys. Rev. B 85, 224521 (2012)

TT 36.12 Wed 12:30 H18

**Superconducting thin films of As-free pnictide $LaPd_{1-x}Sb_2$ grown by reactive molecular beam epitaxy** — •Reiner Retzlaff, Alexander Buckow, Jose Kurian, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

We use reactive molecular beam epitaxy as synthesis technique for the search of arsenic free pnictide superconductors. Epitaxial thin films of $LaPd_{1-x}Sb_2$ were grown on (100) MgO substrates from elemental sources by simultaneous evaporation of high purity La, Pd and Sb metals by e-gun. $LaPd_{1-x}Sb_2$ belongs to a *novel class* of pnictide superconductors with a peculiar *pnictide square net layer* [1]. Previously, we have reported epitaxial growth of isostructural Bi based compounds [2]. The substitution of Bi by Sb leads to thin films with metallic behavior and room temperature resistivity of about 85 $\mu\Omega$cm. The highest observed transition temperature $T_c$ in$LaPd_{1-x}Sb_2$ is 3.1 K and does not depend on $x$. We discuss strategies to increase $T_c$ in this pnictide subfamily.

[1] H. Mizoguchi *et al.*, Phys. Rev. Lett. **106**, 057002 (2011)
[2] A. Buckow *et al.*, Appl. Phys. Lett. **101**, 162602 (2012).

TT 36.13 Wed 12:45 H18

**Local Mn character and P-derived ligand-hole states in LaMnPO** — •Nils Hollmann[1], Anna Efimenko[1], Zhiwei Hu[1], Maurits Haverkort[2], Jack Simonson[3], Hong-Ji Lin[4], Chien-Te Chen[4], Zhiping Yin[5], Meigan Aronson[3], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada — [3]Department of Physics and Astronomy, Stony Brook University, Stony Brook, USA — [4]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [5]Department of Physics and Astronomy, Rutgers, USA

We have investigated the electronic structure of LaMnPO by means of x-ray absorption and photoelectron spectroscopy, as well as LDA+U bandstructure calculations. From the spectroscopy, we found that the Mn ions have local moments and we also observed the strong presence of P-derived ligand hole states. Using LDA+U, we investigate how pressure can first make the system metallic while retaining local moments before entering a metallic state with weak delocalized moments. We also investigate theoretically how electron doping can quench the magnetism as to perhaps facilitate superconductivity like it is present in the Fe compounds.

# TT 37: Quantum Coherence, Quantum Information Systems 1

Time: Wednesday 9:30–13:15 Location: H19

TT 37.1 Wed 9:30 H19

**Emission spectrum of the driven nonlinear oscillator** — •Stephan Andre[1,2], Lingzhen Guo[1,3], Vittorio Peano[4], Michael Marthaler[1,2], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Department of Physics, Beijing Normal University, Beijing 100875, China — [4]Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA

Motivated by recent "circuit QED" experiments [1,2] we investigate the noise properties of coherently driven nonlinear resonators. By using Josephson junctions in superconducting circuits, strong nonlinearities can be engineered, which lead to the appearance of pronounced effects already for a low number of photons in the resonator.

Based on a master equation approach we determine the emission spectrum and observe for typical circuit QED parameters, in addition to the primary Raman-type peaks, second-order peaks [3]. These peaks describe higher harmonics in the slow noise-induced fluctuations of the oscillation amplitude of the resonator and provide a clear signature of the nonlinear nature of the system.

[1] I. Siddiqi *et al.*, Phys. Rev. B **73**, 054510 (2006)
[2] F.R. Ong *et al.*, Phys. Rev. Lett. **106**, 167002 (2011)
[3] S. André *et al.*, Phys. Rev. A **85**, 053825 (2012)

TT 37.2 Wed 9:45 H19

**Effective spinful Kitaev model and Majorana fermion mediated magnetoelectric phenomena** — •Panagiotis Kotetes[1], Alexander Shnirman[2], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe — [2]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Germany

Current trends in the field of quantum information relate to topological quantum computing based on Majorana fermions. In fact, recent experiments involving a Rashba spin-orbit coupled semiconducting wire in proximity to a conventional superconductor which is under the simultaneous influence of a Zeeman field, have provided striking results that could be associated with the presence of Majorana fermions. In the infinite magnetic field limit, the above system is equivalent to a spinless p-wave superconductor and can be effectively described by Kitaev's celebrated lattice model. This model owes the distinctive property of yielding Majorana fermions which are localized at the edges. So far, a vast number of previous studies were based on this mapping to Kitaev's model, neglecting in this manner the possibility of actively manipulating the spin degree of freedom. To remedy this problem, we construct an effective spinful Kitaev model that can be used for finite magnetic fields. This model opens new perspectives for spin-based quantum computing applications and provides a more general description of Majorana-fermion-mediated magnetoelectric Josephson effects, beyond 1D geometries [1].

[1] P. Kotetes, A. Shnirman and G. Schön, arXiv:1207.2691.

TT 37.3 Wed 10:00 H19

**Output photon statistics in driven dissipative arrays of transmission line resonators** — •Robert Jirschik and Michael Hartmann — TU Munich, Munich, Germany

Arrays of circuit cavities offer fascinating perspectives for exploring quantum many body systems in a driven dissipative regime where photon losses are continuously compensated by coherent laser drives. Here we specifically consider a scenario with input lasers of high intensity and thus high intra-resonator excitation numbers. Two different systems which depend on experimentally well controlable properties are considered:

One is a chain of nonlinear transmission line resonators driven by a single input laser, while the other one contains three transmission line resonator sites with a single non-linearity in the middle and lasers with an adjustable phase difference driving the two outer resonator sites. For both set-ups we provide results for the mean photon number and time-resolved second order correlation function of each individual site depending on their different experimental parameters.

TT 37.4 Wed 10:15 H19

**A Quantum Single Photon Transistor in Circuit Quantum Electrodynamics** — Lukas Neumeier, •Martin Leib, and Michael Hartmann — TU München, 85748 Garching, Germany

We propose a superconducting transmission line setup that acts as a single photon transistor for itinerant microwave signals. Photons are ideal carriers of quantum information as they rarely interact while traveling long distances which opens great possibilities for scaling up from one elementary two photon gate to many. However the advantage of great robustness with respect to environmental perturbations poses a great challenge to generate photon-photon interactions where they are needed. The enhanced light-matter interactions due to the quasi-onedimensional geometry of superconducting transmission lines and the macroscopic dipole moments of superconducting artificial atoms may provide a route out of this dilemma. In our setup a "control"-photon inverts a superconducting qubit which in turn shifts the energy of another superconducting qubit that is coupled to the transmission line of a "target"-photon. The "target"-photon is reflected if the energies of "target"-photon and superconducting qubit are degenerate and transmitted if they are sufficiently detuned. We show that this setup can be realized with flux qubits as well as with transmon qubits.

TT 37.5 Wed 10:30 H19

**Josephson Junction Intersected Transmission Line Resonators** — •Martin Leib and Michael J. Hartmann — TU München, 85748 Garching, Germany

Circuit quantum electrodynamics has gone a long way since the first successful demonstration of the strong coupling regime in 2004 by Andreas Wallraff and coworkers. Coherence times grew dramatically, single qubit gates are routine by now and entangling operations have been shown. The logical next step is to scale up the architectures from a few to many building blocks. The simulation of interacting many-body Hamiltonians is a promising direction of research to pursue with these setups. Every nonlinearity in classical field theory can be interpreted after quantizing the theory as an interaction between the elementary bosonic excitations of the systems which in the case of circuit QED are microwave photons. Therefore we propose as a basic building block for a interacting many body Hamiltonian simulator a transmission line resonator that is intersected by Josephson junctions. We calculate the eigenfrequencies of the transmission line resonator with a transfer matrix technique and quantize the classical theory.

TT 37.6 Wed 10:45 H19

**High-Fidelity Single-Qubit Gates for Two-Electron Spin Qubits** — •Pascal Cerfontaine, Fabian Brings, Tim Botzem, David DiVincenzo, and Hendrik Bluhm — 2nd Institute of Physics C, RWTH Aachen University, 52074 Aachen, Germany

Two-electron spin qubits in double quantum dots are promising candidates for quantum computation. Arbitrary single-qubit gates by electrical manipulation of the exchange interaction between two adjacent electrons while maintaining a magnetic field gradient have been demonstrated. However, simple gate constructions incur systematic gate errors in the presence of realistic experimental constraints.

We show the existence of a set of single-qubit gates obtained from simulations based on a model that reflects the experimentally important imperfections. Without decoherence, they exactly implement the desired gates.

Dephasing effects are minimized by avoiding operating points with large sensitivity to charge noise. Furthermore, we show that the gates can be fine-tuned on the experiment using an iterative optimization protocol based on the bootstrap method demonstrated in [1]. Our results should enable the complete elimination of systematic errors from an experimental realization of the gates.

[1] V. V. Dobrovitski *et al.*, Phys. Rev. Lett. **105**, 077601 (2010).

TT 37.7 Wed 11:00 H19

**Cooper-pair tunneling with a resonant environment** — Vera Gramich, •Björn Kubala, Selina Rohrer, Jürgen Stockburger, and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Cooper-pair tunneling through a Josephson junction can be drastically influenced by the electromagnetic environment. Recent experi-

ments [1,2] managed to combine dc-biased josephson junctions and an on-chip microwave cavity, to design an environment, where resonant coupling is achieved. In such setups, not only is the Josephson current strongly influenced by the environment, but, furthermore, the emission of energy to environmental modes can be directly monitored. The complicated cavity-junction coupling gives rise to complex physical behavior already in a classical regime, as well as in the quantum regime, which this talk will focus on.

[1] M. Hofheinz, F. Portier, Q. Baudouin, P. Joyez, D. Vion, P. Bertet, P. Roche, and D. Esteve, Phys. Rev. Lett. **106**, 217005 (2011)
[2] M. Blencowe, A. Armour, and A. Rimberg, arXiv:1106.5945.

**15 min. break**

TT 37.8 Wed 11:30 H19

**Dissipatively driven Entanglement of two Nuclear Spin Ensembles in a Double Quantum Dot** — •Martin J. A. Schuetz, Eric M. Kessler, Juan Ignacio Cirac, and Geza Giedke — Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany

Typically, quantum information schemes have been discussed in the context of isolated many-body systems subject to unitary dynamics. Here, dissipation has been identified as a mechanism that corrupts the useful quantum properties of the system under study. Recently, however, with the advent of novel ideas such as dissipative engineering, a paradigm shift could be observed in quantum physics. More and more approaches actively utilize dissipation as a driving force behind the emergence of coherent quantum phenomena. In this spirit, we propose a transport scheme for an electrically defined double quantum dot in which the two nuclear ensembles in the host environment are actively pumped into an entangled target state. Based on a self-consistent Holstein-Primakoff approximation, we derive an effective quantum master equation for the nuclear spins which features an unique entangled steady state; accordingly, long lasting entanglement is created deterministically. Prospects for the experimental realization of this proposal are briefly discussed.

TT 37.9 Wed 11:45 H19

**Decoherence of a central spin coupled to a fluctuating spin bath** — •Alexandre Faribault and Dirk Schuricht — Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA - Fundamentals of Future Information Technology, 52056 Aachen, Germany

When using the spin of a single electron trapped in a quantum dot as an implementation of a qubit, its hyperfine coupling to the environmental nuclear spins ultimately leads to the decoherence of any prepared state. Using the Algebraic Bethe Ansatz in conjunction with a Monte Carlo sampling procedure, we study how the electron's spin coherence factor evolves with time due to the presence of an unprepared randomly fluctuating nuclear spin bath.

TT 37.10 Wed 12:00 H19

**All optical control of the spin state in the $NV^-$-center in diamond** — •Florian Hilser — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We describe an all-optical scheme for spin manipulation in the ground-state triplet of the negatively charged nitrogen-vacancy (NV) center in diamond. Virtual optical excitation from the $^3A_2$ ground state into the $^3E$ excited state allows for spin rotations by virtue of the spin-spin interaction in the two-fold orbitally degenerate excited state. We derive an effective Hamiltonian for optically induced spin-flip transitions within the ground state spin triplet due to off-resonant optical pumping. Furthermore, we investigate the spin qubit formed by the Zeeman sub-levels with spin projection $m_S = 0$ and $m_S = -1$ along the NV axis around the ground state level anticrossing with regard to full optical control of the electron spin. Next we focus on cavity mediated coupling of different $NV$ centers by extending this scheme to derive an effective spin-spin-interaction between separate $NV$ center ground states due to exchange of a (virtual) cavity photon [1].

[1] Phys. Rev. B **86** 125204

TT 37.11 Wed 12:15 H19

**Nonequilibrium Landau-Zener-Stückelberg spectroscopy in a double quantum dot** — •Peter Nalbach[1], Johannes Knörzer[1], and Stefan Ludwig[2] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany — [2]Center for NanoScience and Fakultät für Physik, Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, D-80539 München, Germany

We study theoretically nonequilibrium Landau-Zener-Stückelberg (LZS) dynamics in a driven double quantum dot (DQD) including dephasing and, importantly, energy relaxation due to environmental fluctuations. We derive effective nonequilibrium Bloch equations. These allow us to identify clear signatures for LZS oscilations observed but not recognized as such in experiments [1] and to identify the full environmental fluctuation spectra acting on a DQD given experimental data as in [1]. Herein we find that super-Ohmic fluctuations, typically due to phonons, are the main relaxation channel for a detuned DQD whereas Ohmic fluctuations dominate at zero detuning.

[1] Petersson et al., Phys. Rev. Lett. 105, 246804 (2010)

TT 37.12 Wed 12:30 H19

**Dynamic Generation of Thermally Stable Surface Code** — •Daniel Becker[1], Tetsufumi Tanamoto[2], Adrian Hutter[1], Fabio Pedrocchi[1], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Corporate R & D center, Toshiba Corporation, Saiwai-ku, Kawasaki 212-8582, Japan

Quantum memories that are based on surface codes with local qubit interactions such as Kitaev's toric code are vulnerable to thermal fluctuations. By inducing strongly non-local interactions between the qubits via a coupling to, e.g, cavity modes [1] or the spins of a ferromagnet [2], the lifetime of encoded states in the presence of a thermal environment increases exponentially with the code's size. We propose a scheme to dynamically realize such a stable quantum memory based on the toric code for qubit systems with typical two-body interactions (Ising, $XY$, Heisenberg), using periodic, NMR-like pulse sequences. It allows both to prepare codewords without measurements and to protect them dynamically against the time evolution of the physical qubit system. Thermal stability is achieved by weakly coupling the qubits to an additional cavity mode. We investigate how the fidelity, with which the toric code is realized, depends on the period length $T$ of the pulse sequence and the magnitude of possible pulse errors. This allows to optimize tunable system parameters, such as $T$, in the presence of pulse errors and decoherence.

[1] F. Pedrocchi et al., Phys. Rev. B **83**, 115415 (2011)
[2] F. Pedrocchi et al., arXiv:1209.5289

TT 37.13 Wed 12:45 H19

**Measuring ultrasmall time delays of light by joint weak measurements** — •Grégory Strübi and Christoph Bruder — University of Basel, Basel, Switzerland

We propose to use weak measurements away from the weak-value amplification regime to carry out precision measurements of time delays of light. Our scheme is robust to several sources of noise that are shown to only limit the relative precision of the measurement, and not set a limit on the smallest measurable phase shift contrary to standard interferometry and weak-value based measurement techniques. Our idea is not restricted to phase-shift measurements and could be used to measure many small effects using a similar protocol.

TT 37.14 Wed 13:00 H19

**Singlet-triplet qubits embodied by multi-electron quantum dots** — •Sebastian Mehl[1,2] and David P. DiVincenzo[1,2] — [1]Peter Grünberg Institut (PGI 2), Forschungszentrum Jülich, D-52428 Jülich — [2]Institute for Quantum Information, RWTH Aachen, D-52056 Aachen

Singlet-triplet qubits (STQs) have attracted attention as one possible realization scheme of a logical qubit in a spin based quantum computer [1]. Commonly, the singlet and spinless triplet level of two single occupied quantum dots are defining the qubit states in these system. We describe an alternative approach to implement STQs using multi-electron quantum dots [2]. Instead of employing singly occupied quantum dots, we fill both quantum dots with three electrons. The qubit states have identical charge configurations for specific external parameters, which protects a STQ from dephasing phenomena affecting only the charge sector. Such qubits are perfectly immune gate voltages fluctuations produced by charge noise [3]. We specify the protection criteria and relate them to available materials and fabrication techniques. Furthermore, we describe full single qubit control of the three electron STQ, while pulsing via electric bias between two regimes immune to charge noise. We discuss limitations and experimental difficulties in realizing

our proposed manipulation scheme.

[1] J.R. Petta et al., Science 309, 2180 (2005), A.C. Johnson et al., Nature 435, 925 (2005)

[2] L.P. Kouwenhoven et al., Rep. Prog. Phys. 64, 701 (2001)
[3] X. Hu and S. Das Sarma, PRL 96, 100501 (2006)

# TT 38: Correlated Electrons: Metal-Insulator Transition 1

Time: Wednesday 9:30–13:15 Location: H20

TT 38.1 Wed 9:30 H20

**Verwey Transition in epitaxial $Fe_3O_4$ thin films studied by Raman spectroscopy** — •Mehrdad Baghaie Yazdi[1], Kwang-Yong Choi[2], Dirk Wulferding[3], Peter Lemmens[3], and Lambert Alff[1] — [1]TU Darmstadt, Materialwissenschaft — [2]Chung-Ang University, Department of Physics, Seoul, Korea — [3]TU Braunschweig, Institut für Festköperphysik

Magnetite has served as the model material for metal insulator transitions for more than seven decades. However, the origin and nature of the Verwey transition remains debated to this day. Recent disputes over the interpretation of measurement data [1,2] have reignited the question over the fundamental driving force behind the Verwey transition. Currently two major models try to explain the origin of this phenomenon, namely one that postulates that the transition is structurally driven [3] while the other sees the ordering of the $t_{2g}$ orbitals of the $Fe^{2+}$ ions at the octahedral sites as the main cause for both charge localization and structural transformation. Using epitaxial thin films of magnetite grown on $Al_2O_3$ and MgO which exhibit different Verwey transition temperatures, 128 K and 119 K respectively, we have investigated the evolution of ordering peaks in Raman spectroscopy. These peaks have been correlated to the global magnetic and electric properties of the films measured by SQUID and four-point electrical transport measurements.

[1] A. Tanaka *et al.*, Phys. Rev. Lett. **108**, 227203 (2012).
[2] S. B. Wilkins *et al.*, Phys. Rev. B **79**, 201102(R) (2009).
[3] G. Kh. Rozenberg *et al.*, Phys. Rev. Lett. **96** 045705 (2006).

TT 38.2 Wed 9:45 H20

**Strongly Correlated Material under Voltage: The Electrical Breakdown in $V_2O_3$ at the Insulator to Metal Transition** — •Stefan Guénon[1], Sebastian Scharinger[2], Siming Wang[1], Juan Gabriel Ramírez[1], Dieter Koelle[2], Reinhold Kleiner[2], and Ivan K. Schuller[1] — [1]Department of Physics and Center for Advanced Nanoscience, University of California San Diego — [2]Physikalisches Institut and Center for Collective Quantum Phenomena and their Applications in LISA+, Universität Tübingen

We have investigated the electrical properties of a $V_2O_3$ thin film micro bridge. Discontinuous jumps to lower voltages in the current voltage characteristic (IV) followed by an approximately constant voltage progression for high currents indicate an electrical breakdown of the device. In addition, the IV curves show hysteresis and a training effect, i.e. the subsequent IV loops are different from the first IV loop after thermal cycling. Low temperature scanning electron microscopy (LTSEM) reveals that the electrical breakdown over the whole device is caused by the formation of electro-thermal domains (ETDs), i.e. the current and temperature redistribution. On the contrary, at the nanoscale, the electrical breakdown causes the insulator to metal transition of individual domains. In a numerical model we considered these domains as a network of resistors and we were able to reproduce the electro-thermal breakdown as well as the hysteresis and the training effect in the IVs.

This work was supported by AFOSR grant number FA9550-12-1-0381.

TT 38.3 Wed 10:00 H20

**Nanodomain formation and electronic transport near the 1st-order Mott-Hubbard transition** — Qinyong Liu and •Johann Kroha — Physikalisches Institut, Universität Bonn

In the vicinity of the 1st-order metal-insulator transition (MIT) in Mott-Hubbard systems metallic and insulating phases coexist. Since the MIT occurs not only at temperature $T = 0$, but persists to finite $T$, in the coexistence region the thermodynamically stable state consists of thermal excitations of insulating nanodomains within the metal and vice versa. The existence of such nanodomains has been demonstrated experimentally in $VO_2$. We calculate the size distribution of nanodomains as a function of $T$ and Hubbard repulsion $U$. To that end, the electronic spectra and the free energy per site are determined in metallic and in insulating regions as well as across a metal-insulator domain wall, using the generalization of dynamical mean field theory (DMFT) for inhomogeneous systems, with the non-crossing approximation (NCA) as impurity solver. The domain-size distribution is then obtained from the resulting free energy difference, including volume and domain wall energies. It exhibits non-trivial, non-monotonic behavior. The 1st-order MIT of Mott-Hubbard systems may, hence, be viewed as a percolation problem with self-generated domain disorder. We calculate the electric resistivity $\rho(T)$ by mapping this problem of random nanodomains onto a random resistor network. Within the phase coexistence region, $\rho(T)$ exhibits anomalous linear $T$ depenence.

TT 38.4 Wed 10:15 H20

**Phase transitions induced by the cooperative Jahn-Teller effect: A multi-scale study of $KCuF_3$** — •Joaquin Miranda Mena[1], Erik Koch[1], and Eva Pavarini[2] — [1]German Research School for Simulation Sciences, Forschungszentrum Jülich and RWTH Aachen University — [2]Institute for Advanced Simulation and JARA, Forschungszentrum Jülich

We study the transition temperature for the structural and the orbital ordering in $KCuF_3$. We first obtain temperature dependent dynamical matrices (TDM) of the crystalline phase by computing the energy displacements of fluorines with density functional theory (DFT) within the LSDA+U framework. Because of the Coulomb interactions, the TDM tend to be quite long ranged. To minimize the required amount of DFT calculations, we subtract the long rang Coulomb (LRC) interaction to obtain short ranged TDM that can be transformed to the disorder systems. The transition temperature is found through Monte Carlo simulations. Here the fluorine positions are sampled using the short-ranged TDM adding back the LRC by an Ewald summation; as a result disorder states can be computed fast and efficiently regardless of the size of system.

TT 38.5 Wed 10:30 H20

**Electronic structure of $Nb_{0.75}O_{0.75}$** — •Anna Efimenko[1,2], Nils Hollmann[1], Katharina Höfer[1], Jonas Weinen[1], Alexander C. Komarek[1], Zhiwei Hu[1], A.Agung Nugroho[3], Hui-Huang Hsieh[4], Hong-Ji Lin[4], Chien-Te Chen[4], Aurora Diana Rata[1], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]II.Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Institut Teknologi Bandung, Jl. Ganesa 10 Bandung, 40132, Indonesia — [4]National Synchrotron Radiation Research Center (NSRRC), 101 Hsin-Ann Road, 30077 Hsinchu, Taiwan

We report on our angle-resolved photoemission (ARPES) study of $Nb_{0.75}O_{0.75}$ single crystals. NbO crystallizes in a rocksalt structure with 25% of ordered vacancies on both Nb - and O - sublattices. We compare our experimental data with the electronic structure calculated by density functional theory. Experimentally obtained bands are assigned to bulk and plausible surface electronic states. The effect of the so called "ordered vacancies" formation on the electronic structure in this compound is discussed. Our results demonstrate the shortcomings of the ionic model for $Nb_{0.75}O_{0.75}$ and the importance of metal-metal bonds for the structural stability. We provide insight into the bonding of Nb and O by constructing the topology of the orbitals from projected Wannier functions.

TT 38.6 Wed 10:45 H20

**Importance of exchange anisotropy and superexchange for the spin-state transitions in $RCoO_3$ (R = rare earth) cobaltates** — •Guoren Zhang[1], Evgeny Gorelov[1], Erik Koch[2,3], and Eva Pavarini[1,3] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]German Research School for Simulation Sciences, 52425 Jülich, Germany — [3]JARA High-Performance Computing

In this work [1], we identify all relevant parameters which shift the energy balance between spin states in rare-earth cobaltates, and determine their trends. We find that the $e_g$-$t_{2g}$ crystal-field splitting increases by $\sim 250$ meV when increasing pressure to 8 GPa, by about 150 meV when cooling from 1000 K to 5 K and by less than 100 meV when La is substituted with another rare earth. Hund's rule coupling is about the same in systems with very different spin-state transition temperature. In addition, the Coulomb-exchange anisotropy and the super-exchange energy-gain play a crucial role. In the $LnCoO_3$ series (Ln=Y or R), super-exchange progressively stabilizes a low-spin ground state as the $Ln^{3+}$ ionic radius decreases. We use a simple model to describe spin-state transitions and show that, at low temperature, the formation of isolated high-spin/low-spin pairs is favored, while in the high-temperature phase, the most likely homogeneous state is high-spin, rather than intermediate spin. An *orbital-selective* Mott state could be a fingerprint of such a state.

[1] G. Zhang, E. Gorelov, E. Koch and E. Pavarini, Phy. Rev. B **86** 184413 (2012)

TT 38.7 Wed 11:00 H20

**Dielectric breakdown of Mott insulators – doublon production and doublon heating** — •Martin Eckstein[1] and Philipp Werner[2] — [1]Max Planck Research Department for Structural Dynamics, University of Hamburg, CFEL — [2]University of Fribourg, Switzerland

Using nonequilibrium dynamical mean-field theory, we study the response of a Mott insulator to strong dc electric fields. Previously, the resulting dielectric breakdown of the insulating state has been studied for isolated bulk systems [1]. Remarkably, in this case a quasi-steady current is observed, although the energy of the system is constantly increasing. In this talk, we show that the current in this nonequilibrium quasi-steady state is related to a field-induced doublon-hole creation mechanism [2]. The induced carriers acquire an infinite-temperature distribution, and hence they do not contribute to the current after the initial pair-creation process. This observation allows to obtain a consistent understanding for the effects of high temperature and dissipation in those systems, which is essential for an understanding of bias-induced metal-insulator transitions in correlated systems.

[1] M. Eckstein, T. Oka, and Ph. Werner, Phys. Rev. Lett. 105, 146404 (2010)
[2] M. Eckstein, and Ph. Werner, arXiv:1211.2698.

**15 min. break**

TT 38.8 Wed 11:30 H20

**Dimensional-crossover-driven Mott transition in the frustrated Hubbard model** — •Marcin Raczkowski and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg

We study the Mott transition in a frustrated Hubbard model with next-nearest neighbor hopping at half-filling [1]. The interplay between interaction, dimensionality and geometric frustration closes the one-dimensional Mott gap and gives rise to a metallic phase with Fermi surface pockets. We argue that they emerge as a consequence of remnant one-dimensional Umklapp scattering at the momenta with vanishing interchain hopping matrix elements. Such a mechanism can also account for the pockets observed in the *spinless* model. In this pseudogap phase, enhanced $d$-wave pairing correlations are driven by antiferromagnetic fluctuations. Within the adopted cluster dynamical mean-field theory on the $8 \times 2$ cluster and down to our lowest temperatures the transition from one to two dimensions is continuous.

[1] M. Raczkowski and F. F. Assaad, Phys. Rev. Lett. **109**, 126404 (2012)

TT 38.9 Wed 11:45 H20

**Effective singlet dynamics in Mott phases of two-dimensional Hubbard models** — •Dominik Ixert and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, Germany

The Hubbard model is one of the paradigm models for the description of strongly correlated electron systems. In this work we focus on the intermediate-coupling regime inside the Mott insulating phase of single-band Hubbard models at zero temperature and at half filling. Recently, several works found indications for exotic spin-liquid phases close to the metal-insulator transition. While the situation on frustrated lattices like the triangular lattice concerning the existence of such interesting intermediate phases seems to be rather settled, the situation on unfrustrated lattices like the honeycomb lattice or the $\pi$-flux square lattice is currently under debate. In all these cases the Mott phase displays a long-ranged ordered antiferromagnet at strong couplings. Here our main focus is a class of two-dimensional systems for which the translational symmetry of the underlying square lattice is broken explicitly and the systems therefore realize a valence bond crystal at strong coupling. Consequently, one expects that the low-energy physics of the full Mott phase is contained in the singlet sector. For such systems we derive effective low-energy spin models using graph-based continuous unitary transformations (gCUTs). The effective spin models are then analyzed in the singlet sector by embedding the graphs within the dimer covering space on larger clusters to describe the singlet dynamics of the hubbard model.

TT 38.10 Wed 12:00 H20

**Dual Fermions + Disorder** — •Patrick Haase[1], Hanna Terletska[2], Shuxiang Yang[2], Thomas Pruschke[1], and Mark Jarrell[2] — [1]Georg-August Universität Göttingen — [2]Louisiana State University

We introduce an extension of the Dual Fermion formalism that allows to tread disordered interacting systems. To derive the formalism, the Replica trick is used. We will show data that compares the method to results obtained within the coherent potential approximation and the dynamical cluster approximation.

TT 38.11 Wed 12:15 H20

**Numerical solution of the t-J model with random coupling in infinite dimensions** — •Junya Otsuki[1,2] and Dieter Vollhardt[1] — [1]Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg — [2]Department of Physics, Tohoku University, Sendai, Japan

To explore the nature of the metallic state near the transition to a Mott insulator, we solve the $t$-$J$ model with random exchange interaction in $d = \infty$ dimensions. A numerically exact solution is obtained by an extension of the continuous-time quantum Monte Carlo (CT-QMC) method to a model with vector bosonic field coupled to the local spin. It is shown that the paramagnetic solution near the Mott insulator describes an incoherent metal with a residual moment, where the single-particle excitations leads to an additional band separated from the Mott-Hubbard band.

TT 38.12 Wed 12:30 H20

**Optical Investigations of the Metal-Insulator Transition in $\kappa$-(BEDT-TTF)$_2$Hg(SCN)$_2$Br** — •Tomislav Ivek[1,2], Rebecca Beyer[1], Rimma N. Lyubovskaya[3], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Institut za fiziku, Zagreb, Croatia — [3]Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Russian Federation

Due to its fundamental character as well as the promise of practical applications, multiferroicity is at the forefront of investigations in solid state physics. Out of many candidate materials there has been a recent increase of interest in the $\kappa$-(BEDT-TTF)$_2$Cu$X$ family of quasi-2D organic conductors due to the pronounced dielectric response found in the magnetically-ordered phase. Puzzlingly, in these compounds the infrared vibrational spectroscopy and NMR do not find the charge disproportionation which is a basic prerequisite for electric dipoles.

On the other hand, a related but still unexplored set of mercury-based materials, $\kappa$-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl,Br, shows evidence of charge disproportionation at low temperatures. We present a detailed investigation of the $\kappa$-(BEDT-TTF)$_2$Hg(SCN)$_2$Br using infrared spectroscopy and dc transport. Below the metal-insulator transition at 80 K a small transport gap of 20 meV is found within the conducting molecular planes. Far- and mid-infrared spectra are taken between 300 K and 8 K along the three crystallographic axes. We discuss the common optical features as well as more exotic ones compared to the Cu-based $\kappa$-materials, particularly temperature dependence of the charge-sensitive vibrational mode $\nu_{27}(B1u)$, in light of recent theoretical descriptions.

TT 38.13 Wed 12:45 H20

**Electric-Field Induced Insulator-Metal Transition in $\alpha$-(BEDT-TTF)$_2$I$_3$** — •Tobias Knoblauch[1], Tomislav Ivek[1,2], Dieter Schweitzer[1], and Martin Dressel[1] — [1]Physikalisches Institut, Universität Stuttgart, Germany — [2]Institut za fiziku, Zagreb, Croatia

Over many decades electric-field induced switching phenomena have been observed in different types of materials, for example, transition metal oxides, inorganic semiconductors as well as organic conductors. In the last mentioned material class, the 2D organic salt $\alpha$-(BEDT-TTF)$_2$I$_3$ is one of the model systems revealing a metal-insulator phase transition at 136 K in a charge-ordered state. We investigated the switching process in $\alpha$-(BEDT-TTF)$_2$I$_3$ from the low conducting (charge-ordered) into the high conducting state triggered by a pulsed electric field in a temperature range from 120 to 133 K. The observed nonlinear current-voltage characteristics show negative differential resistance depending on temperature and on the applied electric field. As the underlying physical mechanism is still under consideration, we have performed time-dependent FTIR measurements to track the switching. It gives us, in combination with the steady-state infrared experiments, the possibility to gain more information about the processes responsible for this effect. Here, we also present possible physical models to explain the observed behavior.

TT 38.14 Wed 13:00 H20

**Mott Metal-Insulator Transition on Compressible Lattices** — •Mario Zacharias[1], Markus Garst[1], and Lorenz Bartosch[2] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Institut für Theoretische Physik, Goethe-Universität, Frankfurt a. M.

In the presence of a coupling to the crystal lattice, the critical properties of the finite temperature Mott end point are drastically altered. While the incompressible Mott transition is analogous to the liquid-gas transition, the compressible Mott transition is a solid-solid transition. Similar as for critical ferroelectrics, the Ising criticality of the electronic system is preempted by an isostructural instability. Long-range shear forces suppress microscopic fluctuations and, thus, the end point is governed by Landau criticality. A hallmark of this effect is the breakdown of Hooke's law of elasticity, i.e. a non-linear strain-stress relation characterized by a mean-field exponent. For the Mott end point of $\kappa$-(BEDT-TTF)$_2$X, we predict critical elasticity to dominate in a temperature range $\Delta T^* \simeq 2.5$ K and over a pressure region of $\Delta p \simeq 50$ bar around the end point.

## TT 39: Focused Session: Frontiers of Electronic Structure Theory 4 (jointly with HL and O)

Time: Wednesday 10:30–13:30 Location: H36

**Topical Talk** TT 39.1 Wed 10:30 H36

**Challenges in data-intensive computational materials design: methodology and infrastructure.** — •Boris Kozinsky — Robert Bosch Research and Technology Center, Cambidge, MA, USA

First-principles high-throughput screening of novel materials requires simultaneously inexpensive and accurate predictive computations of key properties. The first and most difficult challenge is the selection of the appropriate descriptors that are relevant to the material performance, and formulating the computational strategy. We will present examples of the computational design process in the fields of materials screening in batteries, catalysis and ferroelectrics. In each case, the critical issue is the selection of practical methods and validation using available data and higher-level models.

The second challenge is the need to establish a materials* informatics infrastructure able to automatically prepare and execute calculations on large classes of materials, to monitor calculations, and to store, retrieve and analyze complex data. We accomplish this by integrating storage databases with grid-enabled computational workflow into a powerful flexible environment adaptable to diverse purposes. We will discuss the requirements and possible use cases of such infrastructure elements. Together with collaborators, we are developing and making available this open-source software platform named AIDA (*Automated Infrastructure and Database for Atomistic design*) to make computational design efforts faster, easier, and fully integrated with automatic data collection and community sharing.

TT 39.2 Wed 11:00 H36

**DFT+U($\omega$): A simplified approach for dynamical Hubbard corrections to DFT:** — •David D. O'Regan and Nicola Marzari — Theory and Simulation of Materials, EPFL, Switzerland.

Numerous successful techniques have been developed to date, such as DFT+U, in which the screened Coulomb interactions, underestimated by approximate density functionals, are described more accurately via a mapping onto the Hubbard Hamiltonian. Charge screening is a dynamical process, generally, and so to fully realise the capability of such methods for improving optical and quasiparticle spectra, the Hubbard U describing these interactions must gain a frequency dependence.

We introduce a simple and inexpensive approach, named DFT+U($\omega$), and readily implementable within an existing DFT+U or constrained-DFT code, in which the dynamical U tensor appropriate to the rotationally-invariant DFT+U functional is computed and used to correct DFT or static DFT+U spectra perturbatively. The rotationally-invariant DFT+U($\omega$) self-energy interpolates between static DFT+U and GW. We recast the density-functional linear-response approach for the static U, where it is defined as an energy curvature, within the language of many-body perturbation theory. Here, its dynamical generalisation, and its relationship to methods such as constrained RPA, becomes readily apparent. A plasmon-pole type model is used for the inverse dielectric function, whereby low-energy parameters are computed using the appropriately renormalised density-functional linear-response, and high-energy parameters are inexpensively approximated via independent-particle RPA or ALDA.

TT 39.3 Wed 11:15 H36

**Effective onsite interactions for materials with strong nonlocal Coulomb interactions** — •Malte Schüler[1], Alexander Lichtenstein[2], Mikhail I. Katsnelson[3], and Tim Wehling[1] — [1]Institut für Theoretische Physik, Universität Bremen, D-28359 Bremen, Germany — [2]1. Institut für Theoretische Physik I, Universität Hamburg, D-20355 Hamburg, Germany — [3]Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands

*sp*-Electron systems and low-dimensional materials often comprise strong local Coulomb interaction and non-local Coulomb interaction at the same time. Here we report on a method to map a generalized Hubbard model with non-local Coulomb interaction to an effective Hubbard model with strictly local Coulomb terms $U^*$. With the examples of graphene and silicene we show that the non-local Coulomb interaction can reduce the effective local interaction up to a factor of 2. The $U^*$ model is defined by a variational principle with respect to the free energy. In this framework, obtaining the effective interaction requires non-local charge correlation functions for various parameters of the effective Hubbard model, which are calculated by the determinant quantum Monte Carlo method. The temperature dependence of the effective interaction is discussed.

TT 39.4 Wed 11:30 H36

**First-principles calculation of Hubbard *U* parameters for half-metallic ferromagnets** — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Correlation effects play an important role in the electronic structure of half-metallic ferromagnets (HM-FMs). They give rise to non-quasiparticle states above (or below) the Fermi energy at high temperatures [1], which reduce the spin polarization and as a consequence the efficiency of the spintronics devices. Employing the constrained random-phase approximation (cRPA) [2] within the full-potential linearized augmented-plane-wave (FLAPW) method [3], we have calculated the strength of the effective Coulomb interaction (Hubbard $U$) between localized $3d$ electrons in a series of HM-FMs like zincblende MnAs, half- and full-Heusler alloys NiMnSb and Co$_2$MnSi, respectively. The obtained Hubbard $U$ parameters lie between 2.5 and 4.5 eV, being smallest for MnAs (Mn-$3d$) and largest for Co$_2$MnSi (Co-$3d$). The small value of $U$ in the former can be attributed to the efficient screening of the As $p$ electrons. For HM full-Heusler compounds the obtained $U$ values are comparable to the ones in elementary $3d$ transition metals, while for half-Heusler compounds the $U$ is a bit smaller.
[1] M. I. Katsnelson *et al.*, Rev. Mod. Phys. **80**, 315 (2008).
[2] E. Şaşıoğlu *et al.*, Phys. Rev. B **83**, 121101(R) (2011).
[3] http://www.flapw.de

TT 39.5 Wed 11:45 H36

**Magnetic Spectroscopies with DFT + Hubbard (U,V)** — •Emine Kucukbenli[1], Davide Ceresoli[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH) — [2]CNR-ISTM Institute of Molecular Science and Technology, Milan (IT)

Hubbard U corrections to exchange-correlation functionals, introduced to deal with correlated electrons, have been shown to greatly improve the accuracy of DFT calculations of transition-metals, thanks to their ability to restore piecewise linearity of energy as a function of occupations and thus correct self-interaction errors. In addition, U is not a fitting parameter but can be calculated ab initio, using linear-response (LR) formulations.

Nevertheless, transition-metal complexes that display both covalent and ionic character are poorly described by DFT+U. Recently, the addition of an intersite Hubbard V is suggested to restore the accuracy of DFT+U for these cases, while V can be obtained ab initio as well.

In this study we combine DFT+U+V with the gauge-invariant projector augmented wave (GIPAW) method, and calculate magnetic spectroscopic properties of systems with transition metals. We have been implementing this combination in Quantum ESPRESSO package, both for LR and the recently introduced converse approach, that uses a much simpler Berry-phase calculation of the orbital magnetization. We then examine the performance of U+V corrections in determining the structural properties and hyperfine interaction parameters of small transition-metal molecules and complex organometallic systems.

TT 39.6 Wed 12:00 H36

**The magnetization of periodic solids from time-dependent current-density-functional theory.** — •Arjan Berger[1,4], Nathaniel Raimbault[1,2], Paul de Boeij[3], and Pina Romaniello[2,4] — [1]Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier, IRSAMC, CNRS, Toulouse, France — [2]Laboratoire de Physique Théorique, CNRS, Université Paul Sabatier, IRSAMC, Toulouse, France — [3]Scientific Computing and Modeling, Amsterdam, The Netherlands — [4]European Theoretical Spectroscopy Facility

The evaluation of the macroscopic magnetization of solids is problematic when periodic boundary conditions are used because surface effects are artificially removed. This poses a problem unless surface effects can be reformulated in terms of bulk quantities. For example, in case of the macroscopic polarization one can express the contribution of the charge density accumulated at the surface in terms of the bulk current density through the continuity equation. Therefore one can work in the framework of time-dependent current-density functional theory to efficiently calculate the macroscopic polarization [1,2]. In this presentation we will study how also the magnetization can be described within this framework.

[1] F. Kootstra, P. L. de Boeij, and J. G. Snijders, J. Chem. Phys. 112, 6517 (2000).

[2] J. A. Berger, P. Romaniello, R. van Leeuwen, and P. L. de Boeij, Phys. Rev. B 74, 245117 (2006)

TT 39.7 Wed 12:15 H36

**Structure, charge order, phonons and IR spectra of magnetite** — •Charles Patterson — School of Physics, Trinity College Dublin, Dublin 2, Ireland.

The structure and charge order of magnetite ($Fe_3O_4$) below the Verwey transition have been contentious issues for over 70 years. An x-ray refinement for the full 112 atom, $Cc$ space group crystal structure of magnetite was reported only recently [1]. Previous refinements were hampered by multiple domain twinning in samples, whereas the recent study was performed on a micron-sized sample with two domains. Here we report hybrid density functional theory (DFT) calculations for the crystal structure, charge order, vibrations and IR spectra of magnetite in the $Cc$ (112 atom) and $P2/c$ (56 atom) unit cells. Charge order in the $Cc$ structure is found to consist of Fe trimerons, both in experiment [1] and calculations.

[1] M. S. Senn, J. P. Wright and J. P. Attfield, Nature 481, 173 (2012).

TT 39.8 Wed 12:30 H36

**Crystalline and Magnetic Anisotropy of the 3*d* Transistion-Metal Oxides** — •Andreas Schrön[1], Claudia Rödl[1,2], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau, France

The 3*d* transition-metal oxides (TMOs) are subject of debate since many decades due to their extraordinary properties, such as the formation of an antiferromagnetic ordering AFM2 below their Néel temperature. Many studies, both experimental and theoretical, focus only on MnO and NiO, where the crystalline anisotropy is solely driven by exchange striction along the unique symmetry axis in the [111] direction and where the magnetic anisotropy is explained in terms of magnetic dipole interactions. In the other TMOs, FeO and CoO, however, orbital magnetization and spin-orbit interaction play an additional, yet crucial role for both crystalline and magnetic anisotropy.

We present density-functional theory (DFT) studies including an on-site interaction $U$ of the crystalline and magnetic anisotropy of the electronic systems with non-collinear spins. The influence of the (semi-)local description of exchange and correlation (XC) by means of the local density approximation (LDA) and generalized gradient approximation (GGA) on the orbital moments in FeO and CoO and the implications on the aforementioned properties is investigated. We discuss the quenching of the orbital magnetization due to the gradient corrections.

TT 39.9 Wed 12:45 H36

**Electronic Structure and Magnetic interactions in 5*d* Ir oxide compounds** — •Vamshi Mohan Katukuri[1], Viktor Yushankhai[2], Radu Coldea[3], Liviu Hozoi[1], and Jeroen van den Brink[1] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr. 20 01069 Dresden, Germany — [2]Joint Institute for Nuclear Research, Joliot-Curie 6, 141980 Dubna, Russia — [3]Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom

We investigate the correlated *d*-level electronic structure and magnetic interactions of 5*d* Ir oxide compounds by fully *ab initio* quantum-chemical many-body calculations on finite embedded clusters. The wave-function quantum-chemical methods provide a promising alternative to density-functional-based approaches to the electronic structure of solids. The computed *d*-*d* excitations in square-lattice, honeycomb, pyrochlore, and chain-like iridates compare well with recent RIXS (resonant inelastic x-ray scattering) data. We also perform a detailed analysis of the relativistic spin-orbit wave functions and compute observables such as the $\langle \mathbf{L}\cdot\mathbf{S}\rangle$ ground-state expectation value of the spin-orbit operator. The latter is in principle accessible from x-ray absorption and provides information on the role of $t_{2g}$–$e_g$ couplings in the ground-state wave function and on the strength of non-cubic fields that lift the degeneracy of the $t_{2g}$ levels. As concerns to the magnetic structure, we find, in honeycomb lattice structures, $A_2IrO_3$, the magnetic interactions strongly deviate from the proposed Kitaev-Heisenberg model, due to low-symmetry crystal fields.

TT 39.10 Wed 13:00 H36

**Bulk electronic structure of the diluted magnetic semiconductor GaMnAs through hard x-ray angle resolved photoemission** — •Jan Minar[1], Igor diMarco[2], J. Braun[1], H. Ebert[1], A.X. Gray[3], and Ch. Fadley[3] — [1]University of Munich, Munich, Germany — [2]University of Upsalla, Upsalla, Sweden — [3]UC Davis, Davis, USA

A detailed understanding of the origin of the magnetism in diluted magnetic semiconductors is crucial to their development for applications. Using hard X-ray angle-resolved photoemission [1] at 3.2 keV, we investigate the bulk electronic structure of the prototypical diluted magnetic semiconductor GaMnAs, and the undoped reference system GaAs [2]. The fully self-consistent combination of LSDA and dynamical mean field theory (DMFT) [3,4] and its combination with the one-step model of photoemission has been used to explain the experimental findings. Distinct differences are found between angle-resolved, as well as angle-integrated, valence spectra of GaMnAs and GaAs, in good agreement with theory. In addition to the standard LSDA based calculations the LSDA+DMFT approach shows an important effect of electronic correlations on the states close to the Fermi level. The combination of LSDA+DMFT and corresponding the Monte-Carlo simulations indicates an origin of ferromagnetism in GaMnAs and provides us a rather unifying picture of this controversial material.

[1]A. Gray et al., J. Minar et al., Nat. mat. 10, 759 (2011) [2] A. Gray, J. Minar et al., Nat. mat. 11, 957 (2012) [3] J. Minar, J. Phys.: Cond. Mat. (Topical Review) 23, 253201 (2011)

TT 39.11 Wed 13:15 H36

**Magnetic state of pyrochlore $Cd_2Os_2O_7$ emerging from strong competition of ligand distortions and longer-range crystal**

**anisotropy** — •Nikolay Bogdanov[1], Remi Maurice[2], Ioannis Rousochatzakis[1], Jeroen van den Brink[1], and Liviu Hozoi[1] — [1]IFW Dresden, Germany — [2]Groningen University, The Netherlands

We investigate the correlated $d$-level electronic structure of $Cd_2Os_2O_7$, a spin $S=3/2$ pyrochlore, by fully *ab initio* quantum-chemical many-body calculations on finite embedded clusters. The wave-function quantum-chemical methods provide a promising alternative to density-functional-based approaches to the electronic structure of solids. We describe the local Os $d^3$ multiplet structure, the precise mechanism of second-order spin-orbit coupling and zero-field splitting (ZFS), and determine the parameters of the effective spin Hamiltonian, i.e., the single-ion anisotropy, nearest-neighbor Heisenberg exchange as well as the Dzyaloshinskii-Moriya interactions.

The results indicate that local ligand distortions and the anisotropic Cd-ion coordination strongly compete, rendering the magnetic interactions and ordering crucially depend on these geometrical features. Without trigonal distortions a large easy-plane magnetic anisotropy develops. Their presence, however, reverses the sign of the ZFS and causes a large easy-axis anisotropy ($D \simeq -6.8$ meV), which in conjunction with the antiferromagnetic exchange interaction ($J \simeq 6.4$ meV) stabilizes an all-in/all-out magnetic order. The competition uncovered here is a generic feature of 227 pyrochlore magnets and opens new perspectives on the basic magnetism in these materials.

## TT 40: Poster Session Correlated Electrons

Time: Wednesday 15:00–19:00 Location: Poster D

TT 40.1 Wed 15:00 Poster D

**NRG calculations for Kondo-type models as a way to characterize the magnetic properties of deposited molecules** — •Henning-Timm Langwald and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, Bielefeld, Deutschland

Magnetic molecules offer a variety of interesting properties which may be used for future technologies. For such applications a molecule might be deposited on a substrate with which it then interacts. Thus in general, when describing the magnetic properties of the deposited molecule, the interaction with the substrate has to be taken into account and needs to be modeled in a suitable way.

We use Numerical Renormalization Group (NRG) calculations for certain single-impurity Kondo models as a way to access the magnetic properties of such deposited molecules. By analyzing simple model systems such as a dimer (an impurity consisting of two spins) coupled to a single site of a substrate lattice we want to gain insight into the specific behavior of deposited molecules and the ways we can describe them. Our focus is on thermodynamic observables such as the magnetization and their dependence on temperature and magnetic field.

TT 40.2 Wed 15:00 Poster D

**Bosonic NRG using an Optimised Basis Set of Coherent States** — •Christian Kleine and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

The bosonic numerical renormalisation group (bNRG) has been developed to investigate the spin-boson model which exhibits a quantum phase transition between a localised and delocalised phase in the sub-ohmic regime.
Since the bNRG must always use a truncated bosonic basis set, we investigate the influence of the different choices of such finite sets onto the NRG level flow and the prediction of the critical exponents. We propose to use a coherent basis set close to the quantum phase transition to estimate the divergent displacements properly. We compare the predictions for the critical coupling $\alpha_c$ with respect to the different basis sets: (1) standard bNRG fock space occupation eigenbase, (2) displaced oscillator occupation eigenbase and (3) coherent base.

TT 40.3 Wed 15:00 Poster D

**Time Dynamics of the Two-Impurity Kondo Model** — •Benedikt Lechtenberg and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

The equilibrium properties of various two-impurity Kondo models (TIKM) have been investigated extensively in the literature. We study the non-equilibrium dynamics of the TIKM employing the time-dependent numerical renormalization-group (TD-NRG). The TD-NRG was developed to treat the real-time dynamics of quantum-impurity systems. We are interested in the real-time response of the the second spin $\vec{S}_2$ as a function of the initial condition of the first spin $\vec{S}_1$ and their distance $R$. We determine the relevant time scale and relaxation rates. The particle-hole symmetric model exhibits a quantum phase transition at a critical anti-ferromagnetic coupling. We investigate the change in the dynamics as function of the coupling constant close to QPT.

TT 40.4 Wed 15:00 Poster D

**Hybrid NRG-DMRG approach to real-time dynamics of quantum impurity systems** — •Fabian Güttge and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

We present a non-equilibrium hybrid method which uses the numerical renormalization group (NRG) to generate an effective low energy Hamiltonian. This Hamiltonian is then solved with the density-matrix renormalization group (DMRG). By considering systems with two Wilson chains patched together we reduce discretization errors. As the NRG reduces the effective bandwidth of the system the time scales accessible by the DMRG are exponentially increased. We employ the hybrid method to simulate the real-time dynamics of the interacting resonant level model (IRLM) after a sudden local quench. For $U = 0$ the method recovers the exact results. In the limit $U \to \infty$ we compare the hybrid method results to results obtained by a strong coupling treatment of the IRLM. We find an excellent agreement. Furthermore, the hybrid method is capable of treating the IRLM in the whole parameter regime.

TT 40.5 Wed 15:00 Poster D

**Real space Correlations of Impurities in a Dissipative Environment** — •Etienne Gärtner and Ralf Bulla — Institute for theoretical Physics, University of Cologne, Germany

We investigate a model in which two magnetic impurities couple to a one-dimensional lattice of bosons. Since the system is treated quantum-mechanically there can show up the phenomena of coherence between different states and that of entanglement between e.g. the impurities. It is investigated in which way the entanglement between the impurities varies as the distance between the impurities in real space is altered. The models under investigation cannot be solved analytically and are numerically very demanding. It is treated within the Numerical Renormalization Group (NRG) approach that is adapted to deal with multiple bosonic baths which show up in the transformations performed in the NRG.

TT 40.6 Wed 15:00 Poster D

**Towards a Numerical Renormalization Group description of the steady-state nonequilibrium single-impurity Anderson model using Lindblad driving** — •Frauke Schwarz[1], Ireneusz Weymann[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]Institute of Physics, Adam Mickiewicz University, Poznań

Wilson's Numerical Renormalization Group (NRG) allows to describe the single-impurity Anderson model (SIAM) in equilibrium in a non-perturbative way. However, treating situations of steady-state nonequilibrium, such as transport through a quantum dot at finite source-drain bias, remains a challenge for NRG. To model such situations, we consider two additional baths, which are coupled to the left and right leads, respectively. The effect of these baths on the leads can be described by using Lindblad operators [1] in the Liouville equation for the density matrix of the dot and the leads. The action of these operators can, in principle, be chosen such that the left and right leads are effectively held in separate thermal equilibrium at different chemical potentials or temperatures, despite the flow of current. An efficient way of solving this Liouville equation is to use the stochastic quantum trajectory method [1]. The intermediate time evolution needed to gen-

erate such trajectories can be done with time-dependent NRG (tNRG) based on complete basis sets. Here we present our preliminary results illustrating the above ideas.

[1] C.W. Gardiner, P. Zoller, Quantum Noise (Springer, Berlin, 2000)

TT 40.7 Wed 15:00 Poster D

**Conductance scaling in Kondo correlated quantum dots: role of level asymmetry** — •Lukas Merker[1], Theo Costi[1], Enrique Muñoz[2], and Stefan Kirchner[3] — [1]Forschungszentrum Jülich (PGI-2 / IAS-3), Jülich, Germany — [2]Pontificia Universidad Católica de Chile, Santiago, Chile — [3]MPI PKS & CPfS, Dresden, Germany

The low temperature electrical conductance through correlated quantum dots provides a sensitive probe of the physics (e.g., of Fermi-liquid vs non-Fermi-liquid behavior) of such systems. Here, we investigate the role of level asymmetry (gate voltage) and local Coulomb repulsion (charging energy) on the low temperature and low field scaling properties of the linear conductance of a quantum dot described by the single level Anderson impurity model. We use the numerical renormalization group [1] and renormalized superperturbation theory [2] to quantify the regime of gate voltages and charging energies where universal Kondo scaling may be observed and also quantify the deviations from this universal behavior with increasing gate voltage away from the Kondo regime and with decreasing charging energy. Our results could be a useful guide for detailed experiments on conductance scaling in semiconductor and molecular quantum dots exhibiting the Kondo effect [3,4].

[1] L. Merker, et al., preprint (2012)
[2] E. Muñoz, C. J. Bolech, S. Kirchner, Phys. Rev. Lett. (in press), arXiv:1111.4076
[3] A. V. Kretinin, et al., Phys. Rev. B**84**, 245316 (2012)
[4] G. D. Scott, et al., Phys. Rev. B**79**, 165413 (2009)

TT 40.8 Wed 15:00 Poster D

**Kondo regime of the non-equilibrium time evolution of an Anderson quantum dot** — •Sebastian Bock[1,2], Denes Sexty[1,2], and Thomas Gasenzer[1,2] — [1]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany — [2]ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany

We study the Kondo regime of the non-equilibrium time evolution of an Anderson quantum dot. The quantum dot is coupled between two leads forming a chemical-potential gradient and the tunneling to the leads is taken into account exactly. We apply the functional-integral approach based on the Schwinger-Keldysh closed time path integral to derive the Kadanoff-Baym dynamic equations from the two-particle irreducible (2PI) effective action. The dynamic equations are derived in non-perturbative approximation of the resummation of direct, particle-particle, and particle-hole channels. The effect of the resummation leads to the introduction of a frequency-dependent 4-point vertex. The method allows the determination of the transient as well as stationary transport through the quantum dot. We study, in particular, the Kondo regime of strong on-site repulsion and low leads-temperature, focusing on the narrowing of the Kondo resonance.

TT 40.9 Wed 15:00 Poster D

**Spin-boson coupling in continuous-time quantum Monte Carlo** — •Junya Otsuki — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg — Department of Physics, Tohoku University, Sendai, Japan

A vector bosonic field coupled to the electronic spin is treated by means of the continuous-time quantum Monte Carlo method. In the Bose Kondo model with a sub-Ohmic density of states $\rho_B(\omega) \sim \omega^{-s}$, two contributions to the spin susceptibility, the Curie term $T^{-1}$ and a bosonic fluctuating term $T^{-s}$, are observed separately. By including the fermionic bath, a quantum phase transition is identified between the Kondo screened state and the bosonic fluctuating state, at which the effective moment and the local Fermi-liquid energy scale vanish. It is demonstrated that the energy scale of the bosonic fluctuation is not affected by the existence of the quantum phase transition.

[1] J. Otsuki, arXiv:1211.5935.

TT 40.10 Wed 15:00 Poster D

**Hybridisierungs-CT-QMC mit großen U** — •René John Kerkdyk und Thomas Pruschke — Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Mit dem Hybridisierungs-CT-QMC-Algorithmus wird das Multiorbital-Einstörstellen Anderson Modell im Bereich sehr großer U untersucht. Dabei stößt man auf Ergodizitäts- und Effizienzprobleme, die diskutiert werden. Verbesserte Updates ermöglichen das Umgehen energetisch ungünstiger Zustände und erlauben so eine drastische Reduktion der Autokorrelationszeit. Damit verhindern sie auch ein Einfrieren der Besetzung der verschiedenen Orbitale im Einstörstellen Anderson Modell, was sich in fehlender Ergodizität äußert. Mit den zusätzlichen Updates kann man verläßlich Spektralfunktionen auch für extreme Parameter erzielen.

TT 40.11 Wed 15:00 Poster D

**$\pi$ fluxes near the edge of a quantum spin Hall insulator** — •Manuel Weber and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Inserting a $\pi$ flux into a quantum spin Hall insulator creates four spin-charge separated states in the bandgap - two spin fluxons, which form a Kramers doublet, and two charge fluxons. They lead to a characteristic Curie law in the magnetic susceptibility of both free and interacting systems. We study single $\pi$ fluxes in close distance to the edge states of the Kane-Mele model on a ribbon. Numerical investigations of the susceptibility in the noninteracting model show the Curie law down to low temperatures even for $\pi$ fluxes located directly at the edge. This can be interpreted as a consequence of the $\pi$ fluxes' quantum numbers, which inhibit coupling to the edge mode in the absence of interactions. Using CTQMC simulations we investigate the coupling of the $\pi$ flux to the edge states, when correlations are taken into account.

TT 40.12 Wed 15:00 Poster D

**Preparation chain of single crystal intermetallic compounds under UHV-compatible conditions** — Andreas Bauer, •Georg Benka, Marein Rahn, Frederik Goerg, Christian Franz, and Christian Pfleiderer — Physik Department E21, Technische Universität München, D-85747 Garching, Germany

High quality single crystals are perhaps the most important technical requirement for major advances in condensed matter physics. To achieve the highest purity it is crucial to avoid contaminations at any of the preparational steps of the crystal growth process. We report the development of an Ar glove-box with a load-lock system that allows to go from the cutting of the starting elements to the initial synthesis of polycrystals with RF heating or arc-melting in a pure Ar environment. This forms the starting point for single-crystal growth by means of rod casting and optical float-zoning under UHV compatible conditions [1]. The improvements in sample preparation achieved with our glove-box are illustrated in terms of exploratory studies of selected rare-earth compounds.

[1] A. Neubauer et al., RSI **82**, 013902 (2011)

TT 40.13 Wed 15:00 Poster D

**A pressure study of $CePt_3B$** — •Daniela Rauch[1], Steffen Hartwig[1,2], Stefan Süllow[1], Hiroyuki Hidaka[3], Seigo Yamazaki[3], Hiroshi Amitsuka[3], and Ernst Bauer[4] — [1]Institute of Condensed Matter Physics, University of Technology Braunschweig, Braunschweig, Germany — [2]BENSC, Helmholtz Zentrum Berlin, Berlin, Germany — [3]Department of Physics, Hokkaido University, Sapporo, Japan — [4]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria

$CePt_3B$ is isostructural to the non-centro symmetric heavy-fermion superconductor $CePt_3Si$. In contrast to the latter system, $CePt_3B$ exhibits a complex magnetically ordered state at low temperatures, with an antiferromagnetic phase below $T_N = 7.8$ K and a weakly ferromagnetic transition below $T_C \approx 5$ K. As demonstrated in Ref. [1] $CePt_3B$ can be understand as a low pressure variant of $CePt_3Si$.

Here we report a study of $CePt_3B$ by means of high pressure magnetization measurements, this way in particular accessing the pressure evolution of the ferromagnetic transition temperature $T_C$. From our investigation up to about 40 kbar we observe an almost constant transition temperature $T_C$ with pressure. This behavior we will discuss in the context of alloying studies on this material.

[1] D. Rauch *et al.*, Phys. Rev B, in print (2012).

TT 40.14 Wed 15:00 Poster D

**Momentum dependence of the almost quantum critical spin fluctuations in $CeCu_2Si_2$** — •Zita Huesges[1], Oliver Stockert[1], Hirale S. Jeevan[1], Karin Schmalzl[2], and Frank Steglich[1] —

[1]Max Planck Institute CPfS, Dresden, Germany — [2]Jülich Center for Neutron Science, outstation at Institut Laue-Langevin, Grenoble, France

The heavy-fermion superconductor $CeCu_2Si_2$ is located close to a quantum critical point. The spin fluctuations at the nesting wave vector $Q_{AF}$ in the normal state are quasielastic and show considerable slowing down. The magnetic response also exhibits scaling expected for a 3D spin-density-wave quatum critical point. We present here the first measurement of the momentum dependence of these almost quantum critical fluctuations. The temperature dependence of the linewidth of the spin fluctuations in reciprocal space is studied and compared to theoretical expectations, which arise from the connection of momentum width and energy width via the dynamical critical exponent z.

TT 40.15 Wed 15:00 Poster D

**Spin-orbit-coupling-induced $j_{\mathrm{eff}}$ states in perovskite iridates studied by photoemission spectroscopy** — •Atsushi Yamasaki[1,2], Ozan Kirilmaz[2], Michael Sing[2], Akira Sekiyama[3,4], Masaaki Isobe[5], Shigemasa Suga[3,4], and Ralph Claessen[2] — [1]Konan University, Kobe, Japan — [2]Universität Würzburg, Würzburg, Germany — [3]Osaka University, Osaka, Japan — [4]RIKEN SPring-8 Center, Hyogo, Japan — [5]National Institute for Materials Science, Tsukuba, Japan

Novel physics induced by strong spin-orbit coupling has attracted lots of attention from both theory and experiment in recent years. $Sr_2IrO_4$ has a canted antiferromagnetic insulating state which seems to be driven by the strong spin-orbit coupling and relatively weak Coulomb interaction. The electronic structure near the Fermi level is characterized by $j_{\mathrm{eff}} = \frac{1}{2}$ states which have a partially quenched, but still finite angular momentum due to the spin-orbit coupling effect in the $O_h$ crystal field. In order to provide deeper insight into these induced states, we have carried out high energy-resolution photoemission spectroscopy with h$\nu$=8.4-8000 eV photons on perovskite iridates. Photoemission spectroscopy in a wide range of excitation energies enables us to identify the bulk and surface electronic structure including their origin in the valence band. Hard-x-ray photoemission spectroscopy reveals genuine bulk $j_{\mathrm{eff}}$ states due to the large photoionization cross section of the Ir 5*d*-orbitals and the large photoelectron mean-free path. Our results are compared with LDA+DMFT calculations.

TT 40.16 Wed 15:00 Poster D

**Strong Spin-Orbital Coupling and Polarization as origin of the Insulating State in $Sr_2IrO_4$** — •Markus Aichhorn[1], Cyril Martins[2], Loig Vaugier[2], and Silke Biermann[2] — [1]Institut für theoretische Physik - Computational Physics, TU Graz, Austria — [2]CPHT, Ecole Polytechnique, France

We discuss the notions of spin-orbital polarization and ordering in paramagnetic materials, and address their consequences in transition metal oxides. Extending the combined density functional and dynamical mean field theory (DMFT) scheme to the case of materials with large spin-orbit interactions, we investigate the electronic excitations of the paramagnetic phases of $Sr_2IrO_4$ and $Sr_2RhO_4$. We show that the interplay of spin-orbit interactions, structural distortions and Coulomb interactions suppresses spin-orbital fluctuations. As a result, the room temperature phase of $Sr_2IrO_4$ is a paramagnetic spin-orbitally ordered Mott insulator. In $Sr_2RhO_4$, the effective orbital degeneracy is reduced, but the material remains metallic, due to both, smaller spin-orbit and smaller Coulomb interactions. We find excellent agreement of our ab-initio calculations for $Sr_2RhO_4$ with angle-resolved photoemission.

TT 40.17 Wed 15:00 Poster D

**Preparation of $SrIrO_3$ thin films by using metal-organic aerosol deposition technique** — •Sebastian Esser, Melanie Schneider, Vasily Moshnyaga, and Philipp Gegenwart — 1. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The interplay between spin-orbit coupling and electronic correlations could lead to interesting novel states in iridium oxide materials. We focus on the perovskite phase of $SrIrO_3$ because Moon et al. [1] showed by using optical spectroscopy and first-principles calculations that the last member of the Ruddlesden-Popper series $Sr_{n+1}Ir_nO_{3n+1}$ ($n = \infty$) is close to the Mott transition. By using metal-organic aerosol deposition technique we have grown $SrIrO_3$ thin films on (111)-oriented $SrTiO_3$ substrates. The cubic symmetry of the $SrTiO_3$ substrate ensured that the $SrIrO_3$ thin film grew in the monoclinic perovskite phase [1,2]. The X-ray diffraction results suggest that $SrIrO_3$ thin films in perovskite structure were obtained and these show out of plane epitaxy with monoclinic $(002)_m$-orientation. The temperature dependence of the electrical resistivity of these $SrIrO_3$ thin films were investigated and metallic behavior was observed down to 50 K.

This work is supported by the German Science foundation through SFB 602, TP A19.

[1] S. J. Moon *et al.*, Phys. Rev. Lett. **101** 226402 (2008)
[2] A. Sumi *et al.*, Thin Solid Films **486**, 182 (2005)

TT 40.18 Wed 15:00 Poster D

**Effect of hydrostatic pressure on $Yb(Rh_{1-x}Fe_x)_2Si_2$** — •Sebastian-Horst Hübner, Yoshi Tokiwa, Hirale S. Jeevan, Maik Schubert, and Philipp Gegenwart — I. Physik. Institut, Georg-August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The temperature scale, $T^*(K)$, in undoped $YbRh_2Si_2$ have gathered much attention due to its different interpretations. Substituting Fe on the Rh site in $YbRh_2Si_2$ causes a combined effect of chemical pressure and hole doping. By increasing Fe-doping, both the Kondo temperature and Neél temperature $T_N$ ( = 70 mK for $x$=0) decrease, with a critical concentration of $x \sim 0.08$, which suppresses $T_N$ to zero. Since positive pressure enhances $T_N$ in Yb-based materials, the hole doping is most likely responsible for the supression. Along with the suppression of $T_N$, $T^*(K)$ also decreases with Fe-doping and dissappears around the same critical concentration, $x$=0.08.

Application of hydrostatic pressure on $Yb(Rh_{1-x}Fe_x)_2Si_2$ with $x > 0.08$ may cause a reappearance of antiferromagnetic order and it is highly interesting wheather or not the $T^*(K)$ scale also reappears. Here, we present resistivity of $Yb(Rh_{1-x}Fe_x)_2Si_2$ with $x$=0.105 under hydrostatic pressure and discuss our results in terms of the proposed interpretations.

TT 40.19 Wed 15:00 Poster D

**Magnetic cooling through quantum criticality** — •Stefan Doerschug, Bernd Wolf, Natalia van Well, Franz Ritter, Robert Schindler, Wolf Assmus, and Michael Lang — Physikalisches Institut, Goethe-UniversitätFrankfurt (M), Germany

Close to a magnetic field-induced quantum-critical point the entropy at finite temperature exhibit a strong variation upon changing the magnetic field. We demonstrate that this accumulation of entropy can be used for realizing an efficient magnetic cooling. Our proof-of-principle demonstration is based on measurements and theoretical calculations of the magnetothermal properties of low-dimensional antiferromagnets close to their field-induced quantum-critical points. Here we present results of the magnetocaloric effect $\Gamma_B = T^{-1}(\Delta T/\Delta B)_S$ of different xy-antiferromagnets as a function of both field and temperature in the vicinity of the quantum-critical point and discuss various performance characteristics, such as the range of operation, efficiency and hold time. The corresponding figures of the quantum critical systems are compared with those of a state-of-the-art paramagnetic coolant. In addition, we present the experimental set-up, which is used to determine the magnetocaloric effect. The focus is particularly on the construction of a sample-holder for high-resolution measurements in the temperature range 0.02 K $< T <$ 2 K.

TT 40.20 Wed 15:00 Poster D

**Candidate for a quantum Griffiths phase in the itinerant ferromagnet $Sr_{1-x}Ca_xRuO_3$** — Dirk Fuchs[1], •Chien-Lung Huang[1,2], Markus Wissinger[1], Rudolf Schneider[1], Jörg Schmalian[3], and Hilbert von Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76031 Karlsruhe, Germany — [3]Karlsruher Institut für Technologie, Institut für Theorie der Kondensierten Materie, 76031 Karlsruhe, Germany

The magnetization $M$, susceptibility $\chi$, and the specific heat $C$ of polycrystalline $Sr_{1-x}Ca_xRuO_3$ was investigated as a function of the Ca substitution $x$. For $x = 0$ a second-order like ferromagnetic (FM) phase transition occurs at $T_C = 162$ K. $T_C$ decreases with increasing $x$. Above the critical concentration $x_c \sim 0.7$, i.e., $x \geq x_c$, the FM order is completely suppressed. For $x > 0$ the susceptibility $\chi(T)$ deviates from a Curie-Weiss law below $T_C$ of $SrRuO_3$ which indicates a Griffiths phase (GP) behavior. $\chi$, $M$, and $C$ are analyzed in detail with respect to the Griffith exponent $\lambda$ and the GP regime within the phase diagram of $Sr_{1-x}Ca_xRuO_3$.

TT 40.21 Wed 15:00 Poster D

**Field-induced quantum criticality in $CeCu_{6-x}Au_x$** — •Kai Grube[1], Sebastian Zaum[1,2], Felix Eilers[1], Diego Zocco[1], Veronika Fritsch[2], Roland Schäfer[1], Oliver Stockert[3], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

The heavy-fermion system $CeCu_{6-x}Au_x$ is an archetype for pressure-induced quantum criticality at the onset of antiferromagnetic order. Up to now, investigations focused mainly on the behavior close to the critical concentration $x_c \approx 0.1$. The antiferromagnetic order of samples with higher Au content can, however, be also suppressed by magnetic fields. We studied the field-induced quantum critical behavior of samples with Au contents $x = 0.3$, 0.5 and 1.0 in fields applied along the magnetic easy axis by using thermal expansion and magnetostriction measurements. Due to their high sensitivities these measurements are especially suited to expose deviations from Fermi-liquid behavior. The measurements have been performed for temperatures ranging between 20 mK and 10 K, and in magnetic fields up to 14 T. With increasing Au content and critical field $B_c$ they show strongly varying critical behavior. We discuss our results taking into account the field-dependent Zeeman splitting of the CEF ground-state doublet, which manifests itself as a Schottky-like anomaly at low temperatures and fields larger than $B_c$.

TT 40.22 Wed 15:00 Poster D

**Spin excitations in CePdAl** — •S. Woitschach[1], O. Stockert[1], A. Wildes[2], V. Fritsch[3], H. v. Löhneysen[3], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]Karlsruher Institut für Technologie, Physikalisches Institut, Karlsruhe, Germany

Hexagonal CePdAl is a geometrically frustrated heavy-fermion compound that orders antiferromagnetically below $T_N = 2.7$ K in an incommensurate structure. Magnetic order can be continuously suppressed, e.g. by Ni doping on the Pd site. At a Ni content of $\approx 14\%$ the transition is fully suppressed and a quantum critical point is reached. Due to geometrical frustration only 2/3 of the magnetic moments show long-range ordering (LRO), while 1/3 only exhibit short-range order (SRO). In thermodynamic measurements a strong anisotropy between the *c*-axis and the *ab*-plane has been observed. Here we present our neutron diffraction investigations of the (anisotropic) q-space dependence of the LRO and SRO signal in CePdAl below and above $T_N$.

TT 40.23 Wed 15:00 Poster D

**A microscopic study of $Nb_{1-y}Fe_{2+y}$** — •Daniela Rauch[1], Mathias Kraken[1], Jochen Litterst[1], Stefan Süllow[1], and F. Malte Grosche[2] — [1]Institute of Condensed Matter Physics, University of Technology Braunschweig, Braunschweig, Germany — [2]Cavendish Laboratory, University of Cambridge, Cambridge, UK

The C14 laves phase system $NbFe_2$ represents a very rare case of spin density wave order (SDW) in a 3d metal compound, which can be suppressed by slight changes to the stochiometry in $Nb_{1-y}Fe_{2+y}$. In particular, stoichiometric $NbFe_2$ exhibits a SDW order with a Néel temperature ($T_N$) around 10K, while slight Fe-excess induces low-moment ferromagnetism, whereas a quantum critical point (QCP) is approached on the Nb-rich side of the composition range. Moreover, samples close to the QCP show non-Fermi liquid behavior ([1]-[4]).

Here we report a microscopic study of the alloying series $Nb_{1-y}Fe_{2+y}$ utilizing $\mu$SR and Mössbauer experiments. From our investigation using $\mu$SR we verify that all magnetic transitions are bulk transitions. Furthermore, combined with the $\mu$SR we present an analysis of the Mössbauer spectroscopy experiments and discuss the nature of the ground state magnetic phase in the light these studies.

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[4] M. Brando *et al.* Phys. Rev Letter **101**, 026401 (2008).

TT 40.24 Wed 15:00 Poster D

**Pressure and field tuning in $CeAgSb_2$ and $NbFe_2$** — •Peter Logg[1], Zhuo Feng[1,2], Takao Ebihara[3], William J Duncan[4], Andreas Neubauer[5], Christian Pfleiderer[5], Hong'En Tan[1], Sven Friedemann[1], Patricia Alireza[1], Swee Goh[1], and F Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]London Centre for Nanotechnology, UCL, London, UK — [3]Dept. of Physics, Shizuoka University, Shizuoka, Japan — [4]Dept. of Physics, Royal Holloway, University of London, Egham, UK — [5]Physik Department E21, Technische Universitat Munchen, Garching, Germany

The intermetallic $CeAgSb_2$ and the dilution series $Nb_{1-y}Fe_{2+y}$ both exhibit *uniaxial* magnetic order which is sensitive to both hydrostatic pressure and transverse magnetic fields. $CeAgSb_2$ is a Kondo-lattice compound which at ambient pressure undergoes a ferromagnetic (FM) transition at $T_C = 9.6$ K. FM is suppressed via the application of either hydrostatic pressure or an *in-plane* tuning field, and extrapolates to zero temperature by pressures exceeding 35 kbar or fields greater than 2.8 T. Contrastingly, slightly iron-rich $Nb_{1-y}Fe_{2+y}$ ($y = 0.015$) undergoes a spin-density wave transition at $T_N = 31$ K, before becoming FM at $T_C = 23$ K. The application of pressure rapidly suppresses both phases, driving the system towards the quantum critical point which may be reached via compositional tuning at around $y$ = -0.015.

We investigate the *HT* and *PT* phase diagrams of both compounds, through a series of high-pressure and field tuned AC and DC susceptibility measurements.

TT 40.25 Wed 15:00 Poster D

**Synthesis and characterization of single-layered manganites** — •Johannes Engelmayer, Oliver Breunig, Holger Ulbrich, Markus Braden, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

Single-layered manganites show a complex interplay between charge, orbital, and magnetic degrees of freedom. For $La_{1-x}Sr_{1+x}MnO_4$ and $Pr_{1-x}Ca_{1+x}MnO_4$ with doping level $x = 0.5$ (half-doping), the Goodenough model is well established. This model proposes a site-centered charge order with a checkerboard pattern of $Mn^{3+}$ and $Mn^{4+}$ ions that is accompanied by an orbital order. This charge and orbital order induces a magnetic order with ferromagnetic three-spin zig-zag chains and antiferromagnetic interchain coupling. For $Pr_{1-x}Ca_{1+x}MnO_4$ and $Nd_{1-x}Sr_{1+x}MnO_4$ with $x = 2/3$, four-spin zig-zag chains could be observed due to a 2:1 ratio of $Mn^{4+}$ and $Mn^{3+}$. In order to study the charge, orbital, and magnetic order in manganites with other dopants, single crystals of $Pr_{1-x}Sr_{1+x}MnO_4$ and $Nd_{1-x}Ca_{1+x}MnO_4$ with $0.5 \leq x \leq 0.75$ were grown and their structural parameters were determined. We present measurements of resistivity, magnetization, and specific heat that show indications for charge order around room temperature. A dopant and doping-level dependence of the ordering temperature is discussed.

Supported by the DFG through SFB 608.

TT 40.26 Wed 15:00 Poster D

**Pulsed Laser and THz Induced Charge Carrier Excitations in $Pr_{0.65}Ca_{0.35}MnO_3$** — •Nils Folchert, Stephanie Raabe, Claus Ropers, and Christian Jooss — Institut für Materialphysik, Göttingen

Quite similar to electric and magnetic fields, optical stimulation of manganites like $Pr_{1-x}Ca_xMnO_3$ (PCMO) can induce transitions from insulating to metallic conductivity. Applying a bias smaller than the threshold voltage of the electrically induced colossal resistance effect (CER), a short laser pulse can melt the charge-ordered state of PCMO yielding to-metal like conductive paths in the illuminated region. This state is preserved until the bias is switched off [1]. PCMO reveals strong correlation effects, i.e., strong electron-electron, electron-phonon and magnetic interactions. The change of these correlations during excitation is a still not very well understood phenomena of perovskite manganites. In order to investigate the transition, we performed time-resolved dc-measurements after pulsed laser excitations with frequencies varying from UV to Thz and at temperatures between 80 K to 300 K. The PCMO samples with $x = 0.35$ were prepared by means of ion-beam-sputtering using single-crystalline MgO substrates. In this poster, we will mainly focus on the relaxation dynamics of the optically excited charge carriers.

[1] M. Fiebig et al., Appl. Phys. Lett. 74, 2310 (1999)

TT 40.27 Wed 15:00 Poster D

**Spin polarized HSE hybrid functional calculations of $VO_2$** — •Udo Schwingenschlögl[1], Ricardo Grau-Crespo[2], and Hao Wang[1] — [1]KAUST, PSE Division, Thuwal, Saudi Arabia —

[2]University College London, London, United Kingdom

We study the rutile (R) and monoclinic (M1) phases of the prototypical compound $VO_2$ by first principles calculations based on density functional theory, employing the Heyd-Scuseria-Ernzerhof (HSE) screened hybrid functional. Our results show that the HSE lowest-energy solutions for both the low-temperature M1 phase and the high-temperature R phase, which are obtained upon inclusion of spin polarization, are at odds with experimental observations. For the M1 phase the groundstate is (but should not be) magnetic, while the groundstate of the R phase, which is also spin-polarized, is not (but should be) metallic. The energy difference between the low-temperature and high-temperature phases is also in strong discrepancy with the experimental latent heat [1].

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TT 40.28 Wed 15:00 Poster D

**Orbital order and phase transitions in $KCrF_3$** — •Carmine Autieri[1,2,3] and Eva Pavarini[1] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]CNR-SPIN, I-84084 Fisciano (SA), Italy — [3]Dipartimento di Fisica "E. R. Caianiello", Università di Salerno, I-84084 Fisciano (SA), Italy

We study the tetragonal to monoclinic structural transition and the origin of the orbital order in $KCrF_3$. We discuss similarities with $KCuF_3$ and $LaMnO_3$. We compare the hopping parameters for the cubic, tetragonal and monoclinic structures of $KCrF_3$ using the both projectors and maximally localised Wannier functions. Moreover, we calculate the Coulomb parameters using a linear response approach. Finally, we study the effects of spin-orbit and the origin of low-temperature weak ferromagnetism.

TT 40.29 Wed 15:00 Poster D

**Vibrational IR-spectroscopy of charge-ordered $\alpha$-$ET_2I_3$ under pressure** — •Armin Dengl[1], Rebecca Beyer[1], Tomislav Ivek[1,2], and Martin Dressel[1] — [1]1. Physikalisches Institut, University of Stuttgart, Germany — [2]Institut za fiziku, P.O. Box 304, HR-10001 Zagreb, Croatia

One of the most important charge-ordered compounds is the quasi-2D organic conductor $\alpha$-$ET_2I_3$. Its structure consists of alternating conducting cation (ET-molecules) and insulating anion ($I_3$) layers. The compound exhibits a first-order metal-insulator phase transition at $T_{MI} = 135$ K which is accompanied by a horizontal striped charge ordering within the ET layer. For ambient pressure the charge distribution has been well investigated, so we turned our attention to pressure-dependent IR-spectroscopy. The asymmetric charge-sensitive vibration $\nu_{27}(B_{1u})$ is the superior mode to determine the molecular charge due to its high sensitivity of resonance frequency on charge.
We performed vibrational reflectance IR measurements under hydrostatic pressure up to 11 kbar for a temperature range from 10 to 300 K. For the insulating charge-ordered phase we determined the molecular charge for the charge rich molecules. By applying pressure, the phase transition gets suppressed to lower temperatures by $(9 \pm 0.5)$ K/kbar towards the metallic phase. The charges of the charge rich molecules do not show any dependence on temperature, but by increasing pressure, a linear shift to lower values can be observed.

TT 40.30 Wed 15:00 Poster D

**Seebeck measurements on Pt-C FEBID nanostructures** — •Heiko Reith[1,3], Roland Sachser[1], Matthias C. Schmitt[2], Friedemann Voelklein[3], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-University, Frankfurt am Main, Germany — [2]Guenter Effgen GmbH, Herrstein, Germany — [3]IMtech, Hochschule Rhein Main, Ruesselsheim, Germany

We investigated the thermo voltage of Pt-C granular metals fabricated by focused electron beam-induced deposition (FEBID) using trimethyl (methylcyclopentadienyl) platinum (IV) as precursor. The FEBID structures were deposited on specially designed microchips that allow measuring the Seebeck-coefficient of the samples. The electronic intergrain-coupling strength of the samples was tuned by post-growth electron-irradiation. Controlled by in situ measurement of the electrical conductivity of the deposits electrical conducting, insulator-to-metal transition and insulating samples were obtained by post-irradiation. We present the used microchip and results of the electrical conductivity and the Seebeck-coefficient measurements of the Pt-C granular samples in a temperature range from room to liquid 4He temperature and compare our results with theory.

TT 40.31 Wed 15:00 Poster D

**Mott correlated states in the underdoped two-dimensional Hubbard model: variational Monte Carlo versus a dynamical cluster approximation** — •Luca F. Tocchio, Hunpyo Lee, Harald 0. Jeschke, Roser Valenti, and Claudius Gros — Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main, Germany

We investigate the properties of the frustrated underdoped Hubbard model on the square lattice using two complementary approaches, the dynamical cluster extension of dynamical mean field theory, and variational Monte Carlo simulations of Gutzwiller-Jastrow wavefunctions with backflow corrections. We compare data for the energy and the double occupancies, as obtained from both approaches. At small dopings, we observe a rapid crossover from a weakly correlated metal at low interaction strength $U$ to a non-Fermi liquid correlated state with strong local spin correlations. Furthermore, we investigate the stability of the correlated state against phase separation. We observe phase separation only for large values of $U$ or very large frustration. No phase separation is present for the parameter range relevant for the cuprates.

TT 40.32 Wed 15:00 Poster D

**Multiplets of the full and simplified Coulomb Hamiltonians in bases of spherical and cubic harmonics** — •Hermann Ulm and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich, and RWTH Aachen University, 52425 Jülich, Germany

Correctly including electron-electron interactions is crucial for the realistic description of strongly correlated materials. Approaches like LDA+U use simplified Dudarev Hamiltonian [1] or full Hamiltonian [2] which are both solved in the HF(mean-field) approximation and rotationally invariant, i.e. independent of the basis. For the QMC often the Kanamori Hamiltonian [3] or a simplified density-density version which is basis dependent is used to avoid the Fermi sign problem. Here we compare the spectra and eigenstates of the full rotationally invariant electrostatic Hamiltonian and its simplified versions.

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[3] J. Kanamori, Prog. Theor. Phys., 275 (1963)

TT 40.33 Wed 15:00 Poster D

**Ab-initio Hubbard parameters for molecular crystals by a symmetry decomposed Ewald method** — •Michael M. E. Baumgärtel and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich, and RWTH Aachen University, 52425 Jülich, Germany

For strongly correlated molecular crystals we determine realistic Hubbard parameters ab-initio. Restricting to electrons in the partially filled bands, screening by the other electrons renormalizes the Hubbard parameters. The intra-molecular screening is treated within DFT, while inter-molecular Coulomb interaction is modeled by a lattice of distributed polarizabilities. Charging of a molecular orbital breaks the periodic symmetry of dipole interactions. By separating the linear response, we obtain a periodic dipole-dipole interaction operator that is independent of the actual polarization pattern. Inverting this operator gives the self-consistent linear screening. In reciprocal space the interaction matrix is low-dimensional, but long-range. However, we obtain rapidly converging matrix elements through an optimized Ewald-summation.

We present eigen-spectra of Fourier transformed dipole interaction matrices. Employed on a Brillouin zone grid our fast diagonalization method yields the Hubbard parameters, both on-site and long-ranged, for any charging of molecular orbitals. We demonstrate our method for Fullerenes as well as TTF-TCNQ crystals.

TT 40.34 Wed 15:00 Poster D

**Effective gauge field description for the bilinear-biquadratic spin-one chain** — •Shijie Hu[1], Ari M. Turner[2], and Frank Pollmann[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]University of Amsterdam, 1090 GL Amsterdam, The Netherlands

We study the one-dimensional bilinear-biquadratic spin-one model. For this model, the possible existence of a nematic phase between the dimerized and the ferromagnetic phase has been debated. An alternative prediction is derived by modeling the nematic as a quantum rotor

model with a Berry's phase. This theory predicts that the long-range nematic phase does not strictly exist, but that the dimerized phase is a version of it that has been disordered by quantum fluctuations. We present evidence for the latter theory by using it to predict the scaling of the correlation length and the dimerization strength, and then testing these scaling laws with large scale infinite system density-matrix renormalization group calculations, suggesting that the dimerization persists (albeit very weakly) all the way to the edge of the ferromagnetic state.

TT 40.35 Wed 15:00 Poster D

**Thermal form factors of the anisotropic Heisenberg chain** — •Maxime Dugave and Frank Göhmann — Bergische Universität Wuppertal

We derive expressions for the form factors of the quantum transfer matrix of the spin-1/2 XXZ chain which allow us to take the infinite Trotter number limit. This solves the longstanding problem of describing analytically the amplitudes in the leading asymptotics of the finite temperature correlation functions of the model. We show how known results for the high-temperature asymptotics are recovered from the form factor expansion. In the zero-temperature limit we derive the 'critical behaviour' of the form factors from our formulae.

TT 40.36 Wed 15:00 Poster D

**Factorisation of correlation functions of the integrable spin-1 Heisenberg chain at finite temperature** — •Dominic Nawrath and Andreas Klümper — Bergische Universität Wuppertal, Theoretische Physik, Gauss-Strasse 20, 42119 Wuppertal

Based on the reduced quantum Knizhnik-Zamolodchikov equation we derive discrete functional equations for the two site density matrix of the isotropic spin-1 Heisenberg chain [1, 2, 3]. This set of equations can be solved by a transcendental two point function that satisfy a three point equation. Furthermore by means of the fusion procedure [6] it seems that the factorization of correlation functions in the spin-1/2 case holds for correlation functions of the spin-1 model [4, 5].

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[2] H. Boos et al., Algebra and Analysis 17 (2005), 115.
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[5] H. E. Boos et al., Nucl. Phys. B 712 (2005), 573.

TT 40.37 Wed 15:00 Poster D

**Spin dynamics in Azurite: high-field ESR studies** — •M. Ozerov[1], D. Kamenskyi[1], J. Wosnitza[1], H. Engelkamp[2], F. Wolff-Fabris[3], S. Francoual[4], M. Jaime[5], and S. Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden - Rossendorf, Germany — [2]High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University, 6525 ED Nijmegen, The Netherlands — [3]European XFEL GmbH, 22607 Hamburg, Germany — [4]Deutsches Elektronen-Synchrotron DESY, Hasylab Petra III, 22607 Hamburg, Germany — [5]MPA-CMMS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

The natural mineral azurite ($Cu_3(CO_3)_2(OH)_2$), a spin-1/2 chain system with a distorted diamond structure, has been probed by means of electron spin resonance and far-infrared spectroscopy in magnetic fields up to 50 T. The observed spectra revealed a very complex picture of magnetic excitations including the co-existence of monomer and dimer excitations, as well as their high-energy bound states. The observation of the bound monomer-dimer states is of particular importance, illuminating the limitation of the simple *isolated* dimer-monomer chain model employed for the description of magnetic properties of Azurite previously. The peculiarities of the resonance absorption in Azurite are discussed.

This work was partly supported by the DFG and EuroMagNET (EU contract No. 228043).

TT 40.38 Wed 15:00 Poster D

**Exploring the Magnetic Phase Diagram of the Frustrated Chain Cuprate $PbCuSO_4(OH)_2$ - Linarite** — •M. Schäpers[1], A. U. B. Wolter[1], F. Lipps[1], V. Kataev[1], S.-L. Drechsler[1], S. Nishimoto[1], R. Beyer[2], M. Uhlarz[2], J. Wosnitza[2], B. Willenberg[3,5], M. Reehuis[3], K. C. Rule[3], B. Ouladdiaf[4], S. Süllow[5], and B. Büchner[1] — [1]Leibniz-Institut IFW Dresden, Dresden, Germany — [2]Dresden High Magnetic Field Laboratory, Dresden, Germany — [3]HZB, Berlin, Germany — [4]ILL, Grenoble, France — [5]IPKM, TU Braunschweig, Braunschweig, Germany

We present a detailed experimental and theoretical study of the frustrated s = $\frac{1}{2}$ spin-chain compound Linarite, $PbCuSO_4(OH)_2$, with competing nearest-neighbor and next-nearest-neighbor exchange interactions. Our experimental data are described using various theoretical approaches to obtain the magnetic exchange interactions resulting in a frustration ratio $\alpha \approx 0.36$ close to the 1D critical point [1]. ESR and NMR at elevated temperatures indicate a highly frustrated system with the onset of magnetic correlations far above the long range magnetic ordering temperature $T_N = 2.8$ K. Below $T_N$ the ground state was found to be an elliptical, incommensurate spin spiral [2]. Linarite shows a multiplicity of magnetic field induced phases which could be identified by neutron- and NMR-measurements.

This work has partially been supported by the DFG under Contracts No. WO 1532/3-1 and No. SU229/10-1.

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[2] B. Willenberg *et al.*, Phys. Rev. Lett. **108,** 117202 (2012)

TT 40.39 Wed 15:00 Poster D

**Synthesis and magnetic characterization of $Cu_3(OH)_4SO_4$** — •Jung Hwan Chun[1], Joseph M. Law[2], and Reinhard K. Kremer[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart — [2]Dresden High Magnetic Field Laboratory, Bautzner Landstrasse 400, 01314 Dresden

We report the successful synthesis and magnetic characterization of $Cu_3(OH)_4SO_4$ which contains Cu triple chains of two non-equivalent $Cu^{2+}$ ions, Cu1 and Cu2[1]. Antlerite, $Cu_3(OH)_4SO_4$, was proposed to be a candidate of an idle-spin magnetic system, with long-range ferromagnetic ordering in the Cu2 central chains and AFM ordering between Cu2-Cu1-Cu2 chains[2]. Recently, it was proposed that the central chains of Cu1 also contribute to field-induced phases. Then it is questioning the proposed picture of Antlerite being an idle spin system[3]. We employed hydrothermal synthesis methods to prepare a phase pure microcrystalline Antlerite polycrystalline sample which we characterized by X-ray diffraction, magnetic susceptibility, heat capacity and high field magnetization measurements.

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TT 40.40 Wed 15:00 Poster D

**Magnetic Frustration in a Quantum Spin Chain: The Case of Linarite** — •Britta Willenberg[1,2], Markus Schäpers[3], Kirrily Rule[5], Anja Wolter[3], Manfred Reehuis[1], Bachir Ouladdiaf[4], Hanjo Ryll[1], Bastian Klemke[1], Klaus Kiefer[1], and Stefan Süllow[2] — [1]Helmholtz-Zentrum Berlin, Germany — [2]IPKM, TU Braunschweig, Germany — [3]IFW, Dresden, Germany — [4]Institute Laue Langevin, Grenoble, France — [5]ANSTO, Bragg institute, Australia

The natural mineral linarite $PbCuSO_4(OH)_2$ is a realization of a frustrated one dimensional spin chain. Residual interchain coupling leads to a magnetically ordered state for temperatures below $T_N$=2.8 K with an unusual critical behavior at the transition. A rich magnetic phase diagram for an applied magnetic field along the chain direction was found [1] which we characterized by neutron diffraction and thermodynamic measurements.

This work has partially been supported by the DFG under contracts WO 1532/3-1 and SU229/10-1.

[1] B. Willenberg et al., Phys. Rev. Lett. **108**, 117202 (2012)

TT 40.41 Wed 15:00 Poster D

**Spin dynamics in swedenborgites** — •Stefan Buhrandt — Universität Köln

Swedenborgites are magnetic systems of stacked Kagome and triangular lattices that exhibit strong geometric frustration due to antiferromagnetic coupling between all ions. In the most simple model, these systems are described with only two distinct antiferromagnetic next neighbor interactions, one inside and one out of the Kagome layers. Depending on their ratio, the groundstate is either unique or highly degenerated. In the latter case, these systems show interesting dynamics in the sense that one finds flat bands in spin-wave calculations as well as zero-mode signatures in the specific heat within classical Monte Carlo simulations. We discuss the appearance of these zero-modes in dependence on the ratio of the antiferromagnetic couplings and com-

pare to experimental findings on the compund $CaBaCo_2Fe_2O_7$.

TT 40.42 Wed 15:00 Poster D

**Pulsed-field experiments on the quasi-2d antiferromagnet $Cs_2CuBr_4$** — •Lars Postulka, Bernd Wolf, Pham Thanh Cong, Natalia van Well, Franz Ritter, Wolf Assmus, and Michael Lang — PhysikalischesInstitut, Goethe-Universität Frankfurt (M), SFB/TR 49, D-60438Frankfurt (M), Germany

We present pulsed-field measurements up to 50 T of the longitudinal elastic constant $c_{11}$ for 1.5 K $< T <$ 4.2 K on single crystalline samples of $Cs_2CuBr_4$, aiming at identifying the signatures of the proposed spin liquid in the material's elastic properties. A large softening, caused by the coupling of the quasi-2d spin fluctuations to the phonon system, is observed for magnetic fields smaller than the critical field $B_c \sim 31$ T ($B//$a), an effect which is more pronounced for lower temperatures. As expected, in the fully-polarized state the $c_{11}$ mode is field independent for all temperatures. We compare the magnetoelastic properties of $Cs_2CuBr_4$ with those of $Cs_2CuCl_4$ which is less frustrated and according to neutron scattering data can be characterized as a spin liquid. In the latter material the quantum-critical point is located at $B_c = 8.5$ T ($B//$a). In addition, we present a set-up for high precision-magnetization measurements in pulsed fields. The results of the experiments on $Cs_2CuBr_4$ will be discussed in connection with the ultrasonic data.

TT 40.43 Wed 15:00 Poster D

**Magnetic susceptibility measurements in the metal-organic spin-dimer system TK91 at very low temperatures** — •S. Becker[1], U. Tutsch[1], B. Wolf[1], Y. Tsui[1], A. Brühl[1], T. Kretz[2], H.-W. Lerner[2], M. Wagner[2], S. Wessel[3], T. Saha-Dasgupta[4], H. Jeschke[5], R. Valentí[5], and M. Lang[1] — [1]Phys. Inst., Goethe-Universität, 60438 Frankfurt — [2]Inst. f. Anorg. Chemie, Goethe-Universität, 60438 Frankfurt — [3]Inst. f. Theor. Festkörperphysik, RWTH Aachen, 52056 Aachen — [4]S.N. Bose National Centre for Basic Sciences, Salt Lake City, Kolkata 700098, India — [5]Inst. f. Theor. Physik, Goethe-Universität, 60438 Frankfurt

Low-dimensional quantum spin systems show interesting properties at very low temperatures and sufficiently high magnetic fields. According to first principle Density Functional Theory calculations, the compound $C_{36}H_{48}Cu_2F_6N_8O_{12}S_2$ (TK91) is expected to be a 2-dimensionally (2d) coupled spin-1/2 dimer system with an intradimer interaction of $J_1/k_B \sim 10$ K and interdimer couplings of $J_i/k_B \sim 1$ K. We report on high-resolution ac-susceptibility measurements on TK91 as function of magnetic field $B \leq 8\ T$ and temperature 0.04 K $\leq T \leq$ 1 K. Quantum Monte Carlo simulations for various interdimer coupling schemes fit the data very well for the 2d model whereas significant deviations are observed for all other cases thus confirming TK91 as a 2d spin-dimer system. In particular, we identify a range in the $B$-$T$ phase diagram where the system shows distinct 2dXY behaviour accompanied by the formation of vortices and antivortices in the effective spin configuration.

TT 40.44 Wed 15:00 Poster D

**Local probe studies (ESR and NMR) on the $BaAg_2Cu[VO_4]_2$ quantum magnet** — •Y. Krupskaya[1], M. Schäpers[1], E. Vavilova[1,2], A.U.B. Wolter-Giraud[1], H.-J. Grafe[1], V. Kataev[1], A. Möller[3], and B. Büchner[1] — [1]IFW Dresden, Germany — [2]ZPhTI, Kazan, Russia — [3]University of Houston, USA

$BaAg_2Cu[VO_4]_2$ contains Cu(II) $S = 1/2$ on a distorted triangular lattice. DFT band structure calculations, quantum Monte-Carlo simulations, and high-field magnetization measurements show that the physics of this compound is determined by a superposition of ferromagnetic and antiferromagnetic uniform spin chains with nearest neighbour exchange couplings of $J_{\rm FM} = -19$ K and $J_{\rm AFM} = 9.5$ K [1]. Here we report the study of $BaAg_2Cu[VO_4]_2$ by High-Field/Frequency Electron Spin Resonance (HF-ESR) and Nuclear Magnetic Resonance (NMR) spectroscopies, which probe the local magnetic properties. In the HF-ESR measurements, we observe an anisotropic ESR spectrum typical for the Cu(II) ions and determine the $g$-tensor, $g_{\rm paral} = 2.38$ and $g_{\rm perp} = 2.06$. Moreover, we see a substantial shift of the ESR lines at temperatures below 40 K indicating the presence of short range magnetic correlations. NMR methods allowed for the investigation of local magnetic fields, the $T_1$ and $T_2$ relaxation times of the $^{51}$V sites. A pronounced broadening of the NMR line is observed at temperatures below 60 K which is consistent with the ESR results. We discuss the local probe results with relation to the thermodynamic studies and theory calculations.

[1] A.A. Tsirlin et al. *Phys. Rev. B* **85**, 014401 (2012)

TT 40.45 Wed 15:00 Poster D

**Superconducting energy gap of the organic charge-transfer salts $\kappa$-$(ET)_2Cu[N(CN)_2]Br$ and $\kappa$-$(ET)_2Cu(NCS)_2$ studied by point-contact spectroscopy** — •Severin Schad, Benedikt Hartmann, and Jens Müller — Physikalisches Institut, Goethe Universität, Frankfurt, Germany

The organic charge transfer salts (BEDT-TTF)$_2$X form crystalline structures with alternating conducting and insulating layers serving as model systems for two-dimensional metals with strong electronic correlations. Different electronic phases are realised for example by varying the anion X. Compounds with X=Cu[N(CN)$_2$]Br and Cu(NCS)$_2$ show metallic behaviour with a superconducting transition at temperatures of 11.5 K and 9.5 K, respectively.
Although intensively studied, both the anomalous normal conducting state and the nature of superconductivity (regarding the order parameter symetry and the mechanism of cooper pairing) remain unresolved [1]. We use the technique of soft point contact spectroscopy for investigating the superconducting gap structure. Meaningful results require the creation of small interfaces between the superconductor and a normal metal in order to obtain $\frac{\mathrm{d}I}{\mathrm{d}V}$ vs. V curves. The poster will provide information about measurement and various fabrication techniques. Experimental results of both temperature and magnetic-field dependences are presented as well as the discussion of zero-bias conductance curves.

[1] N. Toyota, M. Lang and J. Müller, *Low-Dimensional Molecular Metals*, Solid State Science, Springer-Verlag Berlin Heidelberg (2007)

TT 40.46 Wed 15:00 Poster D

**Thin films of the organic charge transfer compounds TMP-$F_4$TCNQ and TMP-DTF** — •Kai Ackermann[1], Milan Rudloff[1], Michael Bolte[2], Harald Jeschke[3], Matthias Wagner[2], Roser Valenti[3], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Straße 1, 60438 Frankfurt am Main — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität, Max-von-Laue-Straße 7, 60438 Frankfurt am Main — [3]Institut für Theoretische Physik, Goethe-Universität, Max-von-Laue-Straße 1, 60438 Frankfurt am Main

We present results of our investigations on thin films of the organic charge transfer compounds TMP-$F_4$TCNQ [(4,5,9,10-Tetramethoxypyrene)-(2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane)] and TMP-DTF [(4,5,9,10-Tetramethoxypyrene)-(9-Dicyanomethylene-2,4,7-trinitrofluorene)]. The films were grown on silicon dioxide, silicon nitride, sodium chloride and gold substrates by using organic molecular beam deposition (OMBD). The growth properties were investigated by atomic force microscopy (AFM), scanning electron microscopy (SEM) and X-ray diffractometry. The structure analysis of TMP-$F_4$TCNQ shows a triclinic symmetry with a mixed stack configuration and a layered structure of donor and acceptor molecules. First X-ray diffractograms of TMP-$F_4$TCNQ films suggest preferential growth perpendicular to the stacking direction on silicon dioxide. Capacitance, conductivity and field effect measurements of both materials are presented and discussed in conjunction with band structure calculations within the framework of density functional theory.

TT 40.47 Wed 15:00 Poster D

**Scanning Tunneling Spectroscopy at Surfaces of Superconducting Charge-Transfer Salts** — •Sandra Diehl[1,2,3], Torsten Methfessel[2,3], Jens Müller[2,4], Michael Lang[2,4], and Hans-Joachim Elmers[2,3] — [1]Graduate School Materials Science in Mainz, 55099 Mainz — [2]SFB/TR 49 — [3]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz — [4]Physikalisches Institut, Goethe-Universität, 60438 Frankfurt am Main

Superconducting materials based on organic charge-transfer salts are regarded as candidates for unconventional superconductors because their properties strongly deviate from the BCS theory, similar to the high-temperature superconductors. We study $\kappa$-[ET]$_2$Cu[N(CN)$_2$]Br-crystals. Previous measurements showed a surface contamination of the crystals. Because of that we developed an in-situ cleaving mechanism for the preparation of clean surfaces. Measurements on these cleaved crystals show an improved signal-to-noise ratio in the measured $I(U)$ spectra and atomic flat surfaces in the topographic images (nanometer scale in the height profile). All investigations were done under UHV-conditions ($5 \cdot 10^{-11}$ mbar) using a scanning tunneling

microscope at 5 K.

TT 40.48 Wed 15:00 Poster D

**New insight in the glass-like dynamics of the organic charge-transfer salts $\kappa$-(BEDT-TTF)$_2$X from fluctuation spectroscopy** — •Benedikt Hartmann[1], Robert Rommel[1], Jens Brandenburg[1], John Schlueter[2], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt (M) — [2]Argonne National Laboratory, Materials Science Division, Argonne, IL, USA

The organic molecular conductors $\kappa$-(BEDT-TTF)$_2$X are model systems for studying the physics of correlated electrons in reduced dimensions. Recently, the influence of intrinsic disorder on the Mott metal-to-insulator transition (MIT) has been in the focus of experimental and theoretical studies. Fortunately, the degree of intrinsic disorder can be systematically studied through a structural glass-like transition related to the ethylen-endgroups of the BEDT-TTF molecules.
The common method of choice to study the fundamentals of this transition would be dielectric spectroscopy, which due to the materials' high conductivity, however, is not applicable.
In this contribution we demonstrate that fluctuation (noise) spectroscopy is a suitable technique to access the intrinsic properties of the glass-like transition. The temperature dependence of $1/f$-type fluctuations around this transition can be described by a Vogel-Fulcher-Tamman law. Thereby new insight in the glass-like transition is gained and enables one to classify the $\kappa$-(BEDT-TTF)$_2$X-salts as highly fragile glasses.

TT 40.49 Wed 15:00 Poster D

**Exploring the full phase diagram of TTF-CA under pressure** — •Armin Dengl[1], Tobias Knoblauch[1], Rebecca Beyer[1], Tomislav Ivek[1,2], Gabriele Untereiner[1], and Martin Dressel[1] — [1]1. Physikalisches Institut, University of Stuttgart, Germany — [2]Institut za fiziku, P.O. Box 304, HR-10001 Zagreb, Croatia

Tetrathiafulvalene-p-chloranil (TTF-CA) is a 1D organic charge-transfer complex exhibiting a neutral-to-ionic phase transition (NIT), which can be induced both by temperature and pressure. At ambient pressure the phase transition occurs at the critical temperature $T_{\mathrm{NIT}} = 81$ K. It is a first order transition with a jump in ionicity from $\mathrm{CA}^{-0.3}$ to $\mathrm{CA}^{-0.6}$. For a long time the pressure induced NIT was assumed to be continuous, but subsequent studies were able to show a small jump in ionicity. Above a pressure of about 8 kbar, a second sort of CA with a slightly different ionization evolves, an effect which is not yet well investigated.
Most studies on this compound were done either with a dependance on temperature or pressure. We performed vibrational reflectance IR-spectroscopy under hydrostatic pressure up to 11 kbar for a temperature range from 10 to 300 K. To determine the average ionicity per CA molecule we took advantage of the $b_{1u}$ C=O stretching vibration which has a strong dependence of resonance frequency on ionicity. By applying pressure, the NIT shifts to higher temperatures by (25.2 ± 1) K/kbar and the transition becomes broader. For the first time we show the ionicity of CA as a function of both temperature and pressure throughout the whole phase diagram.

TT 40.50 Wed 15:00 Poster D

**Thin film growth and characterization of the neutral-ionic phase transition system tetrathiafulvalene-p-chloranil** — •Achim Rippert, Milan Rudloff, Kai Ackermann, Lukas Keller, and Michael Huth — Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main

Tetrathiafulvalene-p-chloranil (TTF-QCl4) thin films have been prepared by physical vapor deposition of the pre-reacted source material on the substrate materials NaCl, SiO2 and Au. We studied the growth characteristics and electronic transport properties with a view to the influence of substrate-induced effects, such as clamping and strain, on the electronic properties of the layers. TTF-QCl4 is a mixed-stack organic charge transfer compound that shows a temperature-driven paraelectric-to-ferroelectric phase transition associated with a charge of the charge transfer degree at 81 K. This phase transition could be observed in our thin films during electronic transport measurements, as well as in frequency dependent capacity measurements. Furthermore, a color change of the materials could be noticed at the transition temperature. Our research aims for taking advantage of thin-film specific control mechanisms, such as induced biaxial strain and electrostatic field effects, and thus providing a new perspective on the neutral-ionic phase transition in the one-dimensional, mixed-stack organic charge transfer compounds.

TT 40.51 Wed 15:00 Poster D

**Resistivity and Hall-Effect Measurements on $LaAlO_3/SrTiO_{3-\delta}$ Heterostructures** — •Ahmed Sleem[1,2], Dirk Fuchs[1], Philipp Müller[3], Rudolf Schneider[1], Dagmar Gerthsen[3], and Hilbert von Löhneysen[1,4] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [2]Fakultät für Physik, Karlsruher Institut für Technologie, 76031 Karlsruhe, Germany — [3]Laboratorium für Elektronenmikroskopie, Karlsruher Institut für Technologie, 76031 Karlsruhe, Germany — [4]Physikalisches Institut, Karlsruher Institut für Technologie, 76031 Karlsruhe, Germany

The influence of the oxygen partial pressure $p(O_2)$ during film deposition on the transport properties of $LaAlO_3/SrTiO_{3-\delta}$ heterostructures was analyzed by resistivity and Hall-effect measurements. To this end, thin films of $LaAlO_3$ were grown epitaxially by pulsed laser deposition on $TiO_2$ terminated <001> oriented $SrTiO_3$ substrates at different oxygen partial pressure $p(O_2)$, i. e., $10^{-3}$ mbar $\geq p(O_2) \geq 10^{-5}$ mbar. Electrical contacts to the interface were prepared by argon ion-etching and subsequent filling by sputtering of Pt pads. Resistivity measurements were carried out in Van-der-Pauw geometry for 4.2 K $\leq$ T $\leq$ 300 K. The charge carrier concentration, $n_e$, and mobility, $\mu_e$, were deduced from the Hall-constant, $R_H$, and conductivity, $\sigma$ , at room temperature and 4.2K. With decreasing $p(O_2)$ the resistivity changes from an insulating/semi-conductive to a metallic behavior. Experimental results with respect to the sheet resistance $R_S$, $n_e$, and $\mu_e$ versus $p(O_2)$ will be presented and discussed.

TT 40.52 Wed 15:00 Poster D

**Wetting an oxide heterostructure: influence of surface water adsorbates on the electronic properties of $LaAlO_3/SrTiO_3$ studied by in situ photoelectron spectroscopy** — •Philipp Scheiderer[1], Florian Pfaff[1], Judith Gabel[1], Mihaela Gorgoi[2], Michael Sing[1], and Ralph Claessen[1] — [1]Universität Würzburg, Physikalisches Institut — [2]BESSY II., Albert-Einstein-Strasse 15, Berlin

Oxide heterostructures display many interesting phenomena, one example being the formation of a two-dimensional electron system (2DES) at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface beyond a critical thickness of 4 monolayers (ML) of the polar LAO [1,2]. An explanation for this behavior is the so-called electronic reconstruction. In this context it was recently shown that polar adsorbates can enhance the conductivity of the 2DES [3]. Besides their electrostatic influence it was discussed that surface defects/adsorbates can also act as a charge reservoir [4]. To examine the impact of surface adsorbates on the 2DES we performed in situ photoelectron spectroscopy on 6ML thick LAO/STO heterostructures exposed to a defined amount of water vapor. In response to the adsorbed water we observe an increase of charge carriers at titanium sites. Furthermore a comparison between bulk and interface sensitive measurements indicates that the additional charge carriers are located at the interface.

[1] Ohtomo et al., Nature **427**, 423 (2004)
[2] Thiel et al., Science **313**, 1942 (2006)
[3] Xie et al., Nature Comm. **2**, 494 (2011)
[4] Bristowe et al., Phys. Rev. B **83**, 205405 (2011)

TT 40.53 Wed 15:00 Poster D

**Localized and delocalized interface states in $LaAlO_3/SrTiO_3$ heterostructures as probed by resonant inelastic x-ray scattering** — •Florian Pfaff[1], Hidenori Fujiwara[2], Yoshito Nishitani[3], Yoshihisa Harada[4], Shigemasa Suga[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg — [2]Graduate School of Engineering Science, Osaka University — [3]Department of Physics, Konan University — [4]Institute for Solid State Physics, University of Tokyo

The interface between the two band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) hosts a two-dimensional electron system of *itinerant* charge carriers above a critical LAO overlayer thickness of 3 monolayers. Interface ferromagnetism coexisting with superconductivity has been found and attributed to *local* moments. Recently, two peaks in resonant inelastic x-ray scattering (RIXS) indeed have been correlated with *delocalized* and *localized* charge carriers [1]. To shed light on the coexistence of the two types of Ti 3d carriers we performed RIXS on LAO/STO heterostructures with different overlayer thicknesses and different concentrations of oxygen vacancies. While there is an in-

crease of the total charge seen in RIXS with increasing film thickness for samples showing the critical thickness behavior, surprisingly, the spectrum remains unchanged for samples that have been intentionally doped with oxygen vacancies. We discuss this in terms of the electronic reconstruction scenario and a possible non equilibrium situation due to the generation of electron-hole pairs during irradiation.

[1] Ke-Jin Zhou et al., Phys. Rev. B 83, 201402(R) (2011)

TT 40.54 Wed 15:00 Poster D

**Growth and physical properties of $La_8Cu_7O_{19}$ single crystals** — •Ashwin Mohan[1], Surjeet Singh[2], Wolf Schottenhamel[1], Giacomo Prando[1], Sven Partzsch[1], Valentina Bisogni[1], Abdel-Hafez Mahmoud[1], Jochen Geck[1], Sabine Wurmehl[1], Christian Hess[1], and Bernd Büchner[1] — [1]IFW Dresden, Germany — [2]IISER Pune, India

Spin ladder compounds are valuable in understanding the physics of crossover from one dimensional to the two dimensional nature of spin systems. They have been known to show interesting magnetic ground states and even superconductivity upon doping. Gapped and ungapped spin excitation spectra have been predicted and experimentally verified for spin ladders with even and odd number of ladder-legs respectively. Therefore, this class of materials has been of particular interest in the field of low dimensional quantum magnets. It is known that in the thermodynamic phase diagram of $La_2O_3$-CuO there exists a compound whose spin structure resembles that of a five leg ladder, though there has not been much progress towards understanding its magnetism as it is challenging to grow it as a single crystal. Here, we have used the travelling floating zone method to grow single crystals of $La_8Cu_7O_{19}$ and measured some of its physical properties. This compound magnetically orders below 103K and shows anisotropic magnetic behavior, the nature of which is not yet clear.

TT 40.55 Wed 15:00 Poster D

**Phase diagram of the effective Ising spin-1/2 chain compound $CoNb_2O_6$ in transverse magnetic field** — •Simon Scharffe, Oliver Breunig, Johanna Frielingsdorf, Martin Valldor, Markus Garst, Eran Sela, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

$CoNb_2O_6$ is a model system to investigate the quantum phase transition of Ising spins in a transverse magnetic field. The interesting physics exclusively takes place within the magnetic $CoO_6$ layers, separated by non-magnetic $NbO_6$ layers. The edge-sharing oxygen octahedrons link the $Co^{2+}$spins and form 1D ferromagnetic chains along the $c$ axis. Due to crystal field effects an easy-axis anisotropy is present, which leads to an effective spin-1/2 system described by the Ising model. Small inter-chain couplings $J_{||} \approx 0.01 \cdot J_{\perp}$ cause long-range antiferromagnetic order, which is incommensurate below $T_{N1}$=2.95 K and becomes commensurate at $T_{N2}$=1.97 K. A magnetic field parallel to the $b$ axis is normal to the easy axis and allows to study the quantum phase transition in transverse field. Above 5 T the system is driven through its quantum critical point to a quantum paramagnet. Only few studies of the transverse field case are available. We present measurements of specific heat and magnetization in a temperature range from about 0.3 up to 10 K and discuss the phase diagram. We compare our measurements with the theoretical predictions of the 1D Ising model in a transverse field.

This work was supported by the DFG through SFB 608.

TT 40.56 Wed 15:00 Poster D

**Coexistence of anomalous and normal diffusion in integrable Mott insulators** — •Robin Steinigeweg[1,2], Jacek Herbrych[2], Peter Prelovšek[2], and Marcin Mierzejewski[3] — [1]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig — [2]Department of Theoretical Physics, Jožef Stefan Institute, SI-1000 Ljubljana — [3]Institute of Physics, University of Silesia, PL-40-007 Katowice

We study the finite-momentum spin dynamics in the one-dimensional XXZ spin chain within the Ising-type regime at high temperatures using density autocorrelations within linear response theory and real-time propagation of nonequilibrium densities. While for the nonintegrable model results are well consistent with normal diffusion, the finite-size integrable model unveils the coexistence of anomalous and normal diffusion in different regimes of time. In particular, numerical results show a Gaussian relaxation at smallest nonzero momenta which we relate to nonzero stiffness in a grand canonical ensemble. For larger but still small momenta normal-like diffusion is recovered. Similar results for the model of impenetrable particles also help to resolve rather conflicting conclusions on transport in integrable Mott insulators.

TT 40.57 Wed 15:00 Poster D

**Quantum phases of a frustrated four-leg spin tube** — Marcelo Arlego[1], Wolfram Brenig[2,3], •Yousef Rahnavard[2,3], Björn Willenberg[2,3], Hector Rosales[1], and Gerardo Rossini[1] — [1]Departamento de Fisica, Universidad Nacional de La Plata, C.C. 67, 1900 La Plata, Argentina — [2]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — [3]Niedersächsische Technische Hochschule, NTH

We study the ground state phase diagram of a frustrated spin-1/2 four-leg tube. Using a variety of complementary techniques, namely density matrix renormalization group, exact diagonalization, Schwinger boson mean field theory, quantum Monte-Carlo and series expansion, we explore the parameter space of this model in the regime of all-antiferromagnetic exchange. In contrast to unfrustrated four-leg tubes we uncover a rich phase diagram. Apart from the Luttinger liquid fixed point in the limit of decoupled legs, this comprises several gapped ground states, namely a plaquette, an incommensurate, and an antiferromagnetic quasi spin-2 chain phase. The transitions between these phases are analyzed in terms of total energy and static structure factor calculations and are found to be of (weak) first order. Despite the absence of long range order in the quantum case, remarkable similarities to the classical phase diagram are uncovered, with the exception of the icommensurate regime, which is strongly renormalized by quantum fluctuations. In the limit of large leg exchange the tube exhibits a deconfinement cross-over from gapped magnon like excitations to spinons.

TT 40.58 Wed 15:00 Poster D

**Tuning frustrated antiferromagnetism in intermetallic $AFe_4X_2$ systems** — •Katharina Weber[1,2], Nandang Mufti[1], Til Goltz[2], Theo Woike[3], Hans-Henning Klauss[2], Christoph Bergmann[1], Inga Kraft[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, Dresden University of Technology, Dresden, Germany — [3]Institute for Structural Physics, Dresden University of Technology, Dresden, Germany

Magnetic systems with reduced dimensionality or frustration are attracting strong interest because these features lead to an increase of quantum fluctuations which often results in unusual, very interesting properties. Here we present a detailed study of the intermetallic $AFe_4X_2$ compounds ($A$ = Sc, Y, Lu, Zr; X = Si, Ge) crystallizing in the $ZrFe_4Si_2$ structure type in which the Fe-sublattice is formed by chains of edge-linked tetrahedra. We synthesized polycrystalline samples of all these compounds and investigated their magnetic, thermodynamic, structural and transport properties. Our results indeed evidence this family of compounds to cover the whole regime from frustrated antiferromagnetic (AFM) order up to the quantum critical point separating the AFM ground state from the paramagnetic ground state. All compounds with trivalent $A$ elements show frustrated AFM order. Replacement of trivalent $A$ by tetravalent Zr shifts the system towards an unstable magnetic state. Since $YFe_4Si_2$ and $ZrFe_4Si_2$ present peculiar features, we also studied the influence of different annealing conditions and slight off-stoichiometry on their unusual properties.

TT 40.59 Wed 15:00 Poster D

**Phase Space Berry Phases and Electronic Transport in Magnetic Whirl Structures** — •Robert Bamler and Achim Rosch — Universität zu Köln, Cologne, Germany

We present a semi-classical theory of electronic transport in magnetic whirl structures with spin-orbit coupling. Our theory predicts that the magnetic whirls carry an electric charge due to a non-vanishing Berry phase curvature in phase space.

In magnetic materials without inversion symmetry (e.g. MnSi), the spin-orbit coupling can lead to smooth whirls (skyrmions) in the magnetization. The magnetic whirls give rise to an emergent magnetic field that can be measured as a so-called "topological" contribution to the Hall signal. The emergent magnetic field is usually explained with the picture that conduction electrons that transverse the system pick up a Berry phase because their spin follows adiabatically the direction of the local magnetization. This explanation neglects the influence of spin-orbit coupling. However, the anomalous Hall effect in MnSi is known to be large, indicating that spin-orbit coupling may be relevant in this material.

In our work, we develop a semi-classical theory of electronic trans-

port in magnetic whirl structures under the influence of spin-orbit coupling. In addition to the emergent magnetic field and the anomalous velocity known from the anomalous Hall effect, new cross-terms arise in the equations of motion and the skyrmions acquire an electric charge due to Berry phases picked up on closed trajectories in mixed coordinate and momentum space.

TT 40.60 Wed 15:00 Poster D

**Transverse susceptibility of high-quality single crystal MnSi** — •Felix Rucker[1], Andreas Bauer[1], Alfonso Chacón[1], Maximilian Hirschberger[2,1], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik-Department E21, D-85748 Garching, Germany — [2]Department of Physics, Princeton University, Jadwin Hall, Princeton, USA

We have developed a bespoke ac susceptometer which is mounted to a computer controlled rotator. Our susceptometer permits low temperature measurements in applied magnetic fields as a function of angle ranging from a purely longitudinal to a purely transverse set up, i.e., the excitation field may be varied from a parallel to a perpendicular orientation with respect to the applied field, respectively. To demonstrate the operation of our susceptometer we have measured the ac susceptibility of high-quality single crystal MnSi, which reveals several unexpected features of the transverse susceptibility across the magnetic phase diagram. We discuss our results in the context of the comprehensive theoretical framework developed for the helical order and field-induced phases in B20 compounds.

TT 40.61 Wed 15:00 Poster D

**Linear magnetoelectric effects in the cubic ferrimagnetic helimagnet $Cu_2OSeO_3$: phenomenological theory** — Maria Eleni Belesi[1,2], •Ioannis Rousochatzakis[2], Mohamed Abid[1,3], Ulrich Rössler[2], Helmut Berger[1], and Jean-Philippe Ansermet[1] — [1]Institut de Physique de la Matiére Condensée, Ecole Polytechnique Fédérale de Lausanne, Station 3, CH-1015 Lausanne-EPFL, Switzerland — [2]Leibniz Institute for Solid State and Materials Research, Helmholtzstrasse 20, 01069 Dresden, Germany — [3]King Saud University, Riyadh 11451, Saudi Arabia

We present a phenomenological Landau-Ginzburg theory for the linear magnetoelectric (ME) effect in the spin 1/2 compound $Cu_2OSeO_3$. Single-crystal ME data show two additional phases below the 3up-1down ferrimagnetic state. We demonstrate that these are related to the field-driven evolution of a long-period helical phase, which is stabilized by the chiral Dzyaloshinskii-Moriya term $D\mathbf{M}\cdot(\nabla\times\mathbf{M})$ that is present in this noncentrosymmetric compound. The theory is in excellent agreement with experiment, and shows three main features: (i) the polarization P has a uniform as well as a long-wavelength component that follows the magnetic twisting; (ii) the uniform component points along $(H_yH_z, H_zH_x, H_xH_y)$; and (iii) its strength is proportional to $\eta_\parallel^2-\eta_\perp^2/2$, where $\eta_\parallel$ and $\eta_\perp$ are the longitudinal and transverse components of the magnetic order. Hence, the field dependence of P provides a clear signature of the evolution of a conical helix under a magnetic field. A similar theory is discussed for the magnetocapacitance.

TT 40.62 Wed 15:00 Poster D

**Skyrmionic exictations in magnetoelectric $Cu_2OSeO_3$** — •Steffen Harms[1], Maria Belesi[2], Helmuth Berger[3], Jean-Philippe Ansermet[3], Christoph Grams[1], Daniel Niermann[1] und Joachim Hemberger[1] — [1]2. Physikalisches Institut, University of Cologne, Germany — [2]Leibniz Institute for Solid State and Material Research, Dresden, Germany — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Skyrmions are topologically protected spin textures that can be characterized by their winding number. Since their discovery in MnSi, skyrmions are of special interest because of their high potential for applications in spintronics [1]. The magnetoelectric helimagnetic insulator $Cu_2OSeO_3$ undergoes a phase transition from the helical magnetic phase into the skyrmion phase at 57.5 K around 200 Oe. It was recently shown, that the excitation of these phases can be seen in the microwave absorption spectra where an AC magnetic field was coupled to the sample [2]. We present the results of our broadband dielectric spectroscopy measurements up to 4 GHz, in which we measured the excitiations created by coupling an AC electric field to the sample for different magnetic fields at fixed temperatures of 57.5 K and 40 K.

Work supported by the DFG through SFB 608.

[1] C. Pfleiderer and A. Rosch., Nature 465, 880 (2010)
[2] Y. Onose et al., Phys. Rev. Lett. 109, 037603 (2012)

TT 40.63 Wed 15:00 Poster D

**Vibrating-coil magnetometry in rare-earth pyrochlore compounds** — •Christopher Krey[1], Stefan Legl[1], Sarah R. Dunsiger[1], Jason S. Gardner[2], Jennifer M. Roper[3], Hanna A. Dabkowska[4], Jose A. Rodriguez[5], Graeme M. Luke[5], and Christian Pfleiderer[1] — [1]Physik-Department E21, Technische Universität München, Garching — [2]Department of Physics, Indiana University, Bloomington, USA — [3]Los Alamos National Laboratory, New Mexico, USA — [4]Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada — [5]Department of Physics and Astronomy, McMaster University, Hamilton, Canada

An important characteristic of the spin ice systems $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ as well as the spin liquid system $Tb_2Ti_2O_7$ is the observation of spin freezing below a few hundred mK. We report vibrating coil magnetometry down to mK temperatures of these systems, addressing the evidence for field-induced transitions [1,2]. Of particular interest is evidence of putative magnetisation avalanches in the spin-frozen state, which for the case of $Dy_2Ti_2O_7$ have been interpreted as magnetic monopole avalanches [3].

[1] C. Krey *et al.*, Phys. Rev. Lett. **108**, 257204 (2012)
[2] S. Legl *et al.*, Phys. Rev. Lett. **109**, 047201 (2012))
[3] D. Slobinsky *et al.*, Phys. Rev. Lett. **105**, 267205 (2010)

TT 40.64 Wed 15:00 Poster D

**Versatile module for fast experiments with focussing neutron guides** — •Tim Adams[1], Georg Brandl[1], Alfonso Chacon[1], Marein Rahn[1], Sebastian Mühlbauer[2], Robert Georgii[2], Peter Böni[1], and Christian Pfleiderer[1] — [1]Physik-Department E21, Technische Universität München, 85748 Garching — [2]ZWE FRM II, Technische Universität München, 85748 Garching

We report the development of a versatile module that permits fast and reliably the use of focussing neutron guides. We report the procedure of setting up the instrument and typical artefacts under non-ideal conditions. Exploiting gain factors of intensity by an order of magnitude we demonstrate the functionality of the module in a study of the effects of uniaxial stress on the spin-flip transition in single crystal Cr.

TT 40.65 Wed 15:00 Poster D

**Preparation and characterization of doped spin ice** — •Peter Laschitzky, Martin Hiertz, Oliver Breunig, Gerhard Kolland, Johanna Frielingsdorf, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

The magnetic Dy sites in $Dy_2Ti_2O_7$ form a pyrochlore lattice consisting of corner-sharing tetrahedra. A strong crystal field results in an Ising anisotropy of the magnetic moments of the Dy site which align along their local easy axes in the {111} directions pointing either into or out of the tetrahedra. As a consequence, the spin system is geometrically frustrated even in the groundstate. The magnetic excitations in spin ice are discussed as magnetic monopoles. We synthesized the mother compound $Dy_2Ti_2O_7$ and the doped compounds $Dy_{2-x}Y_xTi_2O_7$ with $x = 0.1, 0.2, 1, 2$ and $Dy_2Ti_{1.8}Zr_{0.2}O_7$. Large, high-quality single crystals were grown by the floating-zone method. To characterize the grown crystals, we measured the magnetization, the specific heat and the thermal conductivity for various magnetic-field directions. Doping with non-magnetic Y has a strong influence on the magnetic subsystem. For example, the magnetic contribution $\kappa_{\mathrm{mag}}$ to the thermal conductivity[1] can be completly suppressed by Y doping. Substitution of the non-magnetic Ti by larger Zr ions reduces the phononic thermal conductivity, whereas the magnetic contribution is essentially conserved.

Supported by the DFG through SFB 608

[1] Kolland *et. al.*, Phys. Rev. B **86**, 060402 (2012)

TT 40.66 Wed 15:00 Poster D

**Investigations of the Magnetic Properties in the Pyrochlore $Ho_2Ti_2O_7$** — •Rico Schönemann[1], Thomas Herrmannsdörfer[1], Elizabeth Lauren Green[1], Richard Skrotzki[1,2], Zhaosheng Wang[1], Hiroshi Kaneko[3], Haruhiko Suzuki[3], and Joachim Wosnitza[1] — [1]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Chemistry and Food Chemistry, TU Dresden, Dresden, Germany — [3]Faculty of Mathematics and Physics, Kanazawa University, Kanazawa, Japan

Pyrochlore compounds such as $R_2Ti_2O_7$ (where $R$ is Ho or Dy) have an highly degenerate ground state where the $R^{3+}$ moments obey the "ice rules". This provides access to study extraordinary physical phenom-

ena, like the formation of magnetic monopoles. Recent publications evidence monopoles which can be probed using high frequency (adiabatic) susceptibility measurements [1]. We performed ac susceptibility measurements on a single-crystal $Ho_2Ti_2O_7$ sample at low temperatures down to 30 mK and magnetic fields up to 14 T. Based on isothermal frequency sweeps we were able to determine spin relaxation rates. Both the real and imaginary parts of the temperature-dependent magnetic susceptibility measurements show the spins freezing below 1 K and provide insight into the magnetic-monopole density.

This research has been funded in part by EuroMagNET II (EU contract No. 228043).

[1] L. Bovo et al., arXiv:1210.0106v1 (2012)

TT 40.67 Wed 15:00 Poster D

**Thermodynamic properties of spin-S boundary defects in antiferromagnetic Heisenberg chains** — •Björn Willenberg[1,3], Jan Grelik[2,3], Wolfram Brenig[1,3], and Holger Frahm[2,3] — [1]Institute for Theoretical Physics, Technische Universität Braunschweig — [2]Institute for Theoretical Physics, Leibniz Universität Hannover — [3]Niedersächsische Technische Hochschule, NTH

We investigate magnetic spin-S impurities in contact to isotropic and anisotropic S=1/2 Heisenberg chains with open boundary conditions and an impurity coupling beyond simple superexchange. We employ finite temperature Quantum Monte-Carlo methods based on Stochastic Series Expansion. Results will be presented for thermodynamic properties as functions of temperature, exchange-coupling constants, anisotropy, magnetic fields, and system size. For particular choices of parameters the models we investigate are exactly solvable by means of Bethe Ansatz techniques which will be used to obtain quantities like energy, magnetization, and susceptibility at zero temperature. In this limit we will compare our findings from both methods.

TT 40.68 Wed 15:00 Poster D

**Optical phonons in multiferroic $CuCrO_2$, studied by Raman and Far-Infrared spectroscopy** — •Michael Eichberger[1], Jean Geurts[1], Michael Schmidt[2], Vladimir Tsurkan[2,3], and Joachim Deisenhofer[2] — [1]Institute of Physics, University of Würzburg, Germany — [2]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [3]Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Moldova

$CuCrO_2$ is an example for a multiferroic material, in which the ferroelectric order is driven by a proper-screw type magnetic order, occurring below $T_N \sim 24$ K. While the magnetic order and its coupling with the ferroelectricity has been in the focus of most research activities on this system, we investigated the optical phonons and the possible effect of spin ordering, employing Raman and FIR spectroscopy. As the $CuCrO_2$ crystal structure (space group $R\bar{3}m$) has an inversion centre, Raman spectroscopy gives access to the g-modes, while FIR probes the u-modes. All expected optical modes ($A_{1g}$, $E_g$, $2A_{2u}$, $2E_u$) were observed. No mode splitting or emergence of new modes occurs when entering the magnetically ordered state. The $E_g$ mode shows a slight softening in the low temperature range, which may indicate a weak spin-phonon coupling. This mode is modulating the Cr-O bonding and thereby affecting the overlap of the participating wavefunctions. At the same time, this overlap is responsible for the antiferromagnetic interaction between the Cr-atoms and hence establishing the magnetic order within the Cr-plane.

TT 40.69 Wed 15:00 Poster D

**The spin Drude weight in the spin-1/2 XXZ chain: a combined exact diagonalization and time-dependent DMRG study** — •Johannes Hauschild[1], Christoph Karrasch[2], Stephan Langer[1,3], and Fabian Heidrich-Meisner[1,4] — [1]LMU Munich — [2]University of California, Berkley — [3]University of Pittsburgh, USA — [4]FAU Erlangen-Nuremberg

Various theoretical approaches predict a finite Drude weight D for spin transport in the gapless phase of the spin-1/2 XXZ chain, suggesting ballistic transport properties. Here we address two open questions: first, the temperature dependence of the Drude weight and second, the particular point of an SU(2) symmetric exchange, for which there is no agreement as to whether D is finite or not. We compute the Drude weight at finite temperatures with two approaches [1]: time-dependent density matrix renormalization group simulations using purification [2] and exact diagonalization. For the latter, we compare finite-size data obtained in either the grand-canonical or the canonical ensemble. We argue that the grand-canonical data, obtained from averaging over all subspaces with different magnetizations, have a more systematic finite-size dependence than the canonical one. The results for D(T) from exact diagonalization and tDMRG are in good quantitative agreement in the massless phase.

We acknowledge support from the DFG through FOR 912.

[1] C. Karrasch, J. Hauschild, S. Langer, F. Heidrich-Meisner, in preparation
[2] C. Karrasch, J. H. Bardarson, and J. E. Moore, Phys. Rev. Lett. 108, 227206 (2012)

TT 40.70 Wed 15:00 Poster D

**Kinetic description of the thermalization dynamics of weakly interacting quantum systems** — •Michael Stark and Marcus Kollar — Theoretical Physics III, Center for electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg

After a sudden disruption, weakly interacting quantum systems first relax to a prethermalized state [1] that can be described by perturbation theory and a generalized Gibbs ensemble [2]. Using these properties of the prethermalized state we perturbatively derive a kinetic equation which becomes a quantum Boltzmann equation in the scaling limit of vanishing interaction [3]. Applying this to interaction quenches in the fermionic Hubbard model [4] we find that the momentum distribution relaxes to the thermal prediction of statistical mechanics. For not too large interaction, this two-stage scenario can thus provide a quantitative understanding of the time evolution leading from a pure initial state to the thermal state.

[1] M. Moeckel and S. Kehrein, PRL **100**, 175702 (2008); Ann. Phys. (New York) **324**, 2146 (2009)
[2] M. Kollar, F. A. Wolf, and M. Eckstein, PRB **84**, 054304 (2011)
[3] L. Erdös, M. Salmhofer, H.-T. Yau, J. Stat. Phys. **116**, 367 (2004)
[4] M. Eckstein, M. Kollar, and P. Werner, PRL **103**, 056403 (2009); PRB **81**, 115131 (2010)

TT 40.71 Wed 15:00 Poster D

**Quasiparticle parameterization of meanfields, Galilean invariance and universal conserving response function** — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP), Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The form of meanfield and density functional parameterization in terms of current, energy and density are examined by the restriction of Galilean invariance. It is found that besides a density functional only one parameter remains which is usually condensed in the effective mass. The universal response with respect to density, momentum and energy is found in the sense that the response becomes independent on actual parameterization of the local equilibrium provided the conservation laws are enforced. The sum rules by frequency moments and the compressibility sum rule impose further restrictions which determines the last parameter.

TT 40.72 Wed 15:00 Poster D

**Electronic structure of Cu: An LDA+DMFT approach** — •Kathrin Garb[1], Wilhelm Appelt[1], Joseph-Andreas Weber[2], Michael Leitner[3], Christoph Hugenschmidt[2,4], Peter Böni[2], Igor Di Marco[5], and Liviu Chioncel[6,1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Technische Universität München, Physik Department E21, D-85748 Garching, Germany — [3]Technische Universität München, Physik Department E13, D-85748 Garching, Germany — [4]Technische Universität München, FRM II, 85747 Garching, Germany — [5]Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120, Uppsala, Sweden — [6]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

Although DFT calculations predict the overall band structure of Cu correctly, the entire d-bands' manifold is experimentally found at energies about 0.5 eV lower than the calculated ones. We apply state-of-the-art LDA+DMFT calculations and discuss several technical aspects of the implementation that can be used to explain the picture of weak correlation provided by the Fermi surface results with the intrinsic in-band shift of 0.5 eV.

TT 40.73 Wed 15:00 Poster D

**Electronic correlations in FeAl: an LDA+DMFT study**

— •Anna Galler[1], Ciro Taranto[1], Merzuk Kaltak[2], Giorgio Sangiovanni[3], Alessandro Toschi[1], Georg Kresse[2], and Karsten Held[1] — [1]Institut für Festkörperphysik, Technische Universität Wien, Vienna, Austria — [2]Department of Computational Materials Physics, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We applied the local density approximation combined with dynamical mean-field theory (LDA+DMFT) to the intermetallic compound FeAl. This material shows unexpected magnetic properties. In fact, experimentally it is known to be nonmagnetic while conventional LDA calculations give a ferromagnetic solution.

We claim that this feature is an effect of nontrivial electronic correlations due to the presence of narrow Fe d bands at the Fermi level. The low energy part of the Hamiltonian was projected onto a set of 9 maximally localized Wannier orbitals, and the interaction parameters were computed using the constrained random-phase approximation (cRPA) approach. A continuous-time quantum Monte Carlo in the hybridization expansion was used as impurity solver for the DMFT. In analogy with the iron pnictides, our results show the important role played by the Hund's coupling, that places FeAl in the class of the so called Hund's metals.

TT 40.74 Wed 15:00 Poster D

**The LDA+RISB and LDA+DMFT method: A juxtaposition** — •Christoph Piefke[1], Daniel Grieger[1,2], and Frank Lechermann[1] — [1]1. Institut für Theoretische Physik, Universität Hamburg, Germany — [2]SISSA, via Bonomea 265, 34136 Trieste, Italy

The LDA+RISB (Rotationally Invariant Slave Bosons) and LDA+DMFT (Dynamical Mean-Field Theory) methods are nowadays well established tools describing effects of strong electronic correlations in realistic materials from first principles. Their general concept is to add many-body physics to effective one-particle band structure calculations. Both of them have specific advantages and disadvantages concerning accuracy, numerical efficiency and types of physical effects that can be described. This presentation aims at giving an overview of the theoretical and technical details of both LDA+methods in question, as well as showing the respective strengths and problems via comparing results for a selection of materials. Special attention is given to charge self-consistency[1], which allows for a direct feedback of the respective many-body method onto the LDA part.

[1] D. Grieger, C. Piefke, O. E. Peil and F. Lechermann, Phys. Rev. B 86, 155121 (2012)

TT 40.75 Wed 15:00 Poster D

**Variational Cluster Approximation for broken symmetry phases in strongly correlated electron systems** — •Benjamin Lenz, Piet Dargel, and Thomas Pruschke — Institut für theoretische Physik, Georg-August-Universität, 37077 Göttingen, Germany

The variational cluster approximation (VCA) allows to study broken symmetry phases of various lattice models at zero temperature. We present results for s-type superconductivity of the attractive two-dimensional Hubbard model in the infinite-cluster size limit of VCA. They are discussed in comparison to results from dynamical mean-field theory in combination with the numerical renormalization group method. As a second example, we give an outlook to the investigation of antiferromagnetism and superconductivity in a paradigmatic model for heavy fermions – the Kondo lattice model.

TT 40.76 Wed 15:00 Poster D

**Quantification of correlations in an exactly solvable model of harmonically interacting particles** — Jan Skolimowski[1], •Krzysztof Byczuk[1], and Dieter Vollhardt[2] — [1]Faculty of Physics, University of Warsaw, Hoza 69, 00-681 Wrszawa, Poland — [2]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We employ the relative von Neumann entropy to quantify correlations in a system of interacting particles. The interaction between the particles is harmonic potential-like, making the model exactly solvable. The exact expression for the relative entropy is expanded in the coupling constant, which allows us to classify the different contributions to correlations in terms of Feynman diagrams or correlation functions.

TT 40.77 Wed 15:00 Poster D

**A slave rotor approach to the dynamical screening of Coulomb interactions** — •Igor Krivenko[1,2], Silke Biermann[2], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany — [2]Centre de Physique Théorique (CPHT), École Polytechnique, 91128 Palaiseau Cedex, France

We present a new theoretical approach to lattice and impurity models of strongly correlated electrons with the dynamically screened Coulomb interactions. The method is based on a slave rotors decoupling of the screened interaction and provides a consistent description of quantum impurities with both fermionic and bosonic bath. It is shown, that the simplest meaningful approximation within this method coincides with the dynamic atomic limit approximation (DALA). More refined approximations beyond DALA are constructible in a regular way using a saddle-point or perturbative treatment of the rotor degrees of freedom. The proposed method gives a computationally cheap way to apply existing quantum impurity solvers for unscreened static interactions to the cases of frequency-dependent interactions. It allows to calculate thermal Green's functions and higher-order correlation functions of the impurity models. These functions then can be used as building blocks of modern perturbative approaches to lattice models involving phonons, magnons and other bosonic excitations.

TT 40.78 Wed 15:00 Poster D

**Functional RG study of Goldstone fluctuations in the ground state of a fermionic superfluid** — •Benjamin Obert, Christoph Husemann, and Walter Metzner — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

We analyse the effect of Goldstone fluctuations in the superfluid ground state of the attractive Hubbard model. We apply a coupled bosonic-fermionic functional renormalization group approach to investigate the infrared behaviour in the symmetry-broken state. Bosonic fluctuations, especially Goldstone fluctuations lead to several divergencies in the infrared, which partially cancel due to symmetry. Our results capture the exact infrared behaviour of the interacting Bose gas.

TT 40.79 Wed 15:00 Poster D

**Two-particle Green functions calculated by continuous time quantum Monte Carlo simulations** — •Markus Wallerberger[1], Emanuel Gull[2], Nico Parragh[3], Giorgio Sangiovanni[3], Alessandro Toschi[1], and Karsten Held[1] — [1]Technische Universität Wien, Austria — [2]University of Michigan, Ann Arbor MI, USA — [3]Universität Würzburg, Germany

While dynamical mean field theory (DMFT) has provided fundamental insights into the physics of strongly correlated materials, its approximations break down in low dimensional systems and near second-order phase transitions. Diagrammatic extensions of DMFT like the dynamical vertex approximation (DΓA) and the dual fermion approach which attempt to tackle this problem have the local two-particle Green function as central ingredient. Besides, this quantity is also needed for vertex corrections to response functions.

A state-of-the-art method for solving the DMFT impurity problem is the continuous-time quantum Monte Carlo (CT-QMC) method in its hybridization expansion formulation (CT-HYB). The sheer amount of information encoded in two-particle quantities, however, makes their computation very demanding in this framework. We improve on the naïve measurement by using fast Fourier transformations as well as symmetries of the Hamiltonian and of the vertex. We have implemented this method into the CT-HYB solver [1] using the Krylov method and provide benchmarks and examples for up to seven correlated orbitals.

[1] N Parragh et al., arXiv:1209.0915v1

TT 40.80 Wed 15:00 Poster D

**Reduced Density Matrix Functional Theory- A suitable vehicle to import explicit correlations** — •Ebad Kamil[1], Thomas Pruschke[1], and Peter E. Bloechl[2] — [1]Institute for Theoretical Physics, University of Goettingen, Goettingen, Germany — [2]Institute for Theoretical Physics, Clausthal University of Technology, Clausthal, Germany

A variational formulation for the calculation of interacting fermions system based on density matrix functional theory is presented. This formulation allows importing explicit many particle effects into standard density functional theory based calculations and also avoids ambiguities of double counting terms inherent to other approaches. Local approximation for explicit correlations is introduced and the resulting local density matrix functional is calculated using resolvent expansion/Quantum Master equation technique developed in the field of

Open quantum system.

TT 40.81 Wed 15:00 Poster D

**Measurement of the full three-dimensional Fermi surface at room temperature by angular correlation of positron annihilation radiation** — •Josef Andreas Weber[1], Hubert Ceeh[1], Liviu Chioncel[4], Kathrin Anna Garb[4], Christoph Hugenschmidt[1,3], Michael Leitner[2], and Peter Böni[1] — [1]Technische Universität München, Physik Department E21, D-85748 Garching, Germany — [2]Technische Universität München, Physik Department E13, D-85748 Garching, Germany — [3]FRM II, Technische Universität München, D-85747 Garching, Germany — [4]University of Augsburg, Theoretical Physics III, D-86135 Augsburg, Germany

The two-dimensional measurement of the angular correlation of the positron annihilation radiation (2D-ACAR) is a powerful tool to investigate the electronic structure of materials. Here we present the full three-dimensional Fermi surface obtained by temperature dependent 2D-ACAR measurements in combination with common reconstruction algorithms. Although copper is believed to be a well understood system we find discrepancies between measurement and recent ab-initio calculations.

TT 40.82 Wed 15:00 Poster D

**Development of high frequency measurement methods for Fermi surface studies under high pressure** — •Hui Chang, Sven Friedemann, and Malte Grosche — Cavendish Laboratory, J J Thomson Avenue, Cambridge CB3 0HE, UK

The observation of quantum oscillatory phenomena in high magnetic field, for example of the electrical resistivity (Shubnikov-de Haas), can help resolve the electronic structure of challenging materials. Important progress is expected in a number of areas of current interest, when the Fermi surface can be tracked near to or across pressure and field-induced quantum phase transitions. These include Mott metal-insulator transitions, magnetic or charge density wave transitions and the orbitally selective Mott transition - or Kondo volume collapse - discussed in f-electron metals.

High sensitivity measurements at elevated pressures in anvil cells are hindered by the need to make reliable and robust high quality contacts to submillimetre samples. Radio frequency tank oscillator methods based on tunnel diode or proximity detector based circuits offer an attractive alternative, because they avoid the need to make contacts and at the same time offer supreme relative sensitivity. Further simplification is possible by patterning the detection coil onto the high pressure anvils[1]. We present recent progress in developing such contactless methods for use in high pressure cells and illustrate this by test measurements of quantum oscillations in low carrier density materials.

[1] O. P. Welzel and F. M. Grosche, Rev. Sci. Instrum. 82, 033901 (2011)

TT 40.83 Wed 15:00 Poster D

**Electron-hole pair condensation at the semimetal-semiconductor transition: a BCS-BEC crossover scenario** — •Holger Fehske[1], Bernd Zenker[1], Franz Xaver Bronold[1], Dieter Ihle[2], Van-Nham Phan[3], and Klaus Becker[4] — [1]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, D-17487 Greifswald — [2]Institut für Theoretische Physik, Universität Leipzig, D-04109 Leipzig — [3]Institute of Physics, Vietnamese Academy of Science and Technology, PO Box 429, 10000 Hanoi — [4]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden

We act on the suggestion that an excitonic insulator state might separate - at very low temperatures - a semimetal from a semiconductor and ask for the nature of these transitions. Based on a detailed analysis of electron-hole pairing in the extended Falicov-Kimball model, we show that tuning the Coulomb attraction between both species, a continuous crossover between a BCS-like transition of Cooper-type pairs and a Bose-Einstein condensation of preformed tightly-bound excitons might be achieved in a solid-state system. The precursor of this crossover in the normal state might cause the transport anomalies observed in several strongly correlated mixed-valence compounds.

TT 40.84 Wed 15:00 Poster D

**Coexistance of phase transition and hysteresis near BEC** — •Michael Maennel[1], Klaus Morawetz[1,2,3], and Pavel Lipavsky[4] — [1]Muenster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP), Federal University of Rio Grande do Norte, Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [3]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

Multiple phases occurring in a Bose gas with finite-range interaction are investigated. In the vicinity of the onset of Bose-Einstein condensation (BEC) the chemical potential and the pressure show a van-der-Waals like behavior indicating a first-order phase transition although there is no long-range attraction. Furthermore the equation of state becomes multivalued near the BEC transition. For weak interactions described by a hard-sphere (Hartree-Fock) or Popov (Hartree-Fock-Bogoliubov) approximation such a multivalued region can be avoided by the Maxwell construction. However, for strong interaction described by the many-body T-matrix there remains a multivalued region even after a Maxwell construction which is interpreted as a density hysteresis. This unified treatment becomes possible due to the recently found scheme to eliminate self-interaction in the T-matrix approximation which allows to calculate properties below and above the critical temperature.

TT 40.85 Wed 15:00 Poster D

**Anisotropic superfluidity of bosons in optical Kagome superlattice** — •Xuefeng Zhang[1], Tao Wang[1], Axel Pelster[2], and Sebastian Eggert[1] — [1]Department of the Physics,Univ. Kaiserslautern, Kaiserslautern, Germany — [2]Hanse-Wissenschaftskolleg, Germany

We study the quantum phase transitions for the extended Bose-Hubbard model with bosons on a Kagome superlattice which can be implemented by enhancing the long wavelength laser in one direction of the optical lattice. To this end we combine the virtues of a Mean-Field theory with the Laudau theory and work out of a decoupled effective potential method by comparing the corresponding analytic results with extensive quantum Monte Carlo simulations, we find that several striped solids emerge in this system. Due to the blockade effect of such a striped order, the resulting superfluid density turns out to be anisotropic and thus, reveal its tensional property. Finally, we discuss the complete quantum phase diagram.

TT 40.86 Wed 15:00 Poster D

**Controlled manipulations of fermionic doublon states in the Hubbard model** — •Karsten Balzer and Martin Eckstein — Max Planck Research Department for Structural Dynamics, University of Hamburg (CFEL), Building 99, Luruper Chaussee 149, 22761 Hamburg, Germany

External fields can cause interesting phases and phase transitions in strongly correlated quantum systems [1-3].

In this contribution, we study the dynamics of the Hubbard model at strong coupling and show that a specifically tailored time-dependent electric field can separate a localized doublon into two electrons with a given lattice spacing and also to gradually move one or more doublons through the lattice without destroying the spaciotemporal coherence.

Furthermore, we demonstrate that the same mechanism can be used to create a charge-ordered state (of doublons) starting from a band insulator. This may be of importance for initial state preparations, manipulations and measurements in cold-atom experiments involving optical lattices.

[1] S. Sachdev, K. Sengupta and S.M. Girvin, Phys. Rev. B **66**, 075128 (2002)
[2] J. Simon, W.S. Bakr, R. Ma, M.E. Tai, P.M. Preiss and M. Greiner, Nature **472**, 307 (2011)
[3] Ph. Werner, N. Tsuji and M. Eckstein, Phys. Rev. B **86**, 205101 (2012).

TT 40.87 Wed 15:00 Poster D

**Cooperative phenomena in superconducting atom-chips** — •Sebastian Fuchs, Björn Kubala, and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

We theoretically investigate the physics of hybrid quantum systems, where a cloud of cold atoms is coupled to superconducting microstructures, so called superconducting atom-chips. Coherent enhancement, due to the large number of atoms in the cloud, opens a path to the study of strong coupling effects, like superradiance/Dicke-physics in a decohering environment [1]. A structured environment can be designed by embedding a Cooper pair box within the cavity. Moreover, in such a

system the transfer of quantum information between the atomic cloud and the superconducting solid state system can be studied.

[1] K. Henschel, J., J. Schmiedmayer, and H. Ritsch, Phys. Rev. A **82**, 033810 (2010)

TT 40.88 Wed 15:00 Poster D

**localization-delocalization transition in double-well optical lattices** — •gang wang — Max Planck Institute for the Physics of Complex Systems

Ultracold atoms in optical lattices allow for the study of localization of quantum waves. Within the framework of 1D incommensurate optical lattice, a sharp transition from all eigenstates being extended to all being localized occurs in one dimension, so-called self-duality in the Harper model. This transition has been observed with ultracold atoms loaded in optical lattices. We investigated the localization properties of ultracold atoms loaded in double-well optical lattices, perturbed by a secondary incommensurate lattice to induce the deterministic disorder potential. We found the localization-delocalization transition qualitatively different from those of the Harper model, signaled by the appearance of energy-dependent mobility edges and broken duality.

TT 40.89 Wed 15:00 Poster D

**Negative absolute temperature for motional degrees of freedom and expansion of interacting bosons in optical lattices** — •Simon Braun[1,2], Philipp Ronzheimer[1,2], Michael Schreiber[1,2], Sean Hodgman[1,2], Daniel Garbe[1,2], Immanuel Bloch[1,2], and Ulrich Schneider[1,2] — [1]Ludwig-Maximilians-Universität München — [2]Max-Planck-Institut für Quantenoptik, Garching

Absolute temperature is usually bound to be strictly positive. However, in systems with an upper energy bound, negative absolute temperature states are possible, where the occupation probability of states increases with their energy. We realized a negative absolute temperature state for motional degrees of freedom with ultracold bosonic $^{39}$K atoms in an optical lattice, by implementing the attractive Bose-Hubbard Hamiltonian. This new state strikingly revealed itself by strong occupation peaks at maximum kinetic energy. We found that the negative absolute temperature state is close to degeneracy and as stable as the corresponding positive temperature state.

Additionally, we investigated the out-of-equilibrium expansion dynamics of interacting bosons in one- and two-dimensional Hubbard systems. We found that the fastest, ballistic expansions occur in the integrable limits. In 1D, these are both the non-interacting and the strongly interacting limit where the system enters into the hard-core boson regime. For intermediate interactions, the expansion slows down significantly. In 2D, the system expands ballistically only in the non-interacting case, and even small interactions lead to strongly diffusive behavior. We also mapped out the transition between 1D and 2D.

## TT 41: Spintronics / Quantum Information: Materials and Methods (jointly with HL)

Time: Wednesday 15:00–18:45 Location: H2

TT 41.1 Wed 15:00 H2

**Onsager relations in a two-dimensional electron gas with spin-orbit coupling** — •Cosimo Gorini[1,2], Roberto Raimondi[3], and Peter Schwab[1] — [1]Institut für Physik, Universität Augsburg — [2]CNRS and Université de Strasbourg — [3]Dipartimento di Fisica, Università di Roma Tre

Theory predicts for the two-dimensional electrons gas with only Rashba spin-orbit interaction a vanishing spin Hall conductivity and at the same time a finite inverse spin Hall effect. We show how these seemingly contradictory results are compatible with the Onsager relations: the latter do hold for spin and particle (charge) currents in the two-dimensional electron gas, although (i) their form depends on the experimental setup and (ii) a vanishing bulk spin Hall conductivity does not necessarily imply a vanishing spin Hall effect. We also discuss the situation in which extrinsic spin orbit from impurities is present and the bulk spin Hall conductivity can be different from zero.

[1] - C. Gorini, R. Raimondi, P. Schwab, arXiv:1207.1289 (to appear in PRL)

TT 41.2 Wed 15:15 H2

**On the misinterpretation of the temperature dependence of $T_2^*$ in time-resolved Faraday rotation** — •Sebastian Kuhlen[1], Ralph Ledesch[1], Carla Schenk[1], Matthias Althammer[2], Sebastian T. B. Gönnenwein[2], Matthias Opel[2], Rudolf Gross[2], and Bernd Beschoten[1] — [1]II. Physikalisches Institut A, RWTH Aachen University, Aachen — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching

Time-resolved Faraday rotation (TRFR) is a well-established optical pump probe technique to generate and to probe spin coherence in semiconductors. Spin dephasing times $T_2^*$ can easily be determined from TRFR if their values are comparable to the available pump-probe-delay. If, however, $T_2^*$ exceeds the laser repetition time resonant spin amplification (RSA) can equally be used to extract $T_2^*$. We demonstrate that in ZnO these techniques have several tripping hazards resulting in deceptive results for $T_2^*$. We show that the temperature dependence of the amplitude ratio of two separate spin species can easily be misinterpreted as a strongly temperature dependent $T_2^*$ of a single spin ensemble, while the two spin species have $T_2^*$ values which are nearly independent of temperature. Additionally, consecutive pump pulses can significantly diminish the spin polarization, which remains from previous pump pulses. While this barely affects $T_2^*$ values extracted from delay line scans, it results in seemingly shorter $T_2^*$ values in RSA.

Work supported by DFG through SPP 1285.

TT 41.3 Wed 15:30 H2

**All-electrical time-resolved spin generation and coherent spin manipulation in n-InGaAs** — •Ivan Stepanov[1,2], Sebastian Kuhlen[1,2], Manfred Ersfeld[1,2], Stefan Göbbels[1,2], Mihail Lepsa[2,3], and Bernd Beschoten[1,2] — [1]II. Physikalisches Institut, RWTH Aachen University, 52056 Aachen, Germany — [2]JARA: Fundamentals of Future Information Technology, 52074 Aachen — [3]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich

Creation and manipulation of coherent spin information by electrical means are key tasks in semiconductor spintronics.

Here we demonstrate that a coherent spin polarization can be created and manipulated by two successive electric field pulses in n- InGaAs epilayer at zero external magnetic field. The first electric pulse || $[1\bar{1}0]$ creates a current induced spin polarization (CISP) which is oriented in the plane of the sample. The subsequent electric field pulse || [110] generates a perpendicular magnetic field pulse [1] leading to a coherent precession of this spin polarization with 2-dimensional electrical control over the final spin orientation. Spin precession is measured by time-resolved Faraday rotation. We determine the build-up time of CISP during the first field pulse and extract the spin dephasing time and internal magnetic field strength during the spin manipulation pulse. The results are in good agreement with optical pump-probe experiments on the same device.

Work supported by DFG through FOR 912.

[1] S. Kuhlen *et al.*, Phys. Rev. Lett. 109, 146603 (2012).

TT 41.4 Wed 15:45 H2

**Long hole spin lifetime in InGaAs/GaAs quantum wells probed by high field cyclotron resonance spectroscopy** — •Oleksiy Drachenko[1], Dmitry Kozlov[2], Anton Ikonnikov[2], Kirill Spirin[2], Vladimir Gavrilenko[2], Harald Schneider[1], Manfred Helm[1], and Jochen Wosnitza[3] — [1]Helmholtz Zentrum Dresden Rossendorf, Inst Ion Beam Phys & Mat Res, D-01314 Dresden, Germany — [2]Russian Acad Sci, Inst Phys Microstruct, Nizhnii Novgorod 603950, Russia — [3]Helmholtz Zentrum Dresden Rossendorf, Dresden High Magnet Field Lab HLD, D-01314 Dresden, Germany

In this paper, we report long, milli-second range, hole spin relaxation time in InGaAs/GaAs quantum wells probed by cyclotron resonance-spectroscopy in high pulsed magnetic fields. In our experiments, we found strong hysteresis in the spectral weights of cyclotron resonance absorption lines when rapidly changing magnetic field is used for the experiment. The hysteresis vanishes when a much slower changing magnetic field is used. We attribute this behavior to a long energy relaxation time between two lowest spin-split hole Landau levels, i.e. a long hole spin relaxation time. We also present transition frequen-

cies calculated using a 4x4 Luttinger Hamiltonian, which confirm our findings.

TT 41.5 Wed 16:00 H2

**Magneto-optical study of the sp-d exchange interaction on 1.4 nm diameter $Mn^{2+}$ doped $(CdSe)_{13}$ clusters** — Rachel Fainblat[1], •Dino Iavarone[1], Jiwoong Yang[2], Taeghwan Hyeon[2], and Gerd Bacher[1] — [1]Werkstoffe der Elektrotechnik and CeNIDE, Universität Duisburg-Essen, Germany — [2]Nanomaterials Laboratory, Seoul National University, Korea

Magnetical doping of chemically synthesized nanostructures combines the optical and electronic properties of the host semiconductor with the magnetic characteristics of the doping ions. The mechanism of colloidal nanocrystal doping can be classified into doping at the "growth" or at the "cluster" stage and, in particular, the doping efficiency in small nanocrystals is controversially discussed. On one hand, the statistical adsorption of an impurity is expected to decrease with decreasing nanocrystal size [1], whereas a recent model points out that the dopant adsorption onto the sites of small clusters (d < 2 nm) is more efficient than the adsorption on larger nanocrystals (d > 5 nm) [2].

Here, we report on low temperature (T = 5 K) magneto-optical effects in so-called "magic size" $Mn^{2+}$ doped $(CdSe)_{13}$ clusters. Both absorption and magnetic circular dichroism (MCD) spectra are dominated by a resonance peak related to the heavy hole excitonic transition at 3.65 eV. From the pronounced MCD signal a giant Zeeman splitting of about 15 meV at 1.5 T is extracted supporting the theory that the $Mn^{2+}$ ions are doped directly into the $(CdSe)_{13}$ clusters.

[1] S. Erwin et al., Nature 436, 91-4 (2005)
[2] T. Singh et al., Appl. Phys. Lett. 100, 053105 (2012)

TT 41.6 Wed 16:15 H2

**Influence of strong quantum confinement on the magnetic dopant-carrier exchange coupling in $Mn^{2+}$ doped CdSe nanoribbons** — Rachel Fainblat[1], •Franziska Muckel[1], Julia Frohleiks[1], Jung Ho Yu[2], Jiwoong Yang[2], Taeghwan Hyeon[2], and Gerd Bacher[1] — [1]Werkstoffe der Elektrotechnik and CeNIDE, Universität Duisburg-Essen, Germany — [2]Nanomaterials Laboratory, Seoul National University, Korea

Key materials for future spintronic applications might be magnetically doped semiconductors with a substantial coupling between the dopants and charge carriers of the host semiconductor. This interaction is expected to be significantly altered by quantum confinement, an issue which is controversially discussed since more than a decade.

Here, we report on a clear evidence of a quantum confinement induced modification of both, s-d and s-p exchange interaction in two dimensional 1.4 nm thick $Mn^{2+}$ doped CdSe quantum nanoribbons [1]. Both absorption and magnetic circular dichroism spectra are dominated by spectrally well-separated resonance peaks related to the heavy and the light hole excitonic transition. This allows a separate study of the s-d and the p-d exchange interaction constants. Taking into account the optical selection rules and the statistical orientation of the nanoribbons on the substrate, a remarkable change of the s-d exchange constant with respect to bulk is indicated. Room-temperature studies revealed an unusually high effective g-factor up to ∼13 encouraging the implementation of the nanoribbons for spintronic applications.

[1] R. Fainblat et al., Nano Letters 12, 5311 (2012)

TT 41.7 Wed 16:30 H2

**Electron spin-flip Raman scattering in a CdTe/(Cd,Mg)Te quantum well** — •Dion Braukmann[1], J. Debus[1], D. Dunker[1], V. F. Sapega[2], D. R. Yakovlev[1,2], G. Karczewski[3], T. Wojtowicz[3], J. Kossut[3], and M. Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Science, 194021 St. Petersburg, Russia — [3]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland

The Raman scattering of the electron spin in a neutral exciton has been studied in a CdTe/(Cd,Mg)Te quantum well (QW). The mechanism of the electron spin-flip Raman scattering (SFRS) is experimentally evaluated from the circular polarization properties of the scattered light as well as dependence of the electron-SFRS line intensity on the magnetic field direction with respect to the QW growth axis. The spin-flip process is governed by acoustic phonon interaction and anisotropic electron-heavy-hole exchange interaction. The probability of the anisotropic exchange interaction depends on the $g$ factors of the involved carriers. It shows a strong angular dependence due to the anisotropic heavy-hole $g$ factor. Moreover, by application of above-barrier illumination in addition to the resonant excitation of the neutral QW excitons the intensity of the electron-SFRS line can be modulated significantly.

**Coffee break**

TT 41.8 Wed 17:00 H2

**Ultrafast Spin Noise Spectroscopy** — •Hendrik Kuhn, Fabian Berski, Jan G. Lonnemann, Petrissa Zell, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover

Spin Noise Spectroscopy (SNS) is a powerful experimental technique which explores the full dynamics of stochastically oriented carrier spins close to thermal equilibrium [1]. With the conventional spin noise probing scheme relying on continuous wave (cw) laser probing, the detectable temporal spin dynamic is limited by the electrical bandwidth of the photoreceiver. We advance all optical spin noise spectroscopy in semiconductors to detection bandwidths of several hundred gigahertz by employing an ingenious scheme of pulse trains from ultrafast laser oscillators as an optical probe [2]. As all SNS techniques, ultrafast SNS avoids the need for optical pumping. It enables nearly perturbation free measurements of extremely short spin dephasing times, e.g at high temperatures. We expand our measurements on highly n-doped (n = 8.2 x $10^{17}$ $cm^3$) bulk GaAs towards room temperature and demonstrate the feasibility of ultrafast SNS for spin lifetimes down to the order of a few ten picoseconds.

[1] G. M. Müller, M. Oestreich, M. Römer, and J. Hübner Physica 43, 569-587 (2010).
[2] F. Berski et al., arXiv:1207.0081v1 [cond-mat.mes-hall].

TT 41.9 Wed 17:15 H2

**Spin Noise Spectroscopy: Towards Solid-State Entanglement** — •Fabian Berski[1], Agnes Beichert[1], Jens Hübner[1], Andreas Wieck[2], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Ruhr-Universität Bochum, Angewandte Festkörperphysik, Universitätsstr. 150, D-44780 Bochum, Germany

We study spin dynamics of naturally confined, non-interacting donor electrons in Gallium Arsenide at low temperatures by means of all optical spin noise spectroscopy [1]. The MBE grown sample shows the intriguing feature of localised spins in an environment of stochastically oriented magnetic moments: The orientation of the electron spin is lost on two different timescales which results from the interplay between the spin degree of freedom of the lattice and of the electron. The first timescale is attributed to the transversal component of the electron spin with respect to the nuclear magnetic field inside the donor volume and is determined to 4.5+-3ns. The second timescale is at least two orders of magnitude longer and is linked with the longitudinal component. An extension of the electron spin relaxation time would be possible via initilizing the surrounding spin bath by dynamic nuclear polarization which simplifies the generation and verification of entanglement [2].

[1] G. M. Müller, et al., Physica E: **43**, 569 (2010).
[2] S. Simmons, et al., Nature: **470**, 69 (2011).

TT 41.10 Wed 17:30 H2

**Single Molecule Magnets meet Graphene** — •Christian Cervetti[1], Andrea Cornia[4], Eberhard Ulrich Stützel[2], Stephan Rauschenbach[2], Fernando Luis[5], Martin Dressel[1], Marko Burghard[2], Klaus Kern[2,3], and Lapo Bogani[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Max Planck Institut für Festkörperforschung — [3]Institute de Physique de la Matière Condensée, Ecole Polytechnique de Lausanne, Switzerland — [4]Dipartimento di Chimica, Università di Modena e Reggio Emilia, Italy — [5]Instituto de Ciencia de Materiales de Aragón, Spain

Graphene has a strong potential as component of novel spintronics devices. Besides its use as conducting channel for coherent spin transport, graphene is furthermore of interest for the detection and manipulation of the spin within molecule magnets. This task requires an appropriate coupling between the sheets and the single molecular magnets. Here, we describe the assembly of a functionalized Fe4 cluster compound on graphene exploiting non-covalent $\pi$-stacking interaction. We demonstrate the control over the organization of the molecules by tuning the deposition parameters and the type of graphene. The graphene phononic environment is found to influence the magnetization dynamics of the molecular magnets as evidenced by $\mu$-SQUID

study at mK-temperatures. Finally, preliminary spin-transport experiments at low-temperature are presented.

TT 41.11 Wed 17:45 H2

**Enhanced Infrared Magneto-Optical Response of the Nonmagnetic Semiconductor BiTeI Driven by Bulk Rashba Splitting** — •L. Demko[1], G. A. H. Schober[3], V. Kocsis[4], M. S. Bahramy[5], H. Murakawa[5], J. S. Lee[2], I. Kezsmarki[4], R. Arita[2], N. Nagaosa[2], and Y. Tokura[1] — [1]Multiferroics Project, ERATO, JST, c/o Department of Applied Physics, University of Tokyo, Japan — [2]Department of Applied Physics, University of Tokyo, Japan — [3]Institute for Theoretical Physics, University of Heidelberg, Germany — [4]Department of Physics, Budapest University of Technology and Economics and Condensed Matter Research Group of the Hungarian Academy of Sciences, Hungary — [5]CMRG and CERG, RIKEN ASI, Japan

We study the magneto-optical (MO) response of the polar semiconducting BiTeI with giant bulk Rashba spin splitting at various carrier densities. Despite being nonmagnetic, the material is found to yield a huge MO activity in the infrared region under moderate magnetic fields (up to 3 T). Our first-principles calculations show that the enhanced MO response of BiTeI comes mainly from the intraband transitions between the Rashba-split bulk conduction bands. These transitions connecting electronic states with opposite spin directions become active due to the presence of strong spin-orbit interaction and give rise to distinct features in the MO spectra with a systematic doping dependence. We predict an even more pronounced enhancement in the low-energy MO response and dc Hall effect near the crossing (Dirac) point of the conduction bands.

TT 41.12 Wed 18:00 H2

**Transport of dynamically generated pure spin current in single-layer graphene** — •Masashi Shiraishi[1], Zhenyao Tang[1], Hiroki Ago[2], Kenji Kawahara[2], Yuichiro Ando[1], and Teruya Shinjo[1] — [1]Graduate School of Engineering Science, Osaka Univ., Japan — [2]Institute of Materials Chemistry and Engineering, Kyushu Univ., Japan

Electrical spin injection and generation of a pure spin current in graphene using non-local electrical technique has opened a new frontier in molecular spintronics [1-3], after the achievements, a number of interesting physics related with spin transport and spin relaxation have been studied. However, there are still many issues in spin transport in graphene that need to be clarified, and the establishment of a novel technique for spin injection and generation of a pure spin current in graphene is strongly desired for discussing spin transport phenomena in graphene. Here, we show a new approach for generating and transporting pure spin current in single-layer graphene at room temperature, the dynamical spin pumping method [4]. The dynamical spin transport was successfully demonstrated, and the estimated spin coherence in CVD-grown graphene at room temperature (RT) was 1.36 micrometers.This study is partly supported by JSPS "Nano Carbon Terahertz Science" program.

[1] M. Ohishi, M. Shiraishi et al., JJAP 46, L605 (2007). [2] N. Tombros et al., Nature 448, 571 (2007). [3] M. Shiraishi et al., Adv. Func. Mat. 19, 3711 (2009). [4] Z. Tang, M. Shiraishi et al., Adv. Func. Mat. submitted.

TT 41.13 Wed 18:15 H2

**Investigation of spin drift effect in highly doped Si** — •Masashi Shiraishi[1], Makoto Kameno[1], Yuichiro Ando[1], Eiji Shikoh[1], Toshio Suzuki[2], Tohru Oikawa[3], and Tomoo Sasaki[3] — [1]Graduate School of Engineering Science, Osaka Univ., Japan — [2]AIT, Akita Industrial Technology Center, Japan — [3]TDK Corporation, Japan

Spin drift, which is usually negligible in spin transport in metallic systems, contributes significantly to spin transport and spin accumulation voltages in semiconductors like Si. Since an electric field gives rise to spin drift, investigating spin accumulation voltages as a function of the bias electric field (bias voltage) in Si spin devices can clarify how spin drift governs spin transport and accumulation properties. In this presentation, we report on quantitative analyses of spin drift effect and electric field dependence of spin injection signals in Si [1,2].

[1] M. Shiraishi et al., Phys. Rev. B83, 241204(R) (2011). [2] M. Kameno, M. Shiraishi et al., Appl. Phys. Lett. 101, 122413 (2012).

TT 41.14 Wed 18:30 H2

**Investigation of ordinal and inverted Hanle spin signals in highly-doped Si** — •Masashi Shiraishi[1], Makoto Kameno[1], Yasunori Aoki[1], Yuichiro Ando[1], Eiji Shikoh[1], Toshio Suzuki[2], Tohru Oikawa[3], and Tomoo Sasaki[3] — [1]Graduate School of Engineering Science, Osaka Univ., Japan — [2]AIT, Akita Industrial Technology Center, Japan — [3]TDK Corporation, Japan

Spin injection and spin transport in Si has been attracting much attention in recent several years, and spin physics in Si at room temperature is intensively argued. Whereas non-local 3-terminal method (NL3T) has been widely used for showing spin accumulation at room temperature (RT) [1], heated discussion is arising since the NL3T does not completely exclude spurious signals [2]. For proving spin injection and transport, observation of magnetoresistance in the NL-4T method (NL4T) and Hanle-type spin precession provide the most powerful evidence, and our group exhibited the first transport of pure spin current at RT [3]. In this presentation, we show the results of the detailed study on Hanle effects in NL3T by comparing that in NL4T, which strongly suggests that the results obtained by using NL3T has much room for discussion about their interpretations [4]. [1] S. Dash et al., Nature 462, 491 (2009). [2] M. Tran et al., 102, 036601 (2009). [3] T. Suzuki, M. Shiraishi et al., APEX4, 023003 (2011). [4] Y. Aoki, M. Shiraishi et al., Phys. Rev. B86, 081201(R) (2012).

## TT 42: Quantum Coherence, Quantum Information Systems 2

Time: Wednesday 15:00–19:15 Location: H18

TT 42.1 Wed 15:00 H18

**Magnetic hysteresis effects in superconducting coplanar microwave resonators** — •D. Bothner[1], T. Gaber[1], M. Kemmler[1], M. Grünzweig[1], B. Ferdinand[1], S. Wünsch[2], M. Siegel[2], P. Mikheenko[3], T. H. Johansen[3], D. Koelle[1], and R. Kleiner[1] — [1]Universität Tübingen, Germany — [2]Karlsruher Institut für Technologie, Germany — [3]University of Oslo, Norway

We present experimental data regarding the impact of external magnetic fields on quality factor and resonance frequency of superconducting microwave resonators in a coplanar waveguide geometry. In particular we focus on the influence of magnetic history and show with the assistance of numerical calculations that the found hysteretic behaviour can be well understood with a highly inhomogeneous microwave current density in combination with established field penetration models for type-II superconducting thin films. Furthermore we have used magneto-optical imaging techniques to check the field distribution which we have assumed in our calculations. Finally, we demonstrate that and how the observed hysteretic behaviour can be used to optimize and tune the resonator performance for possible hybrid quantum sytems in magnetic fields [1].

[1] D. Bothner et al., Phys Rev. B 86, 014517 (2012)

TT 42.2 Wed 15:15 H18

**Anisotropic rare-earth spin ensemble strongly coupled to a superconducting resonator** — •Sebastian Probst[1], Hannes Rotzinger[1], Ivan Protopopov[2], Stefan Wünsch[3], Philipp Jung[1], Markus Jerger[1], Michael Siegel[3], Alexey V. Ustinov[1], and Pavel Bushev[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, D-76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruher Institut für Technologie, D-76021 Karlsruhe, Germany — [3]Institut für Mikro- und Nanoelektronische Systeme, Karlsruher Institut für Technologie, D-76189

We report on ESR spectroscopy of an erbium spin ensemble strongly coupled to a superconducting lumped element microwave resonator. $Er^{3+}$ ions are distinct from other spin ensembles due to their optical transitions inside the telecom C-band at 1.54 $\mu m$. This feature makes them most attractive for interfacing optical and microwave photons by using a hybrid quantum architecture [1]. However, in contrast to NV-centers or ruby crystals, rare-earth ions possess a magnetic anisotropy due to the host crystal field. This results in a strong angular dependence of the spin g-factor and of the collective coupling strength with

respect to the orientation of the DC magnetic field. We have probed this anisotropy at millikelvin temperatures by performing on-chip ESR spectroscopy. The strong coupling regime with a collective coupling of 36 MHz and 11 MHz linewidth has been reached at a resonator frequency of 4.9 GHz for spin transitions with a g-factor of 1.4.

[1] P. Bushev et al., Phys. Rev. B 84, 06051 (R) (2011)

TT 42.3 Wed 15:30 H18

**Tunable Coupling between Two Resonators Controlled by a Flux Qubit: the Quantum Switch** — •E. Hoffmann[1], M. Haeberlein[1], A. Baust[1], M. Schwarz[1], E.P. Menzel[1], H. Huebl[1], David Zueco[2], J.-J. García Ripoll[3], E. Solano[4], F. Deppe[1], A. Marx[1], and R. Gross[1] — [1]TU München, Garching and Walther-Meißner-Institut, Germany — [2]CSIC-Universidad de Zaragoza, Spain — [3]IFF-CSIC, Madrid, Spain — [4]Universidad del Pais Vasco UPV/EHU and Ikerbasque, Spain

Superconducting quantum circuits have developed into a promising platform for quantum information processing. To this end, systems consisting of a few qubits and/or harmonic oscillator circuits have been investigated. When scaling up these systems, elements allowing for a controlled coupling/decoupling of circuit parts are mandatory. A possible implementation of such an element is the Quantum Switch, where a controllable coupling between two superconducting transmission line resonators is mediated by a superconducting flux qubit. In this presentation, the experimental characterization of such a device and spectroscopic evidence for the switching behavior will be discussed.

This work is supported by DFG via SFB 631, the German Excellence Initiative via NIM, as well as EU projects CCQED, PROMISCE and SOLID, the Basque Foundation for Science, Basque Government IT472-10, Spanish MICINN FIS2009-12773-C02-01, and DZ granted by ARAID

TT 42.4 Wed 15:45 H18

**Tunable gradiometric flux qubits in circuit-QED experiments** — •J. Goetz[1], M. J. Schwarz[1], Z. Jiang[1,2], F. Sterr[1,2], M. Häberlein[1], F. Deppe[1,2], A. Marx[1], and R. Gross[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching — [2]Physik Department, TU München, Garching

Gradiometric flux qubits with tunable minimal transition frequency have strong potential for scalable quantum circuits as well as for the realisation of various coupling schemes between qubits and coplanar waveguide resonators. We have systematically studied the tuning of the minimal transition frequency, the so called qubit gap, of single qubits depending on fabrication parameters [1]. In addition we investigate how the special geometry of these qubits allows us to switch between the ultrastrong-coupling regime and negligible coupling strength. We discuss the application of tunable gradiometric flux qubits in establishing strong $\sigma_x$ coupling between a resonator mode and the qubit enabling the simulation of relativistic quantum systems.

This work is supported by the DFG via SFB 631, the Excellence Initiative via NIM, as well as by the EU-projects CCQED and PROMISCE.

[1] M. J. Schwarz et al., arXiv:1210.3982

TT 42.5 Wed 16:00 H18

**Path Entanglement of Continuous-Variable Quantum Microwaves** — •E. P. Menzel[1], R. Di Candia[2], F. Deppe[1], P. Eder[1], L. Zhong[1], M. Ihmig[4], M. Haeberlein[1], A. Baust[1], E. Hoffmann[1], D. Ballester[3], K. Inomata[5], T. Yamamoto[5,6], Y. Nakamura[5,7], E. Solano[2], A. Marx[1], and R. Gross[1] — [1]Walther-Meissner-Institut and TU Muenchen, Germany — [2]Universidad del País Vasco UPV/EHU and Ikerbasque, Spain — [3]University College London, UK — [4]TU Muenchen, Germany — [5]RIKEN Advanced Science Institute, Japan — [6]NEC Smart Energy Research Laboratories, Japan — [7]The University of Tokyo, Japan

Entanglement is a quantum mechanical phenomenon playing a key role in quantum communication and information processing protocols. Here, we report on frequency-degenerate entanglement between continuous-variable quantum microwaves propagating along two separated paths. In our experiment, we combine a squeezed and a vacuum state via a beam splitter. We reconstruct the squeezed state and, independently from this, detect and quantify the produced entanglement via correlation measurements[1]. Our work paves the way towards quantum communication and teleportation with continuous variables in the microwave regime.

This work is supported by DFG via SFB 631, the German Excellence Initiative via NIM, EU projects SOLID, CCQED and PROMISCE, MEXT Kakenhi "Quantum Cybernetics", JSPS FIRST Program, the NICT Commissioned Research, EPSRC EP/H050434/1, Basque Government IT472-10, and Spanish MICINN FIS2009-12773-C02-01.

[1] E. P. Menzel *et al.*,arXiv:1210.4413

TT 42.6 Wed 16:15 H18

**Fast microwave beam splitters from superconducting resonators** — •M. Haeberlein[1,2], D. Zueco[3], P. Assum[2], T. Weissl[4], E. Hoffmann[1,2], B. Peropadre[5], J.J. García-Ripoll[5], E. Solano[6], F. Deppe[1,2], E. Xie[1,2], A. Marx[1], and R. Gross[1,2] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Technische Universität München, Garching, Germany — [3]CSIC-Universidad de Zaragoza, Spain — [4]CNRS, Grenoble, France — [5]CSIC-Instituto de Física Fundamental, Madrid, Spain — [6]Universidad del País Vasco and IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Coupled superconducting transmission line resonators have potential applications in quantum information processing. Experimentally, high coupling strength are often desirable. One example is the fabrication of fast beam splitters, which however is hampered by non-negligible two-mode squeezer terms. In this work, we experimentally study superconducting microstrip resonators which are coupled over one third of their length. We alter position of this coupling region, thereby changing the relative weight between inductive and capacitive coupling. As a consequence, the beam splitter terms reach a coupling strength of 800 MHz, which is a significant fraction of the resonance frequency of 5.44 GHz. Nevertheless, the relative weight of the two-mode squeezer terms decreases to 20%, enabling the construction of a fast beam splitter.

This work is supported by DFG via SFB 631, the German excellence Initiative via NIM, EU projects SOLID; CCQED, and PROMISCE, Basque Government IT472-10, Spanish MICINN FIS2009-12773-C02-01, and DZ granted by ARAID.

TT 42.7 Wed 16:30 H18

**Coupling a donor based spin ensemble to superconducting circuits** — •Christoph W. Zollitsch[1,2], Moritz Greifenstein[2], Alexander Backs[2], Felix Hoehne[3], Martin S. Brandt[3], Rudolf Gross[1,2], and Hans Huebl[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching — [2]Physik-Department, Technische Universität München, Garching — [3]Walter Schottky Institut, Technische Universität München, Garching

The realization of solid state based quantum systems has been successful using various approaches, e.g. superconducting qubits, NV centers or quantum dot systems. The coupling of different systems in hybrid systems allows to exploit their individual advantages. To allow a coherent information transfer between two quantum systems strong coupling is required, i.e. the effective coupling $g_{\text{eff}}$ needs to exceed the loss mechanisms of both contributing systems. We study the coupling between a superconducting coplanar niobium microwave resonator and an ensemble of uncoupled electron spins of phosphorus donors in natural silicon. We perform microwave transmission spectroscopy of the resonator at millikelvin temperatures as a function of the magnetic field and observe the onset of an avoided level crossing. By analyzing the evolution of the linewidth near the level degeneracy we find $g_{\text{eff}}/(2\pi) = 1.3$ MHz. The loss rate of the spin system and the resonator are determined to $\gamma/(2\pi) = 10$ MHz and $\kappa/(2\pi) = 0.3$ MHz, respectively. We also discuss the temperature and power dependence of $g_{\text{eff}}$.

Financial support via SFB 631 and NIM is gratefully acknowledged.

**15 min. break**

**Invited Talk** TT 42.8 Wed 17:00 H18

**Orbitronics in Silicon** — •Gabriel Aeppli — London Centre for Nanotechnology, University College London, UK

Control of magnetic interactions as well as localised spin sates is a prerequisite for spin-based quantum computing. Interactions can be induced via photons or exchange interactions mediated through atomic orbitals. We have consequently carried out optical and scan probe measurements demonstrating control over donor impurity orbitals in silicon and at its surface. The experiments are analogous to experiments performed in atom traps, where silicon plays the role of the vacuum and the impurity that of the atoms.

[1] N. Q. Vinh et al., PNAS **105**, 10649 (2008); and submitted (2012)
[2] P. T. Greenland et al., Nature **465**, 1057 (2010)

[3] S. R. Schofield et al., submitted (2012)

TT 42.9 Wed 17:30 H18

**Decoherence due to quasiparticle tunneling in circuit QED** — •Andreas Heimes[1], Michael Marthaler[1], Juha Leppäkangas[2], and Gerd Schön[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, Wolfgang-Gaede-Str. 1, D-76128 Karlsruhe, Germany — [2]Microtechnology and Nanoscience, MC2, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

In recent years great effort in screening envoironmental decoherence sources lead to an increased coherence time of Josephson based qubits. Temperature dependent decay time measurements in phase and transmon qubits suggest that nonequilibrium quasiparticles have become one of the major limiting factors. We theoretically investigate this nonequilibrium situation and show that quasiparticle tunneling through Josephson junctions influences the excitation and relaxation dynamics of such quantum information devices.

TT 42.10 Wed 17:45 H18

**Making optimal control work for superconducting qubits** — Daniel Egger[1], Fadi Abu Dagga[1], Daniel Sank[2], and •Frank K. Wilhelm[1,3] — [1]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken — [2]Physics Department, University of California, Santa Barbara, USA — [3]IQC and Department of Physics and Astronomy, University of Waterloo, Canada

Optimal control is a powerful tool to find pulse sequences and shapes that implement quantum gates on given realistic hardware, such as superconducting qubits. For practical applicability, the intense filtering as well as the challenge of precise calibration need to be met. We illustrate this challenge along the example of the implementation of a controlled phase shift gate between transmon qubits coupled by a resonator. The pulse sequence reaches a high fidelity gate in short time but is highly sensitive to the characterization of the transmon frequencies. We show how a combination of robust optimal control, genetic algorithms, and plain debugging help meet these challenges.

**15 min. break**

TT 42.11 Wed 18:15 H18

**Quantum process tomography of phase and energy relaxation through adaptive measurements** — •Markku Stenberg[1] and Frank Wilhelm[1,2] — [1]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, 200 University Avenue West, Waterloo, ON, N2L 3G1, Canada

Quantum process tomography tends to be very time consuming when multiple degrees of freedom are studied simultaneously. We present a method of efficient quantum process tomography to estimate the phase and energy relaxation rates in qubits. The method applies Bayesian inference to adaptively choose measurements based on the previously obtained measurement outcomes. We adopt sequential Monte-Carlo approach to perform the Bayesian updates and make use of a fast numerical implementation of the algorithm. We compare the performance of our method to conventional offline (implemented after experimental data collection) strategies and illustrate how our method can speed up quantum process tomography.

TT 42.12 Wed 18:30 H18

**Generation of Nonclassical States of Microwave Radiation via Single Photon Detection** — •Luke C.G. Govia, Emily J. Pritchett, and Frank K. Wilhelm — Saarland University, Saarbrücken, Germany

We describe the creation of nonclassical states of microwave radiation via single photon detection, using an ideal dichotomic detector. Ideally, such a detector only indicates the presence or absence of photons and, as such, will have a back action in the form of the subtraction operator. Using the non-linearity of this back action, it is possible to create nonclassical states of microwave radiation, including squeezed and cat-like states, starting from a coherent state. One such dichotomic single photon detector is the Josephson Photomultiplier (JPM), as discussed in [1]. We discuss the implementation of this protocol using JPMs and their necessary regime of experimental operation.

[1] Phys. Rev. A 86, 032311 (2012)

TT 42.13 Wed 18:45 H18

**Understanding and utilizing phase qubit decoherence channels for microwave photon detection** — •Emily Pritchett, Luke Govia, and Frank Wilhelm — Saarland University

Superconducting phase qubits are a leading platform for storing and processing quantum information. While extremely promising, phase qubits experience unexpectedly short lifetimes as compared to other superconducting qubits (e.g, the transmon), which is explained by the experimental observation of densely packed anti-crossings in the phase qubit's spectrum. While currently thought the result of interactions between the qubit and spurious defects in its environment, we show that these anti-crossings exist between the qubit state and other nearly-degenerate eigenstates of the circuit even before interaction with the environment is considered. We discuss how the instability introduced by these in-circuit resonances can be utilized for high-efficiency, high-bandwidth single microwave photon detection.

TT 42.14 Wed 19:00 H18

**Engineered circuit QED with dense resonant modes** — •Daniel Egger and Frank Wilhelm — Universität des Saarlandes, Saarbrücken, Germany

Meta-materials are systems engineered at a wavelength smaller than the radiation considered but larger than the atomic scale; they gain their properties from their structure. Of notable interest are left-handed meta-materials. They exhibit negative permittivity and permeability[1]. On chip quantum optics routinely use right-handed transmission lines, made of a microwave strip-line, as information mediators[2]. In this work, we discuss the properties of a left-handed/right-handed hybrid transmission line. The resulting mode structure presents a mode pile-up at a lower cut-off frequency. Placing a qubit near the hybrid line results in strong to ultra-strong coupling to a quasi-continuum of modes. This system generates strongly entangled multi-mode states and also serves as quantum simulator for a spin-boson model with a sub-sub-ohmic density of states.

[1] V. Veselago, Sov. Phys. Usp. **10**, 517 (1968)
[2] A. Blais *et al.*, PRA **69** 062320 (2004)

## TT 43: Correlated Electrons: Metal-Insulator Transition 2

Time: Wednesday 15:00–16:30 Location: H19

TT 43.1 Wed 15:00 H19

**Charge self-consistent DFT+DMFT approach to strong correlation effects in transition-metal oxides** — •Frank Lechermann[1], Daniel Grieger[1], Oleg. E. Peil[2], and Christoph Piefke[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Department of Condensed Matter Physics, University of Geneva

One of the most suited class of materials to study the physics of strongly correlated electron systems in a realistic scenario is provided by a group of transition-metal oxides. The specific chemistry of these compounds allows for rather localized states in the solid state, giving rise to a variety of intricate phenomena. Large-gap insulators, systems close to a metal-insulator transition as well as metals with an enormously high conductivity all belong to these materials. It will be shown that the newly developed charge self-consistent combination of density functional theory (DFT) and dynamical mean-field theory (DMFT) based on the projected-local-orbital interface between a mixed-basis pseudopotential method and the continuous-time quantum Monte Carlo impurity solution to DMFT [1], is capable of addressing the vast characteristics among correlated transition-metal oxides. For instance, the metal-insulator transition in $V_2O_3$ will be discussed.

[1] D. Grieger, C. Piefke, O. E. Peil and F. Lechermann, PRB **86**, 155121 (2012)

TT 43.2 Wed 15:15 H19

**Orbital and spatial correlations in $LiVS_2$ from a two-particle perspective** — •Lewin Boehnke and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg

The compound $LiVS_2$ shows a transition from a paramagnetic metal to a trimerized valence bond solid insulator phase [1] at 310K. Such a behaviour is already known from its neighbouring compound $LiVO_2$. In contrast to previous studies that concentrated on the symmetry-broken insulating phase [2], our attention is on the emergence of this low-temperature phase from the high-temperature phase. We employ the formalism outlined in [3] to calculate lattice spin- and charge-susceptibilities for this system on top of density functional theory + dynamical mean-field theory (DFT+DMFT) calculations for a detailed investigation of non-local two-particle correlations in view of the orbital ordering and trimerization effects that are observed.

[1] N. Katayama, *et al.*, PRL **103**, 146405 (2009)
[2] H. Pen, *et al.*, PRL **78**, 1323 (1997)
[3] L. Boehnke, *et al.*, PRB **84**, 075145 (2011)

TT 43.3 Wed 15:30 H19

**Correlation effects and spin-orbit interaction in $Sr_3Ru_2O_7$: LDA+DMFT study** — •Evgeny Gorelov, Guoren Zhang, and Eva Pavarini — IAS-3, Forschungszentrum Jülich, 52425 Jülich

The layered ruthenates of the Ruddlesden-Popper family $Sr_{n+1}Ru_nO_{3n+1}$ are interesting examples of strongly correlated transition metal compounds. Due to competing kinetic and Coulomb energies, that are of the same order for Ru 4*d* electrons, these compounds have very rich phase diagram, including Mott-insulator, ferro- and meta-magnetic phases. Among layered ruthenates the bilayered compound $Sr_3Ru_2O_7$ is particularly interesting. It is known to be a paramagnetic metal close to ferro-magnetism and exhibits a metamagnetic behavior in external magnetic field. By using the LDA+DMFT (local-density approximation + dynamical mean-field theory) approach, we study magnetic properties and electron mass renormalization due to correlation effects. In our LDA+DMFT scheme we use maximally-localized Wannier orbitals obtained from Linearized Augmented Plane Wave (LAPW) calculations to build a low-energy Hubbard model for the Ru *d* bands; we use the weak-coupling CT-quantum Monte Carlo method to solve the quantum impurity problem. We take into account the full rotationally-invariant Coulomb interaction, as well as full on-site self-energy matrix in orbital space with spin-orbit coupling.

[1] E. Gorelov, G. Zhang, and E. Pavarini, Correlation effects and spin-orbit coupling in $Sr_{n+1}Ru_nO_{3n+1}$ compounds (in preparation)

TT 43.4 Wed 15:45 H19

**LDA+DMFT calculations of the Knight shift and relaxation rate in $VOMoO_4$** — •Amin Kiani and Eva Pavarini — Institute for Advanced Simulation and JARA, Forschungszentrum Jülich, 52425 Jülich, Germany

By using the LDA+DMFT approach and the local vertex approximation, we calculate the magnetic linear response function of strongly correlated transition-metal oxides. From the susceptibility we obtain Knight shift and relaxation rate. We present results for the frustrated system $VOMoO_4$. In particular we investigate how the Knight shift and the relaxation time behave in different temperature and correlation regimes.

TT 43.5 Wed 16:00 H19

**DFT + DMFT calculations for epitaxially strained $LaTiO_3$** — •Krzysztof Dymkowski and Claude Ederer — Materials Theory, ETH Zurich, Switzerland

Even though bulk $LaTiO_3$ is a Mott insulator [1], metallic properties have been reported for thin films of $LaTiO_3$ grown on $SrTiO_3$ [2]. Such metallicity, can be due to a number of factors such as: electronic reconstruction at the interface, defects, or substrate-induced structural deformations. In order to identify the origin of the observed metallicity, we perform density functional theory plus dynamical mean field theory (DFT + DMFT) calculations for epitaxially strained $LaTiO_3$. First, we use standard DFT to accurately relax the structure under the epitaxial constraint, and we monitor hopping amplitudes and crystal-field splitting as a function of strain. Then, we calculate the electronic properties for the strained structures using DMFT. Based on our results we address the question whether the strain-induced structural modifications of $LaTiO_3$ are enough to change this insulator into a metal.

[1] E. Pavarini et al., Phys. Rev. Lett. 92, 176403 (2004)
[2] F. J. Wong et al., Phys. Rev. B 81, 161101 (2010); C. He et al., Phys. Rev. B 86, 081401 (2012)

TT 43.6 Wed 16:15 H19

**Magnetic susceptibility of the orbital-selective Mott phase** — •Markus Greger, Michael Sekania, Marcus Kollar, and Dieter Vollhardt — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg

We analyze the low-energy physics of multi-orbital Hubbard models in the orbital-selective Mott phase within Dynamical Mean-Field Theory. Our main focus lies on the calculation of dynamical two-particle quantities, e.g., susceptibilities. They are of particular interest in these systems since the coupling between the orbitals is not due to a hybridization, but is caused by two-particle processes originating from the interaction, i.e., the Hund's rule coupling $J$ and the inter-orbital repulsion $U_1$. Employing the Numerical Renormalization Group as an impurity solver we obtain diverging spin-susceptibilities $\chi^{sp}_{i,j}(\omega)$ at $\omega = 0$; here $i, j$ are orbital indices. This corresponds to a divergent density of states for magnetic excitations, indicative of an instability of the phase. An explanation based on a Kondo-type Hamiltonian is given. These results also provide a better characterization of the known non-Fermi liquid properties of the phase.

## TT 44: Focused Session: Majorana Fermions in Condensed Matter (jointly with DS, HL, MA, and O)

Majorana fermions arise as quasi-particle excitations in condensed matter systems which exhibit non-Abelian exchange statistics. This property makes them a fundamentally new type of particles, and possibly allows topological quantum computing in this system. In the last few years, the study of Majorana fermions has rapidly evolved from being a mere theoretical concept to a practical realization: Following theoretical proposals involving hybrid nanosystems consisting of conventional superconductors and semiconducting nanowires, experiments have now found signatures of Majorana fermions. This Focused Session will discuss various aspects of Majorana fermions and the hybrid systems hosting them, including both theoretical and experimental contributions.

Organizers: Fabian Hassler (RWTH Aachen), Michael Wimmer (Leiden University)

Time: Wednesday 15:00–18:00 Location: H20

**Invited Talk** TT 44.1 Wed 15:00 H20

**Subgap States in Majorana Wires** — •Piet Brouwer — Freie Universität Berlin

A one-dimensional spin-orbit coupled nanowire with proximity-induced pairing from a nearby s-wave superconductor may be in a topological nontrivial state, in which it has a zero energy Majorana bound state at each end. In this talk, I will discuss how non-idealities in this proposal, such as potential disorder, deviations from a strict one-dimensional limit, or details concerning the termination of the wire, affect the topological phase and its signatures in a current-voltage measurement. In particular, I'll argue that the topological phase can persist at weak disorder or for multichannel wires, although some of the signatures of the presence of Majorana fermions are obscured.

**Invited Talk** TT 44.2 Wed 15:30 H20

**New Measurements on Nanowire Majorana Systems** —

•Charles Marcus[1,3], Hugh Churchill[2,3], Mintang Deng[4], and Hongqi Xu[4] — [1]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Copenhagen, DK — [2]Department of Physics, MIT, Cambridge, MA USA — [3]Department of Physics, Harvard University, Cambridge, MA USA — [4]Division of Solid State Physics, Lund University, Lund, Sweden

This talk will present recent measurements on gated InSb nanowires coupled to a superconducting film. This set-up is one designed to detect Majorana end states. We show data similar to that seen in other groups recently, and also extend measurements in a number of directions, including higher field and higher conductance. Oscillatory structure suggesting interacting end-state Majoranas is found. We also identify transport regimes where even-odd Kondo-like features are evident, combined with Andreev bound states.

This research is sponsored by Microsoft Project Q, the Danish National Research Foundation, and Harvard University.

**Topical Talk** TT 44.3 Wed 16:00 H20

**Adaptive Tuning of Majorana Fermions in a Quantum Dot Chain** — •Anton Akhmerov — Harvard University, USA

I will explain how to overcome the obstacles that disorder and high density of states pose to the creation of unpaired Majorana fermions in one-dimensional systems. This is achieved by splitting the system into a chain of quantum dots, which are then tuned such that the chain can be viewed as an effective Kitaev chain with maximally localized Majorana fermions. Resonant Andreev spectroscopy allows us to make this tuning adaptive, so that each pair of dots may be tuned independently of the other. Our numerical simulations show that already in three quantum dots it is possible to have almost completely decoupled Majorana fermions.

**15 min. break**

**Topical Talk** TT 44.4 Wed 16:45 H20

**Majorana Fermions in Disordered Quantum Wires** — •Alexander Altland — Institute for Theoretical Physics, Zülpicher Str. 77, 50937 Köln

Proximity coupled spin-orbit quantum wires have recently been shown to support midgap Majorana states at critical points. We show that in the presence of disorder these systems are prone to the buildup of a second bandcenter anomaly, which is of different physical origin but shares key characteristics with the Majorana state: it is narrow in width, insensitive to magnetic fields, carries unit spectral weight, and is rigidly tied to the band center. Depending on the parity of the number of subgap quasiparticle states, a Majorana mode does or does not coexist with the impurity generated peak. The strong 'entanglement' between the two phenomena may hinder an unambiguous detection of the Majorana by spectroscopic techniques.

**Topical Talk** TT 44.5 Wed 17:15 H20

**Parity Effects and Crossed Andreev Noise in Transport through Majorana Wires** — •Bernd Rosenow[1], Björn Zocher[1,2], and Mats Horsdal[1] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04009 Leipzig, Germany — [2]Max-Planck-Institute for Mathematics in the Sciences, D-04103 Leipzig, Germany

One of the defining properties of a topologically ordered state is the ground state degeneracy on surfaces with nonzero genus. In semiconductor-superconductor hybrid structures, a phase transition between regular and topologically nontrivial superconductivity is expected as a function of chemical potential or magnetic field strength. The difference in ground state degeneracies of the two phases is reflected in the parity and magnetic flux dependence of nonlinear Coulomb blockade transport through a ring shaped structure.

In nanowires of finite length, topologically non-trivial superconductivity is expected to give rise to Majorana bound states at the ends of the wire. The non-locality of Majorana bound states opens the possibility of crossed Andreev reflection with nonlocal shot noise, due to the injection of an electron into one end of the superconductor followed by the emission of a hole at the other end. When coupling the end states to leads via quantum dots with resonant levels, in the space of energies of the two resonant quantum dot levels we find a four peaked clover-like pattern for the strength of noise due to crossed Andreev reflection, distinct from the single ellipsoidal peak found in the absence of Majorana bound states.

TT 44.6 Wed 17:45 H20

**Majorana qubit rotations in microwave cavities** — •Thomas L. Schmidt, Andreas Nunnenkamp, and Christoph Bruder — Department of Physics, University of Basel, CH-4056 Basel, Switzerland

Majorana bound states have been proposed as building blocks for qubits on which certain operations can be performed in a topologically protected way using braiding. However, the set of these protected operations is not sufficient to realize universal quantum computing. We show that the electric field in a microwave cavity can induce Rabi oscillations between adjacent Majorana bound states. These oscillations can be used to implement an additional single-qubit gate. Supplemented with one braiding operation, this gate allows to perform arbitrary single-qubit operations.

## TT 45: Superconductivity: (General) Theory

Time: Wednesday 15:00–16:45 Location: H21

TT 45.1 Wed 15:00 H21

**Density Functional Theory for Superconductors** — •Antonio Sanna, Andreas Linscheid, and E.K.U. Gross — Max-Planck Institute for Microstructure Physics, Halle

Superconducting density functional theory (SCDFT) is a fully parameter-free approach to superconductivity. We review the method discussing the main theoretical advantages and disadvantage of the approach as compared to standard Green's functions methods. We present results for several conventional and unconventional superconductors, and in particular we will discuss the special case of surface superconductivity considering the case of Pb on Si(111). Then we will report on the most recent extensions of the method: to incorporate in a correct way the Migdal's theorem; compute the excitation spectrum; describe a coexistence with magnetism.

TT 45.2 Wed 15:15 H21

**Two-particle self-consistent approach to unconventional superconductivity** — •Junya Otsuki — Department of Physics, Tohoku University, Sendai, Japan — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg

A non-perturbative approach to unconventional superconductivity is developed based on the idea of the two-particle self-consistent (TPSC) theory[1]. An exact sum-rule which the momentum-dependent pairing susceptibility satisfies is derived. Effective pairing interactions between quasiparticles are determined so that an approximate susceptibility should fulfill this sum-rule, in which fluctuations belonging to different symmetries mix at finite momentum. The mixing leads to a suppression of the $d_{x^2-y^2}$ pairing close to the half-filling, resulting in a maximum of $T_c$ away from half-filling.

[1] J. Otsuki, Phys. Rev. B **85**, 104513 (2012).

TT 45.3 Wed 15:30 H21

**Response and collective modes in two–band superconductors** — •Nikolaj Bittner[1] and Dietrich Einzel[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]Walther-Meißner-Institut für Tieftemperaturforschung, Bayerische Akademie der Wissenschaften, Walther-Meißner-Straße 8, D-85748 Garching, Germany

We present a systematic study of the response properties of two–band (multi–gap) superconductors with conventional and unconventional spin–singlet pairing correlations. Particular emphasis is on the existence, the dispersion and the general role of a new massive order parameter collective mode, the so–called Leggett mode, which arises as a consequence of interband pairing correlations. The subtle interplay between the gauge mode or Nambu–Goldstone Boson and the Leggett mode is studied in view of both the validity of the charge conservation law and the participation in the Higgs mechanism. The

occurrence of the Leggett–mode is analyzed with respect to its experimental observability in all physically relevant spin-independent collisionless response functions like the Lindhard density response, the dielectric function, the supercurrent response (condensate dynamic conductivity) and the electronic Raman response. Possible applications of this theory include systems like various cuprates, $MgB_2$, pnictides and non–centrosymmetric superconductors.

TT 45.4 Wed 15:45 H21

**Establishing Theoretically the Capacity of Resonant Inelastic X-ray Scattering to Probe the Phase and Excitations of the Superconducting Order Parameter** — •Pasquale Marra[1], Steffen Sykora[1], Krzysztof Wohlfeld[1], and Jeroen van den Brink[1,2] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, D-01069 Dresden, Germany — [2]Department of Physics, TU Dresden, D-01062 Dresden, Germany

The capability to probe the dispersion of elementary spin, charge, orbital, and lattice excitations has positioned Resonant Inelastic X-ray Scattering (RIXS) at the forefront of photon science. Here we develop the scattering theory for RIXS on superconductors, calculating its momentum-dependent scattering amplitude. Considering unconventional superconductors with different pairing symmetries and, in particular, evaluating the theoretical RIXS spectra for cuprate and pnictide-like systems, we show that the low-energy scattering is strongly affected by the superconducting gap and coherence factors. This establishes RIXS as a tool to disentangle pairing symmetries and to probe the elementary excitations of unconventional superconductors.

TT 45.5 Wed 16:00 H21

**Effects of randomness on the critical temperature in quasi-1D and quasi-2D superconductors** — •Enver Nakhmedov[1,2], Oktay Alekperov[2], and Reinhold Oppermann[1] — [1]Institut für Theoretische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Physics, Azerbaijan National Academy of Sciences, H. Cavid str. 33, AZ1143 Baku, Azerbaijan

Effects of non-magnetic disorder on the critical temperature Tc and on diamagnetism of quasi-1D and quasi-2D superconductors (SCs) are reported. The organic SCs are modeled as superconducting wires or layers connecting each others through the Josephson coupling. The Josephson energy is considered to be random parameter with Gaussian distribution. The phase of the order parameter is averaged over thermodynamic fluctuations as well as over disorder by employing the replica method. We show that the randomness destroys phase coherence between wires in quasi-1D SCs and that Tc vanishes discontinuously at a critical disorder-strength. Nevertheless the disorder of arbitrary high strength in quasi-2D organic SCs can not destroy completely the superconducting phase. The interplay between disorder and quantum phase fluctuations is shown to result in quantum critical behavior at T=0 in quasi-1D SCs, which manifests itself as a superconducting-normal metal phase transition of first-order at a critical disorder strength. The parallel and transverse components of the penetration-depth are evaluated. They diverge at different critical temperatures, which correspond to pair-breaking and phase-coherence breaking respectively. Our theory agrees well with the experimental measurements.

TT 45.6 Wed 16:15 H21

**Stability of super-currents and condensates in type I superconductors** — •Klaus Morawetz[1,2,3], Pavel Lipavsky[4], Bretislav Sopik[4], and Michael Maennel[1] — [1]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP), Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

Excitations of Cooper pairs into non-condensed bound pairs are similar to excitations of true bosons out of the Bose-Einstein condensate. Using the Landau criterion of superfluidity we evaluate the critical current above which these pair-excitations would lead to a finite resistivity. The predicted value strongly depends on the chosen approximation. The Kadanoff-Martin theory which is in many aspects equivalent to the BCS theory, leads to zero critical velocity, what is in conflict with the mere existence of super-currents. In contrast, the T-matrix with multiple scattering corrections provides the critical velocity of pair excitation which is $\sqrt{3}$-times larger than the critical velocity of pair breaking. This agrees with the experimentally well established fact that super-currents in type I superconductors are limited by pair breaking, not by pair excitation.

TT 45.7 Wed 16:30 H21

**Vacuum phonon squeezing in femtosecond-laser excited noble metals** — •Fairoja Cheenicode Kabeer, Eeuwe S. Zijlstra, and Martin E. Garcia — Universität Kassel, Kassel, Germany

The interaction of a femtosecond-laser pulse with a material can either strengthen or weaken the interatomic potential, which may give rise to many interesting ultrafast structural phenomena. Using electronic-temperature dependent density functional theory we demonstrate that the noble metals copper and silver show laser-induced bond hardening and that this can be used to achieve vacuum phonon squeezing. For the squeezed states we predict optimal squeezing factors at the L-point longitudinal mode which are orders of magnitude greater than what has been achieved so far[1].

[1] G. A. Garrett et al., Science 275, 1638 (1997)

## TT 46: Graphene - SiC Substrates and Intercalation (jointly with DS, HL, MA, and O)

Time: Wednesday 16:00–19:15 Location: H17

TT 46.1 Wed 16:00 H17

**Molecular Doping of Epitaxial Graphene on SiC with flouro-fullerenes** — •Martina Wanke[1,2], Anton Tadich[3], Mark Edmonds[4], Yaou Smets[4], Chris Pakes[4], and Thomas Seyller[1,2] — [1]Institut für Physik, Technische Universität Chemnitz, Reichenhainer Strasse 70, 09126 Chemnitz, Germany — [2]LS Technische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erwin-Rommel-Strasse 1, 91058 Erlangen — [3]Soft-X-Ray-Beamline, Australian Synchrotron, 800 Blackburn Road, Clayton, VIC 3168, Australia — [4]Scholl of Physics, La Trobe University, Physical Sciences 1, Bundoora, VIC 3086, Australia

Epitaxial graphene (EG) on SiC(0001) is intrinsically n-type doped due to charge transfer from the substrate surface [1,2]. Charge transfer doping with F4-TCNQ reduces the carrier concentration and increases the carrier mobility [2], but the stability of the molecular layer in ambient conditions is not given [2]. Molecules with a sufficiently high electron affinity are needed in order to achieve a significant reduction of the electron concentration in EG by surface transfer doping. The mechanism of surface transfer doping of diamond with $C_{60}F_{48}$ is well understood [3]. Using ARPES we investigated the surface transfer doping of EG with $C_{60}F_{48}$. A net p-type doping of EG was observed for higher coverages of the $C_{60}F_{48}$.
[1] T.Ohta et al., Science **313** (2006) 951; [2] J.Jobst et al., PRB **81** (2010) 195434; W.Chen et al., JACS **129** (2007) 10418; C. Coletti et al., PRB **81** (2010) 235401. [3] M. T. Edmonds et al., JCP 136 (2012) 124701.

TT 46.2 Wed 16:15 H17

**Transport properties of epitaxially grown graphene nanostructures** — •Jens Baringhaus, Frederik Edler, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The patterning of graphene into small stripes, the so called graphene nanoribbons, is an essential task for the development of future graphene based electronic devices. For such ribbons with a well-ordered edge geometry the presence of one-dimensional edge states has been predicted. The fabrication of these well-defined structures requires the avoidance of any damaging post-processing. To overcome this obstacle we use a selective graphitization process on SiC-mesa structures, producing monolayer graphene nanoribbons of 40 nm to 100 nm in width and of several micrometers in length. The local electronic properties of the ribbons are investigated by means of a 4-tip STM. The self-assembled graphene nanoribbbons show metallic behav-

ior and can be clearly distinguished from the non-metallic substrate. Conductances close to $G_0 = e^2/h$ are observed for a wide temperature range from 30 K up to room temperature. Description within the Landauer formalism is possible assuming ballistic transport dominated by a single ballistic channel. This is a strong indication for spin-polarized transport through the edge-states of the ribbons. These edge states also show up in scanning tunneling spectra. At higher temperatures the conductance increases due to the occupation of the next subband. Remarkably all investigated ribbons exhibit very large mean free paths up to 15 $\mu m$.

TT 46.3 Wed 16:30 H17

**Local investigation of transport properties and morphology of epitaxially grown 2d graphene** — •Frederik Edler, Jens Baringhaus, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

Graphene has a peculiar band structure and special transport properties. The transport is strongly affected by imperfections of the graphene films, e.g atomic steps and impurities located at the interface between graphene and its support. A reliable control of these parameters is possible by epitaxial grown graphene on SiC. To characterize the epitaxial growth and correlate the structure with transport properties, the sheet resistance of graphene grown on SiC(0001) and SiC(000$\bar{1}$) have been studied via a 4-tip STM/SEM system. The SEM allows precise positioning of feedback controlled STM tips, enabling transport measurements on a nm-scale. While STM is used to characterize atomic size defect structures, step-bunches and nano-inhomogeneities can be identified in SEM. Sheet resistances were found to be independent from probe spacing indicating a 2d transport behavior but highly depending on ex-situ processing steps. Further in-situ annealing led to sheet resistances around $6 - 8$ k$\Omega/\square$. These values can be explained by diffusive transport theory [1] and correlate with the concentration of the nano-inhomogeneities. Structural defects induce a mobility gap as deduced from temperature-dependent transport measurements. The sheet resistance increased by a factor of three for elastically bend graphene layers across SiC step-bunches. [1] Adam *et al.*, PNAS, **104**, 18392 (2007)

TT 46.4 Wed 16:45 H17

**Electronic structure of epitaxial graphene on 3C-SiC(111)** — •Lydia Nemec, Volker Blum, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin

We present a study of the electronic structure of the carbon-rich surface phases on 3C-SiC(111), including quasi-freestanding graphene and intercalated phases. Our approach is based on density-functional theory (DFT) including van der Waals (vdW) dispersion terms in the Tkatchenko-Scheffler approach [1]. We use semilocal DFT (PBE+vdW functional) for our first-principles structure predictions. For the oxygen intercalated bilayer graphene, we consider an oxygen-rich interface passivating the Si dangling bonds [2]. Based on the predicted geometries, hybrid functionals (HSE06 and PBE0) are used to assess the electronic structure of: (1) the partially sigma-bonded "buffer layer" phase, (2) quasi-freestanding graphene up to three monolayers, and (3) hydrogen- and oxygen intercalated graphene phases. For the different phases, we discuss the changes of the electronic structure, addressing the influence of the intercalated material on the doping of the graphene and the charge transfer from the substrate to the graphene layer. We observe that in the intercalated phases graphene is decoupled from the substrate, making intercalation a promising approach for further studies.

[1] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).
[2] M.H. Oliveira *et al.*; Carbon **52**, 83-89 (2013).

TT 46.5 Wed 17:00 H17

**Graphene on cubic and hexagonal SiC: A comparative theoretical study** — Oleg Pankratov, •Stephan Hensel, Paul Götzfried, and Michel Bockstedte — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudstr. 7B2, D-91058 Erlangen

Epitaxial graphene grows on different SiC polytypes which possess distinct band gaps. We investigate the influence of polytypes on the graphene electronic spectrum employing density functional calculations with LDA and hybrid HSE functionals. We consider different buffer layer-graphene layer stackings as well as different substrate terminations.[1] We find a systematic displacement of the Dirac point relative to the valence-band edge as a function of the polytype hexagonality. The HSE values are in good agreement with available experimental results,[2,3] while LDA corroborates the trends. The Dirac point, the interface-related states, and the Fermi level follow similar polytype-dependent shifts, hence the graphene doping of the epilayer stays practically the same. For the AB stacked buffer and epilayer on Si-terminated SiC the Dirac spectrum exhibits an energy gap of 25-40 meV (depending on the polytype). On the contrary, for the AA stacking the Dirac cone remains intact. We suggest a symmetry-based analytical model which explains the origin of the gap and its absence for the AA geometry.

[1] Pankratov *et al.* Phys. Rev. B 86, 155432 (2012).
[2] Sonde *et al.*, Phys. Rev. B 80, 241406 (2009).
[3] Ristein *et al.*, Phys. Rev. Lett. 108, 246104 (2012).

TT 46.6 Wed 17:15 H17

**Phonons of graphene on SiC(0001)** — Stefan Fryska[1], Roland J. Koch[1], Felix Fromm[1], Alejandro Molina-Sánchez[2], •Ludger Wirtz[2], Martina Wanke[1,3], and Thomas Seyller[1,3] — [1]FAU Erlangen-Nürnberg — [2]University of Luxembourg — [3]TU Chemnitz

Epitaxial graphene (EG) on SiC(0001) can be grown on a wafer scale [1] but its charge carrier mobility is considerably lower than that of graphene flakes obstained by mechanical exfoliation. A previous study [2] of the temperature dependence of the mobility suggested that it is determined by remote phonon scattering with phonons of the buffer layer at the interface between EG and SiC(0001). The buffer layer, which is identical to the $(6\sqrt{3}\times 6\sqrt{3})R30°$ reconstruction of SiC(0001), consists of a monolayer of carbon atoms in a honeycomb structure. Due to a strong interaction with the substrate, the buffer layer has destorted $\pi$-bands and does not exhibit a Dirac cone [3]. In order to learn more about the phonons of the buffer layer we have carried out a study using high-resolution electron energy loss spectrscopy (HREELS) and Raman spectroscopy, accompanied by *ab-initio* calculations. We observe strong modifications of the phonons of the buffer layer with respect to weakly interacting, quasi-free standing graphene on SiC(0001). In particular, the Kohn anomaly is quenched, which agrees with the lack of a Dirac cone. [1] K. V. Emtsev et al., Nat. Mater. **8** (2009) 203. [2] F. Speck et al., Appl. Phys. Lett. **99** (2011) 122106. [3] K. V. Emtsev et al., Phys. Rev. B **77** (2008) 155303.

TT 46.7 Wed 17:30 H17

**Intercalation of hydrogen at the graphene/Ir(111) interface** — •Thorsten Balgar, Hyunil Kim, and Eckart Hasselbrink — Universität Duisburg-Essen, Universitätsstr. 5, D-45141 Essen

Epitaxially grown graphene on an iridium crystal exhibits a well known moire pattern due to the lattice mismatch of graphene and the Ir(111) surface. This leads to a buckling of the carbon layer and a lateral modulation of the chemical reactivity towards adsorbates [1,2]. Unlike intercalated metal atoms hydrogen cannot be directly detected with surface scientists' standard analysis tool box, namely XPS or AES. In our study we have used vibrational sum frequency generation (SFG) spectroscopy to monitor the stretching vibration of hydrogen chemisorbed on graphene [3]. The results are discussed in view of the intercalation of hydrogen and the local formation of graphane-like structures.

[1] C. Busse et al., Phys. Rev. Lett. 107 (2011) 036101 [2] J. Wintterlin et al., Surf. Sci. 603 (2009) 1841 [3] Kim et al., Chem. Phys. Lett. 546 (2012) 12

TT 46.8 Wed 17:45 H17

**Decoupling of Epitaxial Graphene on Ir(111) by Oxygen Intercalation** — •Søren Ulstrup[1], Rosanna Larciprete[2], Paolo Lacovig[3], Matteo Dalmiglio[3], Marco Bianchi[1], Jens Christian Johannsen[1], Federico Mazzola[1], Liv Hornekær[1], Fabrizio Orlando[4], Alessandro Baraldi[4], Silvano Lizzit[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, Denmark — [2]CNR-Institute for Complex Systems, Roma, Italy — [3]Sincrotrone Trieste, Trieste, Italy — [4]Physics Department and Center of Excellence for Nanostructured Materials, University of Trieste, and IOM-CNR Laboratorio TASC, Area Science Park, Trieste, Italy

Epitaxial growth of graphene on transition metal surfaces is now a well-established method for obtaining extended layers of high quality graphene. However, interactions between graphene and its metal substrate are unwanted in applications typically requiring a mechanical transfer of the graphene. Here we demonstrate a different strategy based on decoupling the graphene from an Ir(111) substrate by oxy-

gen intercalation. More specifically, we present evidence using photoelectron spectroscopy techniques that the intercalation results in an extended layer of hole-doped quasi free-standing graphene (QFG). Analysis of the electronic self-energy near the Fermi level reveals an extremely weak electron-phonon coupling in QFG. Finally, we find that abrupt deintercalation of oxygen occurs at elevated temperatures, which is accompanied by a modest etching of the graphene lattice.

TT 46.9 Wed 18:00 H17

**Transfer-free electrical insulation of epitaxial graphene from its metal substrate** — Silvano Lizzit[1], Rosanna Larciprete[2], Paolo Lacovig[1], Matteo Dalmiglio[1], Fabrizio Orlando[3,4], Alessandro Baraldi[3,4], Lauge Gammelgaard[5], •Lucas Barreto[6], Marco Bianchi[6], Edward Perkins[6], and Philip Hofmann[6] — [1]Sincrotrone Trieste, Italy — [2]CNR-Institute for Complex Systems, Roma, Italy — [3]Physics Department and CENMAT, University of Trieste,Italy — [4]IOM-CNR Laboratorio TASC, Trieste, Italy — [5]Capres A/S, Lyngby, Denmark — [6]Institut for Fysik og Astronomi, Interdisciplinary Nanoscience Center (iNANO), Aarhus Universitet Denmark

High-quality, large-area epitaxial graphene can be grown on metal surfaces, but its transport properties cannot be exploited because the electrical conduction is dominated by the substrate. Here we show how to insulate epitaxial graphene from the Ru(0001) surface it is grown on by a step-wise intercalation of silicon and oxygen, and the eventual formation of a $SiO_2$ layer between the graphene and the metal. The reaction steps are followed by x-ray photoemission spectroscopy. The presence of a $SiO_2$ layer should insulate the metal from the substrate. In order to verify this, lateral transport measurements were performed using a nano-scale multipoint probe technique. The resistance obtained is substantially higher than expected for a clean ruthenium surface but consistent with that expected for graphene. Moreover, the data suggest two-dimensional electronic transport, as expected for graphene.

TT 46.10 Wed 18:15 H17

**Intercalation as a route to atomically sharp graphene/ferromagnet interfaces: Structural and electronic investigations** — •Philipp Leicht, Konstantin Krausert, Lukas Zielke, and Mikhail Fonin — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The interface between graphene (G) and the substrate plays a vital role for the electronic properties of G. Apart from direct growth of G on a small number of substrates, a variety of metals can be intercalated between G and the substrate interface [1,2] and allow for the production of G on a large number of materials. In this work, we present the investigation of Ni intercalation underneath G on Ir(111). The atomic structure and electronic properties were investigated for samples with intercalated Ni ranging from a submonolayer to few monolayers.

For Ni intercalation underneath G/Ir(111), scanning tunneling microscopy shows strongly increased moiré corrugation as well as a decreased average distance of G/Ni/Ir(111) compared to G/Ir(111). The stronger corrugation is accompanied by considerable changes in the electronic structure of the G layer. The intercalation channels including the influence of defects and diffusion of intercalants within the graphene-metal interface are discussed for the two regimes of submonolayer and multilayer intercalation.

[1] M. Sicot et al. ACS Nano 6, 151 (2012) [2] L. Huang et al. Appl. Phys. Lett. 99, 163107 (2011)

TT 46.11 Wed 18:30 H17

**Magnetism of graphene/Ir(111) intercalation systems** — •Régis Decker[1], Jens Brede[1], Nicolae Atodiresei[2], Vasile Caciuc[2], Stefan Blügel[2], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, D-30355 Hamburg — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungzentrum Jülich, D-52425 Jülich

The presence of intercalation compounds in graphite, i.e. impurities or layer(s) trapped between carbon sheets, can lead to changes in the transport, optical and catalytic properties compared to bulk graphite, or even to superconductivity. The intercalation of elements between graphene and its substrate can also influence the properties of graphene. Furthermore, this approach opens a new route to explore the behavior of graphene on a magnetic substrate.

Here, we present the local structure and magnetic properties of graphene on magnetic substrates, resolved by spin-polarized STM. The magnetic substrates are obtained by the intercalation of 3d elements (Co and Fe) between graphene and the Ir(111) surface [1]. In both cases, the atomic structure of the graphene layer is dominated by a highly corrugated Moiré pattern. Within the Moiré pattern different regions are identified. Interestingly, these regions show very different electronic and magnetic signatures in the experiments. The experimental observations are compared to state-of-the-art first principles density functional theory calculations.

[1] Atomic-scale magnetism of cobalt-intercalated graphene. R. Decker et al., accepted in Phys. Rev. B (Rapid Comm.).

TT 46.12 Wed 18:45 H17

**Deuteration kinetics of the graphene** — •Alexei Nefedov[1], Alessio Paris[2], Nikolay Verbitskiy[3,11], Ying Wang[4], Alexander Fedorov[5,6], Danny Haberer[5], Martin Oetzelt[7], Luca Petaccia[8], Dmitry Usachov[6], Denis Vyalikh[6,9], Hermann Sagdev[10], Christof Woell[1], Martin Knupfer[5], Berndt Buechner[5], Lucia Calliari[2], Lada Yashina[3], Stephan Irle[4], and Alexander Grüneis[5,11] — [1]KIT, Leopoldshafen, Germany — [2]FBK-CMM, Trento, Italy — [3]MSU, Moscow, Russia — [4]Nagoya University, Nagoya, Japan — [5]IFW Dresden, Dresden, Germany — [6]St. Petersburg University, St. Petersburg, Russia — [7]BESSY II, Berlin, Germany — [8]Elettra, Trieste, Italy — [9]TU Dresden, Dresden, Germany — [10]MPI für Polymerforschung, Mainz, Germany — [11]University of Vienna, Vienna, Austria

The kinetics of the hydrogenation/deuteration reaction of graphene was studied by time-dependent x-ray photoemission spectroscopy (XPS). The graphene layer was then exposed to hydrogen or deuterium atomic gas beams, obtained by thermal cracking in a tungsten capillary at T=3000 K. After each step XPS of the C1s line was performed in order to measure H/C and D/C ratios. We have observed a strong kinetic isotope effect for the hydrogenation/deuteration reaction leading to substantially faster adsorption and higher maximum D/C ratios as compared to H/C (D/C˜35% vs. H/C˜25%).

TT 46.13 Wed 19:00 H17

**Intercalated thin films on Graphene/Ir(111)** — •Hendrik Vita[1], Stefan Böttcher[1], Yuriy S Dedkov[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin — [2]SPECS Surface Nano Analysis GmbH, Voltastr. 5, D-13355 Berlin

The investigation of graphene/metal systems is interesting from fundamental as well as applications-oriented point of view. Here we report on the interaction of weakly and strongly bound intercalated metals (Cu vs. Ni) with graphene grown on Ir(111), using core and valence level photoemission spectroscopy. Studying the electronic structure of graphene in these interfaces reveals the effect of weak and strong interaction between graphene and the underlying intercalated thin film. The graphene/Ni/Ir(111) system shows a strong hybridization between the graphene $\pi$-band and the Ni 3d valence bands, which leads to the destruction of the graphene Dirac cone. The graphene/Cu/Ir(111) system, on the other hand, shows at first glance the properties of weakly bonded graphene (Dirac cone with a linear dispersion of the $\pi$-band) but with additional doping due to the donation of electrons by the intercalated Cu. Contrary to the weakly bonded scenario we observe a hybridization between the distinct Cu3d states and the graphene $\pi$-band.

# TT 47: Focused Session: Frontiers of Electronic Structure Theory 5 (jointly with HL and O)

Time: Wednesday 16:00–19:30 Location: H36

**Topical Talk** TT 47.1 Wed 16:00 H36

**Screening high throughput density functional theory calculations using simplified models.** — •Georg K. H. Madsen, Ingo Opahle, Alessandro Parma, Eunan J. McEniry, and Ralf Drautz — ICAMS, Ruhr Universität Bochum, Bochum, Germany

Thermoelectric materials can be utilized for an efficient conversion of waste heat to electric power. Thermoelectric properties of known compounds can be rationalized and predicted using only the structure as an input.[1] While this can used to discover potential thermoelectric materials by screening known structures[2], there remains a large challenge in discovering unknown phases computationally. Employing a newly developed high throughput environment we show how the stability of binary transition metal silicides can be reproduced using a systematic replacement technique.[3]

As ternary and higher compounds are considered, a combinatorial explosion of potential structures and combinations must be considered. We have therefore develop ed tight binding models of the electronic structure and datamining methods based on the calculation of binary compounds. It will be discussed how these simplified models can be interpreted and used to pre-screen the stability of higher compounds to limit the number of density functional calculations to be done.

TT 47.2 Wed 16:30 H36

**Tight-binding scale-bridging calculations for steel research** — •Nicholas Hatcher, Georg K H Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum, Germany

Parameterized methods to extend electronic structure calculations to large systems have recently garnered additional attention due to the limits of traditional DFT. The ability to model low carbon content in steel requires the accurate calculation of millions of atoms. However, interatomic potentials have been shown to be inconsistent with DFT in different environments and cannot give an accurate portrayal of chemical bonding or magnetism. Thus, a coherent transferable tight-binding (TB) parameterization was developed for Fe-C by extracting bonding interactions from DFT and finding a suitable interatomic repulsion. This model gives an accurate description of the energy hierarchy of relevant Fe-C structures, elastic properties, and defect energies. We apply this model to determine mechanisms of carbon segregation to grain boundaries and carbon diffusion in iron, including the interaction of multiple defects under tension and pressure. Furthermore, this intuitive energy functional forms the basis for bond order potentials, thereby extending system sizes to millions of atoms.

TT 47.3 Wed 16:45 H36

**Local atomic energies from optimal atomic orbitals** — •Björn Lange, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

Decomposing the energy of a condensed matter system into atomic contributions is of great use e.g. for understanding the physical origin of defect and surface energetics or for identifying chemically reactive regions in disordered systems. However, commonly employed energy calculations in the framework of density-functional theory (DFT) do not in general provide a natural decomposition into atoms. Here we propose a novel scheme to achieve this based on the recently introduced concept of atom-centered Quamols[1] that are variationally optimized to represent the electronic structure with a minimal basis set, which largely avoids local overcompleteness issues. The spillage resulting from the remaining small incompleteness is segmented according to a space separation derived from the Quamol atomic densities, maintaining the accuracy of the underlying DFT calculation. The total energy is then decomposed by combining this basis set with a local energy density treatment based on the ideas of Chetty and Martin[2]. We demonstrate the performance of our scheme by visualizing and analyzing the energy distribution at surfaces and in amorphous silicon.

[1] PRB 84, 085101, (2011)
[2] Chetty, N. and Martin, Richard M., PRB 45, 6074, (1992)

TT 47.4 Wed 17:00 H36

**Environmental linear-scaling tight-binding for multicomponent metallic alloys** — •Eunan J. McEniry, Georg K. H. Madsen, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany.

The development of accurate and transferable models to describe the behaviour of multicomponent systems is attracting considerable interest in materials modelling. Tight-binding models derived from density functional theory potentially provide an accurate and systematic approach to this problem. We introduce a methodology for environmental tight-binding (ETB) in which both the overlap and environmental contributions to the electronic structure are included. In order to implement the resulting ETB models within linear-scaling tight-binding approaches, a method for the evaluation of the screening matrix has been developed, based on a Chebyshev expansion of the inverse of the overlap matrix. The resultant linear-scaling environmental tight-binding framework has been applied to a number of relevant material systems, and the transferability and scalability of the approach is discussed. The present contribution outlines our attempts to extend the tight-binding approach towards larger-scale molecular dynamics simulations within a linear-scaling framework.

TT 47.5 Wed 17:15 H36

**Spontaneous Electric Polarisation from a Classical Perspective.** — •Paul Tangney — Imperial College London, London, UK

Spontaneous polarisation is a quantity attributed to noncentrosymmetric crystals and is often associated with a macroscopic electric field permeating the bulk of a sample. Its time derivative is measured as a current density during application of an external stimulus, such as temperature, strain, or an electric field. I will argue that such currents do not require the existence of a spontaneous polarisation field or a macroscopic electric field in the bulk of a polar material. They can be explained by symmetry arguments within a purely classical picture and should be calculable from the time dependence of the many-particle position probability density function of the material's constituent charges - a classical quantity. The only macroscopic electric field across any bulk crystal arises from the charges on its surfaces, which in most cases are strongly influenced by surface relaxation/reconstruction and chemical environment and unlikely to be determined by polarization currents. I will show how the classical picture of polarisation presented is consistent with the Modern Theory of Polarisation[1], in all but interpretation. I will illustrate my arguments with simulations of a toy system.

[1] R. Resta and D. Vanderbilt, "Theory of Polarization: A Modern Approach", in Physics of Ferroelectrics: a Modern Perspective C.H. Ahn, K.M. Rabe, and J.M. Triscone, Eds. Springer-Verlag, (2007).

TT 47.6 Wed 17:30 H36

**Potential energy surface of $BaTiO_3$ explored with density-functional theory and classical force fields** — •Joseph Fallon[1], David McComb[2], Arash Mostofi[1], and Paul Tangney[1] — [1]Imperial College London, London, UK — [2]The Ohio State University, Columbus, USA

Much is known about the electronic structure of $BaTiO_3$, its phonon dispersions, and the energetics of its long wavelength lattice distortions. However, there is much more to learn about the potential energy surface (PES) on which the atoms move. We study the PES using a combination of density functional-theory (DFT) and a polarisable ionic model of interatomic bonding. Our force field is in close agreement with DFT on structures, the PES, and phonon frequencies and allows accurate large scale atomistic simulations of domain structures and dynamics to be performed. A key advantage of an atomistic model over the coarse grained models that are often used to simulate domain dynamics is that it allows the simulation of heterogeneous materials (e.g. grain boundaries, point defects). However, we also point out some features of the PES, which may be important to domain dynamics, that effective Hamiltonians based on the transverse optic soft mode eigenvector and the local strain fail to capture.

TT 47.7 Wed 17:45 H36

**Efficient Oscillator-Based Approach for Polarizability and van der Waals Interactions** — •Vivekanand Gobre[1], Robert A. Distasio Jr.[2], Roberto Car[2], Matthias Scheffler[1], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG — [2]Princeton University, USA

The dynamic polarizability measures the response to an applied time-dependent electric field, and its accurate determination is crucial for van der Waals (vdW) interactions and other response properties. First-principles calculations of polarizabilities in principle require a computationally expensive explicit treatment of many-electron excitations, and are only applicable in practice to systems with less than about 100 atoms. In this work, we present an efficient parameter-free approach for calculating accurate frequency dependent polarizabilities for molecules with thousands of atoms, as well as periodic materials. This is achieved by the synergistic coupling of the Tkatchenko-Scheffler method [1], which accurately treats short-range hybridization effects, with the self-consistent screening equation from classical electrodynamics [2,3]. Using only the electron density and free atom reference, we obtain an accuracy of 7% for both static polarizabilities and vdW coefficients for an extensive database of gas-phase molecules and crystals. We analyze the interplay of hybridization and long-range screening effects on the polarizability. [1] Tkatchenko and Scheffler, PRL (2009), [2] Felderhof, Physica (1974), [3] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012).

TT 47.8 Wed 18:00 H36

**Van der Waals interactions in Density Functional Theory and Linear-scaling Density Functional Theory** — •Lampros Andrinopoulos, Nicholas D. M. Hine, and Arash A. Mostofi — Imperial College London, London, United Kingdom

Semilocal functionals in Density Functional Theory (DFT) achieve high accuracy simulating a wide range of systems, but miss the effect of dispersion (vdW) interactions, important in weakly bound systems. We study two different methods to include vdW in DFT: First, we investigate a recent approach [1] to evaluate the vdW contribution to the total energy using maximally-localized Wannier functions. Using a set of simple dimers, we show that it has a number of shortcomings that hamper its predictive power; we then develop and implement a series of improvements [2] and obtain binding energies and equilibrium geometries in closer agreement to quantum-chemical coupled-cluster calculations. Second, we implement the vdW-DF functional [3], using Soler's method [4], within ONETEP [5], a linear-scaling DFT code, and apply it to a range of systems. This method within a linear-scaling DFT code allows the simulation of weakly bound systems of larger scale, such as organic/inorganic interfaces, biological systems and implicit solvation models. [1] P. Silvestrelli, J.P.C. A 113, 5224 (2009). [2] L. Andrinopoulos et al, J.C.P. 135, 154105 (2011). [3] M. Dion et al, P.R.L. 92, 246401 (2004). [4] G. Roman-Perez, J.M. Soler, P.R.L. 103, 096102 (2009). [5] C. Skylaris et al, J.C.P. 122, 084119 (2005).

TT 47.9 Wed 18:15 H36

**Microscopic van der Waals Interactions with Localized and Metallic States** — •Victor Gonzalo Ruiz, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG

Several promising methods have been developed in recent years for an efficient modeling of van der Waals (vdW) interactions in molecules and solids. However, essentially all of these methods rely on an localized model for the polarizability, ignoring the rather strong interplay between localized and metallic electronic states. Such states are present in many relevant materials, including transition metals, hybrid organic/metal interfaces, and topological insulators. Here we show how to extend the Tkatchenko-Scheffler method [1] for vdW interactions to treat localized and itinerant electronic states on equal footing by using the gradient of the electron density. In our model, the vdW correction vanishes for the homogeneous electron gas as it should in density-functional theory built upon the local-density approximation. To illustrate the performance of the newly developed microscopic model, we study the cohesive properties of coinage metals and the binding of organic molecules on metals. [1] A. Tkatchenko and M. Scheffler, PRL 102, 073005 (2009).

TT 47.10 Wed 18:30 H36

**Self-Consistent Density Functional Including Long-Range van der Waals Interactions** — •Nicola Ferri[1], Robert A. Distasio JR.[2], Roberto Car[2], Matthias Scheffler[1], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Princeton University, USA

Van der Waals (vdW) interactions are significant for a wide variety of systems, from noble-gas dimers to complex organic/inorganic interfaces. The long-range vdW energy is a tiny fraction (∼0.001%) of the total energy, hence it is typically assumed that vdW interactions do not change electronic properties. Although the vdW-DF functional self-consistently includes the effect of the vdW energy on electronic structure [1], the influence of "true" long-range vdW interactions is difficult to assess since a significant part of vdW-DF energy arises from short distances. Here, we present a self-consistent implementation of the long-range Tkatchenko-Scheffler (TS) density functional [2], including its extension to surfaces [3]. The analysis of self-consistency for rare-gas dimers allows us to reconcile two different views on vdW interactions: (i) Feynman's view that advocates changes in the electron density, and (ii) atoms separated by an infinite barrier. In agreement with previous work [1], we find the contribution from self-consistency to be negligible in the structure and stability of vdW-bound complexes. However, a closer look at complex organic/inorganic interfaces reveals notable modification of the energy levels when using the self-consistent TS vdW density functional. [1] Thonhauser *et al.*, PRB (2007), [2] Tkatchenko and Scheffler, PRL (2009), [3] Ruiz *et al.*, PRL (2012).

TT 47.11 Wed 18:45 H36

**Many-Body van der Waals Interactions from Isotropically Damped Coupled Quantum Harmonic Oscillators** — •Alberto Ambrosetti[1], Robert A. DiStasio Jr.[2], and Alexandre Tkatchenko[1] — [1]Fritz-Haber institut der MPG, Faradayweg 4-6 14195 Berlin, Germany — [2]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA

The current interest in functional materials with increasing size and complexity demands high accuracy in first-principles calculations. In these systems, the collective many-body (MB) description of van der Waals (vdW) interactions is indispensable to reach the highly coveted "chemical accuracy". The recently introduced DFT+MBD method (PRL **108**, 236402 (2012); PNAS **109** 14791 (2012)) for the dispersion energy based on a coupled set of quantum harmonic oscillators (QHOs) was shown to reach chemical accuracy for gas-phase molecules and molecular solids. Its formulation, however, makes the derivation of interatomic forces and a fully self-consistent DFT+MBD implementation non-trivial. We propose here a simplified approach, making use of a set of QHOs with isotropically damped dipole–dipole coupling, which provides an effective random-phase approximation treatment of their vdW interaction (arXiv:1210.8343). This allows for a simple analytical treatment of interatomic forces, yet providing high efficiency and accuracy. Application over a wide range of systems shows a consistent improvement with respect to pairwise approximations, particularly for the most extended systems.

TT 47.12 Wed 19:00 H36

**Interplay between H bond symmetrization and spin transition in $\epsilon$-FeOOH: insights from first principles** — •Carmen Quiroga and Rossitza Pentcheva — Dept. of Earth and Environmental Sciences, University of Munich

Structural and electronic spin transitions in high-pressure $\epsilon$-FeOOH are studied using density functional theory calculations including an on-site Coulomb repulsion term. A high-spin to low-spin transition in trivalent iron is predicted at $\sim$ 58 GPa, in agreement with previous theoretical study [1] and experimental indications [2]. The spin transition is heralded by a second order $P2_1nm$ to $Pnnm$ phase transition at $\sim$ 43 GPa, driven by hydrogen bond symmetrization at the critical hydrogen bond $O\cdots O$ limit of $\simeq$ 2.4 Å. Our results give indications of a possible connection between the symmetry of hydrogen bonds in $\epsilon$-FeOOH and the spin state of $Fe^{3+}$, with important implications in disclosing the influence of water content in the mantle redox state.

Funding by DFG SPP1236 (PE883/8-1) is acknowledged.

[1] Otte et al. Phys. Rev. B **80**, 205116 (2009).
[2] Gleason et al. In preparation.

TT 47.13 Wed 19:15 H36

**From spheres to iso: Implementing implicit solvation in FHI-aims** — •Ran Jia, Chunsheng Liu, Daniel Berger, Harald Oberhofer, and Karsten Reuter — Department Chemie, Technische Universität München, Lichtenbergstr. 4, D-85747 Garching, Germany

At the cost of reduced accuracy, implicit solvation models yield strong speedups compared to explicit solvent simulations. Here, we report on the implementation of the multipole moment expansion (MPE) solvent continuum model into the density-functional theory (DFT) program package FHI-aims. Characterizing the surrounding solvent mainly by its dielectric constant and density, the form of the cavity employed for the solute and the description of the reaction field created by the polarized solvent are the two central characteristics of any implicit sol-

vation approach. In MPE the reaction field is computed as a truncated multipolar expansion. In our implementation we discard the prevalent cavity representation in form of a set of overlapping spheres centered around the solute atoms in favor of an electron isodensity surface. This allows for more flexible shapes with increased physical meaning. In particular, it paves the way towards the description of one- or two-dimensional periodic systems, and therewith to complex solid-liquid interfaces.

## TT 48: Correlated Electrons: Quantum-Critical Phenomena - Theory

Time: Wednesday 16:45–18:45 Location: H19

**Topical Talk** TT 48.1 Wed 16:45 H19

**Transport as a sensitive indicator for quantum criticality** — •Gernot Schaller, Malte Vogl, and Tobias Brandes — Institut für Theoretische Physik, TU Berlin, Berlin, Germany

Quantum-critical systems exhibit a non-analytic behavior of the ground state with respect to an external control parameter, separating macroscopically different phases. At zero temperature, this is transfered to order parameters such as e.g. the energy or other observables. However, when dealing with fragile quantum systems one has to take the inevitable interaction with a reservoir into account. The fate of the quantum criticality in this regime is less understood.

We argue that due to the closure of the energy gap above the ground state, at finite reservoir temperatures the non-analytic ground state properties will be suppressed in most observables. This can also be expected in non-equilibrium setups, where the system is placed in contact with multiple thermal reservoirs at different temperatures. In contrast, we propose the stationary current through the quantum-critical system itself (e.g. the heat current transferred between the reservoirs through the system) to be much more sensitive to quantum criticality: We expect signatures in the stationary current even in the far from equilibrium regime. These findings are made explicit at a toy model for adiabatic computation corresponding to a first order quantum phase transition and at the quantum Ising model in a transverse field with a second order quantum phase transition.

[1] M. Vogl, G. Schaller, and T. Brandes, Phys. Rev. Lett. (in press), arXiv:1208.5989 (2012).

TT 48.2 Wed 17:15 H19

**Conductivity close to antiferromagnetic criticality** — Sergey Syzranov and •Jörg Schmalian — Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie

We study the conductivity of a three dimensional disordered metal close to an antiferromagnetic instability within the framework of the spin-fermion model[1]. We calculate the interaction correction to the conductivity, assuming that the latter is dominated by disorder scattering, and the interaction is weak. Although the fermionic scattering rate shows critical behaviour on the entire Fermi surface, the interaction correction is dominated by processes near the hot spots, narrow regions of the Fermi-surface corresponding to the strongest spin-fermion scattering. We discuss the scaling behavior of the conductivity as function of frequency and temperature and the role of quantum corrections to the semi-classical Boltzmann theory of transport.

[1] S. Syzranov, and J. Schmalian, Phys. Rev. Lett. 109, 156403 (2012)

TT 48.3 Wed 17:30 H19

**Universal short time dynamics after a quantum quench in the vicinity of a quantum critical point** — •Pia Gagel, Peter Orth, and Jörg Schmalian — Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie

We investigate the dynamical evolution of the order parameter after a quantum quench from the ordered state to the quantum critical point. The calculation is done for a model relevant for quantum magnets and bosons near the superfluid insulator transition. The short time dynamics after a quantum quench is, similar to quenches near classical phase transitions, characterized by a new universal exponent. We determine this exponent using a 4-d-z and 1/N expansions and by mapping the system onto boundary layer problems. Here d is the space dimension, z the dynamic scaling exponent, and N the number of components of the order parameter. Thermalization of the post quantum quench dynamics then leads to a sequence of distinct temporal regimes that are qualitatively distinct from classical quenches. Our results demonstrate that the post quench dynamics can be used to determine the universality class of a quantum critical point.

TT 48.4 Wed 17:45 H19

**Kondo breakdown in RKKY-coupled two- and multi-impurity Kondo systems** — •Ammar Nejati, Katinka Ballmann, and Johann Kroha — Universität Bonn

The driving mechanisms for magnetic quantum phase transitions in different heavy fermion systems have remained obscure. One difficulty is the lack of theoretical methods for treating a possible breakdown of Kondo screening and of heavy quasiparticles without invoking magnetic order. We consider a dense system of Kondo impurities and develop a novel renormalization group technique for the local Kondo coupling $J_i$ on a given impurity site $i$. At the one-loop level, the $\beta$ function for $J_i$ includes RKKY corrections due to the coupling to the surrounding impurities $j \neq i$, which arises in order $O(J_i J_j)$ from the local couplings $J_i$ and $J_j$. In this way, double counting of RKKY operators is avoided. This method allows to determine the single-impurity Kondo screening scale $T_K(y)$ as a function of the dimensionless RKKY coupling $y$ (determined alone by the conduction electron response function), without invoking magnetic ordering fluctuations. The solution of the RG equation indicates a breakdown of Kondo screening when $y$ exceeds a critical value $y_c$, where the latter can be expressed in a universal way in terms of the bare Kondo temperature $T_K(y = 0)$. For $y < y_c$ the RKKY-corrected single-impurity Kondo screening scale $T_K(y)/T_K(0)$ is a universal function of $y/y_c$ [1]. We compare these predictions with recent experiments on heavy fermion [1] and two-impurity [2] systems.

[1] M. Klein *et al.*, PRL **101**, 266404 (2008)
[2] J. Bork *et al.*, Nature Physics **7**, 901 (2011)

TT 48.5 Wed 18:00 H19

**Quantum Criticality in the two-channel pseudogap Anderson model** — •Farzaneh Zamani[1,2], Tathagata Chowdhury[3], Pedro Ribeiro[1,2], Kevin Ingersent[3], and Stefan Kirchner[3] — [1]Max Planck Institute for the Physics of Complex System, Nöthnitzer Str. 38, D-01187 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, D-01187 Dresden, Germany — [3]Department of Physics, University of Florida, Gainesville, Florida 32611-8440, USA

The two-channel Anderson impurity model with a density of states $\rho(E) \propto |E|^r$ that vanishes at the Fermi energy (E = 0) is of current interest in connection with impurities in graphene and in unconventional superconductors. We study the dynamical properties of the two-channel Anderson model using the non-crossing approximation (NCA), and compare our results against the numerical renormalization-group (NRG) method. This model shows continuous quantum phase transitions between weak- and strong-coupling phases. The NCA is shown to reproduce the correct qualitative features of the pseudogap model, including the phase diagram, and to yield critical exponents in excellent agreement with the NRG and exact results. The forms of the dynamical magnetic susceptibility and impurity Green's function at the fixed points are suggestive of frequency-over-temperature scaling, another aspect associated with interacting quantum critical points.

TT 48.6 Wed 18:15 H19

**Charge order in the Falicov-Kimball model - a dual fermion approach** — •Andrey Antipov[1,2], Emanuel Gull[3], and Stefan Kirchner[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [3]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA

We study charge ordering in the Falicov-Kimball model in 2,3,4, and infinite dimensions within the dynamical mean field theory (DMFT) and its recently developed dual fermion extension, which allows for the systematic diagrammatic description of the spatial corrections to the DMFT solution. We focus on the critical properties of the model

and compare various levels of approximations. The Falicov-Kimball model is particularly well suited to this purpose as the reducible n-point vertices entering a dual fermion calculation can be constructed analytically from the exactly solvable DMFT limit. We make a comparison to exactly known results.

TT 48.7 Wed 18:30 H19

**Matrix Product States with Long-Range Localizable Entanglement** — •Thorsten Wahl[1], David Pérez-García[2], and Ignacio Cirac[1] — [1]Max-Planck Institut für Quantenoptik, Hans-Kopfermann-Str. 1, Garching, D-85748, Germany — [2]Departamento de Analisis Matematico, Universidad Complutense de Madrid, 28040 Madrid, Spain

Localizable entanglement is the maximum amount of entanglement that can be generated between two spins of a spin chain by measuring the remaining ones. The case of long-range localizable entanglement, where this amount is finite even if the two spins are infinitely far apart, constitutes a hidden long-range order and is important for quantum repeaters and the characterization of quantum phase transitions. A criterion will be presented which characterizes the full set of Matrix Product States with long-range localizable entanglement.

## TT 49: Superconductivity: SQUIDs & Cryodetectors

Time: Wednesday 17:00–19:00 Location: H21

TT 49.1 Wed 17:00 H21

**Dc SQUIDs with asymmetric shunt resistors** — •Matthias Rudolph[1], Joachim Nagel[1], Johannes Maximilian Meckbach[2], Matthias Kemmler[1], Konstantin Ilin[2], Michael Siegel[2], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut - Experimentalphysik II and Center for Collective Quantum Phenomena in LISA$^+$,Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [2]Institut für Mikro- und Nanoelektronische Systeme, Karlsruhe Institute of Technology, Hertzstr. 16, D-76187 Karlsruhe, Germany

We have investigated asymmetrically shunted Nb/Al-AlO$_x$/Nb dc SQUIDs. Simulations based on the coupled Langevin equations predict that the optimum energy resolution $\epsilon$, and thus also the noise performance of such an asymmetric SQUID, can be 3-4 times better than that of its symmetric counterpart. While keeping the total resistance $R$ identical to a comparable symmetric SQUID with $R^{-1} = R_1^{-1} + R_2^{-1}$, we shunted only one of the two Josephson junctions with $R = R_{1,2}/2$. Both types of SQUIDs were characterized with respect to their transport and noise properties at temperature $T = 4.2\,K$, and we compared the experimental results with numerical simulations. Experiments yielded $\epsilon \approx 32\,\hbar$ for an asymmetric SQUID with an inductance $L = 22\,\mathrm{pH}$, whereas a comparable symmetric device achieved $\epsilon = 110\,\hbar$.

TT 49.2 Wed 17:15 H21

**Nb nanoSQUIDs for detection of small spin systems** — •R. Wölbing[1], J. Nagel[1], M. Kemmler[1], R. Kleiner[1], D. Koelle[1], O. Kieler[2], T. Weimann[2], J. Kohlmann[2], A. Zorin[2], A. Buchter[3], F. Xue[3], M. Poggio[3], D. Rüffer[4], E. Russo-Averchi[4], A. Fontcuberta i Morral[4], R. Huber[5], P. Berberich[5], and D. Grundler[4,5] — [1]Physikalisches Institut, Universität Tübingen, Germany — [2]Fachbereich 2.4 "Quantenelektronik", PTB Braunschweig, Germany — [3]Department of Physics, University of Basel, Switzerland — [4]Laboratoire des Matériaux Semiconducteurs, EPF Lausanne, Switzerland — [5]Physik-Department E10, Technische Universität München, Germany

We report on the realization of highly sensitive dc nanoSQUIDs for the investigation of small spin systems in moderate magnetic fields. The Nb SQUIDs are based on normal metal Josephson junctions made of HfTi and patterned by e-beam lithography. We demonstrate stable operation up to $B = \pm 50\,\mathrm{mT}$ without degradation of rms flux noise ($S_\Phi^{1/2} \leq 280\,\mathrm{n}\Phi_0/\sqrt{\mathrm{Hz}}$). We also present a multifunctional system combining a Nb nanoSQUID and a low-temperature magnetic force microscope (LTMFM) with a Ni nanotube as a scanning tip. This system allows for magnetization measurements of the Ni tube by using both, LTMFM and SQUID readout. Furthermore, the measurement of magnetic flux $\Phi$ vs. position of the particle provides an experimental determination of the coupling factor $\phi_\mu = \Phi/\mu$ between SQUID and Ni tube with magnetic moment $\mu$. The results confirm our predictions from numerical simulations, taking into account the SQUID geometry.

TT 49.3 Wed 17:30 H21

**Low-noise $YBa_2Cu_3O_7$ nanoSQUIDs for the detection of small spin systems operating in Tesla magnetic fields** — •Tobias Schwarz, Joachim Nagel, Roman Wölbing, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut - Experimentalphysik II and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany

We investigated the noise performance of $YBa_2Cu_3O_7$ (YBCO) nanoSQUIDs with grain boundary Josephson junctions in high magnetic fields. On $SrTiO_3$ [001] bicrystal substrates YBCO films were grown by pulsed laser deposition and covered by an in-situ evaporated gold layer to provide non-hysteretic IV-curves. SQUIDs with line widths down to 100nm were fabricated by focused ion beam milling. A constriction next to the SQUID allows on-chip modulation of the magnetic flux coupled into the SQUID loop. The SQUID we present here can be operated in Tesla magnetic fields applied parallel to the SQUID loop. The white flux noise level increases only slightly from $S_\Phi^{1/2} = 1.3\,\mu_B/Hz^{1/2}$ at $B = 0$ to $S_\Phi^{1/2} = 2.3\,\mu\Phi_0\Phi_0/Hz^{1/2}$ at $B = 1\mathrm{T}$. Assuming that a point-like magnetic particle is placed on top of the constriction, we calculate a spin sensitivity $S_\mu^{1/2} = 62\,\mu_B/Hz^{1/2}$ at $B = 0$ and $S_\mu^{1/2} = 110\,\mu_B/Hz^{1/2}$ at $B = 1\mathrm{T}$. Further we show that by optimizing the parameters of the presented SQUID geometry spin sensitivities of a few $\mu_B/Hz^{1/2}$ should be feasible.

TT 49.4 Wed 17:45 H21

**Experiments with Tunable Josephson Metamaterials** — •Susanne Butz[1], Philipp Jung[1], Valery Koshelets[2], and Alexey V. Ustinov[1,3] — [1]Physikalisches Institut , Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Kotel'nikov Institute of Radio Engineering and Electronics RAS, Moscow 125009, Russia — [3]National University of Science and Technology MISIS, Moscow 119049, Russia

We will report on experiments investigating a tunable metamaterial consisting of rf-SQUIDs. A metamaterial is a medium constructed of artifical elements, so-called meta-atoms, that interact in a specific way with an incoming electromagnetic wave. The size of the individual meta-atom is much smaller than the wavelength. Our metamaterial consists of an array of rf-SQUIDs which is placed into a coplanar waveguide. The rf-SQUIDs couple to the magnetic field component of the propagating microwave. In a frequency range around the resonance frequency, the magnetic permeability $\mu_r$ of the metamaterial deviates strongly from the typical value of $\mu_r = 1$. By using an additional constant magnetic field bias, the inductance of the Josephson junction and thereby the resonance frequency of our meta-atom is changed. We show that the magnetic permeability of such a SQUID metamaterial is tunable in situ and compare the experimental results with numerical simulations.

TT 49.5 Wed 18:00 H21

**MRX Measurement Setup Employing a Directly-Coupled High-$T_c$ SQUID With Slotted Pickup Loop** — •Alexander Guillaume, Frank Ludwig, Jan M. Scholtyssek, and Meinhard Schilling — Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, Technische Universität Braunschweig, Hans-Sommer-Str. 66, D-38106 Braunschweig, Germany

Magnetic nanoparticles (MNP) are employed in a wide range of medical and industrial applications. Besides other characterization techniques, magnetorelaxometry (MRX) is well established. In our MRX setup, we employ a directly-coupled high-$T_c$ SQUID with a slotted pickup loop as magnetic field sensor.

The whole setup is installed in a magnetically shielded room. The MNP sample, which is attached to a glass dipstick containing the SQUID, is magnetized by a pair of Helmholtz-coils. In order to prevent flux vortices from entering the SQUID, the sensor is aligned parallel to the magnetizing field so that only the stray field of the MNP is mea-

sured. The aligning process is accomplished by using three alignment screws. Hence, the SQUID only measures 1 ppm of the magnetizing field which is in the order of several mT. Since the magnetic nanoparticles are placed in liquid nitrogen, the relaxation time constant increases in comparison to a measurement of the particles at room temperature allowing to investigate particle sizes down to 10 nm.
Here, we present our MRX setup and the employed SQUID design. We evaluate its performace by carrying out MRX measurements on immobilized MNPs.

TT 49.6 Wed 18:15 H21

**AC susceptometry on the single-molecule magnet $Ni_2Dy$** — •Pascal Wendler[1], Alexander Sundt[1], Amin Khan[2], Yanhua Lan[2], Annie K. Powell[2], and Oliver Waldmann[1] — [1]Physikalisches Institut, Universität Freiburg, Germany — [2]Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, Germany

Molecular nanomagnets are molecules which show novel and fascinating magnetic properties. The best known phenomenon is the observation of magnetic hysteresis on the molecular scale in the single-molecule magnets (SMMs), such as $Mn_{12}$ac. In addition, quantum mechanical effects, such as the tunneling of the magnetization, can be observed in bulk samples of SMMs. A key goal for understanding the underlying physics is the measurement of the magnetization dynamics, which can be accomplished using ac susceptometry. However, the magnetic moments of samples of SMMs are weak since the volume density of the magnetic ions is very small as compared to e.g. inorganic compounds.

In this talk we will describe the construction of an ac susceptometer suitable for investigating molecular nanomagnets. A particular goal was to reach frequencies of the ac field of 100 kHz, extending the frequency range of commercial devices typically used in this research area by two decades. The device can be operated in the temperature range of 1.5 to 300 K and was characterized by comparing data recorded on $Mn_{19}$ with available literature results. Lastly, we will present our experimental results on the novel SMM $Ni_2Dy$ and discuss the different magnetic relaxation regimes observed in it.

TT 49.7 Wed 18:30 H21

**Effect of the wire geometry and an externally applied magnetic field on the detection efficiency of superconducting nanowire single-photon detectors** — •Robert Lusche[1], Alexey Semenov[1], Heinz-Willhelm Hübers[1], Konstantin Ilin[2], Michael Siegel[2], Yuliya Korneeva[3], Andrey Trifonov[3], Alexander Korneev[3], and Gregory Goltsman[3] — [1]DLR, Institut für Planetenforschung, Berlin, Germany — [2]Karlsruher Institut für Technologie — [3]Moscow State Pedagogical University, Russia

The interest in single-photon detectors in the near-infrared wavelength regime for applications, e.g. in quantum cryptography has immensely increased in the last years. Superconducting nanowire single-photon detectors (SNSPD) already show quite reasonable detection efficiencies in the NIR which can even be further improved. Novel theoretical approaches including vortex-assisted photon counting state that the detection efficiency in the long wavelength region can be enhanced by the detector geometry and an applied magnetic field. We will present spectral measurements in the wavelength range from 350-2500nm of the detection efficiency of meander-type TaN and NbN SNSPD with varying nanowire line width from 80 to 250nm. Due to the used experimental setup we can accurately normalize the measured spectra and are able to extract the intrinsic detection efficiency (IDE) of our detectors. The results clearly indicate an improvement of the IDE depending on the wire width according to the theoretic models. Furthermore we experimentally found that the smallest detectable photon-flux can be increased by applying a small magnetic field to the detectors.

TT 49.8 Wed 18:45 H21

**maXs: Metallic Magnetic Calorimeters for High-Resolution X-ray Spectroscopy in Atomic Physics** — •Daniel Hengstler[1], Sönke Schäfer[1], Christian Pies[1], Sebastian Kempf[1], Simon Uhl[1], Sebastian Heuser[1], Jeschua Geist[1], Nadine Foerster[1], Matthäus Krantz[1], Emil Pavlov[1], Sebastian Georgi[2], Thomas Wolf[1], Loredana Gastaldo[1], Andreas Fleischmann[1], and Christian Enss[1] — [1]Kirchhoff-Institut für Physik, Heidelberg — [2]Max-Planck-Institut für Kernphysik, Heidelberg

We are presently developing the detector array maXs, which will allow for benchmark experiments in x-ray spectroscopy to challenge bound-state QED calculations. maXs will consist of 32 Metallic Magnetic Calorimeters (MMCs), operated at temperatures around 30 mK in a dry $^3He/^4He$ dilution refrigerator. In such a MMC the energy of an absorbed photon leads to an increase of the detector temperature accompanied by a change in magnetization of a paramagnetic temperature sensor which is detected by a SQUID-magnetometer. One fourth of the detectors of the array will have an energy resolution of 3 eV for photon energies up to 20 keV. Three fourth of the detectors are designed for the detection of photons with energies up to 200 keV with a resolution of 40 eV. We discuss how to minimize the thermal and electromagnetic crosstalk between the detectors and how to remove the heat that is produced within the two-dimensional array without degrading the energy resolution. We consider how to ensure equal detector response despite a position-dependent absorption of high energy photons. Furthermore we present latest results of present prototype arrays.

## TT 50: Exciton Polaritons and their Condensates (jointly with HL)

Time: Thursday 9:30–12:15 Location: H2

TT 50.1 Thu 9:30 H2

**Polariton lasing in III-nitride based microcavities: How far are we from the Mott-transition?** — •Georg Rossbach, Jacques Levrat, Etienne Giraud, Eric Feltin, Jean-Francois Carlin, Raphael Butte, and Nicolas Grandjean — ICMP, Ecole Polytechnique Fdérale de Lausanne, 1015 Lausanne, Switzerland

Non-equilibrium polariton condensates producing a coherent light source referred to as polariton laser have attracted a lot of interest as they should allow the realization of ultralow threshold coherent light-emitting devices due to the release of the population inversion condition. Polariton lasing under ambient conditions was demonstrated for the first time in a III-nitrid based microcavity, where the increased exciton stability and oscillator strength facilitate the strong coupling regime even for high carrier injection. Nevertheless, the generally observed emission energy blueshift toward the polariton lasing threshold indicates a significant altering of the light-matter coupling with increasing carrier density. Such non-linearities arise from the interacting excitonic fraction of cavity-polaritons.

Based on the investigation of the Mott-transition occurring in GaN/AlGaN single quantum wells and the microcavity bare active medium by means of non-resonant photoluminescence, the impact of the exciton renormalization on the polariton branch dispersion is discussed. Contrary to the usually assumed picture the exciton energy shift is shown to play a negligible role, while saturation effects emerging from phase space filling and exchange interaction govern the polariton renormalization already far below threshold.

TT 50.2 Thu 9:45 H2

**Weak periodic modulation of exciton-polariton condensates** — •Edgar Cerda-Mendez[1], Dipankar Sarkar[2], Klaus Biermann[1], Dmitry Krizhanovski[2], Maurice Skolnick[2], and Paulo Santos[1] — [1]Paul Drude Institut for Solid State Physics, Berlin, Germany — [2]Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom

Macroscopic quantum behavior manifest when bosonic particles undergo a phase transition to a condensate state described by a single quantum wavefunction. Such behavior also occurs in microcavities containing quantum wells (QWs), where quasiparticles called polaritons arise from the strong coupling of photons and the QW excitons. In this work, we study the properties of polariton condensates in a shallow square lattice created via acoustic modulation. We demonstrate the formation of an extended state with negative effective mass at the corners (i.e. M-points) of the square lattice mini-Brillouin Zone. Also, optical threshold intensities for condensation are reduced, which is attributed to the lower density of states at the M-points and to the negative effective mass which compensates polariton drift induced by repulsive interactions. Both effects may allow to reach the critical density for condensation more efficiently than at the center of the MBZ (i.e. the $\Gamma$ point). Finally, the momentum spread of the M-point states is independent from the area covered by the MCP, showing that the

wavefunction of the MCP has a self-induced intrinsic coherence length. This work opens the way for investigation of polariton quantum phases such as a Bose Glass, Mott insulator or bright gap solitons.

TT 50.3 Thu 10:00 H2

**Coherent Propagation of blue Polaritons in $Cu_2O$** — •Johannes Schmutzler, Dietmar Fröhlich, and Manfred Bayer — Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany

The lowest excitons in $Cu_2O$ are intensively studied as they are considered as candidates for Bose-Einstein Condensation. The excitons of the so-called yellow and green series are of even parity and thus only quadrupole allowed. There are, however, two other series of excitons (blue and violet series) which are dipole allowed and should thus exhibit a pronounced polariton structure.

Despite the fact that $Cu_2O$ has inversion symmetry we report sum-frequency generation of blue exciton polaritons. This is possible since in our case the SFG is of quadrupole-dipole type. Typically the observation of non-linear effects requires power levels in the kW to MW range, necessitating pulsed laser sources. Here, we achieve strong sum-frequency (SF) signals far above the bandgap by spectrally narrow excitation of two exciton-polariton resonances in $Cu_2O$ with two continuous wave lasers in the mW to W power range.

In the case of an antiparallel laser beam configuration pronounced oscillations of the SF-signal can be observed. We attribute these oscillations to a phase matching effect. This observation is rather surprising since the absorption length in one-photon absorption is in the range of 150 nm [1]. The occurrence of oscillations clearly indicates the creation of coherent exciton-polaritons, the damping of which is suppressed.

[1] S. Brahms et al., Physics Letters. 21, 31 (1966)

TT 50.4 Thu 10:15 H2

**Polariton condensates in GaAs-based microcavities: influence of the spot size** — •Matthias Salewski[1], Marc Assmann[1], Jean-Sebastian Tempel[1], Franziska Veit[1], Sven Höfling[2], Martin Kamp[2], Alfred Forchel[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund — [2]Technische Physik, Physikalisches Institut, Universität Würzburg, 97074 Würzburg

Microcavity-polaritons consist of excitons strongly coupled to the photon field of the cavity. Photons leaking out of the cavity show the same energy-momentum dispersion as the polariton, which allows for easy experimental accessibility of the polariton states. It has been shown, that microcavity polaritons are able to undergo Bose-Einstein condensation.

Here, we investigated the influence of the excitation-spot size on the threshold carrier density necessary to create polariton condensates in a GaAs-based quantum-well microcavity. Different cavity-exciton detunings were examined.

By measuring the far-field emission of the cavity, we mapped the polariton dispersion relation as a function of the excitation power. Carriers were created by two excitation spots of different sizes. First, the intensity of the larger spot was varied. Second, while keeping the intensity of the larger spot fixed, the intensity of the second, much smaller spot was increased in the sub-milliwatt range. This way, we could measure the excitation efficiency of different spot sizes. Different results are observed for various detunings.

TT 50.5 Thu 10:30 H2

**Optically and structurally trapped exciton-polariton systems** — •Tom Michalsky, Helena Franke, Chris Sturm, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

The formation and properties of exciton-polaritons in microcavities (MCs) have been intensively investigated in the last years, since they can undergo a Bose-Einstein condensation (BEC). In this work we present the investigation of the momentum and spatial distribution of polaritons in the uncondensed as well as in the condensed phase for planar ZnO-based MCs with a wedge-shaped cavity layer and also in mesa structures. In the mesa structures we found an enhancement of the trapping as a result of the reduced potential energy therein. For MCs without mesa structures we demonstrate the manipulation of propagation of condensed polaritons. It turns out that for small negative detuning values the condensate is trapped by the excitation laser spot whereas for larger negative detunings an acceleration of the polaritons out of the pumping region accompanied by ballistic propagation [1] is observed.

[1] M. Wouters, I. Carusotto and C. Ciuti, Phys. Rev. B **77**, 115340 (2008)

**Coffee break**

TT 50.6 Thu 11:00 H2

**Influence of disorder on the propagation of polariton BEC** — •Martin Thunert[1], Helena Franke[1], Chris Sturm[1], Rüdiger Schmidt-Grund[1], Alexander Janot[2], Bernd Rosenow[2], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig — [2]Universität Leipzig, Institut für Theoretische Physik, Brüderstr. 16, 04103 Leipzig

We report on the influence of disorder effects on the propagation of exciton-polariton Bose-Einstein condensates (BEC) in a ZnO-based bulk planar microcavity (MC). Due to their composite nature, the spatial distribution is affected by electronic (inhomogeneous carrier distribution) as well as photonic (thickness fluctuations, rough interfaces) disorder. The energy($E$)-$k$-space emission patterns of the condensate show in dependence on temperature ($T$) and detuning ($\Delta$) two different regimes: 1) ballistic polariton propagation for low ($T$,$\Delta$) values and 2) disorder effects for increasing ($T$,$\Delta$) values, which are reflected by a fragmentation of the ($E$,$k$) emission patterns. This can be explained by interference of localized condensates or by propagating condensates with different discrete velocities determined by scattering events at the disorder potential. For each ($T$,$\Delta$) parameter set increasing pump power causes an increase of the fragmentation parameter which is deduced quantitatively from the ($E$,$k$) emission patterns. A theoretical investigation shows that a non-equilibrium exciton-polariton condensate remains stiff at finite length scales only. This indeed suggests a scenario of fragmentation caused by the interplay of disorder and gain-loss of the condensate.

TT 50.7 Thu 11:15 H2

**Exciton-polariton pseudospin polarization in a planar microcavity** — •Steffen Richter, Chris Sturm, Helena Franke, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

Exciton-polaritons are composite quasi-particles which arise from strong coupling between excitons and photons. An interesting feature is their pseudospin. It expresses at the same time the average exciton spin orientation and the photonic light polarization of a polariton ensemble.

A planar ZnO-based microcavity of thickness $\lambda/2$ was investigated by angle-resolved photoluminescence experiments. A slight wedge shape of the cavity allows probing of different detunings. The Stokes vector of the emission from the lower polariton branch was determined under non-resonant excitation. The energetic splitting between the TE- and TM-polarized eigenmodes is found to increase with in-plane wavevector $k_{||}$ until the polariton becomes mostly exciton-like. It reaches about 20meV at most. Contrary to expectations, a circular polarization degree of up to 5% is found in the emission from these supposedly linear modes. The extent of this circular polarization reveals the same $k_{||}$-dependence as the TE-TM splitting.

The pseudospin model and the impact of related effective magnetic fields are discussed in order to explain the observed polarization behavior. Influences by different detunings, crystal quality and local anisotropic effects are considered.

TT 50.8 Thu 11:30 H2

**Magnetic field interaction of exciton-polariton-condensates in a GaAs-quantum-well microcavity** — •Julian Fischer[1], Ingo Lederer[1], Alexander Chernenko[2], Sebastian Brodbeck[1], Arash Rahimi-Iman[1], Matthias Amthor[1], Alfred Forchel[1], Christian Schneider[1], Martin Kamp[1], and Sven Höfling[1] — [1]Technische Physik, Physikalisches Institut, Universität Würzburg and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432 Russia

In this work we investigate the interaction of exciton-polaritons with an external magnetic field in a GaAs-quantum-well-microcavity. The magnetic field up to B=5T is applied in Faraday configuration. We focus on measurements of the Zeeman-splitting for the three regimes of our quantum-well microcavity: uncondensed exciton-polariton at low excitation power, exciton-polariton-condensate and a photon dom-

inated regime above the mott density of excitons. For the uncondensed polaritons we measure the expected linear dependence of the Zeeman-splitting on the magnetic field, while we observed a quenching of the Zeeman-splitting for the condensate case, referred to as "Spin-Meissner-effect". Above the mott-density the Zeeman-splitting is not measurable anymore due to the negligible excitonic content. Hence, the Zeeman-splitting is a reliable tool to distinguish a polaritonic system from a photonic one.

TT 50.9 Thu 11:45 H2

**Electroluminescence from spatially confined exciton polaritons in a textured microcavity** — •Karol Winkler[1], Christian Schneider[1], Julian Fischer[1], Arash Rahimi-Iman[1], Matthias Amthor[1], Alfred Forchel[1], Stephan Reitzenstein[1,2], Sven Höfling[1], and Martin Kamp[1] — [1]Wilhelm Conrad Röntgen Center for Complex Material Systems, Technische Physik, Universität Würzburg — [2]Institut für Festkörperphysik, Technische Universität Berlin

Strong coupling between microcavity photons and quantum well excitons results in the formation of exciton polaritons. Spatial trapping of these quasi-particles in three dimensions allows for the observation of long-range coherence phenomena and could be exploited for new kind of coherent or non-classical light sources.

While electrical injection of quasi-2D-polaritons has been already archived, we report on electrically pumped formation of spatially confined polaritons. The trapping scheme is based on an elongated textured cavity which results in a three-dimensional confinement potential for the photonic part of the polaritons. An external bias can be used for fast manipulation of the exciton energy through the quantum confined stark effect with a simultaneous read out via resonant photocurrent measurements.

TT 50.10 Thu 12:00 H2

**Zeeman split nonlinear emission from electrically injected exciton-polaritons** — •Matthias Amthor[1], Christian Schneider[1], Arash Rahimi-Iman[1], Na Young Kim[2,3], Julian Fischer[1], Matthias Lermer[1], Martin Kamp[1], Stephan Reitzenstein[1,4], Alfred Forchel[1], Yoshihisa Yamamoto[2,5], and Sven Höfling[1] — [1]Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Am Hubland, Germany. — [2]E.L. Ginzton Laboratory, Stanford University, Stanford CA, 94305, USA. — [3]Institute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan. — [4]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany. — [5]National Institute of Informatics, Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan.

We report on magneto-optical measurements of an electrically driven GaAs based exciton-polariton light-emitting diode. The system under investigation is a p-i-n GaAs microcavity with a stack of four InGaAs quantum wells in the center of a one-lambda cavity, etched into circular pillars with diameters of 20 $\mu$m. Three different regimes occur in the energy-momentum dispersion characteristics. Subject to an applied magnetic field in Faraday configuration, we observe two distinct nonlinearities in the excitation power dependent output characteristics. Additionally, we prove the conservation of the strong coupling regime above the first threshold by investigating the Zeeman splitting of the cavity resonance in the non-linear regime.

## TT 51: Correlated Electrons: General Theory 1

Time: Thursday 9:30–12:30 Location: H6

TT 51.1 Thu 9:30 H6

**Electronic Entanglement in Late Transition Metal Oxides** — •Patrik Thunström[1], Igor Di Marco[2], and Olle Eriksson[2] — [1]TU Wien, Vienna, Austria — [2]Uppsala University, Uppsala, Sweden

We present a study of the entanglement in the electronic structure of the late transition metal monoxides – MnO, FeO, CoO, and NiO – obtained by means of density-functional theory in the local density approximation combined with dynamical mean-field theory. Two main sources of entanglement are resolved. The interplay of crystal field effects and Coulomb interaction are shown to give the entanglement in CoO a particularly intricate form.

TT 51.2 Thu 9:45 H6

**Interface spin polarization of Half-metal/Semiconductor heterostructures** — •Andreas Held[1], Stanislav Chadov[2], Igor Di Marco[3], and Liviu Chioncel[4,1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nothnitzer Str. 40, 01187 Dresden, Germany — [3]Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [4]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

Half-metallic/Semiconductor interfaces ($Co_2MnAl$/CoMnVAl) have been recently proposed as efficient spin injectors based on Heusler materials [1]. We discuss the impact of electronic correlation within the mean field (+U) and beyond (+DMFT) upon the electronic and magnetic properties in this interface. Our results suggest that typical correlations strength encountered in the family of Heusler compounds does not lead to a dramatic depolarization effect.

[1] S. Chadov et. al. PRL 107, 047202 (2011)

TT 51.3 Thu 10:00 H6

**Comparing GW+DMFT and LDA+DMFT for the testbed material $SrVO_3$** — •Ciro Taranto[1], Merzuk Kaltak[2], Nicolaus Parragh[3], Giorgio Sangiovanni[3], Georg Kresse[2], Alessandro Toschi[1], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We have implemented the GW+dynamical mean field theory (DMFT) approach in the Vienna ab initio simulation package. Employing the interaction values obtained from the locally unscreened random phase approximation (RPA), we compare GW+DMFT and LDA+DMFT against each other and against experiment for $SrVO_3$. We observed a partial compensation of stronger electronic correlations due to the reduced *GW* bandwidth and weaker correlations due to a larger screening of the RPA interaction, so that the obtained spectra are quite similar and well agree with experiment. Noteworthily, the GW+DMFT better reproduces the position of the lower Hubbard side band.

TT 51.4 Thu 10:15 H6

**Calculation of total energies and forces in correlated materials** — •Ivan Leonov[1], Vladimir I. Anisimov[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia

We present a computational scheme for the investigation of complex materials with strongly interacting electrons which is able to treat atomic displacements, and hence structural relaxation, caused by electronic correlations. It combines *ab initio* band structure and dynamical mean-field theory and is implemented with the linear response formalism regarding atomic displacements [1,2]. We employ this approach to compute the equilibrium crystal structure and phase stability of several correlated electron materials, such as elemental hydrogen, $SrVO_3$, and $KCuF_3$. We find an excellent agreement between the results for the equilibrium atomic positions in these materials obtained from calculation of total energy and forces, respectively. The approach presented here allows one to study the structural properties of materials with strongly correlated electrons such as lattice instabilities observed at correlation induced metal-insulator phase transitions from first principles.

[1] I. Leonov *et al.*, Phys. Rev. Lett. **101**, 096405 (2008)
[2] I. Leonov *et al.*, Phys. Rev. B **81**, 075109 (2010).

TT 51.5 Thu 10:30 H6

**Effective crystal field and Fermi surface topology in correlated multi-orbital systems** — Nico Parragh[1], Giorgio

Sangiovanni[1], Philipp Hansmann[2], Stefan Hummel[3], Karsten Held[3], and •Alessandro Toschi[3] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Centre de Physique Théorique, École Polytechnique, France — [3]Institut für Festkörperphysik, Technische Universität Wien, Austria

The electronic correlation effect of enhancing/reducing the effective crystal field in multi-orbital correlated materials can be crucial in determining the topology of the Fermi surface and, hence, the physical properties of these systems. Consequently, an accurate theoretical prediction of the Fermi surface structure is a very desirable goal, in particular for the emerging field of engineering new correlated heterostructures. In this respect, however, the application of one of the most powerful ab-initio scheme, i.e. the merger between the local density approximation (LDA) and the dynamical mean field theory (DMFT), can give contractdicting results: In recent studies of Ni-based heterostructure, the predicted Fermi surface is totally different depending on whether less correleated $p$ orbitals are or are not included in the calculation[1,2]. The LDA+DMFT model study we present here aims at a clarifying the origin of this problem and at identifying the key parameters, which control the Fermi surface properties of these systems.

[1] P. Hansmann, A. Toschi, Xiaoping Yang, O.K. Andersen, and K. Held, Phys. Rev. B **82**, 235123 (2010)
[2] M. J. Han, Xin Wang, C. A. Marianetti, and A. J. Millis, Phys. Rev. Lett. **107**, 206804 (2011).

TT 51.6 Thu 10:45 H6

**Quasi continuous-time impurity solver for dynamical mean-field theory with linear scaling in the inverse temperature** — •Daniel Rost[1], Fakher Assaad[2], and Nils Blümer[1] — [1]Institute of Physics, Johannes Gutenberg-University, Mainz — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg

Diagrammatic quantum Monte Carlo impurity solvers (CT-QMC) provide numerically exact solutions for dynamical mean-field theory (DMFT), at a computational cost that scales *cubically* with the inverse temperature $\beta$. In contrast, a recently proposed approach [1], based on a hamiltonian representation of the bath Green function and the BSS quantum Monte Carlo algorithm [2], scales *linearly* with $\beta$, but introduces a bias due to Trotter discretization. We present an algorithm, based on multigrid extrapolations of Green functions, that combines the advantages of both methods: (i) it retains the superior linear scaling of BSS and (ii) is free of significant Trotter errors. The accuracy of this quasi continuous-time method is established for the metal-insulator transition in the 1-band Hubbard model, in comparison with CT-QMC and exact diagonalization. We also analyze the impact of the bath discretization and conclude that the new method appears most promising for cluster DMFT studies at low temperatures.

[1] E. Khatami et al., PRE **81**, 056703 (2010); QUantum Electron Simulation Toolbox, http://www.cs.ucdavis.edu/∼bai/QUEST_public/.
[2] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981).

**15 min. break**

TT 51.7 Thu 11:15 H6

**Using Dual Bosons to go beyond EDMFT** — •E.G.C.P. van Loon[1,2], A.B.J. Wilhelm[1], H. Hafermann[3], A.N. Rubtsov[4], M.I. Katsnelson[2], and A.I. Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg — [2]Institute of Molecules and Materials, Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [3]Centre de Physique Théorique, Ecole Polytechnique, CNRS, F-91128 Palaiseau Cedex, France — [4]Department of Physics, Moscow State University, 119992 Moscow, Russia

DMFT is widely used to study models of condensed matter. A problem of interacting particles is mapped onto a self-consistent impurity problem. It is exact in infinite dimension but in finite dimension it does not describe non-local effects. Dual fermions provide a way to incorporate these non-local effects beyond DMFT. Dual bosons can then be used to describe collective modes. In zeroth order, Dual Bosons correspond to EDMFT. Plasmons in Hubbard-like models can be studied using these theories. We present a new technique to use the method of Dual Bosons to self-consistently calculate the effects of these collective bosonic modes in a two dimensional Hubbard model on a square lattice. The hybridization solver from the ALPS project is used to solve an impurity model with retarded interaction. Self-energy diagrams are calculated with the resulting quantities to include non-local effects. We first present benchmark results. Then our results are compared with EDMFT results.

TT 51.8 Thu 11:30 H6

**Non-perturbative precursors of the Mott-Hubbard transition at the two-particle level** — •Thomas Schaefer[1], Georg Rohringer[1], Karsten Held[1], Olle Gunnarsson[2], Sergio Ciuchi[3], Giorgio Sangiovanni[4], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Universita degli Studi de l'Aquila, L'Aquila, Italy — [4]Institute of Physics and Astrophysics, University of Würzburg, Würzburg, Germany

Amongst plenty other successes, DMFT is able to cover the Mott-Hubbard metal-to-insulator transition (MIT), which is an intrinsic non-perturbative phenomenon. At the MIT the local spin susceptibility diverges, following Curie's law in the insulating phase, whereas the local charge susceptibility remains finite at the transition [1]. However, these divergencies are not the only hallmarks of the MIT at the two-particle level. In fact, the first non-perturbative precursors of the MIT can be identified well inside the metallic phase in the frequency structures of the irreducible vertex functions [2,3]. The strong enhancements of the irreducible vertex functions, characterising this precursor, stem from local scattering processes and can be traced up to the limit of high temperatures (i.e. the atomic limit).

[1] A. Georges et al., Rev. Mod. Phys. 68, 13-125 (1996)
[2] G. Rohringer et al., Phys. Rev. B 86, 125114 (2012)
[3] T. Schaefer et al., in preparation (2012)

TT 51.9 Thu 11:45 H6

**Non-perturbative derivation of effective models using graph-based continuous unitary transformations** — •Kris Cöster and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I , TU Dortmund, 44221 Dortmund, Germany

Unitary transformations are an essential tool in many-body physics mapping the original model to a simpler effective model in a better suited basis. One way to schematically derive such unitary transformations is given by the so-called continuous unitary transformations (CUTs). For lattice models of finite dimension, these CUTs can be combined with graph theory to capture all zero-temperature fluctuations within a controlled spatial range (gCUTs) providing a robust non-perturbative scheme to derive effective low-energy models when at least one degree of freedom is gapped. This method has already been succesfully applied to various systems and the aim is to increase both the understanding and the accuracy of this novel tool. To this end we introduce a general recipe on each graph respecting all symmetries of the graphs. Furthermore, an intuitive truncation on each graph is gained. One particular challenge for gCUTs is that the graphs typically have less symmetries than the full lattice model. The impact of this reduced symmetry on the effective low-energy Hamiltonian is studied focussing on possible remedies. These aspects are tested for one-dimensional and two-dimensional quantum spin systems.

TT 51.10 Thu 12:00 H6

**Revealing the breakdown of spin-charge separation in spin-imbalanced fermions in one dimension using quench dynamics** — •Michael Sekania[1] and Paata Kakashvili[2] — [1]Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, Germany — [2]Department of Physics and Astronomy, Rutgers University, USA

Recently, spin-imbalanced fermions in one dimension have attracted considerable attention both theoretically and experimentally. This system was successfully simulated using ultracold atoms in optical lattices. The phase diagram was measured and found to be in agreement with exact analytical calculations. It was also established theoretically that the spin-charge separation, an important property of Luttinger liquids, is absent. Low-energy bosonic excitations do not carry spin and charge separately due to the interaction between spin and charge degrees of freedom. Based on our numerical (time-dependent Density-Matrix Renormalization Group method) and analytical calculations (Bethe Ansatz, Bosonization) on the Hubbard model, we propose quench experiments which not only reveal the breakdown of spin-charge separation but also make it possible to study the so called "string" bound states in this system.

TT 51.11 Thu 12:15 H6

**Conserved quantities of SU(2)-invariant interactions for correlated fermions and the advantages for quantum Monte Carlo simulations** — Nicolaus Parragh[1], Alessandro Toschi[2], Karsten Held[2], and •Giorgio Sangiovanni[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg, Deutschland — [2]Institut für Festkörperphysik, Technische Universität Wien, Vienna, Österreich

In the context of realistic calculations for strongly correlated materials with $d$ or $f$ electrons the efficient computation of multi-orbital models is of paramount importance. Here we introduce a set of invariants for the SU(2)-symmetric Kanamori Hamiltonian, which allows us to massively speed up the calculation of the fermionic trace in hybridization-expansion continuous-time quantum Monte Carlo algorithms. We show that by exploiting this set of good quantum numbers the study of the orbital-selective Mott transition in systems with up to seven correlated orbitals becomes feasible.

[1] N. Parragh, A. Toschi, K. Held, and G. Sangiovanni, Phys. Rev. B **86**, 155158 (2012)

## TT 52: Transport: Spintronics, Magnetotransport 1 (jointly with HL and MA)

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

TT 52.1 Thu 9:30 H18

**A relativistic implementation of the non-equilibrium Green's function formalism for layered systems** — •S Wimmer[1], M Ogura[2], H Akai[2], and H Ebert[1] — [1]Department Chemie, Ludwig-Maximilians-Univeristät München — [2]Department of Physics, Graduate School of Science, Osaka University

The non-equilibrium Green's function formalism has been implemented within the Korringa-Kohn-Rostoker (KKR) multiple scattering theory following previous work [1,2]. First results for the transport in layered systems are presented and compared to available results of other authors [1–3]. Using a fully relativistic approach within the Dirac-formalism allows us to investigate the influence of spin-orbit coupling. This will be discussed for various transport properties including the spin-transfer torque.

[1] C. Heiliger et al., J. Appl. Phys. **103**, 07A709 (2008)
[2] S. Achilles, Ph.D. thesis, Martin-Luther-Universität Halle-Wittenberg (2012)
[3] P. M. Haney et al., Phys. Rev. B **76**, 024404 (2007)

TT 52.2 Thu 9:45 H18

**Persistent Spin Helix Conditions in Two-Dimensional Electron and Hole Gases** — •Tobias Dollinger, Andreas Scholz, Paul Wenk, John Schliemann, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg

We discuss magnetotransport in systems with nonnegligable cubic in momentum Dresselhaus Spin Orbit Interaction (SOI). The latter has been found responsible for diminishing and shifting the parameter regime where weak localization signatures, attributed to the so called "Persistent Spin Helix"(PSH) symmetry [1,2], are detected in magnetoconductance traces [3]. Building on the electronic results, we present an effective model for the heavy hole band of a confined twodimensional hole gas, where typically SOI terms with cubic structure are relevant. We investigate numerically and analytically the magnetotransport propery of this model, in which we can identify an analogue to the PSH.

[1]J. Schliemann et al., PRL **90** 146801 (2003)
[2] Bernevig et al., PRL **97** 236601 (2006)
[3] Kohda et al., PRB **86** 081306 (2012)

TT 52.3 Thu 10:00 H18

**Aharonov-Casher effect in quantum rings: geometric phase shift by in-plane magnetic field** — Diego Frustaglia[1], •Henri Saarikoski[2], Klaus Richter[2], Fumiya Nagasawa[3], and Junsaku Nitta[3] — [1]Departamento de Física Aplicada II, Universidad de Sevilla, Sevilla, Spain — [2]Department of Theoretical Physics, Regensburg University, Germany — [3]Department of Materials Science, Tohoku University, Sendai, Japan

We study transport through Rashba spin-orbit coupled quantum rings where the spin-orbit field causes the Aharonov-Casher effect [1, 2]. The ring is subject to an in-plane magnetic field which gives rise to a shift in the geometric phase. We show that the in-plane field allows control of the geometric phase independently from the dynamic phase and without competing with Aharonov-Bohm phases. We use perturbation theory to calculate the resulting phase shift in quasi-1D rings for weak in-plane fields. The resulting phase shift is quadratic in the in-plane field. Numerical Recursive Green's function algorithm is used to study the effect in multi-mode quantum rings and in the case of large in-plane fields. We demonstrate the effect in InGaAs/InAlAs based quantum rings where the Rashba spin-orbit field is modulated by an external gate. As the in-plane magnetic field is increased we find a quadratic phase shift in the Aharonov-Casher effect towards lower spin-orbit fields in good agreement with calculations.

[1] F. Nagasawa, J. Takagi, Y. Kunihashi, M. Kohda, and J. Nitta, Phys. Rev. Lett. 108, 086801 (2012)
[2] K. Richter, Physics 5, 22 (2012).

TT 52.4 Thu 10:15 H18

**Quantum Feedback in nuclear spin-assisted electronic transport** — •Klemens Mosshamer and Tobias Brandes — Institut für theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

We investigate theoretically the electronic transport through quantum dot systems that interact with the nuclear environment via the hyperfine interaction. We show that the non-linear dynamics arising due to the hyperfine interaction can be controlled via closed-loop feedback operations, such as time-dependent modifications of the tunneling rate.

TT 52.5 Thu 10:30 H18

**Projective Boltzmann approach to thermal drag in spin-1/2-ladder systems coupled to phonons** — •Christian Bartsch and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig

We quantitatively investigate the spin-phonon drag contributions to the thermal conductivity of a two-leg-spin-1/2-ladder coupled to lattice vibrations in a magnetoelastic way. By applying suitable transformations the system is mapped onto a weakly interacting quantum gas model of bosonic spin excitations (magnons) and phonons. We adequately construct a collision term of a linear(ized) Boltzmann equation from the underlying quantum dynamics by means of a pertinent projection operator technique. From the Boltzmann equation we obtain concrete numerical values for the drag conductivity and relate it to the individual thermal conductivities of magnons and phonons for parameter ranges which are typical for certain material classes.

TT 52.6 Thu 10:45 H18

**Rashba spin-orbit-interaction-based quantum pump in graphene** — •Dario Bercioux[1], Daniel F. Urban[2,3], Francesco Romeo[4], and Roberta Citro[4] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [3]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany — [4]Dipartimento di Fisica "E. R. Caianiello" and Spin-CNR, Università degli Studi di Salerno, I-84084 Fisciano (Sa), Italy

We present a proposal for an adiabatic quantum pump based on a graphene monolayer patterned by electrostatic gates and operated in the low-energy Dirac regime [1]. The setup under investigation works in the presence of inhomogeneous spin-orbit interactions of intrinsic- and Rashba-type and allows to generate spin polarized coherent current. A local spin polarized current is induced by the pumping mechanism assisted by the spin-double refraction phenomenon [2].

[1] Citro, Appl. Phys. Lett. **101**, 122445 (2012)
[2] D. Bercioux, A. de Martino, Phys. Rev. B **83**, 012106 (2011)

TT 52.7 Thu 11:00 H18

**First-principles calculation of ballistic transport in single-atom contacts** — •Fabian Otte[1], Björn Hardrat[1], Frank Freimuth[2], Yuriy Mokrousov[2] und Stefan Heinze[1] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-

Universität zu Kiel, 24098 Kiel, Germany — [2]Peter-Grünberg-Institut, Forschungszentrum Jülich, 520425 Jülich, Germany

Recently, the spin-valve effect of single-atom contacts has been demonstrated using scanning tunneling microscopy [1]. In these measurements a magnetic tip approaches magnetic adatoms on a surface and the distance-dependent conductance and magnetoresistance is obtained. Here, we report first-principles calculations of ballistic transport in model systems of such single-atom contacts using our recently developed approach [2] which allows to include spin-orbit coupling and non-collinear spin structures. We present the conductance between two ferromagnetic Co monowires terminated by single Mn apex atoms while varying the distance between the two Mn atoms. Due to frustration of exchange interactions a non-collinear spin state is favorable in the contact regime. We show that it leaves a fingerprint in the distance-dependent conductance and magnetoresistance [3]. We also study the ballistic anisotropic magnetoresistance from the tunneling to the contact regime for leads whose structure is modeled with Fe monowires.

[1] M. Ziegler et al., New J. Phys. 13, 085011 (2011)
[2] B. Hardrat et al., Phys. Rev. B 85, 245412 (2012)
[3] B. Hardrat et al., Phys. Rev. B 86, 165449 (2012)

**15 min. break**

TT 52.8 Thu 11:30 H18

**A carbon nanotube quantum dot in the intermediate coupling regime: Conductance and tunnel magnetoresistance** — •Alois Dirnaichner, Johannes Kern, and Milena Grifoni — Universität Regensburg

We discuss transport through carbon nanotube quantum dots with intermediate coupling to ferromagnetic leads. In a density matrix approach we sum up infinite-order corrections due to charge fluctuations within the dressed second order approximation (DSO) [1], allowing us to go beyond the sequential tunneling regime. From the master equation we deduce conductance and tunnel magnetoresistance (TMR). The results are compared to experimental data with a pronounced gate modulation of the TMR and negative TMR features in particular.

[1] J. Kern and M. Grifoni, arXiv:1209.4995v1

TT 52.9 Thu 11:45 H18

**Spin transport in carbon nanotubes in the Fabry-Perot regime** — •Miriam del Valle and Milena Grifioni — Institute of Theoretical Physics, University of Regensburg

We investigate the spin-dependent transport through carbon nanotubes connected to two ferromagnetic leads in the ballistic regime. The effect and origin of the phases acquired by electrons upon scattering at the contact interfaces are analyzed. These phases greatly determine the Fabry-Perot patterns obtained in this transport regime. With stress on the nanotube fingerprints, the magneto-resistance is calculated with the inclusion of spin-orbit effects, which are not negligible due to the finite curvature of the nanotubes.

TT 52.10 Thu 12:00 H18

**Investigation of spin transfer torques in $Mn_{1-x}Fe_xSi$** — •Christoph Schnarr, Robert Ritz, Andreas Bauer, Christian Franz, and Christian Pfleiderer — Technische Universität München, Physik-Department E21, D-85748 Garching, Germany

Small angle neutron scattering and Hall effect measurements recently revealed sizeable effects of spin transfer torques in the skyrmion lattice phase of MnSi [1,2]. The associated critical current densities of $\sim 10^6$ A/m$^2$, are exceptionally small and about 5 orders of magnitude smaller than the spin transfer torque observed in conventional systems. The low critical current density is due to a very efficient gyromagnetic coupling exhibited by a topological Hall contribution that arises in the topologically non-trivial magnetic structure of a skyrmion lattice. We report spin transfer torque experiments, measuring the Hall effect in $Mn_{1-x}Fe_xSi$ for a wide range of $x$, where the topological Hall effect increases by up to a factor of ten characteristic of a much more efficient coupling of the electric currents to the magnetic structure. The dependence of $j_c$ on the doping concentration is discussed in view of the increased topological Hall effect as well as the increased pinning by disorder.

[1] F. Jonietz *et al.*, Science **330**, 1648-1651 (2010)
[2] T. Schulz *et al.*, Nat Phys **8**, 4, 301-304 (2012)

TT 52.11 Thu 12:15 H18

**Magnetotransport along a boundary: From coherent electron focusing to edge channel transport** — •Thomas Stegmann, Dietrich E. Wolf, and Axel Lorke — University of Duisburg-Essen, Department of Physics and CENIDE

In a two dimensional electron system with a boundary, electrons are injected at one point on the boundary and focussed by a perpendicular magnetic field $B$ onto another voltage probe on the boundary. Using the nonequilibrium Green's function approach we study theoretically the 4-point Hall resistance $R_{xy}$ as a function of $B$. For low fields, $R_{xy}$ shows the characteristic equidistant peaks observed in the experiment, which can also be explained by simple classical trajectories: The electrons are guided on cyclotron orbits, are reflected speculary at the boundary, and end finally at the collector when a multiple of the cyclotron diameter equals the distance between injector and collector. In a strong magnetic field, the current is carried by edge channels parallel to the boundary and the typical fingerprint of the quantum Hall effect is observed. Here, we study the transition from the classical cyclotron motion to the edge channel transport and discuss its influence on the focussing spectrum. In intermediate fields, we find that $R_{xy}$ shows sets of oscillations, which are neither periodic in $B$ (such as the magnetic focussing peaks) nor in $1/B$ (quantum Hall effect). These oscillations can be understood as interference between adjacent edge states.

TT 52.12 Thu 12:30 H18

**Entanglement detection in Cooper pair splitters based on carbon nanotubes in magnetic fields** — •Pablo Burset[1,2], Bernd Braunecker[1], and Alfredo Levy Yeyati[1] — [1]Departamento de Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, E-28049 Madrid, Spain — [2]Institute for Theoretical Physics and Astrophysics, University of Wuerzburg, Am Hubland, 97074 Wuerzburg, Germany

The production of entangled electron pairs in a solid state device from the splitting of a Cooper pair is currently attracting much attention. Recent experiments have shown that Cooper pairs can be split in a controlled fashion in double quantum dot structures. In this talk I will describe how spin-orbit interaction in carbon nanotubes presents unique characteristics for the study of the entanglement of injected pairs of electrons.

I will briefly introduce the double dot Cooper pair splitter device based on carbon nanotubes. In this setup, I will review the form of spin-orbit interaction and demonstrate that it leads to a perfect spin filter with spin orientations tunable by external fields. Tunable spin-orbit induced spin-filtering allows to implement entanglement detectors, such as probing a Bell inequality. These detectors can rely on conductance measurements alone and do not require the precise knowledge of the spin orientations of the spin filter. Yet if in addition the spin orientations are known, the same setup can be used for full quantum state tomography.

TT 52.13 Thu 12:45 H18

**Electronic correlations in magnetic heterostructures.** — •Liviu Chioncel[1,2] and Junya Otsuki[2,3] — [1]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [3]Department of Physics, Tohoku University, Sendai, Japan

Heterostructures that contain semiconducting and magnetic monolayers offer the possibility to adjust simultaneously band-gap and magnetic properties. Dynamical Mean Field Theory is a necessary theoretical tool to address physical properties of multilayer systems containing correlated electrons. Here we solve a simplified Hubbard model within DMFT using the recently developed CT-QMC solver, for several magnetic monolayers embedded into semiconducting/insulating host. Our approach is relevant for the Cr/Mn-doped semiconducting heterostructures. We discuss possible half-metallic properties in these systems in the presence of dynamic correlations at finite temperatures.

# TT 53: Correlated Electrons: Heavy Fermions

Time: Thursday 9:30–13:00 Location: H19

TT 53.1 Thu 9:30 H19

**Formation of the coherent heavy fermion liquid at the 'hidden order' transition in $URu_2Si_2$** — Shouvik Chatterjee[1], •Jan Trinckauf[2], Torben Hänke[2], Daniel E. Shai[1], John W. Harter[1], Travis J. Williams[3], Graeme M. Luke[3], Kyle M. Shen[1,4], and Jochen Geck[2] — [1]Laboratory of Atomic and Solid State Physics, Department of Physics, Cornell University, Ithaca, New York 14853, USA — [2]Leibniz Institute for Solid State and Materials Research IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]Dept. of Physics and Astronomy, McMaster University, 1280 Main St. West, Hamilton, Ontario L8S 4M1, Canada — [4]Kavli Institute at Cornell for Nanoscale Science, Ithaca, New York 14853, USA

We present angle-resolved photoemission (ARPES) spectra of the heavy-fermion superconductor $URu_2Si_2$. Detailed measurements as a function of both excitation photon energy and temperature allow us to disentangle a variety of spectral features, revealing the evolution of the low energy electronic structure at the hidden order transition. We directly observe that precisely at THO, localized and fluctuating electronic states rapidly hybridize with light conduction states, forming a well-defined heavy band coincident with a dramatic reduction in the scattering rate. We thereby demonstrate that in $URu_2Si_2$, the formation of the coherent heavy fermion liquid occurs via a thermodynamic phase transition into the HO phase. This behavior is in stark contrast with the gradual crossover expected in Kondo lattice systems, suggesting the possibility of multiple pathways towards the creation of heavy fermionic states.

TT 53.2 Thu 9:45 H19

**High field Hall measurements on $UPt_2Si_2$ at very low temperatures** — •Dirk Schulze Grachtrup[1], Ilya Sheikin[2], Stefan Süllow[1], and John A. Mydosh[3] — [1]Institut für Physik der Kondensierten Materie, Braunschweig, Germany — [2]Grenoble High Magnetic Field Laboratory, Grenoble, France — [3]Kammerlingh Onnes Laboratory, Leiden, The Netherlands

Tetragonal $UPt_2Si_2$ is a moderately mass enhanced antiferromagnet with a transition temperature $T_N = 32$ K in zero magnetic field. Moreover, in magnetization and resistivity measurements in high magnetic fields multiple features indicating new field induced phases have been observed. These features, together with signs of Fermi surface effects point to a significant role of the Fermi surface in $UPt_2Si_2$ [1].

Here, we present new magnetoresistivity and Hall effect data on $UPt_2Si_2$ at temperatures 50 mK to 2 K in magnetic fields up to 34 T. For the $a$ axis this field range only covers the AFM phase. Instead, for the $c$ axis, we observe a broad maximum in the magnetoresistivity in the field range $\sim 25$ to $\sim 33$ T indicating the transition into one of the high field phases. Additionally, the magnetoresistivity is hysteretic at all temperatures, with multiple steps appearing at temperatures below $\sim 530$ mK. Moreover, in the Hall signal we observe a significant change with an increase of the Hall coefficient by about 40% in the field range 23 - 26 T, this independent of temperature. These findings are discussed in the context of the proposed magnetic phase diagrams and the possibility of the occurence of a Lifshitz transition.

[1] D. Schulze Grachtrup *et al.*, Phys. Rev. B **85**, 054410 (2012)

TT 53.3 Thu 10:00 H19

**Quasiparticles and Fermi surface of $UPt_2Si_2$** — •Zübeyir Cakir and Gertrud Zwicknagl — Institut für Mathematische Physik, TU Braunschweig, Braunschweig, Germany

U intermetallic compounds exhibit highly complex phase diagrams at low temperatures with unusual and often enigmatic orders. The high sensitivity with respect to variations in external parameters like pressure or magnetic field reflect the strong correlations within the U 5f shell. The present contribution focusses on the tetragonal compound $UPt_2Si_2$. We calculate the quasi-particle dispersion comparing the results for itinerant and (partially) localized U 5f electrons. The role of the local geometry is emphasized.

TT 53.4 Thu 10:15 H19

**The magnetic phase diagram of $CeAu_2Ge_2$** — •Felix Eilers[1], Diego Zocco[1], Chien-Lung Huang[1,2], Veronika Fritsch[2], Kai Grube[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie, Institut für Festkörperphysik — [2]Karlsruher Institut für Technologie, Physikalisches Institut, Karlsruhe, Germany

$CeAu_2Ge_2$ hosts one of the lighter heavy-fermion systems located far on the magnetic side of the Doniach phase diagram. Being a strongly uniaxial antiferromagnet, its metamagnetic transition is of the spin-flip type. Recent neutron diffraction measurements [1] indicate several commensurate and incommensurate magnetic structures in the magnetically ordered state. In order to map out a detailed phase diagram we measured magnetostriction and thermal expansion on a $CeAu_2Ge_2$ single crystal. We found several phase transitions. The crystal under study has a Néel temperature of 9 K and a critical magnetic field around 3.4 T for $B \parallel c$ [2]. The uppermost transition changes from continuous to discontinuous at temperatures below approximately 6 K. At temperatures below 0.5 K the phase-transition lines fan out and exhibit increased hysteresis. The Néel temperature of $CeAu_2Ge_2$ changes very little with hydrostatic pressure [3]. Using the Ehrenfest relation and the Clausius-Clapeyron relation we extracted the uniaxial pressure dependencies of the Néel temperature and the critical magnetic field.

[1] D. K. Singh et al., Physical Review B 86, 060405(R) (2012)
[2] V. Fritsch et al., Physical Review B 84, 104446 (2011)
[3] C. L. Huang et al., Physical Review B, in print (2012)

TT 53.5 Thu 10:30 H19

**Strong enhancement of the thermopower of $YbRh_2Si_2$ by La substitution** — •Ulrike Stockert[1], Heike Pfau[1], Cornelius Krellner[1,2], Steffen Wirth[1], Christoph Geibel[1], and Frank Steglich[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Present address: Physikalisches Institut Goethe-University Frankfurt, 60438 Frankfurt (Main)

$YbRh_2Si_2$ orders antiferromagnetically below $T_N = 70$ mK and $B_c \approx 60$ mT $\perp c$. In addition, a crossover from a small Fermi surface (FS) at low fields to a large FS incorporating the $4f$ electrons at high fields takes place at $T^*(B)$. Rather large values are found for the absolute thermopower divided by temperature $|S/T|$. The different regions of the phase diagram are characterized by specific $T$ and $B$ dependencies, e.g. a broadened step-like increase of $|S/T|$ upon crossing $T^*(B)$.

Substitution of 2 % La on the Yb site of $YbRh_2Si_2$ results in a suppression of $T_N$ to below 20 mK, while $T^*(B)$ is not altered. Moreover, additional scattering centers are introduced. This leads to a lowering of the thermal conductivity in $Yb_{0.98}La_{0.02}Rh_2Si_2$. By contrast, $|S/T|$ is strongly enhanced below 1 K, but falls rapidly below the value for $YbRh_2Si_2$ already in moderate magnetic fields. In order to evaluate the origin of this unexpected behavior we studied in detail the field-dependence of the low-$T$ thermopower of $Yb_{0.98}La_{0.02}Rh_2Si_2$. Our results suggest, that the enhancement of the absolute thermopower upon La substitution and the strong field dependence are related to modifications of the band structure upon doping into the $4f$ sublattice.

TT 53.6 Thu 10:45 H19

**Magnetic phases in $Yb(Rh_{0.42}Co_{0.58})_2Si_2$** — •A. Hannaske[1], O. Stockert[1], C. Klingner[1], C. Krellner[1,2], S. Matas[3], M.-H. Lemee-Cailleau[4], L. Pedrero[1], M. Brando[1], C. Geibel[1], and F. Steglich[1] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Goethe-Universität Frankfurt, Frankfurt a. M., Germany — [3]Helmholtz-Zentrum Berlin, Berlin, Germany — [4]Institut Laue-Langevin, Grenoble, France

The heavy fermion compound $YbRh_2Si_2$, which orders antiferromagnetically below $T_N = 70$ mK, has attracted particular interest due to its anomalous properties such as pronounced non-Fermi-liquid behaviour, the divergence of the magnetic Grüneisen ratio as well as strong ferromagnetic fluctuations when approaching the quantum critical point. For a better understanding of this unique behaviour we started to investigate the microscopic magnetic structure in $Yb(Rh_{1-x}Co_x)_2Si_2$. For $x = 1$ and 0.68 we found an incommensurate propagation vector $\tau_1 \approx (0.25\ 0.08\ 1)$ below $T_N$ followed by a change to a commensurate structure at a lower $T_L$ with $\tau_2 = (0.25\ 0.25\ 1)$. Around $x \approx 0.5$, which is close to a minimum in the $(x - T)$-phase diagram, a change of the magnetic structure takes place. This change was investigated by a comprehensive study of magnetisation and neutron diffraction in magnetic fields on $Yb(Rh_{0.42}Co_{0.58})_2Si_2$. While below $T_L \approx 700$ mK the same commensurate propagation vector was found as for the higher Co concentrations, ferromagnetic behaviour was observed for $T_L < T < 820$ mK, which might be connected to the

magnetic order for Co concentrations $x < 0.58$.

TT 53.7 Thu 11:00 H19

**Electronic Structure of $LuRh_2Si_2$ - reference to $YbRh_2Si_2$** — •Pascal Reiss[1], Swee K. Goh[1], F. Malte Grosche[1], Zachary Fisk[2], Michael Sutherland[1], Patrick M.C. Rourke[3], Gertrud Zwicknagl[4], and Sven Friedemann[1] — [1]Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, CB3 0HE Cambridge, United Kingdom — [2]Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575, USA — [3]National Research Council Canada, 1200 Montreal Road, Ottawa, Ontario, K1A 0R6, Canada — [4]Institute for Mathematical Physics, TU Braunschweig, Mendelssohnstraße 3, 38106 Braunschweig, Germany

The intermetallic compound $LuRh_2Si_2$ is of interest as a non-magnetic reference compound to the heavy fermion material $YbRh_2Si_2$. $YbRh_2Si_2$ features an intensively studied quantum critical point (QCP) when small magnetic fields suppress the Neel temperature to zero. Signatures in transport and thermodynamic properties suggest a reconstruction of the Fermi Surface from a small configuration with localised f-electrons in the antiferromagnetic phase to a large configuration with itinerant f-electrons in the paramagnetic phase. Hence isostructural $LuRh_2Si_2$ with its completely filled f-shell and identical lattice parameters is a perfect reference compound for the small Fermi surface configuration. Here we present band structure calculations of $LuRh_2Si_2$ and compare predicted and observed Shubnikov-de Haas frequencies under different angles in dependence of the relative $z/c$ position of the Si atoms.

**15 min. break**

TT 53.8 Thu 11:30 H19

**Eu valence and Fermi-surface development in $EuX_2Si_2$ ($X$ = Co, Rh, Ir) systems** — •K. Götze[1,5], S. Seiro[2], C. Geibel[2], H. Rosner[2], V. Petzold[2], A. Polyakov[1], J. Wosnitza[1], I. Sheikin[3], and A. Suslov[4] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]MPI for Chemical Physics of Solids, Germany — [3]LNCMI-Grenoble, France — [4]National High Magnetic Field Laboratory, Tallahassee, USA — [5]TU Dresden, Institut für Festkörperphysik, Germany

The valence-fluctuating Eu systems $EuX_2Si_2$, with $X$ being the transition metal Co, Ir, or Rh, show different types of ground states, strongly depending on $X$. The instability of the Eu 4f shell underlies this phenomenon and leads among other effects to different valence states ranging from $Eu^{2+}$ over mixed valence and intermediate valence behavior to $Eu^{3+}$ [1]. Investigations on the structure and the magnetic behavior of $EuCo_2Si_2$, $EuIr_2Si_2$, and $EuRh_2Si_2$ have revealed their Eu valence. Further experiments on specific heat and resistivity gave insights to magnetic ordering, electronic correlations, and possible valence fluctuations. We report about a systematic de Haas-van Alphen study on the Fermi-surface development of the $EuX_2Si_2$ compounds in magnetic fields up to 35 T. High-quality single crystals were available for the first time. We will focus on the Fermi-surface topology obtained by angle dependent measurements and discuss a comparison to band-structure calculations.

This work was partly supported by EuroMagNET, EU contract 228043 and DFG within GRK1621.

[1] Z. Hossain et al., Journal of Alloys and Compounds 323-324 (2001).

TT 53.9 Thu 11:45 H19

**Optical study of archetypical valence-fluctuating Eu systems** — V. Guritanu[1], S. Seiro[1], •J. Sichelschmidt[1], N. Caroca-Canales[1], T. Iizuka[2], S. Kimura[2], C. Geibel[1], and F. Steglich[1] — [1]MPI Chemische Physik fester Stoffe, Dresden, Germany — [2]UVSOR Facility, Institute for Molecular Science, Okazaki, Japan

We have investigated the optical conductivity of the prominent valence-fluctuating compounds $EuIr_2Si_2$ and $EuNi_2P_2$ in the infrared energy range to get new insights into the electronic properties of valence-fluctuating systems. For both compounds, we observe upon cooling the formation of a renormalized Drude response, a partial suppression of the optical conductivity below 100 meV and the appearance of a midinfrared peak at 0.15 eV for $EuIr_2Si_2$ and at 0.13 eV for $EuNi_2P_2$. Most remarkably, our results show a strong similarity with the optical spectra reported for many Ce- or Yb-based heavy-fermion metals and intermediate valence systems, although the phase diagrams and the temperature dependence of the valence differ strongly between Eu- and Ce-/Yb-systems. This suggests that the hybridization between $4f$- and conduction electrons, which is responsible for the properties of Ce- and Yb-systems, plays an important role in valence-fluctuating Eu systems.

TT 53.10 Thu 12:00 H19

**Non-Fermi liquid picture and superconductivity in heavy fermion systems** — •Steffen Sykora[1] and Klaus W. Becker[2] — [1]IFW Dresden, D- 01171 Dresden, Germany — [2]Department of Physics, TU Dresden, D-01069 Dresden, Germany

We study the $S = 1/2$ Kondo lattice model which is widely used to describe heavy fermion behavior. In conventional treatments of the model a hybridization of conduction and localized $f$ electrons is introduced by decoupling the Kondo interaction. However, such an approximation has the detrimental effect that a breaking of a local gauge symmetry is imposed which implicates that the local $f$ occupation $n_i^f$ is no longer conserved. To avoid such an artifact, we treat the model in an alternative approach based on the Projective Renormalization Method (PRM). Thereby, within the conduction electron spectral function we identify the lattice Kondo resonance as an almost flat incoherent excitation near the Fermi surface which is composed of conduction electron creation operators combined with localized spin fluctuations. This leads to a new concept of the Kondo resonance without having to resort to a symmetry breaking and Fermi liquid theory. Based on this new picture we develop a microscopic theory for superconductivity in heavy fermion systems. Thereby we study the momentum-dependence of the superconducting order parameter for singlet as well as triplet pairing. We show that in particular the triplet pairing components are strongly affected by the incoherent excitations found to be responsible for the Kondo resonance.

TT 53.11 Thu 12:15 H19

**$YbPt_2Sn$ and $YbPt_2In$: Unusual weak magnetic exchange in two different structure types** — •Thomas Gruner, Dongjin Jang, Alexander Steppke, Manuel Brando, and Christoph Geibel — MPI Chemical Physics of Solids, 01187, Dresden, Germany

We have synthesized the two new compounds $YbPt_2Sn$ (YPS) and $YbPt_2In$ (YPI) and investigated their structural and magnetic properties. Powder diffraction patterns show YPS to crystallize in the same hexagonal $ZrPt_2Al$ structure type as previously known $RPt_2Sn$ and $RPt_2In$ ($R$ = Y, Gd - Tm) compounds, while at 300 K YPI was found to form in the cubic Heusler phase as $ScPt_2In$. Despite very different structure types both compounds show very similar, but peculiar magnetic properties. Analysis of susceptibility $\chi$(T), magnetization $M$(H), specific heat $C$(T) and resistivity $\rho$(T) indicate a stable trivalent $Yb^{3+}$ state, without any sign for a significant Kondo interaction. Nevertheless, $C$(T) data evidence a very low magnetic ordering temperature, of only 240 mK and 180 mK for YPS and YPI, respectively, connected with a very weak intersite magnetic exchange. This very weak exchange makes these compounds candidates for magnetic cooling. Possible origins for and implications of this weak exchange shall be discussed.

The transition from the $ZrPt_2Al$ structure type to the cubic laves phase upon decreasing the size of the $R$-element has been previously reported for the $RPd_2Sn$ and $RPd_2In$ series. Our results allow to generalize this observation to a whole series of $RT_2X$ compounds and indicate that this transition is mainly induced by a size effect and not related to a particular valence electron count.

TT 53.12 Thu 12:30 H19

**Magnetic field dependence of multiple order parameters in $CeB_6$** — •G. Friemel[1], H. Jang[1], A. Schneidewind[2], Y. Li[1], A. V. Dukhhenko[3], N. Y. Shitsevalova[3], N. E. Sluchanko[4], A. Ivanov[5], V. B. Filipov[3], B. Keimer[1], and D. S. Inosov[1] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]FRM-II, Garching, Germany — [3]Institute for Problems of Material Sciences, Kiev, Ukraine — [4]General Physics Institute, Moscow, Russia — [5]Institut Laue-Langevin, Grenoble, France

The heavy fermion (HF) antiferromagnet $CeB_6$ is known for exhibiting an antiferroquadrupolar (AFQ) order below $T_Q = 3.2$ K at $\mathbf{Q} = R(1/2, 1/2, 1/2)$, which was confirmed by resonant x-Ray and polarized neutron diffraction. Furthermore, the compound orders antiferromagnetically (AFM) in a double-$\mathbf{k}$ pattern below $T_N = 2.3$ K, which was so far neglected in the discussion of this compound. Only recently we could observe a spin exciton mode formation in the AFM state at $\hbar\omega = 0.5$ meV by inelastic neutron scattering, which can be understood as a feedback effect of the AFM order on the itinerant spin dynamics. By applying magnetic field the AFM order becomes quickly suppressed

at $B_c = 1\,\mathrm{T}$, whereas the intensity at $R(1/2, 1/2, 1/2)$ stays constant up to $B_Q = 1.7\,\mathrm{T}$, suggesting that it belongs to an unknown phase different from AFM and AFQ, with the latter setting in at $B > B_Q$. The exciton mode energy surprisingly becomes enhanced in field, parallel to the emergence of multiple other modes reaching into the AFQ state. These latter modes show a strong field dependence in energy, but are absent in the zero field AFQ phase above $T_N$.

TT 53.13 Thu 12:45 H19

**Spin excitons in the unconventional superconducting and hidden order state of strongly correlated electrons** — •Alireza Akbari and Peter Thalmeier — Max Planck Institute for the Chemical Physics of Solids, 01187 Dresden, Germany

The formation of collective spin excitons below the single particle continuum is observed in numerous unconventional superconductors. $CeCoIn_5$ is the most well established case for heavy fermion compounds. It is also the first example where the magnetic field splitting of magnetic excitons is observed for fields within the tetragonal plane. Contrary to expectations it is revealed as a doublet excitation. We explain the splitting as the result of a strongly anisotropic spin response described within the context of an Anderson lattice type model. Recently it was shown that collective spin excitations also appear within the hidden order phase of non- superconducting $CeB_6$. It is a signature of the itinerant nature of spin response as opposed to the commonly used localized 4f approach in this compound. We show that the salient features of the spin exciton can be explained in an itinerant quasiparticle model supplemented by hidden and antiferromagnetic order.

[1] A. Akbari and P. Thalmeier, Phys. Rev. B 86, 134516 (2012)
[2] A. Akbari and P. Thalmeier, Phys. Rev. Lett. 108, 146403 (2012)

## TT 54: Focused Session: Magnetism & Superconductivity in Fe-based Pnictides and Chalcogenides (jointly with MA)

Iron-based superconductors and their relation to magnetism is an exciting research field involving condensed matter physics, materials science, and solid state chemistry. In this Focus Session recent advances and results will be presented by leading experts in the field.

Organizers: Joachim Deisenhofer (University of Augsburg), Carsten Honerkamp (RWTH Aachen)

Time: Thursday 9:30–12:45 Location: H20

**Invited Talk** TT 54.1 Thu 9:30 H20

**Fermiology and Order Parameter of Iron-based Superconductors from ARPES** — •Sergey Borisenko — IFW Dresden

We use angle-resolved photoemission at ultra-low temperatures (1K-ARPES) to study iron-based superconductors. A number of materials from the 11, 111, 1111, 122, 245 and 1048 families have been studied. In some of them precise measurements of the superconducting gap as a function of momentum allow us to draw conclusions as for the structure and symmetry of the order parameter. In addition, we single out those details of the low-energy electronic structure which are necessary for the superconductivity itself.

[1] S. V. Borisenko et al., arXiv:1204.1316 (2012)
[2] S. V. Borisenko, Synchrotron Radiation News **25**(5), 6 (2012)
[3] S. V. Borisenko et al., J. Vis. Exp. **68**, e50129, DOI: 10.3791/50129 (2012)

**Invited Talk** TT 54.2 Thu 10:00 H20

**Electron Correlations in Solids from the Dynamical Mean Field Perspective and the Origin Anomalous State of Matter in Iron Chalchogenides** — •Kristjan Haule — Rutgers The State University of New Jersey, Piscataway, NJ, USA

The Dynamical Mean Field Theory in combination with the Density Functional Theory has recently enabled detailed modeling of the electronic structure of complex materials such as heavy fermions, transition metal oxides, chalchogenides and arsenides. Simulations based on this method has recently uncovered the origin of unusual properties of iron based high temperature superconductors and the physics behind the poor metallic conductivity in these systems. Here the Coulomb interaction among the electrons is not strong enough to localize electrons, but it significantly slows them down, such that low-energy emerging quasiparticles have a substantially enhanced mass, and at intermediate temperature and intermediate energy scale show strong deviations from the Fermi liquid theory. This enhanced mass emerges not because of the Hubbard interaction U, but because of the Hund's rule interactions J that tends to align electrons with the same spin but different orbital quantum numbers when they find themselves on the same atom. The ab-initio simulations with the Dynamical Mean Field Theory not only uncover the origin of anomalous properties, but also successfully explains the key properties of these material: such as the mass renormalizations and anisotropy of quasiparticles, the crossover into an incoherent regime above a low temperature scale, the magnetic moments in iron compunds, and dispersion of magnetic excitations.

**Topical Talk** TT 54.3 Thu 10:30 H20

**A Light Scattering Study of the Evolution of Pairing in Fe-based Superconductors** — •Rudi Hackl[1], Florian Kretzschmar[1], Bernhard Muschler[1], Thomas Böhm[1], Hai-Hu Wen[2], Vladimir Tsurkan[3,4], Joachim Deisenhofer[3], and Alois Loidl[3] — [1]Walther-Meissner-Institut, DE-85748 Garching — [2]Nanjing University, Nanjing 210093, China — [3]University of Augsburg, DE-86159 Augsburg — [4]Academy of Sciences of Moldova, MD-2028 Chisinau

The iron-based superconductors are a laboratory for exploring the relevance of electron-electron interactions beyond electron-phonon coupling, being at work in conventional superconductors, since the Fermi surfaces can be varied systematically by atomic substitution. This enables one to systematically study magnetism and superconductivity as a function of the Fermi surface topology. Inelastic light scattering affords a window into the electronic properties of the ordered states. In particular, the evolution of the superconducting pairing upon doping can be probed since light scattering allows access to the anisotropy of the energy gap and, in some cases, of the pairing potential. $Ba_{1-x}K_xFe_2As_2$ is one of those cases since the competition between $s$- and $d$-wave pairing leads to the appearance of exciton-like modes below the gap edges of the various bands. Along with the results from other materials having different Fermi surface cross-sections the data in $Ba_{1-x}K_xFe_2As_2$ support the spin fluctuation scenario driven by interband coupling. The experiments show that there exist alternative routes for the analysis of the pairing interaction in superconductors with unconventional coupling and anisotropic gaps.

**15 min. break**

**Topical Talk** TT 54.4 Thu 11:15 H20

**Theory of Magnetism and Superconductivity for Iron-Chalcogenides** — •Jiangping Hu — Dept. of Physics, Purdue University, West Lafayette, IN, USA — Institute of Physics, Chinese Academy of Sciences, Beijing, China

We discuss the difference on both magnetic and superconducting properties between iron-pnictides and iron-chalcogenides high temperature superconductors and construct a microscopic model based on $S_4$ symmetry that faithfully represents the intrinsic unit cell doubling of the materials. Within this model, we can show that there are two different types of extended S-wave pairing states. One is in the A representation of $S_4$ and the other is in the B representation of $S_4$. The A-phase is well studied $S_\pm$ phase when there are both electron pockets at M points and hole pockets at Γ point. However, the B phase is the new phase which has been ignored by models with one-iron per unit cell. The B phase is characterized by the sign reverse of the superconducting order parameter in real space between top and bottom layers in the building block of the trilayer Fe-As(Se) structure. We show that the B-phase is most likely realized in the electron-doped 122' or strained single layer iron-chalcogenides.

**Topical Talk** TT 54.5 Thu 11:45 H20

**Charge Dynamics in 122 Iron Pnictides** — •Aliaksei Charnukha, Oleg V. Dolgov, Paul Popovich, Dunlu Sun, Chengtian Lin, Alexander Yaresko, Bernhard Keimer, and Alexander V. Boris — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany

We report the full complex dielectric function of high-purity $Ba_{0.68}K_{0.32}Fe_2As_2$ single crystals with $T_c = 38.5$ K determined by broadband spectroscopic ellipsometry at temperatures $10 \leq T \leq 300$ K. We discuss the microscopic origin of superconductivity-induced infrared optical anomalies in the framework of a multiband Eliashberg theory with two distinct superconducting gap energies, $2\Delta_A \approx 6\ k_B T_c$ and $2\Delta_B \approx 2.2\ k_B T_c$. The observed unusual suppression of the optical conductivity in the superconducting state at energies up to 14 $k_B T_c$ can be ascribed to spin-fluctuation–assisted processes in the clean limit of the strong-coupling regime. We further observe a superconductivity-induced suppression of an absorption band at an energy of 2.5 eV, two orders of magnitude above the superconducting gap energy $2\Delta \approx 20$ meV, which challenges one of the central notions of conventional theories of superconductivity. We argue that the observed superconductivity-induced suppression involves a redistribution of electronic population between bands with different orbital character. Our results emphasize the importance of orbital physics for the mechanism of superconductivity in the iron-based superconductors.

TT 54.6 Thu 12:15 H20

**Disentangling Magnetism and Superconductivity in $EuFe_2(As_{1-x}P_x)_2$** — •Sina Zapf[1], Tomislav Ivek[1], Felix Klingert[1], Fabian Pfister[1], Shuai Jiang[1], Dan Wu[1], Hirale S. Jeevan[2], Philipp Gegenwart[2], Reinhard K. Kremer[3], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]I. Physikalisches Institut, Universität Göttingen — [3]Chemical Service Group, MPI-FKF Stuttgart

Due to local magnetic ordering of $Eu^{2+}$, $EuFe_2(As_{1-x}P_x)_2$ is a perfect system to study the interplay between superconductivity (SC) and magnetism in iron pnictides. However, there is still an ongoing debate about the extent of the superconducting dome and the development of the local Eu magnetic ordering with chemical pressure [1,2]. Especially the question whether SC coexists with ferro- (FM) or antiferromagnetic (AFM) $Eu^{2+}$ ordering has drawn tremendous interest.
We have performed a systematic study on a set of high-quality single crystals ($x$ = 0, 0.12, 0.145, 0.15, 0.165, 0.17, 0.26, 0.35 and 1) using DC resistivity, as well as DC and AC magnetic susceptibility measurements along the principal crystallographic directions. By combining these techniques we identify the different phases, prove that AFM interlayer coupling coexists with SC and discuss the complex magnetization behaviour of these compounds. Our investigations reveal the delicate interplay between SC and magnetism.

[1] Jeevan et al., PRB 83, 054511 (2011)
[2] Cao et al., Condens. Matter 23, 464204 (2011)

TT 54.7 Thu 12:30 H20

**Growth and characterization of $Rb_{1-x}Fe_{2-y}Se_2$ single crystals** — •Vladimir Tsurkan[1,2], Joachim Deisenhofer[1], Axel Günther[1], Hans-Albrecht Krug von Nidda[1], Sebastian Widmann[1], and Alois Loidl[1] — [1]Experimental Physics 5, Center for Electronic Correlations and Magnetism, University of Augsburg, D 86159, Augsburg, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028, Chisinau, R. Moldova

Growth of single crystals of Rb-Fe-Se system and their characterization by X-ray powder diffraction, Squid magnetometry, conductivity, and specific heat are presented [1]. The single crystals exhibit an anisotropic antiferromagnetism below 400 K. For 1.53 < Fe < 1.6 the superconducting (SC) behavior is found. The sharp transition into the SC state at 32.4 K is observed for $Rb_{0.8}Fe_{1.6}Se_2$. For the Fe concentrations below 1.5 and above 1.6, respectively, samples show insulating and semiconducting behavior. Magnetic behavior of SC and non-SC samples provides an evidence for the coexistence of superconductivity and static antiferromagnetic order. The evolution of the SC and AFM correlations in the Rb-Fe-Se system is discussed within the constructed phase diagram which includes several structural phases with different magnetic behavior. The coexistence of the superconductivity and antiferromagnetism in $Rb_{0.8}Fe_{1.6}Se_2$ is considered within a scenario of phase separation based on the results of neutron scattering, Mössbauer spectroscopy, optical, $\mu$SR, and nuclear magnetic resonance investigations.

[1] V. Tsurkan, J. Deisenhofer, A. Günther, H.-A. Krug von Nidda, S. Widmann, and A. Loidl, Phys. Rev. B **84**, 144520 (2011)

## TT 55: Correlated Electrons: Low-Dimensional Systems -Materials 2

Time: Thursday 9:30–13:00 Location: H21

TT 55.1 Thu 9:30 H21

**Absence of charge order in the dimerized $\kappa$-phase BEDT-TTF salts** — •Martin Dressel[1], Katrin Sedlmeier[1], Sebastian Elsässer[1], David Neubauer[1], Rebecca Beyer[1], Dan Wu[1], Tomislav Ivek[1,2], Silvia Tomic[2], and John A. Schlueter[3] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Institut za fiziku, Zagreb, Croatia — [3]Material Science Division, Argonne National Laboratory, U.S.A.

Utilizing infrared vibrational spectroscopy we have investigated dimerized two-dimensional organic salts in order to search for possible charge redistribution that might constitute electronic dipoles and ferroelectricity: the quantum spin liquid $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$, the antiferromagnetic Mott insulator $\kappa$-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl, and the superconductor $\kappa$-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br. None of them exhibit any indication of charge disproportionation. Upon cooling to low temperatures all BEDT-TTF molecules remain homogeneously charged within $\pm 0.005e$. No modification in the charge distribution is observed around $T = 6$ K where a low-temperature anomaly has been reported for the spin-liquid material $\kappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$. In this compound the in-plane optical response and vibrational coupling are rather anisotropic, indicating that the tilt of the BEDT-TTF molecules in $c$-direction and their coupling to the anion layers has to be considered in the explanation of the electromagnetic properties.

[1] K. Sedlmeier *et al.*, Phys. Rev. B (in press); arXiv:1208.2652

TT 55.2 Thu 9:45 H21

**Magnetoacoustic and pressure studies of frustrated distorted diamond chain compound azurite** — •P. T. Cong, B. Wolf, R. S. Manna, U. Tutsch, M. de Souza, A. Brühl, and M. Lang — Physikalisches Institut, Goethe-Universität, SFB/TR 49, D-60438 Frankfurt

Measurements of ultrasound, thermal expansion and magnetic susceptibility measurements were carried out on a high-quality single crystal of distorted diamond chain compound azurite. The results show clear signatures of the magnetic energy scales involved [1, 2] and disclose two pronounced anomalies at $\sim 20$ K and $\sim 5$ K in accordance with literature results of magnetic susceptibility and specific heat data [1]. Huge anomaly of acoustic signal and thermal expansivity at $T_N = 1.88$ K demonstrate that in this material the onset of long-range antiferromagnetic (AFM) ordering is accompanied by sizable structural distortions. From the analysis of the temperature dependence of elastic constant and results of the pressure dependence of the magnetic susceptibility an estimate of the strain dependence of the dominant magnetic exchange coupling can be derived. These results highlight the significant role of strain interaction in this compound. The field and temperature dependence of sound velocity and thermal expansion reveal a very complex magnetic structure of azurite at temperature below $T_N$. Based on these measurements we map out a detailed $B-T$ phase diagram.

[1] H. Kikuchi et al. Phys. Rev. Lett. 94, 227201 (2005).
[2] H. Jeschke et al., Phys. Rev. Lett. 106, 217201 (2011)

TT 55.3 Thu 10:00 H21

**Impurity effects in a S=1/2 Heisenberg spin chain probed by $^{63}$Cu NMR** — •Yannic Utz[1], Eva Maria Brüning[1], Franziska Hammerath[1], Christian Rudisch[1], Hans-Joachim Grafe[1], Ashwin Mohan[1], Romuald Saint-Martin[2], Alexandre Revcolevschi[2], Christian Hess[1], Satoshi Nishimoto[1], Stefan-

Ludwig Drechsler[1], and Bernd Büchner[1] — [1]IFW Dresden, Germany — [2]LPCES, Orsay, France

We present $^{63}$Cu NMR measurements on undoped, Ni doped and Mg doped $SrCuO_2$ single crystals. $SrCuO_2$ is a good realization of a one-dimensional S=1/2 Heisenberg spin chain. This is confirmed by the theoretically-expected temperature independent NMR spin-lattice relaxation rate $T_1^{-1}$. Doping with Ni, which can be regarded as a S=1 impurity, has a major impact on the magnetic properties of the spin chains. On the one hand, this is manifested by unusual features in the NMR spectra below 100 K, revealing the existence of an impurity-induced local alternating magnetisation. On the other hand, exponentially decacying spin lattice relaxation rates towards low temperatures indicate the opening of a spin gap similar to Ca doped $SrCuO_2$ [1]. Mg doping (S=0) has, however, no influence on the magnetic properties of the spin chains. Neither the NMR spectra nor the spin lattice relaxation rates differ from those measured on pure $SrCuO_2$. While the different impact of Ni and Mg doping on the spin chains could be explained by their different impurity spins, the opening of a spin gap in case of Ni doping is totally unexpected and not yet understood.

[1] F. Hammerath et al., Phys. Rev. Lett. 107, 017203 (2011).

TT 55.4 Thu 10:15 H21

**Magnetism of $CuX_2$ frustrated chains (X = F, Cl, Br): the role of covalency** — •Stefan Lebernegg[1], Miriam Schmitt[1], Alexander Tsirlin[1,2], Oleg Janson[1], and Helge Rosner[1] — [1]MPI Chemical Physics of Solids, Dresden, Germany — [2]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

Periodic and cluster DFT calculations, including DFT+$U$ and hybrids, are applied to study magnetostructural correlations in spin-1/2 frustrated chain compounds: $CuCl_2$, $CuBr_2$, and a fictitious chain structure of $CuF_2$. The nearest-neighbor and second-neighbor exchange integrals, $J_1$ and $J_2$, are evaluated as a function of the Cu–X–Cu bridging angle $\theta$ in the physically relevant range 80–110°. The ionic $CuF_2$ exhibits ferromagnetic coupling only for $\theta \leq 100°$, according to the Goodenough-Kanamori-Anderson rules. However, both $CuCl_2$ and $CuBr_2$ feature ferromagnetic $J_1$ in the whole angular range studied. This surprising behavior is ascribed to the increased covalency in the Cl and Br compounds, which amplifies the contribution from Hund's exchange on the ligand atoms and renders $J_1$ ferromagnetic. At the same time, the larger spatial extent of X orbitals enhances the antiferromagnetic $J_2$, which is realized via the long-range Cu–X–X–Cu paths. Both, periodic and cluster approaches supply a consistent description of the magnetic behavior which is in good agreement with the experimental data for $CuCl_2$ and $CuBr_2$. Thus, owing to their simplicity, cluster calculations have excellent potential to study magnetic correlations in more involved spin lattices, especially making parameter-free quantum-chemical methods computationally feasible.

TT 55.5 Thu 10:30 H21

**Novel frustrated quantum antiferromagnets in the solid-solution $Cs_2CuCl_{4-x}Br_x$through site-selective halide substitution** — •Bernd Wolf, Pham Thanh Cong, Natalia van Well, Franz Ritter, Wolf Assmus, and Michael Lang — Physikalisches Institut, Goethe-Universität, SFB/TR 49, D-60438 Frankfurt

Depending on the growing conditions, an A-type orthorhombic or a B-type tetragonal structure can be found in the solid solution $Cs_2CuCl_{4-x}Br_x$ ($0 \leqslant x \leqslant 4$). Here we present measurements of the temperature-dependent susceptibility and isothermal magnetization on the B-type compounds x = 1.6 and 2.0 and compare these results with the magnetic properties recently derived for the A-type variant by Cong *et al.*, Phys. Rev. B 83, 064425 (2011). We find that due to their different Cu coordination, these two structural modifications exhibit quite dissimilar magnetic properties. The tetragonal compounds can be classified as quasi-2D ferromagnets characterized by ferromagnetic layers with a weak antiferromagnetic inter-layer coupling, whereas the orthorhombic materials, notably the border compounds x = 0 and 4, are model systems for frustrated 2D Heisenberg antiferromagnets.

TT 55.6 Thu 10:45 H21

**A metal-organic spin-1/2 dimer system yielding a 2d field-induced collectively-coupled dimer phase** — •U. Tutsch[1], B. Wolf[1], T. Kretz[2], H.-W. Lerner[2], M. Wagner[2], S. Wessel[3], T. Saha-Dasgupta[4], H. Jeschke[5], R. Valenti[5], and M. Lang[1] — [1]Phys. Inst., Goethe-Universität, 60438 Frankfurt — [2]Inst. f. Anorg. Chemie, Goethe-Universität, 60438 Frankfurt — [3]Inst. f. Theoret. Festkörperphysik, RWTH Aachen, 52056 Aachen — [4]S.N. Bose National Centre for Basic Sciences, Salt Lake City, Kolkata 700098, India — [5]Inst. f. Theoret. Physik, Goethe-Universität, 60438 Frankfurt

Spin-dimer systems have proven to be very useful in studying magnetic field-induced phase transitions. Here, we present high-resolution susceptibility and specific heat measurements at very low temperatures down to 0.040 K on the metal-organic spin-1/2 dimer system $C_{36}H_{48}Cu_2F_6N_8O_{12}S_2$. The *intra*-dimer coupling between the spins on the Cu sites is $J_d/k_B \approx 10$ K, making field-induced ordering accessible for standard laboratory magnets. *Ab initio* calculations suggest an effective two-dimensional (2d) structure with *inter*-dimer couplings $J_i$ of at least an order of magnitude smaller than $J_d$. This is confirmed by comparison of the experimental data with results form Quantum Monte Carlo simulations for 1d, 2d and strongly anisotropic 3d coupling schemes. We identify a region in the field vs. temperature phase diagram where the system exhibits typical 2dXY behaviour accompanied by the formation of vortices and antivortices in the effective spin configuration. The possibility of a magnetic Berezinskii-Kosterlitz-Thouless transition will be discussed.

TT 55.7 Thu 11:00 H21

**Padé approximations for the magnetic susceptibilities of Heisenberg antiferromagnetic spin chains for various spin values** — •Joseph Law[1] and Reinhard Kremer[2] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The temperature dependence of the spin susceptibilities of $S$=1, $\frac{3}{2}$, 2, $\frac{5}{2}$ and $\frac{7}{2}$ Heisenberg nearest-neighbor antiferromagnetic 1D spin chains was simulated via Quantum Monte Carlo calculations, within the temperature range of $0.005 \leq T^\star \leq 100$ and fitted to Padé approximations with deviations between the simulated and fitted data of the same order of magnitude or smaller than the Quantum Monte Carlo error. To demonstrate the practicality of our theoretical findings, we successfully compared them with the well known 1D chain compound TMMC ($d^5$, $S$=5/2) and the new $S$=1 Heisenberg spin chain $NiTa_2O_6$.

**15 min. break**

TT 55.8 Thu 11:30 H21

**Similarities between the phase diagrams of the $S$=3/2 Heisenberg spin chains $CrXO_4$ [X=V,P]** — •Joseph Law[1], Tobias Foerster[1], Robert Glaum[2], and Reinhard Kremer[3] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Institut für Anorganische Chemie, Universität Bonn, 53121 Bonn, Germany — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

$CrVO_4$ and $CrPO_4$ both adopt the same structure type. They can be well described as $S$=$\frac{3}{2}$ Heisenberg spin chains with predominant nearest-neighbour only spin exchange interaction. We show here an in-depth investigation into the magnetic structures of both compounds which is complimented by magnetic property measurements. Wherein, we've shown that both compounds exhibit a high field phase transition into an unknown state.

TT 55.9 Thu 11:45 H21

**Lattice effects in the 2D valence-bond-solid Mott insulator $EtMe_3P[Pd(dmit)_2]_2$** — •Rudra Sekhar Manna[1], Reizo Kato[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany — [2]RIKEN, Wako, Saitama 351-0198, Japan

$EtMe_3P[Pd(dmit)_2]_2$ is a quasi-twodimensional valence-bond-solid (VBS) Mott insulator where $Pd(dmit)_2$ molecules form dimers in the conducting layer, arranged in a triangular lattice with transfer integrals $t$ and $t'$ ($t'/\ t = 0.87$) and an average inter-dimer exchange coupling $J/k_B \approx 250$ K. Despite this strong spin frustration the system reveals a low-temperature transition into a spin-gapped Mott insulating phase. Here we present results of the uniaxial expansion coefficients $\alpha_i$ on single crystals of $EtMe_3P[Pd(dmit)_2]_2$ for temperatures 1.4 K $\leq T \leq$ 200 K and magnetic fields $B \leq 8$ T. We find a sharp and well-pronounced $\lambda$-type thermal expansion anomaly at 24.1 K corresponding to the second-order phase transition into the low-$T$ VBS phase. The discontinuity in $\alpha_i$ at $T_{VBS}$ reveals a pronounced in-plane ($c$-axis) vs out-of-plane ($b$-axis) anisotropy. Strongly anisotropic expansivities also characterize the state $T > T_{VBS}$. While the in-plane $c$-axis shows a large positive expansivity, as often found in soft organic

materials, the out-of-plane *b*-axis is dominated by a large negative contribution which sets in rather abruptly around 40 K. Measurements in magnetic fields up to 8 T were found to have no effect on the VBS phase transition, *i.e.*, there are no indications of a field-induced melting of the VBS state at this field level.

TT 55.10 Thu 12:00 H21

**Frustrated Cairo lattice in $Bi_4Fe_5O_{13}F$** — •Alexander A. Tsirlin[1], Dmitry Batuk[2], and Artem M. Abakumov[2] — [1]National Institute for Chemical Physics and Biophysics, Tallinn, Estonia — [2]EMAT, University of Antwerp, Belgium

Cairo lattice reveals an unusual topology of frustrated magnetic interactions that form pentagonal units. We present crystal structure and magnetism of $Bi_4Fe_5O_{13}F$, a recently discovered spin-$\frac{5}{2}$ compound, which is one of the few material prototypes of the Cairo spin lattice. Thermodynamic measurements reveal a sequence of phase transitions, with the onset of magnetic order at $T_N = 178$ K and subsequent transformations at $T_1 = 62$ K and $T_2 = 71$ K. The low-temperature magnetic structure is non-collinear and commensurate, in agreement with theoretical expectations for the Cairo-lattice spin model. However, additional magnetic transitions below $T_N$ have not been anticipated by theory. A comparative microscopic analysis of $Bi_4Fe_5O_{13}F$ and the sister compound $Bi_2Fe_4O_9$ will be presented.

Financial support of the Mobilitas program of the ESF is acknowledged.

TT 55.11 Thu 12:15 H21

**Magnetic-ordering transitions of the effective XY-spin-1/2 compound $Cs_2CoCl_4$** — •Oliver Breunig[1], Eran Sela[2], Achim Rosch[2], Benjamin Buldmann[2], Petra Becker[3], Ladislav Bohatý[3], Sandra Niesen[1], Ralf Müller[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln — [3]Institut für Kristallographie, Universität zu Köln

$Cs_2CoCl_4$ is a model system for studying the magnetism of one-dimensional spin chains with an XY-like anisotropy. It contains $CoCl_4$ tetrahedra which form chains along the crystallographic *b* axis. Due to a strong crystal field, an easy-plane anisotropy of magnetization is established. For symmetry reasons, easy planes in $Cs_2CoCl_4$ appear in two orientations. At temperatures between 0.3 and 4 K, the compound is well described by the one-dimensional XXZ model. At lower temperatures magnetic order arises due to finite inter-chain coupling. Our measurements of thermal expansion and specific heat down to 50 mK and in magnetic fields up to 3 T reveal a field-dependent ordering temperature $T_C(H)$. Depending on the orientation of the magnetic field with respect to the easy planes' orientation various ordered phases arise. We present phase diagrams for different field directions and discuss possible ordering mechanisms.

This work was supported by the DFG through SFB 608.

TT 55.12 Thu 12:30 H21

**Magnetic and structural properties of antiferromagnetic $VF_3$** — •Patrick Reuvekamp[1], Reinhard Kremer[1], Roland Eger[1], Gwilherm Nenert[2], and Thomas Hansen[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Institut Laue-Langevin, 38042 Grenoble, France

We report on a magnetic and structural investigation of layered antiferromagnetic system vanadium (III) fluoride. $VF_3$ crystallizes in a distorted $ReO_3$ structure ($R\bar{3}c$) with rotated undistorted $VF_6$ octahedra. The $V^{+3}$ cations are arranged in a triangular lattice with the possibility of exhibiting magnetic frustration. Polycrystalline samples of $VF_3$ were investigated using heat capacity, dielectric, magnetic susceptibility and neutron powder diffraction methods. Combining our results, we confirmed that $VF_3$ undergoes long-range antiferromagnetic order at ∼19 K in accordance with literature [1]. The antiferromagnetic order results in a magnetic structure with the magnetic moments alternating between **a** parallel and **b** parallel alignments in the *ab* plane . A second phase transition can be seen at ∼120 K in the heat capacity [1] and dielectric measurements possibly associated to a minute structural distortion.

[1] A.C. Gossard, H.J. Guggenheim, F.S.L. Hsu, and R.C. Sherwood, AIP Conf. Proc., No. 5, 302 (1971).

TT 55.13 Thu 12:45 H21

**Magnetic anisotropies in the Ising spin-chain compound $BaCo_2V_2O_8$** — •Sandra Niesen, Michael Seher, Gerhard Kolland, Oliver Breunig, and Thomas Lorenz — II. Physikalische Institut, Universität zu Köln

The effective Ising spin 1/2 system $BaCo_2V_2O_8$ consists of $CoO_6$ octahedra that form screw chains along the crystallographic *c* axis which are separated by nonmagnetic $Ba^{2+}$ and $V^{5+}$ ions. Long-range antiferromagnetic order is observed below $T_N = 5.5$ K in zero magnetic field with the spins aligned along *c*. Within the tetragonal *ab*-plane competing exchange interactions are present causing a lower symmetry of the stabilized magnetic structure. Therefore, magnetic domains occur with ferromagnetic alignment of the spins along [100] and an antiferromagnetic one along [010], or vice versa. High resolution zero-field thermal-expansion data show, that the system undergoes a structural transition from tetragonal to orthorombic while entering the Néel phase. Here, the frustration within the *ab*-plane is lifted by a small orthorhombic splitting $(a-b)/(a+b) \neq 0$, that is below the resolution of diffraction techniques. Moreover, detailed investigations of *e.g.* magnetization, thermal expansion, specific heat, and thermal conductivity reveal an additional magnetic-field anisotropy within the *ab*-plane. The corresponding phase diagrams for magnetic fields along [100] and [110] will be presented.

This work is supported by the DFG through SFB 608.

## TT 56: Graphene - Preparation and Characterization 1 (jointly with DS, HL, MA, and O)

Time: Thursday 10:30–13:15 Location: H17

TT 56.1 Thu 10:30 H17

**Synthesis of graphene on $(6\sqrt{3} \times 6\sqrt{3})R30°$ reconstructed SiC surfaces by molecular beam epitaxy** — •Timo Schumann[1], Martin Dubslaff[1], Myriano H. Oliveira Jr.[1], Michael Hanke[1], Felix Fromm[2], Thomas Seyller[2,3], J. Marcelo J. Lopes[1], and Henning Riechert[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Lehrstuhl für Technische Physik, Friedrich-Alexander-Universitt Erlangen-Nürnberg, Erlangen, Germany — [3]Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

We report on the synthesis of graphene on a $(6\sqrt{3} \times 6\sqrt{3})R30°$ reconstructed SiC(0001) surface (a.k.a. *buffer layer*) by means of molecular beam epitaxy (MBE). Raman spectroscopy reveals that the quality of the MBE-grown graphene films increases with growth time and that the average crystallite size exceeds 20 nm. X-ray photoelectron spectroscopy confirms that the thickness of the films increases as a function of the growth time and proves that the buffer layer is preserved during the growth process. In addition, grazing-incidence X-ray diffraction measurements were performed at the beamline ID10 of the ESRF in Grenoble. In-plane reflections of the buffer layer, the SiC, as well as from the MBE-synthesized graphene, were investigated. Strikingly, despite their nanocrystalline nature, it is observed that the graphene films grown by MBE show an in-plane alignment to the substrate, revealing that a conventional epitaxial growth on the buffer layer takes place. The results will be discussed in the context of MBE growth of graphene considering the most recent data reported in the literature.

TT 56.2 Thu 10:45 H17

**Microscopic characterization of CVD grown graphene suspended on TEM grids** — •Florian Studener[1], Luca Bignardi[1], Willem van. Dorp[1], Steffano Gottardi[1], Oleksii Ivashenko[1], Pavel Dudin[2], Alexei Barinov[2], Petra Rudolf[1], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, Netherlands — [2]Sincrotrone Trieste S.C.p.A, 34149 Basovizza, Trieste, Italy

We investigated CVD grown graphene, which was transferred and suspended on a TEM grid. Both electronic and structural properties were investigated. The former were investigated with angle resolved photoelectron spectroscopy and microscopy, while the latter were analysed with Raman spectroscopy and transmission electron microscopy. We could observe that CVD grown graphene has comparable characteris-

tics with free standing graphene produced with micro cleavage, e. g. the Fermi velocity of 1*10-6 m/s is close to the theoretically expected value. Despite the polycrystalline nature of the Cu foil used as a substrate for the graphene growth, the obtained graphene exhibits large single-crystalline domains up to tens of microns. Thus, the presented transfer method can be successfully exploited for clean TEM substrates for further investigations.

TT 56.3 Thu 11:00 H17

**Graphene-enhanced versus Surface-enhanced Raman Scattering** — •Fatemeh Yaghobian, Tobias Korn, and Christian Schüller — Institute of Experimental and Applied Physics University of Regensburg D-93040 Regensburg, Germany

Graphene-enhanced Raman scattering (GERS) is emerging as an important method due to the need for highly reproducible, quantifiable and biocompatible active substrates. As a result of its unique two dimensional carbon structure, graphene provides particularly large enhanced Raman signals of molecules at its surface. In this work, it is demonstrated that graphene works as active substrate for enhanced Raman scattering and has a great potential in biosensing because of its ability to quench interfering fluorescence. Obtained GERS signals of different molecules with reproducible enhancement factors are discussed and compared with surface-enhanced Raman scattering (SERS) signals on highly active substrates, covered with spherical silver nanoparticles. We have also observed an upshift in the frequency of the breathing mode of a test molecule, when adsorbed on graphene, in contrast to measurements on silver nanoparticles, where the frequencies remain unchanged.

TT 56.4 Thu 11:15 H17

**Dynamics of adsorbate layers on freestanding graphene probed by ultrafast low-energy electron diffraction** — •Max Gulde[1], Simon Schweda[1], Manisankar Maiti[1], Hakki Yu[2], Sascha Schäfer[1], and Claus Ropers[1] — [1]Materials Physics Institute and Courant Research Centre, University of Göttingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, University of Göttingen, Germany

Ultrafast structural dynamics in solids and nanostructures can be observed by an increasing number of sophisticated electron and x-ray diffraction techniques. Despite successful implementations of ultrafast reflection high-energy electron diffraction (1,2), the diffractive probing of ultrafast structural processes at surfaces remains an experimental challenge. We have implemented ultrafast low-energy electron diffraction (ULEED) to study structural changes with high temporal resolution and ultimate surface sensitivity, at electron energies from 100 eV to 500 eV. Specifically, we ultilize nanoscopic needle emitters in an electrostatic lens geometry as high-brightness sources of pulsed electrons. With this approach, the ultrafast melting dynamics of ordered adsorbate structures on freestanding graphene is investigated in transmission with a temporal resolution below 5 ps.

(1) A. Hanisch-Blicharski, A. Janzen, B. Krenzer, S. Wall, F. Klasing, A. Kalus, T. Frigge, M. Kammler, and M. Horn-von Hoegen, Ultramicroscopy (accepted) (2012)

(2) S. Schäfer, W. Liang, and A. H. Zewail, J. Chem. Phys. 135, 214201 (2011)

TT 56.5 Thu 11:30 H17

**High-Temperature STM of the Ordering of an Amorphous Carbon Layer into Graphene on Ru(0001)** — Sebastian Günther[1], Sebastian Dänhardt[2], •Martin Ehrensperger[2], Patrick Zeller[2], Stefan Schmitt[3], and Joost Wintterlin[2] — [1]Chemie Department, Technische Universität München, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, Germany — [3]SPECS GmbH, Voltastr. 5, D-13355 Berlin, Germany

An amorphous carbon layer was prepared on Ru(0001) by chemical vapor deposition of ethylene at about 650 K. High-Temperature Scanning Tunneling Microscopy (HTSTM), Low Energy Electron Diffraction and Temperature Programmed Desorption measurements were used to characterize the layer and its formation. The obtained carbon layer then served as amorphous precursor in an ordering transition towards graphene. At temperatures between 920 and 950 K the layer transformed into graphene which was indicated by the evolving moiré pattern. The ordering was monitored *in situ* by HTSTM. The observations revealed a unique mechanism involving mobile, small topographic holes that move through the disordered carbon layer leaving graphene behind. The transport of carbon monomers mediated by these holes opens a low-energy pathway for the ordering transition. In a dense packed graphene layer this mechanism is impossible which can explain the problems of healing defects in chemically synthesized graphene.

TT 56.6 Thu 11:45 H17

***In situ* LEEM Investigations of the Growth of Graphene on Ni(111)-Films** — •Patrick Zeller[1], Michael Weinl[2], Florian Speck[3], Markus Ostler[3], Thomas Seyller[3], Matthias Schreck[2], and Joost Wintterlin[1] — [1]Department Chemie, Ludwig-Maximilians-Universität München — [2]Institut für Physik, Universität Augsburg — [3]Department für Physik, FAU Erlangen-Nürnberg

We report about low energy electron microscopy (LEEM), scanning tunneling microscopy (STM), auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS) investigations of graphene grown on single-crystalline Ni(111) films. The films, which may provide an easy and economical way towards a scalable graphene synthesis, consist of 150 nm thick, heteroepitaxially grown Ni(111) layers on a Si(111) wafer with a YSZ-buffer layer. Monolayer graphene was grown by chemical vapor deposition of ethylene and *in situ* LEEM investigations of the graphene growth were performed. Also the formation of nickel carbide and its transformation into graphene were observed. Furthermore we noticed an involvement of the bulk during the reaction. At the beginning of the ethylene dosing the C atoms dissolve in the bulk, and after nucleation segregation of C atoms starts. We could also observe the healing of rotated graphene towards aligned, high quality graphene in a small temperature range. Also a temperature dependent formation and healing of dislocation lines in the Ni films was observed.

TT 56.7 Thu 12:00 H17

**Growth of graphene on a stepped iridium surface: morphology, domains and electronic fingerprints** — •Iva Šrut[1], Vesna Mikšić Trontl[1], Petar Pervan[1], Fabian Craes[2], Thomas Michely[2], Carsten Busse[2], and Marko Kralj[1] — [1]Institut za fiziku, Bijenička 46, 10000 Zagreb, Croatia — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

A promising route for modification of graphene properties is the growth of graphene on a substrate with a periodic arrangement of steps. We have used scanning tunneling microscopy and spectroscopy (STM/STS) and low energy electron diffraction (LEED) to study the growth of graphene on such periodically stepped Ir(332) surface. We have found that graphene continuously extends over iridium terraces and steps. Moreover, new distinctive mesoscopic features of the underlying surface are formed involving large, flat terraces accompanied by groups of narrower steps [1]. These morphologically different regions are also distinctive by their spectroscopic features found in STS. The distribution of the newly formed terraces as well as the contribution of various graphene orientations is sensitive to the preparation temperature. Below 800°C we find that the terrace width distribution is closer to the intrinsic distribution of clean Ir(332) than for higher temperatures. Additionally, graphene grown at low temperatures has a prominent contribution of a domain rotated by 30° with respect to the substrate. We find that the microscopic shape of steps after graphene formation strongly depends on the orientation of graphene.

[1] I. Šrut, et al., submitted

TT 56.8 Thu 12:15 H17

**Phonons of graphene on Ir(111)** — •Michael Endlich[1], Alejandro Molina-Sánchez[2], Ludger Wirtz[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau — [2]Physics and Material Sciences Research Unit, University of Luxembourg, L-1511 Luxembourg

The phonon dispersion relations of graphene on Ir(111) were determined with angle-resolved inelastic electron scattering. A weak graphene–Ir interaction is inferred from the lifting of the degeneracy of the out-of-plane optical and acoustic dispersion branches at the $\bar{K}$ point of the surface Brillouin zone and from the energy reduction of the out-of-plane optical phonon. Despite this interaction the Kohn anomalies known from graphite of the highest optical phonon branch at $\bar{\Gamma}$ and $\bar{K}$ persist. The experimental dispersion relations are in agreement with density functional calculations.

TT 56.9 Thu 12:30 H17

**Support restructuring during graphene growth on Cu foils triggers the formation of non flat membranes** — •Jürgen Kraus[1], Sebastian Böcklein[2], Robert Reichelt[1], Benito Santos[3], Tevfik O. Mentes[3], Andrea Locatelli[3], and Sebas-

tian Günther[1] — [1]Technische Universität München Chemie Department, D-85748 Garching — [2]Ludwig-Maximilians-Universität, D-81377 München — [3]Sincrotrone Trieste, I-34149 Trieste - Basovizza

Meanwhile the growth of single crystalline graphene flakes on Cu foils at a mm-length scale can be achieved, which provides a potential source for high quality graphene. On the other hand, the g-Cu system still suffers from certain inherent defects: during graphene growth sequences of inclined Cu facets form which are visible in scanning electron microscopy (SEM) images as stripes and which have been observed as well applying atomic force microscopy (AFM) and scanning tunneling microscopy (STM). Since the graphene follows the morphology of the underlying Cu foil the support restructuring leads to the formation of so called nanorippled graphene which persists even if the graphene is transferred on a flat Si wafer. In our study, we identified a sequence of such Cu facets after graphene growth on a Cu foil using low energy electron microscopy (LEEM) and show why the graphene cannot flatten when removed from the support. In addition, we were able to prepare graphene membranes by the local electrochemical removal of the Cu foil underneath the grown graphene. We show that the resulting membranes are exact replicas of the former morphology of the Cu foil during growth, i.e. they are non flat membranes.

TT 56.10 Thu 12:45 H17

**Graphene on Rh(111) and Ru(0001): combined STM/NC-AFM and DFT studies** — •Yuriy Dedkov[1], Torben Haenke[1], Oliver Schaff[1], Andreas Thissen[1], Elena Voloshina[2], and Mikhail Fonin[3] — [1]SPECS Surface Nano Analysis GmbH, Voltastraße 5, 13355 Berlin, Germany — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [3]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

The electronic and crystallographic structure of graphene moiré on Rh(111) and Ru(0001) is studied via combination of density-functional theory calculations and scanning tunneling and noncontact atomic force microscopy (STM and NC-AFM). Whereas the principal contrast between hills and valleys observed in STM does not depend on the sign of applied bias voltage, the contrast in atomically resolved AFM images strongly depends on the frequency shift of the oscillating AFM tip. The obtained results demonstrate the perspectives of application atomic force microscopy/spectroscopy for the probing of the chemical contrast at the surface.

TT 56.11 Thu 13:00 H17

**Epitaxial graphene nanoflakes on Au(111): Structure, electronic properties and manipulation** — •Mikhail Fonin[1], Philipp Leicht[1], Lukas Zielke[1], Elena Voloshina[2], and Yuriy S. Dedkov[3] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [3]SPECS Surface Nano Analysis GmbH, 13355 Berlin, Germany

Graphene nanoribbons and graphene dots have been proposed to exhibit such peculiar phenomena like localized edge states or edge magnetism. The aim of the present study is the investigation of structural and electronic properties of epitaxial graphene nanoflakes on the Au(111) surface.

Upon in situ preparation, we observe a formation of two types of nanoflakes, which are either embedded in the gold surface or sit directly on top of Au(111). In all cases, flakes reveal a moiré contrast, which is modulated by the herring-bone reconstruction of the Au(111) surface with the moiré period depending on the orientation of the graphene sheet in relation to the substrate. We show that quasi-free-standing graphene nanoflakes can be easily manipulated by the STM tip regardless of the flake size. The details of the structure and electronic properites of such quasi-free-standing flakes are discussed upon comparison with graphene dots on Ir(111).

## TT 57: Focused Session: Frontiers of Electronic Structure Theory 6 (jointly with HL and O)

Time: Thursday 10:30–13:15 Location: H36

**Topical Talk** TT 57.1 Thu 10:30 H36

**Atomic-scale design of energy materials** — •Karsten W. Jacobsen — CAMD, DTU Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The design of new materials for more efficient production and use of sustainable and clean energy is of utmost importance for the standard of living all over the World the coming years. In the talk I shall describe some computational efforts to design new materials related to solar energy in particular to the conversion of light into hydrogen fuel through water splitting. We have employed computational screening to search for stable semiconductor materials with an appropriate bandgap, band edge alignment, and with sufficient stability to be relevant for light-induced water splitting. In particular we have focused on materials in the cubic perovskite structure but also more generally materials in the ICSD database. The screening of bandgaps is performed using the so-called GLLB-functional which is shown to give reasonable estimates of light absorption for a number of different systems. The stability of the materials towards dissolution in water is investigated through the construction of Pourbaix diagrams combining DFT calculations and experimental information about solution energies.

The talk will also cover some recent efforts in using machine-learning techniques to develop new electronic density functionals. The functional construction uses Tikhonov regularization to obtain smooth functionals and employs bootstrapping to avoid overfitting. The new functionals are named Bayesian Error Estimation Functionals (BEEF) because they automatically offer error estimation on calculated results.

TT 57.2 Thu 11:00 H36

**A new computational screening approach for co-catalysts for water splitting:**
**Disentangling electron and proton transfer.** — •Harald Oberhofer, Daniel Berger, Ran Jia, and Karsten Reuter — TU München, Germany

Recently, computational screening techniques have made great progress in the identification and classification of promising new materials for (photo-)catalytic water splitting. Yet, contributions of so called co-catalysts—nano-sized particles enhancing the reaction kinetics—have so far not been addressed. In our contribution we present a novel first-principles thermodynamic approach based on earlier work by Nørskov and Rossmeisl [J. Phys. Chem. B **108**, 17886 (2004)] to gauge the efficiency of co-catalyst particles and search for favourable combinations of catalyst surface and co-catalyst particle. Additionally, we study reaction pathways other than the commonly assumed proton-coupled electron transfer. Our results show that these uncoupled paths can lead to new, unexpected behaviour: Catalysts predicted to have a good reactivity considering only coupled mechanisms might actually get stuck in charged intermediates, while others can be much more reactive than anticipated.

TT 57.3 Thu 11:15 H36

**An extended Pareto approach to computational materials design** — •Kurt Lejaeghere[1], Stefaan Cottenier[1,2], and Veronique Van Speybroeck[2] — [1]Center for Molecular Modeling, Ghent University, Zwijnaarde, Belgium — [2]Department of Materials Science and Engineering, Ghent University, Zwijnaarde, Belgium

Because of competing design criteria, it is often hard to decide on one particular material as the best solution for a given need. A multidimensional optimization strategy can already narrow down the initial large set of candidates to a much smaller number of promising materials, the Pareto-optimal set. Quite often, however, this set contains more materials than can be afforded for further systematic examination. An ordering within this set, highlighting the most promising candidates, would be very useful to expedite the design process. Conventional Pareto approaches cannot offer such a ranking. We present an algorithm to do exactly this.

This procedure is applied to a set of binary tungsten alloys to look for a candidate first-wall material for nuclear fusion purposes. Because of the harsh operating conditions inside (future) fusion reactors, materials selection is a critical aspect there. Tungsten is a promising first-wall material, but several issues, such as room-temperature brittleness, are still to be resolved. Alloying tungsten with other elements is one possible way of overcoming these problems. By combining a computational screening study (at the DFT-PBE level) with our ex-

tended Pareto analysis, a select number of alloys is presented as most promising candidates for further experimental investigation.

TT 57.4 Thu 11:30 H36

**Automated system for massive sets of first-principles calculations** — •Atsushi Togo and Isao Tanaka — Department of Materials Science and Engineering, Kyoto University, Yoshida-honmachi, Sakyo-ku, Kyoto, Japan

Large systematic sets of first principles calculations can provide information that cannot be obtained merely by a single calculation. Computation of phonon, cluster expansion, and data mining are typical examples that require massive sets of calculations. If each of single calculation is independent to the others, it is trivial to handle massive calculations consecutively. However it is annoying if a calculation has to wait for the previous calculations to finish. We have been developing an automated system. This system is composed of an automation algorithm and interfaces for a first-principles calculation code (VASP) and a batch-queuing system (grid engine). Small tools are prepared to handle crystal symmetry and dynamical properties. As an application, an algorithm for crystal structure search is implemented. The automation algorithm is as follows. We define 'task'. A task is made of 'task elements', where each task element is designed to be also a task. A task may be composed of a series of task elements. In this case, each task element waits for the previous task element to finish. A task may be composed of task elements that are mutually independent. In this case, all task elements are distributed into computers at the same time. By describing each kind of task in a similar manner, a task is easily built into the other task as a task element.

TT 57.5 Thu 11:45 H36

**Bandgap Engineering via Nanoporosity in ZnO** — Ilker Demiroglu[1], Sergio Tosoni[1], Francesc Illas[1], and •Stefan Bromley[1,2] — [1]Departament de Química Física and Institut de Química Teòrica i Computacional, Universitat de Barcelona (IQTCUB), 08028 Barcelona, Spain — [2]Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, Spain

Following previous studies [1-3], we have mined databases of 4-connected nets to generate novel nanoporous ZnO structures. Using density functional theory and GW calculations, we calculate the energetic stability and band gaps of >80 distinct nanoporous ZnO solids. We find that the degree and type of nanoporosity is inextricably linked with band gap magnitude. Increasing the degree of nanoporosity tends reduce energetic stability and increase the band gap. Within this tendency, we also find significant variations in band gap (˜0.5 eV) for structures with very similar densities or energetic stabilities but different types of nanoporosity (e.g. pore size). We estimate that altering the degree/type of nanoporosity could allow tailored band gap values up to ˜4.2 eV. This proposed nanomorphological approach to band gap engineering potentially opens the door to optoelectronically tunable sensors, solar cells and other unforeseen devices which could take advantage of this versatile combination.

[1] J. Carrasco, F. Illas and S. T. Bromley, PRL 99, 235502 (2007). [2] M. A. Zwijnenburg, F. Illas and S. T. Bromley, PRL 104, 175503 (2010). [3] D. Stradi, F. Illas, S. T. Bromley, PRL 105, 045901 (2010).

TT 57.6 Thu 12:00 H36

**Phonon-mediated quantum processes in materials** — •Emmanouil Kioupakis — University of Michigan, Ann Arbor, MI, USA

Higher-order quantum processes enabled by the coupling of charge carriers to lattice vibrations can play an important role in the operation of modern electronic and optoelectronic devices. First-principles calculations based on density functional theory can provide insight into the fundamental nature of phonon- assisted quantum processes in materials and their impact on device performance. In this talk, I will discuss our recent work on phonon-assisted quantum processes with first-principles techniques. I will show how phonon- assisted Auger recombination gives rise to the observed efficiency loss in nitride light-emitting diodes. Moreover, I will demonstrate that first-principles techniques can accurately reproduce the phonon-assisted optical absorption spectrum of silicon. Last, I will show that phonon-mediated free-carrier absorption leads to optical loss in transparent conducting oxides and semiconductor lasers. The developed techniques are general and can be applied to study phonon-assisted quantum processes in any material. This work was done in collaboration with C. G. Van de Walle, P. Rinke, K. Delaney, A. Schleife, F. Bechstedt, D. Steiauf, H. Peelaers, J. Noffsinger, S. G. Louie, and M. L. Cohen.

TT 57.7 Thu 12:15 H36

**Electron-hole puddles in the absence of charged impurities** — •Marco Gibertini[1,2], Andrea Tomadin[2], Francisco Guinea[3], Mikhail I. Katsnelson[4], and Marco Polini[2] — [1]Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland — [2]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy — [3]Instituto de Ciencia de Materiales de Madrid (CSIC), Sor Juana Inés de la Cruz 3, E-28049 Madrid, Spain — [4]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands

It is widely believed that carrier-density inhomogeneities ("electron-hole puddles") in single-layer graphene on a substrate such as quartz are due to charged impurities located close to the graphene sheet. In this talk we demonstrate by using a Kohn-Sham-Dirac density-functional scheme that corrugations in a real sample are sufficient to determine electron-hole puddles on length scales that are larger than the spatial resolution of state-of-the-art scanning tunneling microscopy.

TT 57.8 Thu 12:30 H36

**Ab-initio transport calculations of functionalized graphene flakes** — •Michael Walz, Alexei Bagrets, and Ferdinand Evers — Institut für Nanotechnologie, Karlsruher Institut für Technologie (KIT), D-76021 Karlsruhe, Germany

These days, nanoelectronics is focused on molecular systems such as single organic molecules, graphene ribbons, functionalized graphene flakes, carbon nanotubes.

In our project, we calculate the transmission and the local current density in graphene flakes which are functionalized by adsorbed atoms. We are especially interested in current patterns associated with the functionalized carbon atoms and the role of quantum interference effects.

Performing such calculations starting from first principles is challenging because of high computational costs. On this account, we work with the parallelized *ab-initio* framework FHI-aims, on top of which we implement our own transport calculations using non-equilibrium Green's functions (NEGF) techniques with standard functionals [1,2]. Such *ab-initio* transport studies already exist for the field of Molecular Electronics. Our effort presents a first step towards the broader scope of meso-sized molecular materials in general.

[1] V. Blum *et al.*, Comput. Phys. Commun. **180**, 2175 (2009).
[2] A. Arnold *et al.*, J. Chem. Phys. **126**, 174101 (2007).

TT 57.9 Thu 12:45 H36

**Thermionic emission from metal surfaces: A first principles study** — •Johannes Voss[1], Sharon Chou[1], Aleksandra Vojvodic[1,2], Igor Bargatin[3], Roger Thomas Howe[1], and Frank Abild-Pedersen[2] — [1]Stanford University, USA — [2]SLAC National Accelerator Laboratory, USA — [3]University of Pennsylvania, USA

The ability to lower the temperatures required for sufficient electronic emission from hot cathodes would lead to more efficient thermionic energy converters and electron guns. Thermionic emission of electrons from metal surfaces is governed by the work function and tunneling probabilities. While the former can be extracted easily from ab initio band structure calculations, for the latter, scattering properties of the surface need to be taken into account.

Here, we present density functional theory calculations of thermionic emission currents based on a non-equilibrium Green's function approach. We compare these results to experiments both for clean and coated metal surfaces. Based on an analysis of interactions in the coating layers, we suggest design pathways for new materials with higher emission current densities.

TT 57.10 Thu 13:00 H36

**Comparative computational study of Li, Na, and Mg diffusion in bulk Si: influence of cooperative effects, vibrations, and atom-centered bases** — •Sergei Manzhos[1], Oleksandr Malyi[1], and Teck L. Tan[2] — [1]Department of Mechanical Engineering, National University of Singapore, Blk EA #07-08, 9 Engineering Drive 1, Singapore 117576 — [2]Institute of High Performance Computing, A*STAR, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632

Si is one of the most efficient anode materials for Li ion batteries. At the same time, for bulk storage and/or high energy density applications, Na and Mg are advantageous due to low cost and abundance of Na and high energy density in the case of Mg. Yet the performance of Si as anode material for Na and Mg batteries is still understudied. We present a comprehensive computational study of diffusion barri-

ers of Li, Na, and Mg in Si including cooperative effects (influence of neighboring metal atoms on the barrier). Interactions between metal atoms in Si cause a significant lowering of the diffusion barrier; this effect is increasing when going from Li to Na to Mg. Zero-point vibrations (ZPE) affect migration barriers strongly and differently for different metals, increasing the barrier for Li diffusion, having little effect on Na, and decreasing the barrier for Mg. Most calculations to date for metal ion diffusion in battery electrodes were done using plane-wave based codes. We present an analysis of the effects due to atomic-centered basis selection. To the best of our knowledge, this is the first study of the effects of ZPE and atomic-centered bases on the computed properties of battery electrodes.

## TT 58: Poster Session Transport & Matter at Low Temperature

Time: Thursday 15:00–19:00 Location: Poster D

TT 58.1 Thu 15:00 Poster D

**Weak localization and magnetoresistance in a two-leg ladder model** — •Michael P. Schneider[1,2], Sam T. Carr[2], Igor V. Gornyi[2], and Alexander D. Mirlin[2] — [1]Max-Born-Institut, 12489 Berlin, Germany — [2]Institut für Theorie der Kondensierten Materie and DFG Center for Functional Nanostructures, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany

We analyze the weak-localization correction to the conductivity of a spinless two-leg ladder model in the limit of strong dephasing $\tau_\phi \ll \tau_{tr}$, paying particular attention to the presence of a magnetic field, which leads to an unconventional magnetoresistance behavior. We find that the magnetic field leads to three different effects: (i) negative magnetoresistance due to the regular weak-localization correction, (ii) effective decoupling of the two chains, leading to positive magnetoresistance, and (iii) oscillations in the magnetoresistance originating from the nature of the low-energy collective excitations. All three effects can be observed depending on the parameter range, but it turns out that large magnetic fields always decouple the chains and thus lead to the curious effect of magnetic-field-enhanced localization [1].

[1] M. P. Schneider, S. T. Carr, I. V. Gornyi and A. D. Mirlin, Phys. Rev. B **86**, 155141 (2012)

TT 58.2 Thu 15:00 Poster D

**Majorana fermions in systems with coexisting density waves and superconductivity** — •Daniel Mendler, Panagiotis Kotetes, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

The recent discovery of topological materials such as HgTe/CdTe quantum wells and Bi-based compounds has motivated the systematic study of topological phases. Among the ten possible topological classes, we find cases in which topological systems admit Majorana bound state solutions which could be used as building blocks for topological quantum computing. In this work, we focus on strongly correlated systems that can exhibit conventional or unconventional density waves and superconductivity. We perform an exhaustive study of the possible phases by inferring their point group symmetry and topological class, in order to identify which of them can support Majorana fermions. Our results can be applied to the hexagonally warped Dirac modes living on a surface of the 3D topological insulator $Bi_2Te_3$, that demonstrates enhanced tendency towards spin density wave instabilities. Superconductivity can also emerge in this system due to correlations or proximity effects. We focus on heterostructures consisting of a superconducting wire on top of a $Bi_2Te_3$ surface and investigate the conditions under which Majorana bound states are accessible.

TT 58.3 Thu 15:00 Poster D

**Majorana modes and localization in a disorderd Kitaev model** — •Hanno Schmiedt, Lars Fritz, and Alexander Altland — Institut für theoretische Physik, Universität zu Köln, Deutschland

The periodic table of topological insulators and superconductors makes predictions about the localization properties as well as the absence or presence of gapless edge modes of systems having a certain type of symmetry. In one dimension it has been established that systems in class D exhibit protected Majorana edge modes. A microscopic realization of this system was introduced by Kitaev in terms of a simple one dimensional tight binding model. Using this lattice model we study (i) the robustness of the Majorana edge modes upon including disorder and increasing the number of parallel channels by computing the topological invariant as well as (ii) the existence or absence of extended zero energy states from the inverse participation ratio.

TT 58.4 Thu 15:00 Poster D

**Spectral properties of disordered multi-channel Majorana wires** — •Patrick Neven, Dmitry Bagrets, and Alexander Altland — Institut für Theoretische Physik, Universität zu Köln, Köln, Germany

Proximity coupled multi-channel spin-orbit quantum wires may support midgap Majorana states at the ends. We study the fate of these Majorana fermions in the presence of disorder in such wires. Inspired by the widely established theoretical methods of mesoscopic superconductivity, we develop a quasiclassical approach which is valid in the limit of strong spin-orbit coupling. A numerical solution of the Eilenberger equation reveals that disordered topological wires are prone to the formation of a zero-energy anomaly (class D impurity spectral peak) in the local density of states which shares the key features of a Majorana peak. We also find that the $\mathbb{Z}_2$ topological invariant distinguishing between the state with and without Majorana fermions (symmetry class B and D, resp.) is related to the Pfaffians of quasiclassical Green's functions.

TT 58.5 Thu 15:00 Poster D

**Energy-charge separation in an electronic interferometer with two-particle collision** — •Guillem Rosselló[1], Mikhail Moskalets[2], and Janine Splettstoesser[1] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen, Germany — [2]Department of Metal and Semic. Physics, NTU "Kharkiv Polytechnical Institute", Ukraine

Quantum wave experiments with electrons were recently reported in mesoscopic devices in the quantum Hall regime, with quantum point contacts as beam splitters and unidirectional edge states as waveguides. They resemble quantum optics experiments but are based on fermions instead of bosons. An important further ingredient is a recently developed single-particle source [1], which permits to inject single particles in a controllable manner into an electronic circuit. This allows to address single-particle coherence properties as well as controlled two-particle exchange effects occurring as "collisions" between particles. On this poster a setup consisting of a Mach-Zehnder interferometer and two synchronized sources is presented, in which collisions of particles strongly influence - and in certain cases even suppress - the single-particle interference pattern [2]. In particular, the signatures occurring in the heat current and the noise are theoretically investigated, complementing the features occurring in the charge current. This study yields further insight into the particle-emission process and the impact of collisions on which-path information.

[1] G. Fève, et al., Science 316, 1169 (2007)
[2] S. Juergens, J. Splettstoesser, and M. Moskalets, EPL 96, 37011 (2011)

TT 58.6 Thu 15:00 Poster D

**Measurement back-action on the dynamics of an interacting quantum dot** — •Jens Schulenborg[1], L.Debora Contreras-Pulido[2], Janine Splettstoesser[1], and Michele Governale[3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [2]Institute of Theoretical Physics, Ulm University, Germany — [3]School of Physical and Chemical Sciences, Victoria University of Wellington, New Zealand

Due to potential applications in nanoelectronics, metrology and quantum information, the study of the *dynamics* of quantum dots has attracted great interest over the past years. Recently, the relaxation rates in the dynamical response of an interacting single-level quantum dot, weakly tunnel coupled to an electronic reservoir and initially brought out of equilibrium, have been investigated [1]. The theoretical study presented on this poster focuses on the readout of the dynamic response of the quantum dot, capacitively coupled to a measuring device. In particular, the influence of measurement back-action effects on the dot's time-evolution is addressed. Starting from a master equa-

tion approach for the quantum dot coupled to the measuring device, the relaxation behavior of the dot (influenced by the measurement) is extracted. The result shows that the back-action of the measurement leads to a significant modification of the dot's relaxation rate for gate voltages close to the electron-hole symmetric point. On top of that, an additional rate governs the time-evolution of the quantum dot, which is closely related to the characteristics of the measuring device.

[1] L. D. Contreras-Pulido et al., Phys. Rev. B **85**, 075301 (2012).

TT 58.7 Thu 15:00 Poster D

**Mechanical characterization of single electron charging in a quantum dot in the Kondo regime** — •Daniel Schmid, Alois Dirnaichner, Peter Stiller, Christoph Strunk, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Detection of the transversal mechanical resonance frequency of a suspended, doubly clamped carbon nanotube resonator can be used to infer changes in the time-averaged charge on the embedded quantum dot at cryogenic temperatures. This method is applied to the case of strong Kondo correlations between the quantum dot and its leads; we observe and model single electron charging as function of the applied gate voltage in a highly regular transport spectrum. Good agreement with theoretical predictions and previous observations in literature in GaAs is observed.

TT 58.8 Thu 15:00 Poster D

**Lab::Measurement — Measurement control and automation with Perl** — Alois Dirnaichner[1], Hermann Kraus[1], Stefan Geissler[1], Christian Butschkow[1], David Kalok[2], Florian Olbrich[1], and •Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, 76100 Rehovot, Israel

For quickly setting up varying and evolving complex measurement tasks involving diverse hardware, graphical logic programming quickly reaches practical limits. We present *Lab::Measurement*, a collection of Perl modules designed to control instruments connected by as various means as GPIB, USB, serial cable, Oxford Instruments IsoBus, or ethernet. Internally, backends as e.g. Linux-GPIB or National Instruments' NI-VISA library are used as well as direct operating system calls. Dedicated instrument driver classes relieve the user from taking care of internal details. Recording a measurement trace, say $I(V_{sd})$, becomes as easy as programming a single for-loop, and much more complex setups can be implemented. At the same time, the modules provide (live) plotting and metadata handling. For simple applications, a graphical control front end is being developed. *Lab::Measurement* has already been successfully used in several low temperature transport spectroscopy setups. It is free software and available at `http://www.labmeasurement.de/`

TT 58.9 Thu 15:00 Poster D

**kwant - A computer program for quantum transport** — Anton Akhmerov[1], Christoph Groth[2], Xavier Waintal[2], and •Michael Wimmer[3] — [1]Harvard University, USA — [2]CEA Grenoble, France — [3]Instituut-Lorentz, Universiteit Leiden, The Netherlands

We discuss methods for computing various quantum transport properties in tight-binding systems. We discuss both Green's function and wave function based methods, and how to implement them in a numerically stable way. In addition, we also discuss practical issues such as convenient data structures for defining the transport problem in a computer program. These algorithms and data structures are implemented in an easy to use, open source python package - kwant.

TT 58.10 Thu 15:00 Poster D

**Fabrication of Au atomic sized contacts and conductivity measurements** — •Karthiga Kanthasamy, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany

Mechanically controllable break junctions offers an inherent stability and repeatability to contact a single atom and measure its electrical properties. We describe the fabrication of Au contacts on thin silicon substrate. Shadow mask technique, Electron Beam lithography and Thermal evaporation are used to fabricate Au contacts. The undercut is done by Reactive Ion Etching and Chemical Etching. The comparison of electrical conductance on Silicon substrate with different etching methods are discussed. Stepwise changes in the conductance measurements are observed for both room and low temperature and conductance histogram graph is studied.

TT 58.11 Thu 15:00 Poster D

**Quantum-point contact based charge read-out for the InAs nanowire tip of a scanning tunneling microscope** — •Sebastian Wüsten[1], Kilian Flöhr[1], Eugen Kaganovitch[1], Nils Freitag[1], Kamil Sladek[2], Mihail Lepsa[2], Hilde Hardtdegen[2], Marcus Liebmann[1], Thomas Schäpers[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut, RWTH Aachen and JARA-FIT, 52074 Aachen, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich and JARA-FIT, 52425 Jülich, Germany

Proximal on-chip read-out of the current of a scanning tunneling microscope (STM) could improve low-current operation of the STM dramatically down to the detection of single tunneling electrons. Recently, we have demonstrated that InAs nanowires work as semiconducting tips for STM providing atomic resolution [1]. The wires grown by metal-organic vapor phase epitaxy (MOVPE) without catalysts are picked up individually with a sharp indium tip exploiting adhesion forces and subsequently, placed on the edge of a GaAs wafer [2]. Further on, this process creates the possibility of circuitry on the wafer, i.e. within $1\mu m$ from the tip apex. As a first step in that direction, we used a quantum point contact (QPC) processed into an AlGaAs/GaAs heterostructure [3]. Different QPC shapes are characterized by low-temperature (>0.3 K) transport measurements with respect to the nanowire read-out.

[1] K. Flöhr, K. Sladek, H. Y. Günel, M. I. Lepsa, H. Hardtdegen, M. Liebmann, Th. Schäpers, M. Morgenstern, Apl. Phys. Lett., accepted (2012)
[2] K. Flöhr et al., Rev. Sci. Instrum. 82, 113705 (2011)
[3] I. Shorubalko et al., Nano Lett. 8, 382 - 385 (2008)

TT 58.12 Thu 15:00 Poster D

**Non-equilibrium quantum dynamics of the magnetic Anderson model** — •Daniel Becker[1,2], Stephan Weiss[3], Michael Thorwart[1], and Daniela Pfannkuche[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg — [2]Department Physik, Universität Basel, 4056 Basel, Schweiz — [3]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

For a Coulomb-interacting single-level quantum dot in contact with two metallic leads and a spin-1/2 magnetic impurity, which is exchange-coupled to the electron spin, a systematical investigation of the mutual dependencies between charge current and impurity relaxation dynamics is provided. To this end, the numerically exact, non-perturbative scheme of iterative summation of path integrals (ISPI)[1] is employed in a regime, where all appearing energy scales are of the same order of magnitude. We observe a significant influence of the non-equilibrium decay of the impurity spin polarization both in the presence and absence of Coulomb interaction. The exponential relaxation is faster for larger bias voltages, electron-impurity interactions and temperatures. Conversely, we find a reduction of the stationary current for increasing coupling to the impurity. Moreover, our approach allows us to systematically distinguish mean-field Coulomb and impurity effects from the influence of quantum fluctuations and flip-flop scattering, respectively. In fact, we find a local maximum of the current for a finite Coulomb interaction due to the presence of the impurity.

[1] D. Becker et al., NJP **14**, 073049 (2012)

TT 58.13 Thu 15:00 Poster D

**Joule heating and current-density profiles during electromigration controled gap formation in nanostructures** — •Birgit Kiessig[1,2], Roland Schäfer[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

For molecular electronics gaps between metallic electrodes not larger than a few nm are needed. However, the structuring of such gaps is still a challenging task. One route towards reliable nanogaps utilizes electromigration which is reported to yield extremely small gaps if current and resistance is carefully monitored during the process. Electromigation leads to a continuous thinning out of metallic nanowires at sufficiently large current densities. The main driving force is the so called electron wind, e.g. the momentum transfer from the direc-

tional flow of conduction electrons to the atomic cores and the resulting displacement of the latter. However, electromigation depends on elevation of temperature due to Joules heating as well. We present our own experience with so called feedback controlled electromigration and discuss the influence of sample geometry and substrate texture on current-density and temperature profiles.

TT 58.14 Thu 15:00 Poster D

**Transport through capacitively coupled carbon nanotube bundles.** — Birgit Kiessig[1,2], •Roland Schäfer[1], Cornelius Thiele[1,3], Ralph Krupke[1,3], 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 Nanotechnologie, 76021 Karlsruhe

We have investigated transport through single walled carbon nanotubes deposited by AC electrophoresis at low temperatures. The samples comprise source and drain electrodes as well as two independent gates. Measurements of current as function of the gate voltages give evidence that transport is due to a bundle of a few tubes which open up several parallel conductance channels. We present a sequential tunneling model in which three quantum dots are connected in parallel to source and drain. Including capacitive coupling between the dots leads to transport characteristics which are in qualitative accord with our measurements.

TT 58.15 Thu 15:00 Poster D

**Anomalous Hall effect in $Mn_5Si_3$ and $Mn_5Si_3C_{0.8}$ films** — Patrick Winkel[1], •Christoph Sürgers[1], Gerda Fischer[1], Inga A. Fischer[2], and Hilbert v. Löhneysen[1,3] — [1]Physikalisches Institut, KIT, Karlsruhe — [2]Institut für Halbleitertechnik, Universität Stuttgart — [3]Institut für Festkörperphysik, KIT, Karlsruhe

Antiferromagnetic $Mn_5Si_3$ ($T_N$ = 100 K) can be tuned ferromagnetically by incorporation of carbon [1]. The highest Curie temperature is observed for $Mn_5Si_3C_{0.8}$ with $T_C$ = 350 K. We investigate the magnetoresistance and Hall effect of 45-nm thick films for temperatures $T = 2 - 400$ K and magnetic fields up to 8 T. For each temperature, the different contributions to the Hall conductivity, $\sigma^0_{xy}$ and $\sigma^{AH}_{xy}$, arising from the ordinary and anomalous Hall effect, respectively, are separated by taking into account the temperature dependence of the magnetoresistance and magnetization $M$.

For ferromagnetic $Mn_5Si_3C_{0.8}$, we find a positive ordinary Hall coefficient and a linear behaviour $\sigma^{AH}_{xy} \propto M$ similar to the isotructural ferromagnet $Mn_5Ge_3$ [2]. In contrast, a negative ordinary Hall coefficient and a nonlinear behaviour of $\sigma^{AH}_{xy}(M)$ is observed for antiferromagnetic $Mn_5Si_3$. While the negative $\sigma^0_{xy}$ is attributed to the change of the electronic structure induced by carbon [3] the nonlinear $\sigma^{AH}_{xy}(M)$ awaits theoretical calculations of the anomalous Hall effect in antiferromagnetic compounds.

[1] C. Sürgers et al., Appl. Phys. Lett. **93**, 062503 (2008)
[2] C. Zeng et al., Phys. Rev. Lett. **96**, 037204 (2006)
[3] I. Slipukhina et al., Appl. Phys. Lett. **94**, 192505 (2009)

TT 58.16 Thu 15:00 Poster D

**Electronic and magnetic properties of NiMnSb/MgO and NiMnSi/MgO interfaces** — •Rui-Jing Zhang[1], Ulrich Eckern[1], and Udo Schwingenschlögl[2] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

The electronic and magnetic properties of the interfaces between the half-metallic Heusler alloys NiMnSb and NiMnSi, and MgO have been investigated using first-principles density-functional calculations with projector augmented wave (PAW) potentials generated with Generalized Gradient Approximation. In all the cases of NiMnSb/MgO(100) and NiMnSb(Si)/MgO(111), the half-metallicity is lost. However, the MnSb/MgO-terminated interface in the NiMnSb/MgO(100) contact keeps a high degree of spin polarization at the Fermi level, which can be up to 77%. The (111) interfaces show a spin polarization at the Fermi level of around 52% at most for NiMnSb/MgO with Sb/O termination, which has more potential in real applications than NiMnSi/MgO(111) with Si/O termination (36% spin polarization).

TT 58.17 Thu 15:00 Poster D

**Rashba spin-orbit interaction in graphene armchair nanoribbons** — Lucia Lenz[1], Daniel F. Urban[2,3], and •Dario Bercioux[1,4] — [1]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [3]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany — [4]Department of Physics, Stanford University, Stanford, California 94305, USA

We study graphene nanoribbons (GNRs) with armchair edges in the presence of Rashba spin-orbit interaction (RSOI). We impose the boundary conditions on the tight binding Hamiltonian for bulk graphene with RSOI by means of a sine transform and use the results to derive different approximations and to investigate their ranges of validity. In addition, we derive an approximation for the lowest two energy bands, which is valid for experimentally available sizes of RSOI. Finally, we address the effect of RSOI on the spin polarization in GNRs. We show that the spin polarization perpendicular to the nanoribbon axis changes sign when reversing the momentum along the GNR. This effect arises from the coupling of the modes induced by RSOI.

[1] L. Lenz, D.F. Urban, D. Bercioux, arXiv:1210.2865.

TT 58.18 Thu 15:00 Poster D

**Spin-resolved scattering in bilayer graphene** — •Linnéa Schätzle and Dario Bercioux — Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, D-79104 Freiburg, Germany

Bilayer graphene in contrast to single layer graphene has a tunable bandgap. This makes it a promising material for a novel kind of field effect transistors. Electrons in bilayer graphene have high mobilities and long spin-relaxtion-lengths that makes it interesting for electronic applications [1].

We are interested in spin-resolved scattering through regions of inhomogeneous spin-orbit interactions. The spin-resolved scattering properties, for the case of single layer graphene with these spin-orbit barriers, are a function of the incident angle [2]. We show that the more complex band structure of bilayer graphene leads to similar results. These can be useful for the implementation of carbon-based spintronics devices.

[1] T.- Y. Yang *et al.*, PRL **107**, 047206 (2011)
[2] D. Bercioux and A. de Martino, Phys. Rev. B **81**, 165410 (2010)

TT 58.19 Thu 15:00 Poster D

**Electronic structure and transport properties of crossed carbon nanotubes** — •Fabian Teichert[1], Andreas Zienert[1], and Jörg Schuster[2] — [1]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

According to their geometric structure carbon nanotubes (CNT) have different electronic properties. The metallic ones could be used for interconnects in future microelectronic devices. During experimental preparation CNTs can not be placed isolated. They get curved and form bundles. Therefore it is necessary to study the interaction of closely neighboring CNTs and its influence on the electronic and transport properties.

In the present work the attention is focused on a special geometry, where two (4,1)-CNTs (one curved and one linear) are aligned at a minimum distance of 3 Å. For this system electron densities, densities of states and transmission spectra are obtained from ab initio simulations. To get the current-voltage characteristic $I(U)$, transmission spectra are calculated for non-zero voltages by the use of non-equilibrium Green's function theory and integrated within the Landauer-Büttiker formalism. All calculations are performed for various angles $\alpha$ between the periodic axes of the two CNTs so that the influences of the crossing and curving effects could be extracted separately. The simulations show that the behavior of $I(U)$ changes with increasing $\alpha$. Furthermore, the reduction of the current with respect to a linear CNT is dominated by the crossing effect for small $\alpha$ and by the curving effect for large $\alpha$.

TT 58.20 Thu 15:00 Poster D

**Model study of vibrationally dependent electron-electron interactions in single-molecule junctions** — •André Erpenbeck[1], Rainer Härtle[1,2], Michel Bockstedte[1], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen- Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Department of Physics, Columbia University, 538 W. 120th St., New York, NY 10027, USA

In a single molecule junction, the interaction of the electrons with the vibrational degrees of freedom gives rise to direct electronic-vibrational

coupling, but results also in vibrationally dependent electron-electron interactions. We derive a general, reduced model that incorporates vibrationally dependent electron-electron interactions and show that it leads to an effective electronic-vibrational coupling, which depends on the population of the electronic states of the molecular bridge. Employing a Born-Markov master equation approach, the influence of the interactions on the transport characteristics is analyzed. In particular, we show that vibrationally dependent electron-electron interactions may result in regimes of purely electronic transport, negative differential resistance, a significant decrease of the vibrational excitation as well as characteristic asymmetries in the gate-voltage dependence of the conductance properties of a molecular contact.

TT 58.21 Thu 15:00 Poster D

**Electrical characterization of single organic molecules via mechanically controllable break junctions** — •Torsten Sendler[1], Matthias Wieser[1], Shou-Peng Liu[2], Samuel Weisbrod[2], Zhou Tang[2], Andreas Marx[2], Jannic Wolf[2], Thomas Kuhn[2], Elke Scheer[2], Francesca Morecso[3], Jochen Grebing[1], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Universität Konstanz, Germany — [3]Max Bergmann Center of Biomaterials, Germany

Molecular electronics has been of big interest for the last years. To allow an electrical characterization of single molecules a reliable contact to gold atoms is required. We ensure this by using single organic molecules with a plain structure, in particular 1,4-Diethoxy-2,5-bis (4-sulfanyl-phenylethynyl)-benzene and single stranded DNA fragments, dissolved in an organic non-polar solvent. For measurements we use the technique of mechanically controllable break junctions. IV-curves taken from single molecules connected to single gold atom contacts show the expected tunneling behavior, from which we gain the energy of the molecular level and the coupling between electrode and molecule.

TT 58.22 Thu 15:00 Poster D

**Combining master-equation and DFT for simulating STM images of single molecules: An ab-initio approach for the coupling-strength** — •Tim Ludwig[1], Carsten Timm[1], Torsten Hahn[2], and Jens Kortus[2] — [1]U Dresden, Dresden, Germany — [2]TU Freiberg, Freiberg, Germany

The power of STM imaging of single molecules lies in the spatial resolution and a well-defined contact with highly controllable contact strength. Traditional methods for simulating STM images, e.g., DFT + Tersoff-Hamann, combine a static single-particle density-of-states description of the scanned object with more or less artificial models for the tunneling amplitude between the object and the contacts. This can be inappropriate for the investigation of single molecules, as for example Coulomb blockade may occur. We propose a new *ab-initio* algorithm for the calculation of the tunneling amplitudes. Together with a master-equation approach, which models the full many-body dynamics of the scanned object, both limitations can be overcome.

TT 58.23 Thu 15:00 Poster D

**Insertable $^4$He sample probe for combined microwave and dc electrical transport measurements** — •Oleksandr V. Dobrovolskiy[1,2], Jörg Franke[1], and Michael Huth[1] — [1]Physikalisches Institut Goethe-Universität, Frankfurt am Main, Germany — [2]Department of Physics, Kharkiv National University, Ukraine

Combined microwave and dc electrical transport measurements at low temperatures represent a valuable experimental method in many research areas. In particular, when samples are conventional superconductors, a typical experiment requires a combination of helium temperatures, a wide range of magnetic fields, and the utilization of coaxial lines along with the usual dc wiring. We report on the general design features and the microwave performance of a home-made low-temperature sample probe, with a measurement bandwidth tested from dc to 20 GHz. Equipped with 6 coaxial cables, a heater, Hall and temperature sensors, the probe fits into a ⌀32 mm shaft. We present our setup, describe the calibration procedures, and give examples of experiments enabled by this system. The proposed setup will be essential for a systematic study of the dc- and ac-response of the vortex dynamics in nanopatterned superconductors subjected to combined dc and microwave stimuli. Besides, it will be valuable for the investigation of a broad class of nonlinear stochastic systems where a combination of dc and high-frequency ac driving in a wide temperature range is necessary.

TT 58.24 Thu 15:00 Poster D

**Negative frequency tuning of a carbon nanotube nanomechanical resonator** — Sabine Kugler, Daniel Schmid, •Peter Stiller, Christoph Strunk, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

The transversal mechanical resonance frequency of a suspended carbon nanotube doubly clamped at its contact points can be tuned with an externally applied gate voltage. In a simple picture, the electrostatic force between the gate and the resonator applies mechanical tension, increasing the resonance frequency at finite voltage. We present data on an unusual resonator where application of a back gate voltage leads to a strong detuning of the mechanical resonance towards *lower* frequencies; we observe a decrease of approximately 30%. Tentative models for this effect are discussed.

TT 58.25 Thu 15:00 Poster D

**Stabilizing Superconducting Qubits by Coupling To A Cavity** — •Christos Bokas and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm

We consider a superconducting qubit capacitively coupled with a one-dimensional cavity. This system can be mapped to a model consisting of a quantum mechanical harmonic oscillator interacting with a two level system.The unavoidable influence of the environment causes the qubit to loose its coherence. Here, we focus on whether and under which conditions, the stability of qubit's states can benefit from being entangled with resonator states. We identify parameters relevant for the experimental realisation, in order to determine the optimal range in which stabilizing takes place. The total system is analyzed in the context of the Jaynes-Cummings-Model, both by applying a RWA and without any approximation.

TT 58.26 Thu 15:00 Poster D

**High cooperativity in a microwave resonator coupled to YIG** — H. Huebl[1], •J. Lotze[1], C. Zollitsch[1,2], F. Hocke[1], S. T. B. Goennenwein[1], and R. Gross[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany

Understanding the coupling of magnetic moments (spins) to light fields (photons) on a quantum level is of fundamental interest. Recent work [1,2] on paramagnetic samples coupled to superconducting resonators has shown coherent coupling between microwave photons and electron spins. This coupling is enhanced compared to a single spin by a factor of $\sqrt{N}$, where $N$ is the number of spins in the ensemble. Here [3], we study a bulk ferrimagnetic Ga-doped yttrium iron garnet (YIG) crystal coupled to a superconducting niobium coplanar waveguide resonator operating at 5.9 GHz. Measuring the transmission through the resonator in a magnetic field $H$, we observe an anticrossing of the spin and photon dispersions with a splitting of 900 MHz. From the $H$ dependence of the resonance linewidths in the interaction regime, we find that the coupling clearly dominates the intrinsic loss rates of the exchange-locked spins and the resonator, with a cooperativity $C = 1350$. This system is therefore well suited for studying the magnon-photon interaction in the strong coupling regime. This work is supported by DFG via SFB 631 and the German Excellence Initiative via NIM.

[1] D. I. Schuster *et al.*, Phys. Rev. Lett. **105**, 140501 (2010)
[2] Y. Kubo *et al.*, Phys. Rev. Lett. **105**, 140502 (2010)
[3] H. Huebl *et al.*, arXiv:1207.6039 (2012)

TT 58.27 Thu 15:00 Poster D

**Scalable chains of coupled superconducting transmission line resonators** — •Ling Zhong[1,2], Lisa Janker[2], Friedrich Wulschner[1,2], Frank Deppe[1,2], Edwin Menzel[1,2], Max Haeberlein[1,2], Alexander Baust[1,2], Elisabeth Hoffmann[1,2], Jan Goetz[1,2], Manuel Schwarz[1,2], Achim Marx[1,2], and Rudolf Gross[1,2] — [1]Walther-Meißner-Institut, D-85748 Garching, Germany — [2]Technische Universität München, D-85748 Garching, Germany

The investigation of many-body Hamitonians is relevant to understand collective quantum behavior in solid state physics. However, solving these many-body Hamitonians can be challenging on a classical computer. For this reason, quantum simulations are an attractive approach to simulate such complex Hamitonians with experimentally easily accessible and well-controlled systems. In our experiment, we use superconducting circuits to take the first steps towards this direction. More precisely, we characterize chains of up to four coupled transmission line

resonators in a scalable layout. After introducing nonlinearities in the form of Josephson junctions and scaling to longer chains, our system can become a quantum simulator for Bose-Hubbard-type Hamitonians.

This work is supported by DFG via SFB 631, the German Excellence Initiative via NIM, as well as EU projects CCQED and PROMISCE.

TT 58.28 Thu 15:00 Poster D

**From strong to ultrastrong coupling in Circuit QED** — •A. Baust[1,2], T. Losinger[2], M. Haeberlein[1,2], E. Hoffmann[1,2], P. Eder[1,2], J. Goetz[1,2], F. Loacker[2], E.P. Menzel[1,2], M.J. Schwarz[1,2], F. Wulschner[1,2], L. Zhong[1,2], F. Deppe[1,2], H. Huebl[1,2], A. Marx[1,2], and R. Gross[1,2] — [1]Walther-Meißner-Institut, Germany — [2]TU München, Garching

In circuit quantum electrodynamics, the light-matter coupling strength can be tuned over several orders of magnitude and can even be increased to a significant fraction of the system energy. For a flux qubit coupled to a transmission line resonator, we have reached the regime of ultrastrong light-matter interaction and show experimental evidence for the breakdown of the Jaynes-Cummings-model [1]. We present spectroscopic measurements for different coupling schemes of flux qubits and transmission line resonators and discuss the possibility to further increase the coupling strength and reach the regime of deep-ultrastrong coupling. For a complete characterization of our qubits we also perform time-domain spectroscopy measurements in order to determine the coherence times of our qubits.

This work is supported by DFG via SFB 631, the German Excellence Initiative via NIM, as well as EU projects CCQED and PROMISCE.

[1] T. Niemczyk et al., Nature Phys. 6, 772-776 (2010)

TT 58.29 Thu 15:00 Poster D

**Hysteresis effects in superconducting resonators** — •Philipp Mayer[1], Fengbin Song[1], Martin Weides[1], Hannes Rotzinger[1], Michael Stüber[2], Harald Leiste[2], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Center for Functional Nanostructures — [2]Angewandte Werkstoffphysik, Karlsruher Institut für Technologie

Superconducting microwave resonators are of considerable interest for quantum circuits. They can be used for many applications in circuit quantum electrodynamics, for example as a readout tool for qubits, a quantum bus or a coupling to spins in crystals. For these purposes, it is important to understand the behavior of superconducting resonators in magnetic fields. Previous studies on resonators made of Nb have shown a hysteretic dependence of quality factor and resonance frequency on applied magnetic field. High quality microwave resonators are made of TiN and can have high internal quality factors in the order of $10^7$ at high and $10^6$ at low photon numbers. Furthermore they were shown to have a large kinetic inductance. In this work, 40 nm thin films of TiN were sputtered on intrinsic Si wafers. The films were patterned by reactive ion etching into resonators of $\frac{\lambda}{2}$, $\frac{\lambda}{4}$ and lumped LC geometry. We investigated their hysteretic behavior in out-of-plane magnetic fields at temperatures ranging from 275 mK up to 1K in both the many photon and single photon limit. We will present and discuss results of our on-going experiments.

TT 58.30 Thu 15:00 Poster D

**Probing the TLS Density of States in Thin a-SiO Films using Superconducting Lumped Element Resonators** — •Sebastian T. Skacel[1,2], Christoph Kaiser[2], Stefan Wünsch[2,3], Hannes Rotzinger[1], Oleksandr Lukashenko[1], Markus Jerger[1], Georg Weiss[1,3], Michael Siegel[2,3], and Alexey V. Ustinov[1,3] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Wolfgang-Gaede-Straße 1, D-76131 Karlsruhe, Germany — [2]Institut für Mikro- und Nanoelektronische Systeme, Karlsruher Institut für Technologie, Hertzstraße 16, D-76187 Karlsruhe, Germany — [3]Center for Functional Nanostructures, Karlsruher Institut für Technologie, Wolfgang-Gaede-Straße 1a, D-76128 Karlsruhe, Germany

In the context of low-loss materials needed for superconducting qubits, we investigated the dielectric loss in the volume of a-SiO thin films at mK temperatures and single photon power levels. Our broadband measurement setup employs multiplexed lumped element resonators as well as suitable power combiner and low noise amplifier. This enables measurements on all resonators to be carried out in one cool down cycle. The results are in good agreement with the temperature and power dependence of the dielectric losses predicted for atomic two-level tunneling systems (TLSs). We find indication that the TLS density of states increases with frequency, which had not been seen in previous loss measurements.

TT 58.31 Thu 15:00 Poster D

**Decoherence of the Majorana fermions** — •François Konschelle and Fabian Hassler — Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

Majorana fermion is one of the possible candidates for future quantum computation implementations. Of interest are their topological properties which protect them from decoherence. More precisely, the delocalization of the Majorana wave function at the two ends of a semi-conducting wire in the proximity with a superconductor allows the parity (i.e. the number of fermions) to be conserved up to some exponential corrections. We want to discuss the decoherence aspects of the Majorana fermion in general terms. To do that, we first establish a toy-model for the calculation of the wave function associated with a delocalized Majorana fermion. Then, we discuss the possibilities for exciting a proximity-induced superconductor. Finally, we discuss the decoherence characteristic times associated with several quantities, the most important of them being the parity of a given part of the wire.

TT 58.32 Thu 15:00 Poster D

**Decoherence due to quasi particle tunneling in superconducting resonators** — •Sebastian Zanker, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie, D-76128 Karlsruhe

We investigate decoherence in superconducting resonators due to quasi particle tunneling. In particular resonators shunted by single Josephson junctions and SQUIDs as well as transmission line embedded Josephson junctions are studied. Quasi particle tunneling is assumed to occur because of the presence non-equilibrium quasi particles and decay times may be used to calculate quasi particle densities.

TT 58.33 Thu 15:00 Poster D

**Solving non-Markovian master equations for N-Qubit-systems** — •Christian Karlewski[1], Michael Marthaler[2], and Gerd Schön[2] — [1]Fakultät für Physik, Universität Bielefeld, Postfach 100131, D-33501 Bielefeld, Germany — [2]Institut für theoretische Festkörperphysik, Karlsruher Institute for Technology, D-76128 Karlsruhe, Germany

We solve non-Markovian master-equations of N-Qubit systems with Born-approximation using Fourier-transformation. With the full solution of the reduced density matrix of the Qubit-system we analyze different noise-spectra and the resulting dynamics. Decoherence and the appearance of dark states can be seen. One special system we have a closer look at is the one-excitation model with one of the N-Qubits in an excited state. By the use of the observable that measures the population of all other qubits and some constraints to the system it is possible to reduce the dynamics of this observable to three ODE.

TT 58.34 Thu 15:00 Poster D

**Current noise in disordered Josephson junctions** — •Pierre-Luc Dallaire-Demers[1], Mohammad Ansari[2], and Frank Wilhelm-Mauch[1] — [1]Universität des Saarlandes, Saarbrücken, Deutschland — [2]Institute for Quantum Computing, Waterloo, Canada

Josephson junctions are one of the fundamental building blocks of mesoscopic superconducting circuits. Despite being dissipationless, spurious low-energy Andreev bound states inside those junctions could provide an intrinsic microscopic mechanism for fluctuations of the current, therefore limiting the coherent operation time of superconducting quantum circuits. Models of bound states arising from pinholes in different models of disorder were investigated and their current noise signatures were characterized with respect to temperature, phase difference and sample-to-sample fluctuations of the conductance. In this theoretical work, it is shown that the low-frequency noise signature of Josephson junctions is a property specific to each individual sample independent of the fabrication process. Furthermore, the comparison of sample-specific noise spectra and characteristic current-voltage relations reveals under which conditions the presence of those disorder-induced bound states may elude detection in a 4-probe measurement but still reveal themselves as dephasing of coherent observables in circuits dominated by inductive energy.

TT 58.35 Thu 15:00 Poster D

**Non-perturbative stochastic method for driven quantum impurity systems** — •Peter Orth[1] and Karyn Le Hur[2] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of

Technology (KIT), 76131 Karlsruhe — [2]Center for Theoretical Physics, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France

We discuss a numerically exact method for investigating the real-time dissipative dynamics of quantum impurities embedded in a macroscopic environment beyond the weak-coupling limit. We focus on the spin-boson Hamiltonian that describes a two-level system interacting with a bosonic bath of harmonic oscillators. Starting from the real-time Feynman-Vernon path integral, we derive an exact stochastic Schrödinger equation that allows to compute the full spin density matrix and spin-spin correlation functions beyond weak coupling. We present an analogy between the dissipative dynamics of a quantum spin and that of a classical spin in a random magnetic field. This analogy is used to recover the well-known Non- Interacting-Blip-Approximation (NIBA) in the weak-coupling limit. As interesting applications of our method, we explore the non-Markovian effects of the initial spin-bath preparation on the dynamics of the coherence $\sigma^x(t)$ and of $\sigma^z(t)$ under a Landau-Zener sweep of the bias field. We also compute to a high precision the asymptotic long-time dynamics of $\sigma^z(t)$ without bias and demonstrate the wide applicability of our approach by calculating the spin dynamics at non-zero bias and different temperatures.

TT 58.36 Thu 15:00 Poster D

**Absorption and transfer properties of quantum aggregates under the influence of Lévy-stable disorder** — Sebastian Möbius[1], •Sebastiaan M. Vlaming[1,2,3], Victor A. Malyshev[2], Jasper Knoester[2], and Alexander Eisfeld[1] — [1]Max Planck Institute for Physics of Complex Systems, Dresden, Germany — [2]Centre for Theoretical Physics and Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands — [3]Department of Chemistry and Center for Excitonics, Massachusetts Institute of Technology, Cambridge, USA

Molecular aggregates exhibit extraordinary absorption properties, depending on their geometrical conformation and inter-monomeric coupling. The narrowing of the absorption band for J-aggregates can be well described by diagonal Gaussian static disorder for individual site energies. Aggregates consisting of large molecules are usually embedded in complex environments, making it impossible to separate individual contributions to the energy fluctuations.

Recent developments in generating and trapping highly excited Rydberg atoms allow for quantum simulations of molecular aggregates. By controlling the environment, e.g. a polar background gas, static disorder besides Gaussian can be studied. We analyze how the environment generates disorder distributions with heavy tails, so called Lévy-stable distributions. These distributions can lead to broadening of the absorption bandwidth [1] as well as subdiffusive exciton transfer.

[1] A. Eisfeld, S.M. Vlaming, V.A. Malyshev, J. Knoester, PRL **105**, 137402 (2010)

TT 58.37 Thu 15:00 Poster D

**Real Time Dynamics in the Central Spin Model: a Chebyshev Polynomial Approach** — •Johannes Hackmann and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

The central spin model describes the dephasing of a single electron spin in a negatively doped semiconductor quantum dot. The real time dynamics of the system are studied using the Chebyshev polynomial expansion for arbitrary initial conditions. Typically, we include a representation of 20 nuclear spins in our simulations. We discuss the influence of different couplings between the central spin and the bath and compare our data to a mean field result. We extend our simulations and include a finite transverse magnetic field. We study the interplay of the Larmor precession and the spin dephasing as function of magnetic field strength. We gauge a simplified mean-field approach for a large number of spins with our numerical data for a small cluster.

TT 58.38 Thu 15:00 Poster D

**Interacting electrons on trilayer honeycomb lattices** — Michael M. Scherer[3], Stefan Uebelacker[1,2], •Daniel D. Scherer[4], and Carsten Honerkamp[1,2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52056 Aachen, Germany — [2]JARA-FIT Fundamentals of Future Information Technology — [3]Institute for Theoretical Physics, Heidelberg University, D-69120 Heidelberg, Germany — [4]Institute for Theoretical Physics, Leipzig University, D-04103, Leipzig, Germany

Few-layer graphene systems come in various stacking orders. Considering tight-binding models for electrons on stacked honeycomb layers, this gives rise to a variety of low-energy band structures near the charge neutrality point. Depending on the stacking order, these band structures enhance or reduce the role of electron-electron interactions. Here, we investigate the instabilities of interacting electrons on honeycomb multilayers with a focus on trilayers with ABA and ABC stackings theoretically by means of the functional renormalization group. We find different types of competing instabilities and identify the leading ordering tendencies in the different regions of the phase diagram for a range of local and non-local short-ranged interactions. The dominant instabilities turn out to be toward an antiferromagnetic spin-density wave (SDW), a charge density wave, and quantum spin Hall (QSH) order. Ab initio values for the interaction parameters put the systems at the border between SDW and QSH regimes. We thus obtain a comprehensive picture of the possible interaction-induced ground states of few-layer graphene.

TT 58.39 Thu 15:00 Poster D

**Zero-Gap State in Organic Conductors** — •Rebecca Beyer[1], Armin Dengl[1], Mohamed Assili[2], Tomislav Ivek[1,3], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]University of Tunis, Tunisia — [3]Institut za fiziku, Zagreb, Croatia

The quasi-two-dimensional molecular crystal $\alpha$-(BEDT-TTF)$_2$I$_3$ exhibits a metallic behavior down to $T_{MI} = 135$ K, at which it undergoes a metal-insulator transition into a charge-ordered state. This transition is very sensitive to hydrostatic pressure: it not only decreases the transition temperature by about 9 K/kbar but also the charge disproportionation gets reduced with increasing pressure. Above a certain pressure of about 15 kbar, the metal-insulator transition is completely suppressed and the material goes into a zero-gap semiconducting (ZGS) state with close similarities to the Dirac-Cone in Graphene. The ZGS-state has been predicted by theory and been supported by dc- and Hall-measurements while the NMR-response shows very exotic features which also have been assigned to ZGS fingerprints.

For further investigation of the ZGS state in $\alpha$-(BEDT-TTF)$_2$I$_3$ we performed infrared optical measurements in the frequency range of 100 cm$^{-1}$ to 8000 cm$^{-1}$ at temperatures as low as 10 K under hydrostatic pressure up to 15 kbar. We were able to follow the decrease of the transition temperature and the closure of the insulating gap with increasing pressure. Calculations were performed predicting the optical conductivity of free charge carriers in a tilted Dirac-Cone, in order to compare experimental results with theory.

TT 58.40 Thu 15:00 Poster D

**Non-perturbative laser effects on the electrical properties of graphene nanoribbons** — •Hernán L. Calvo[1], Pablo M. Pérez Piskunow[2], Horacio M. Pastawski[2], Stephan Roche[3,4], and Luis E. F. Foa Torres[2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [2]Instituto de Física Enrique Gaviola (CONICET) and FaMAF, Universidad Nacional de Córdoba, Argentina — [3]CIN2 (ICN-CSIC), Catalan Institute of Nanotechnology, Universidad Autónoma de Barcelona, Spain — [4]Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain

We study the interplay between lateral confinement and photon-induced non-adiabatic processes on the electronic properties of laser-illuminated graphene nanoribbons. By using Floquet theory applied to realistic models of these nanostructures, we predict a strong dependence on the polarization direction which is averaged out in the bulk limit. Depending on the device setup (edges geometries, ribbon width, polarization direction and metallic/semiconducting character of the sample), a laser with frequency $\Omega$ may either not affect the electronic structure, or induce bandgaps or depletions at $\pm\hbar\Omega/2$, and/or at other energies not commensurate with half the photon energy. Similar features are also observed in the dc conductance, suggesting the use of the polarization direction to switch on and off the graphene device. Our results could guide the design of novel types of optoelectronic nano-devices.

TT 58.41 Thu 15:00 Poster D

**Kondo effect in graphene with isolated vacancies** — •Lars Fritz[1] and Andrew Mitchell[1,2] — [1]Universität zu Köln, Institut für Theoretische Physik — [2]Department of Chemistry, Physical and Theoretical Chemistry, Oxford University,UK

The physics of a reconstructed vacancy in graphene is investigated by a combination of numer- ical renormalization group and analytical techniques. The effective model introduced recently by [1] describes a localized $\sigma$ level hybridized with the $\pi$-band, whose local density of

states is enhanced due to potential scattering. Rich quantum impurity physics is shown to result, with both doublet and triplet powerlaw Kondo phases accessible, depending on microscopic parameters. Thermodynamic quantities and the scattering t matrix are calculated exactly in each phase. The quantum phase transition separating Kondo phases is examined, and the unusual role of particle-hole symmetry breaking is also considered. We show that the asymmetric lo- cal moment phases of simplified Kondo models are not in practice accessible in the full Andersonian model describing the vacancy, and that Kondo screening is always important at low energies.

[1] Cazalilla et al., arXiv:1207.3135 (2012)

TT 58.42 Thu 15:00 Poster D

**De Haas - van Alphen oscillations in graphene** — •Carolin Küppersbusch and Lars Fritz — Institut für Theoretische Physik, Universität zu Köln

De Haas van Alphen oscillations are customarily analyzed using the Lifshitz-Kosevich (LK) formula. This is a phenomenological formula which relates the amplitude of the harmonics to system parameters such as the temperature, disorder strength and the effective mass of the electrons. For systems which can be described within Fermi liquid theory the LK formula holds without modifications when electron-electron interactions are included. The introduction of a renormalized mass is fully effectual. Since graphene cannot be described within Fermi liquid theory for all doping levels, modifications of the LK formula should be expected for this system with electron-electron interactions included. These modifications are investigated.

TT 58.43 Thu 15:00 Poster D

**Kondo effect in a graphene sheet with a vacancy** — •Martin Sprengel and Fakher F. Assaad — Institut für theoretische Physik und Astrophysik, Universtität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We study the influence of a single-atom vacancy in a Graphene lattice using a tight-binding model with nearest neighbour hopping and a Hubbard U term. The vacancy generates a *localised* state, which extends into the bulk with a power law. The question we wish to address is if under correlation effects a local moment is created and if it is ultimately screened by the bulk. To do so, we use continuous-time Quantum Monte Carlo (CT-QMC) simulations to calculate the dependence of the spin susceptibility on temperature, chemical potential and the Hubbard U. For small deviation from half-filling no sign problem occurs which allows us to benefit from the fact that CT-QMC is a numerically exact method. At half filling and down to our lowest temperatures we observe a Curie behaviour of the local spin susceptibility. Away from half filling, the very signature of the local moment is absent within the considered parameter range.

TT 58.44 Thu 15:00 Poster D

**Probing the transport properties of graphene nanostructures produced by local anodic oxidation** — •Nils Freitag[1], Aviral Vaid[2], Marco Pratzer[1], Marcus Liebmann[1], Theresa Hecking[1], Alexander Nent[1], and Markus Morgenstern[1] — [1]II. Physikalisches Institut, RWTH Aachen and JARA-FIT, Otto-Blumethal-Straße, 52074 Aachen — [2]Dept. of Materials Science and Engineering, Indian Institute of Technology Kanpur, India 208016

Graphene flakes exfoliated on 300 nm $SiO_2$/Si and contacted by Indium soldering are modified by local anodic oxidation in an atomic force microscope (AFM). By varying voltage, tip velocity and contact pressure, we produced either cuts or areas appearing as elevations in AFM. The width of the cuts and elevations ranged down to 15 nm and 35 nm respectively. However, the cuts are mostly surrounded by additional elevations. The elevations are insulating at room temperature with an areal resistance of several TΩ and exhibit a D and a 2D peak in Raman spectroscopy.

Transport studies on an Aharanov-Bohm ring with a diameter of 600 nm showed magnetooscillations with a visibility of 0.2 % at 300 mK and a strong peak around 0 T attributed to weak localization within the ring. Transport measurements on a Quantum Dot structure with a diameter of 60 nm and several side gates showed several Coulomb diamonds, however, with addition energies not compatible with the structured dot area. Nevertheless, the plunger gate was six times more effective than the back gate and charge rearrangements were seldom observed.

TT 58.45 Thu 15:00 Poster D

**Back-action of charge detectors on graphene quantum dots** — •Marvin Junk[1], Christian Volk[1,2], Christoph Neumann[1,2], Stephan Engels[1,2], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Peter-Grünberg-Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Graphene quantum devices, such as single electron transistors and quantum dots have received increasing attention over the last years. Quantum dots (QDs) made from graphene have been suggested to be an interesting system for implementing spin qubits. Compared to the well-established GaAs-based quantum dots their advantages are the smaller hyperfine interaction and reduced spin-orbit coupling, which promises more favorable spin coherence times.

Our devices consist of etched graphene QDs surrounded by electrostatic gates and two nearby graphene nanoribbons. Local resonances in these nanoribbons can be successfully used to detect individual charging events in the quantum dot even in regimes where the direct current through the QD is below the detection limit. The current through the QD and the charge detectors (CD) are measured simultaneously. In finite-bias spectroscopy measurements - so-called Coulomb diamonds - the CD is an important tool providing information on the asymmetry of the quantum dot device tunneling barriers. In the presented work we focus on the back-action of graphene CDs on the transport through the graphene quantum dot.

TT 58.46 Thu 15:00 Poster D

**Driven Topological Insulator Quantum Dot: A single-electron spin-source** — •Andreas Inhofer and Dario Bercioux — Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, 79104 Freiburg, Germany

We use the concepts of scattering matrix theory and recent progress in theory and experiment on topological insulators in order to investigate the feasibility of a single-particle spin-source. The basic concept of such a device has been realized by Fève and coworkers as a single electron source (SES) in Ref. [1]. They used a driven quantum dot in a quantum Hall device to allow for the controlled emission of quantized charges into the edge-states of a quantum well. The conducting edge-states exhibit interesting features such as insensitivity to (strong) disorder, providing mainly dissipationless transport. However, these SES require high magnetic fields. Recently, spin-polarized edge-states were theoretically predicted and experimentally observed in two- and three-dimensional topological insulators in the absence of magnetic fields [2]. Such a source could provide quantized spin-currents and become one of the key components for spintronic devices. Further investigations involve the characterisation of the emitted spin-currents with respect to current-noise and entanglement of the counter-propagating electrons.

[1] G. Fève *et al.*, Science **316**, 1169 (2007)
[2] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010)

TT 58.47 Thu 15:00 Poster D

**Majorana single-charge transistor** — •Roland Hützen[1], Alex Zazunov[1], Bernd Braunecker[2], Alfredo Levy Yeyati[2], and Reinhold Egger[1] — [1]Institut für Theoretische Physik, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany — [2]Departamento de Física Teórica de la Materia Condensada C-V and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

We study transport through a Coulomb blockaded topologically nontrivial superconducting wire (with Majorana end states) contacted by metallic leads. An exact formula for the current through this interacting Majorana single-charge transistor is derived in terms of wire spectral functions. A comprehensive picture follows from three different approaches. We find Coulomb oscillations with universal halving of the finite-temperature peak conductance under strong blockade conditions, where the valley conductance mainly comes from elastic cotunneling. The nonlinear conductance exhibits finite-voltage sidebands due to anomalous tunneling involving Cooper pair splitting.

TT 58.48 Thu 15:00 Poster D

**Topological edge states in a HgTe quantum well in proximity to an s-wave superconductor** — •Luzie Weithofer and Patrik Recher — Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

Topological insulators represent a new class of condensed matter systems which are characterized by topologically protected edge states. Two-dimensional topological insulators have been experimentally realized in HgTe quantum wells [1]. In a HgTe quantum well in the

topologically non-trivial phase, two edge states of different spin propagate in opposite directions at the same boundary.

Here, we consider the proximity-induced superconductivity in the bulk of a HgTe quantum well in terms of a four-band model [2]. In addition, we include various symmetry-breaking terms and discuss their consequences on the topological properties of the system, focusing on the existence of edge states.

[1] M. König *et al.*, Science **318**, 766 (2007)
[2] B. Bernevig *et al.*, Science **314**, 1757 (2006)

TT 58.49 Thu 15:00 Poster D

**Quantum dot coupled to a quantum spin Hall edge** — •Benedikt Probst and Patrik Recher — Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

In topological insulators new interesting states of matter are realised. In two dimensional topological insulators the quantum spin Hall effect was predicted and observed [1-3]. In this effect the different spin polarisations propagate in opposite directions, which gives new perspectives for spintronic devices.

We couple a quantum dot in the Coulomb blockade regime to an helical edge, where the quantum dot can be treated as a spin impurity. We discuss the behaviour of the impurity in an open quantum system approach. The helical edge is used as a bath and to manipulate the dot spin. We also discuss the transport signature of this system.

[1] B. A. Bernevig, T. L. Hughes and S.-C. Zhang, *Science* **314**, 1757 (2006)
[2] M. König, S. Wiedemann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi and S.-C. Zhang, *Science* **318**, 766 (2007)
[3] A. Roth, C. Brüne, H. Buhmann, L. W. Molenkamp, J. Maciejko, X.-L. Qi and S.-C. Zhang, *Science* **325**, 294 (2009)

TT 58.50 Thu 15:00 Poster D

**Electrically tunable charge transport in CVD-grown nanostructures of $Bi_2Se_3$** — •Louis Veyrat — IFW-Dresden, Dresden, Germany

Electrical transport in nanostructures of the 3D topological insulator $Bi_2Se_3$ is studied as a function of a back-gate voltage. Shubnikov de Haas oscillations indicate the presence of Dirac fermions, reproducing the results of previous studies based on exfoliated crystals [1], but here with a 4-probe geometry. Besides, the simultaneous measure of both the longitudinal and transverse magneto-resistance allows us to compare the different carrier densities infered from Shubnikov-de-Haas oscillations and the Hall resistance. The strong back gate effect on the longitudinal and Hall resistances shows that we can efficiently tune the total carrier density in a nanostructure. Moreover, we can separate the contributions to the conduction from bulk carriers and surfaces states, and evaluate their different mobilities and densities.

[1] Sacépé et al., Nature Comm. 2, 575, (2011)

TT 58.51 Thu 15:00 Poster D

**Modulation of Majorana induced current cross-correlations by quantum dots** — •Björn Zocher[1,2] and Bernd Rosenow[1] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04103 Leipzig, Germany — [2]Max Planck Institut für Mathematik in den Naturwissenschaften, D-04103 Leipzig, Germany

We study charge transport through a topological superconductor with a pair of Majorana end states, coupled to leads via quantum dots with resonant levels [1]. The non-locality of the Majorana bound states opens the possibility of crossed Andreev reflection with nonlocal shot noise, due to the injection of an electron into one end of the superconductor followed by the emission of a hole at the other end. In the space of energies of the two resonant quantum dot levels, we find a four peaked clover-like pattern for the strength of noise due to crossed Andreev reflection, distinct from the single ellipsoidal peak found in the absence of Majorana bound states. For finite temperatures, we observe a characteristic sign change of the crossed noise for two leafs of the clover-like pattern. We apply our findings to disordered multichannel semiconductor-superconductor heterostructures with Rashba spin-orbit coupling which are predicted to host Majorana bound states [2] and show that the clover-like crossed noise pattern is a robust feature of quasi one-dimensional Majorana wires.

[1] B. Zocher and B. Rosenow, arXiv:1208.4092
[2] J. D. Sau, R. M. Lutchyn, S. Tewari, and S. Das Sarma, Phys. Rev. Lett. **104**, 040502 (2010)

## TT 59: Correlated Electrons: Quantum-Critical Phenomena - Experiments

Time: Thursday 15:00–18:30 Location: H6

TT 59.1 Thu 15:00 H6

**Quasi one-dimensional electronic structure of ferromagnetic heavy fermion $YbNi_4P_2$** — •Sven Friedemann[1], Swee K Goh[1], Michael Sutherland[1], F Malte Grosche[1], Cornelius Krellner[2], Christoph Geibel[3], Helge Rosner[3], Manuel Brando[3], and Frank Steglich[3] — [1]University of Cambridge, Cavendish Laboratory, CB3 0HE Cambridge, United Kingdom — [2]Physikalisches Institut, Goethe-UniversitätFrankfurt, 60438 Frankfurt am Main, Germany — [3]Max PlanckInstitute for Chemical Physics of Solids, 01187 Dresden, Germany

Quantum critical phenomena can be studied in great detail in lanthanide based heavy-fermion systems. Up to now, however, only materials with antiferromagnetic ground state were found. In the new heavy fermion material $YbNi_4P_2$ a clear ferromagnetic transition is observed at $T_C = 0.17$ K. $YbNi_4P_2$ has the prospect for studying ferromagnetic quantum criticality. Above the transition temperature strong evidence is found for the vicinity of $YbNi_4P_2$ to a quantum critical point: the specific heat diverges in a power-law form and the resistivity follows a linear temperature dependence. We present first Shubnikov-de Haas measurements in combination with electronic band structure calculations. The electronic structure is dominated by parallel disconnected sheets in accordance with the crystal structure featuring quasi-one-dimensional chains of Yb. The observed Shubnikov-de Haas oscillations are assigned to small quasi-two-dimensional portions of the Fermi surface. The experimentally observed mass enhancement of these orbits reflects the heavy-fermion character of $YbNi_4P_2$.

TT 59.2 Thu 15:15 H6

**$\mu$SR investigations on the $4f$-derived ferromagnetic quantum quantum critical system $YbNi_4(P_{1-x}As_x)_2$** — •Rajib Sarkar[1], Johannes Spehling[1], Cornelius Krellner[2], Hubertus Luetkens[3], Chris Baines[3], Manuel Brando[4], Christoph Geibel[4], and Hans-Henning Klauss[1] — [1]IFP, TU Dresden, D-01069 Dresden, Germany — [2]Goethe University Frankfurt, D-60438 Frankfurt am Main, Germany — [3]PSI, CH-5232 Villigen PSI, Switzerland — [4]MPI-CPFS, D-01187 Dresden, Germany

Ferromagnetic quantum criticality (FMQC) is one central topic of research in strongly correlated electron systems. Despite adequate research so far there is no concrete evidence of FMQC. In this context, the recently discovered 4f-derived heavy fermion FM metal $YbNi_4P_2$ with $T_c$ =170 mK, a Kondo temperature $T_K$=8 K and a very small ordered moment of $\approx 0.05\ \mu_B$, deserves particular interest [1]. With 8 % As substitution at the P site, $T_c$ goes down to 28 mK and the Grüneisen ratio diverges as $\Gamma(T) \propto T^{-0.22}$, evidencing the presence of FMQC. For $YbNi_4P_2$, zero field $\mu$SR investigations prove static long range magnetic ordering [2] and the ordered moment is strongly suppressed with increasing As-substitution. For 8% As, $\mu$SR time spectra suggest that static ordering appears below 20 mK. Here, we present our recent $\mu$SR results for x $\leq$ 0.13 and discuss the dynamics of the quantum fluctutations at this ferromagnetic quantum critical point.

[1] New J. Phys. 13, 103014 (2011)
[2] Phys. Rev. B 85, 140406 (2012)

TT 59.3 Thu 15:30 H6

**Ferromagnetic Quantum Critical Point in $YbNi_4(P_{1-x}As_x)_2$** — •Cornelius Krellner[1,2], Alexander Steppke[2], Robert Küchler[2], Stefan Lausberg[2], Edit Lengyel[2], Lucia Steinke[2], Robert Borth[2], Thomas Lühmann[2], Michael Nicklas[2], Sven Friedemann[3], Christoph Geibel[2], Frank Steglich[2], and Manuel Brando[2] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Cavendish Laboratory, University of Cambridge, United Kingdom

$YbNi_4P_2$ is a quasi-one-dimensional heavy-fermion system where recently a very low lying ferromagnetic (FM) transition at $T_C = 0.17\,\mathrm{K}$ was observed [1]. Above this transition distinct deviations from the predictions of the Landau-Fermi-liquid theory were observed, indicating the presence of a nearby FM quantum critical point (QCP).

In this contribution, we present a thorough investigation of $YbNi_4(P_{1-x}As_x)_2$ single crystals where the ferromagnetism is further suppresed. We show that the FM phase transition line remains second order down to 30 mK for $x \leq 0.08$ with unexpected power-laws above $T_C$ in all thermodynamic quantities. At $x = 0.08$, we found a power-law divergence of the Grüneisen ratio, demonstrating the existence of a FM QCP.

[1] C. Krellner *et al.*, New J. Phys. **13**, 103014 (2011).

TT 59.4 Thu 15:45 H6

**Quantum criticality in partially frustrated $CePd_{1-x}Ni_xAl$** — •Veronika Fritsch[1], Sarah Woitschach[2], Oliver Stockert[2], Wolfram Kittler[1], and Hilbert v. Löhneysen[1,3] — [1]Physikalisches Institut, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe, Germany — [2]Max-Planck-Institut für chemische Physik fester Stoffe, Dresden, Germany — [3]Institut für Festkörperphysik, Karlsruher Institut für Technologie (KIT), 76021 Karlsruhe, Germany

In the antiferromagnetic (AF) heavy-fermion system CePdAl the magnetic Ce ions form a network of equilateral triangles in the (001) plane, similar to the kagomé lattice, with one third of the Ce moments not participating in the long-range order due to geometrical frustration. The Néel temperature $T_N = 2.7$ K is reduced upon replacing Pd by Ni in $CePd_{1-x}Ni_xAl$, with $T_N \to 0$ for $x \approx 0.14$. At this concentration the specific heat $C$ exhibits a $C/T \propto -\log T$ dependence. This and the linear $T_N(x)$ dependence are indicative of two-dimensional (2D) critical AF fluctuations within the conventional description of quantum criticality after Hertz, Millis and Moriya, in marked contrast to the three-dimensional (3D) magnetic order found by neutron diffraction experiments in CePdAl. We discuss the role of frustration when approaching the quantum critical point in Ni-substituted CePdAl on the basis of measurements of the magnetization, specific heat, electrical resistivity, and neutron diffraction experiments.

TT 59.5 Thu 16:00 H6

**Pressure- and Composition-Induced Structural Quantum Phase Transition in the Cubic Superconductor $(Sr,Ca)_3Ir_4Sn_{13}$** — •Swee K. Goh[1], Lina E. Klintberg[1], Patricia L. Alireza[1], Paul Saines[2], David Tompsett[1], Peter Logg[1], Jinhu Yang[3,4], Bin Chen[3,4], Kazuyoshi Yoshimura[4], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom — [2]Department of Materials Science and Metallurgy, University of Cambridge, United Kingdom — [3]Department of Physics, Hangzhou Normal University, China — [4]Department of Chemistry, Kyoto University, Japan

The quasi-skutterudite superconductor $Sr_3Ir_4Sn_{13}$ has been reexamined recently. In addition to a superconducting transition at $T_c = 5$ K, pronounced anomalies can be seen in magnetic susceptibility and resistivity at $T^* = 147$ K. Using single crystal x-ray diffraction, we identify $T^* = 147$ K as the temperature where the system undergoes a structural transition from a simple cubic parent structure (I-phase) to a superlattice variant (I'-phase) with a lattice parameter twice that of the I-phase. Applying physical pressure or chemical pressure (via the isoelectronic substitution of Ca for Sr) leads to a rapid suppression of $T^* = 147$ K and an enhancement of $T_c$. Furthermore, a quasi-linear temperature dependence of resistivity is observed at the pressure where $T^* = 147$ K extrapolates to 0 K, reminiscent of quantum critical phenomena on the border of magnetism. We argue that the pressure phase diagram of $Sr_3Ir_4Sn_{13}$ features a superlattice quantum critical point.

TT 59.6 Thu 16:15 H6

**Heat and charge transport study of quantum critical behavior in heavy fermion YbAgGe** — •Jinkui Dong[1], Yoshi Tokiwa[1], Maik Schubert[1], Sergey L. Bud'ko[2], Paul C. Canfield[2], and Philipp Gegenwart[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [2]Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

We have performed electrical resistivity and thermal conductivity measurements on the heavy fermion metal YbAgGe to investigate quantum critical behavior and the validity of Wiedemann-Franz law. A power law analysis of electrical resistivity $\rho(T)$, $\rho(T) = \rho_0 + AT^n$ showed that NFL behavior with $n < 2$ persists in fields up to 9 T. A broad maximum of $\rho(H)$ appeared in the vicinity of critical field $H_c \simeq 4.5$ T, where a field-induced quantum critical end point (QCEP) was expected. Far away from this critical region, the Lorenz ratio $L(T)/L_0$ converges to unity in the limit of $T \to 0$. However, near the QCEP, the extrapolation of $L(T)/L_0$ gives $L(T \to 0)/L_0 \simeq 0.91$. We associate this moderate violation of Wiedemann-Franz law at 4.5 T with the strong inelastic scattering of electrons from the quantum critical fluctuations.

**15 min. break**

**Invited Talk** TT 59.7 Thu 16:45 H6

**Electron Spin Resonance (ESR) close to a Quantum Phase Transition: Probing $YbRh_2Si_2$ at mK Temperatures** — •Marc Scheffler[1], Conrad Clauss[1], Mojtaba Javaheri[1], Martin Dressel[1], Jörg Sichelschmidt[2], Cornelius Krellner[2,3], Christoph Geibel[2], and Frank Steglich[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [3]Physikalisches Institut, Goethe-Universität Frankfurt, Frankfurt/Main, Germany

The heavy-fermion material $YbRh_2Si_2$ is a model system for quantum criticality: the very weak antiferromagnetic order below 70 mK can be suppressed e.g. by a small magnetic field of 60 mT. This quantum phase transition results in unusual properties such as pronounced non-Fermi-liquid behavior. Previous electron spin resonance (ESR) studies on $YbRh_2Si_2$ revealed new insights concerning the spin dynamics of Kondo lattices, but were limited to temperatures above 500 mK and could not access the most interesting low-temperature regimes.

We recently developed a new measurement technique which we now use for ESR studies on $YbRh_2Si_2$ single crystals at temperatures down to 40 mK. With a set of ESR frequencies spanning 1.5-13 GHz and ESR fields as low as 30 mT, we address the temperature and field regimes close to the quantum critical point. Our results cover all three phases (antiferromagnet, non-Fermi liquid, field-induced Fermi liquid) and they open new opportunities to gain deeper insight into ESR of heavy-fermion systems and to investigate the quantum critical point.

TT 59.8 Thu 17:15 H6

**Influence of charge carrier doping on the $T^*$-Scale in $YbRh_2Si_2$** — •M.-H. Schubert, Y. Tokiwa, H. S. Jeevan, E. Blumenröther, and P. Gegenwart — I. Physikalische Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

$YbRh_2Si_2$ is a prototype heavy-fermion metal which displays a magnetic, field-induced antiferromagnetic (AF) quantum critical point (QCP). It has attracted much attention due to an additional low-energy scale $T^\star(B)$ merging at the QCP, whose origin is still under discussion. Here, we present our recent thermodynamic, magnetic and electrical transport measurements on different single crystalline samples of charge-carrier doped $Yb(Rh_{1-x}T_x)_2Si_2$ (T=Fe, Ni, Ru) at temperatures down to 15 mK and in magnetic fields up to 7 T. The partial substitution of Rh by either Fe or Ni introduces holes or electrons, respectively. The evolution of the single-ion Kondo scale is similar to isoelectronic Co substitution in accordance with the chemical pressure effect. However, while chemical pressure has little influence on $T^\star(B)$ in isoelectronic doped samples, we observe a drastic reduction or increase of $B^\star(T = 0)$ by Fe- or Ni-doping, respectively. As the AF order is completely suppressed by Fe-doping, a heavy Fermi liquid ground state (without the $T^\star(B)$ anomaly) is observed. These results are compared to measurements on samples where Rh is partially substituted by Ru. Here the chemical pressure effect is minimized in order to investigate the pure charge doping effect.

Work supported by the DFG research unit 960 (Quantum phase transitions).

TT 59.9 Thu 17:30 H6

**Competing Magnetic Anisotropies and Multicriticality: The Case of Co-doped $YbRh_2Si_2$** — •Eric C. Andrade[1], Manuel Brando[2], Christoph Geibel[2], and Matthias Vojta[1] — [1]TU Dresden — [2]MPI-CPfS

Motivated by the unusual evolution of magnetic phases in stoichiometric and Co-doped $YbRh_2Si_2$, we study Heisenberg models with competing single-ion and exchange anisotropies by large scale Monte-Carlo

simulations. Upon also including the competition between ferromagnetic and antiferromagnetic order, we analyze the ingredients required to obtain the characteristic crossing point of susceptibilities observed experimentally in $Yb(Rh_{0.73}Co_{0.27})_2Si_2$. The models possess various multicritical points, which we speculate to be relevant for the behavior of Co-doped $YbRh_2Si_2$. We also make contact with experimental data on $YbNi_2P_4$.

TT 59.10 Thu 17:45 H6

**Evolution of ferromagnetic order in $Yb(Rh_{1-x}Co_x)_2Si_2$ with $x \leq 0.27$** — •Sandra Hamann[1], Stefan Lausberg[1], Lucia Steinke[1], Christoph Klingner[2], Cornelius Krellner[3], Manuel Brando[1], Christoph Geibel[1], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Max Planck Institute of Biochemistry, D-82152 Martinsried, Germany — [3]Institute of Physics, Goethe University Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany

Antiferromagnetic (AFM) order appears in $YbRh_2Si_2$ at $T_N = 70\,\mathrm{mK}$ although strong ferromagnetic fluctuations are observed. The application of chemical pressure $x$ in the series $Yb(Rh_{1-x}Co_x)_2Si_2$ stabilizes the AFM phase, i.e. $T_N$ increases with increasing $x$. A second phase transition at $T_L < T_N$ emerges with increasing $x$ and the strength of the ferromagnetic fluctuations raises up to a maximum for $x \approx 0.27$ [1]. Eventually, in pure $YbCo_2Si_2$ both phase transitions $T_N$ and $T_L$ are of AFM nature with $4f$ local moments aligned along the crystallographic $ab$-plane. However, the sample with $x = 0.27$ reveals only one phase transition at 1.30 K which is surprisingly ferromagnetic with moments parallel to the $c$-axis [2]. This motivates a deeper investigation of the magnetic properties in $Yb(Rh_{1-x}Co_x)_2Si_2$ with the magnetic field along the $c$-axis. Here, we present ac-susceptibilty measurements of single crystals with $x \leq 0.27$ down to a temperature of 25 mK.

[1] C. Klingner *et al.*, Phys. Rev. B. **83**, 144405 (2011)
[2] S. Lausberg *et al.*, arXiv:1210.1345

TT 59.11 Thu 18:00 H6

**NMR as a local probe for ferromagnetic correlation and quantum criticality in 3d systems: $YFe_2Al_{10}$ and $Ta(Fe_{1-x}V_x)_2$** — •P. Khuntia[1], M. Brando[1], A. Strydom[2], M. Aronson[3], G. Kreiner[1], F. Steglich[1], and M. Baenitz[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]Physics Department, University of Johannesburg,South Africa — [3]Brookhaven National Laboratory, New York 11973, USA

Probing the $q$-averaged dynamic susceptibility at low energies, the spin lattice relaxation rate by $T$, $(1/T_1T)$ (SLR) is ideal for the investigation of FM and AFM spin fluctuations. At the verge of magnetic order, unusual scaling laws in $T$ and $H$ dependent SLR could be associated with quantum criticality. In $YFe_2Al_{10}$, fluctuation of Fe moments leads to enhanced $\chi$ and $C/T$ values yielding large Wilson ratio accompanied by $^{27}(1/T_1T) \sim \chi$ reveal the dominant role of FM fluctuations in the spin excitation spectra [1].$Ta(Fe_{1-x}V_x)_2$ undergoes an itinerant AFM order, but for nominal V doping, the magnetic properties are reminiscent of itinerant FM at the verge of a FM instability. The enhanced $M(T \to 0)$ supported by $C/T \sim -\ln T$ behavior suggest the persistence of FM fluctuations.Additionally,the $^{51}(1/T_1T) \sim T^{-0.8}$ dependence in small fields indicates the co-existence of FM and AFM spin fluctuations.The Korringa product implies FM correlation between itinerant moments. Presented systems pose special interest since the bulk and microscopic data support low lying magnetic phase transitions and both are naturally located in the vicinity of FM QCP without any external tuning parameter.

[1] Phys. Rev. B (R), in press (2012)

TT 59.12 Thu 18:15 H6

**High pressure transport studies of quantum critical behaviour close to ferromagnetism** — •Yang Zou[1], Zhuo Feng[1,2], Peter Logg[1], Sven Friedemann[1], Hong En Tan[1], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Department of Physics, University College London, UK

Metals close to a magnetic quantum critical point offer a comparatively clear and well-defined environment to investigate the breakdown of Landau's Fermi liquid theory. The low temperature band ferromagnet $ZrZn_2$ violates the predictions of Fermi liquid theory over a wide temperature range [1]. We present new measurements of the electrical resistivity and thermal conductivity as a function of applied magnetic field. These suggest that the temperature scale below which Fermi liquid behaviour is observed rises rapidly with field and reaches 6 K at $B = 9\,\mathrm{T}$. A different kind of Fermi liquid breakdown is seen in the Kondo lattice ferromagnet $CeAgSb_2$ [e.g. 2]. The ferromagnetic transition temperature $T_C = 9.6\,\mathrm{K}$ is sensitive to the application of both pressure and transverse magnetic fields. Therefore, tuning these parameters could be used to access a magnetic quantum phase transition. We present transport measurements under pressure and field tuning, as well as combined measurements of the specific heat and the magnetocaloric effect which provide a comprehensive transport and thermodynamic study of the system.

[1] Smith et al. Nature **455**, 7217 (2008)
[2] Araki et al. PRB **68**, 024408(2003)

## TT 60: Graphene - Theory (jointly with DS, HL, MA, and O)

Time: Thursday 15:00–17:30 Location: H17

TT 60.1 Thu 15:00 H17

**Influence of non-local exchange-correlation and spin-orbit interaction on electronic and optical properties of graphene, silicene, germanene, and tinene** — •Lars Matthes[1], Olivia Pulci[2], Paola Gori[3], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Dipartimento di Fisica, Università di Roma "Tor Vergata", via della Ricerca Scientifica 1, 00133 Rome, Italy — [3]CNR-ISM, Via Fosso del Cavaliere 100, 00133 Rome, Italy

We present first-principles studies of the optical absorbance of the group-IV honeycomb crystals graphene, silicene, germanene, and tinene. We account for many-body effects on the optical properties by using the non-local hybrid functional HSE06. The optical absorption peaks are blue-shifted due to quasi-particle corrections, while the influence on the low-frequency absorbance remains unchanged and reduces to the universal value $\pi\alpha$,[1,2] where $\alpha$ is the Sommerfeld fine-structure constant. However, in silicene, germanene and tinene an electronic band gap arises at the Dirac-point due to spin-orbit splitting and parabolic bands with a very small effective mass emerge. Consequently, the low-frequency absorbance is modified due to the spin-orbit induced fundamental absorption edge. We demonstrate numerically that the absorbance increases at the fundamental absorption edge.

[1] A. Geim et al., Science 320, 1308 (2008)
[2] F. Bechstedt, L. Matthes et al., Appl. Phys. Lett. 100, 261906 (2012)

TT 60.2 Thu 15:15 H17

**Generalized Hubbard models for two dimensional hybrid materials** — •M. Rösner[1], E. Sasioglu[2], C. Friedrich[2], S. Blügel[2], A. I. Lichtenstein[3], M. I. Katsnelson[4], and T. O. Wehling[1] — [1]Institut für Theoretische Physik, Universität Bremen, D-28359 Bremen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]1. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [4]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525 AJ Nijmegen, The Netherlands

We present effective generalized Hubbard models for the description of novel two dimensional materials. The local and non-local partially screened Coulomb interaction as well as hopping integrals are calculated from first principles for silicene and graphene on a metallic substrate. We consider interactions up to the 6th nearest neighbor in real space and investigate the long range behavior of the dielectric function in k-space. We compare the resulting silicene Hubbard model to the corresponding model for pure graphene. Thereby we find values of $U/t \approx 4.0$ eV for the on-site and $V/t \approx 2.4$ eV for the nearest neighbor partially screened Coulomb interaction in silicene, which are slightly bigger than in freestanding graphene. We further show that the ratio of the local to the non-local Coulomb interaction can be controlled by a

metallic substrate, which efficiently screens non-local Coulomb terms.

TT 60.3 Thu 15:30 H17

**Subgap conductivity in gated bilayer graphene** — •Maxim Trushin — University of Konstanz, 78457 Konstanz

In the present work [1], the subgap electron transport has been investigated in gated bilayer graphene [2] within the two-band effective model using the finite-size Kubo formula. The conductivity does not vanish even though the temperature is set to zero and the chemical potential gets into the middle of the band gap. In contrast to the universal subgap conductivity observed in the 2D topological insulators [3], the subgap conductivity in bilayer graphene turns out to be sensitive to the band gap size and disorder strength.

The effect can be explained in terms of the quantum mechanical interband coherence which turns out to be important for the chiral carriers. At finite temperature, a competition between the temperature-dependent interband decoherence and thermal activation processes results in the non-monotonic conductivity vs. temperature dependence. The non-monotonicity can be seen as a signature of the interband entanglement responsible for the difference between the transport and spectral gaps. The effect can be observed in gapped bilayer graphene sandwiched in boron nitride where the electron-hole puddles and flexural phonons are strongly suppressed.

[1] M. Trushin, Europhys. Lett. **98**, 47007 (2012). [2] E. McCann, Phys. Rev. B **74**, 161403 (2006). [3] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).

TT 60.4 Thu 15:45 H17

**Lattice dynamics of few-layer graphene after ultrashort laser excitation** — •Naira Grigoryan, Eeuwe S. Zijlstra, and Martin E. Garcia — Universität Kassel, Kassel, Germany

Femtosecond laser pulses may induce striking structural effects in solids via electronic excitation. Here we studied the phonon dynamics on the 10 ps timescale in thin graphite films as a function of its thickness after laser interaction using ab initio molecular dynamics simulations including a Van der Waals force correction term to the local density approximation. We implemented the coupling of the hot electrons with the so-called strongly coupled optical phonons (SCOPs) [T. Kampfrath et al., PRL 95, 187403 (2005)] in a semiempirical way . From our simulations we could determine the decay of the SCOPs into other phonon modes, in particular, the out-of-plane lattice vibrations.

TT 60.5 Thu 16:00 H17

**RKKY Interaction in a Graphene Bilayer** — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

RKKY interaction in doped graphene monolayer ($k_F \neq 0$) shows Friedel oscillations decaying as $1/r^2$ [1]. In this work we consider the RKKY interaction in AA- and AB-stacked bilayer graphene using exact low energy Green's functions. Apart from the common site-to-site interaction we discuss impurities located at the bond centers as well as impurities at the center of the hexagonal plaquettes and intercalant-type impurities located in-between the two carbon layers. Similarly to the monolayer case, we find an oscillatory $1/r^2$ decay for on-site impurities in AA-stacked bilayer graphene. The exchange integral separates into the product of an energy dependent oscillation and an additional modulation resulting from the interlayer coupling. Interestingly, for on-site impurities in AB-stacked bilayer graphene this additional modulation vanishes at low Fermi energies. Moreover, due to the interference of the neighboring site-to-site interactions, at high Fermi energies the RKKY interaction between two plaquette impurities shows a $1/r^3$ behavior.

[1] M. Sherafati and S. Satpathy, Phys. Rev. B 84, 125416, 2011

**Coffee break**

TT 60.6 Thu 16:30 H17

***Ab initio* calculations of functionalized graphene nanoribbons** — •Christian Till, Nils Rosenkranz, Christian Thomsen, and Janina Maultzsch — TU Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, 10623 Berlin

Since nearly 30 years the discovery and subsequent research on fullerenes, carbon nanotubes, and graphene fuel expectations on carbon-based nanoelectronics. In this context, thin stripes of the two-dimensional material graphene, so-called graphene nanoribbons (GNRs), draw broad interest as well. In this work, we present a comprehensive ab initio study of the structural, electronic and vibrational characteristics of a 7-armchair GNR with hydroxyl functionalized edges. Our results show AGNRs with increasing hydroxyl saturation to be particularly stable. In addition, we find a variation of the ribbon geometry under functionalization. An increasing degree of functionalization leads to a compression perpendicular to the ribbon axis. As a consequence we find a linear shift of the band gap with growing edge hydroxylation. With regard to a possible experimental determination of the degree of functionalization, we indicate fingerprint vibrational modes of the hydroxyl groups as well as a substantial shift of Raman active phonons.

N. Rosenkranz, C. Till, C. Thomsen, and J. Maultzsch, Phys. Rev. B **84**, 195438 (2011).

TT 60.7 Thu 16:45 H17

**Phonon dispersions of AB- and ABC-stacked graphene trilayers and multilayers** — •Bart Verberck[1,2], Karl H. Michel[1], and Björn Trauzettel[2] — [1]Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Recently, it was experimentally confirmed that the electronic structure of graphene multilayers crucially depends on how they are stacked. The simplest multilayer for which different stackings can be realised is the trilayer. The ABA variant features both linearly and quadratically dispersed electronic bands near the K-point, while the ABC variant has cubic electronic dispersion. At the same time, the difference between the phonon dispersions for ABA and ABC trilayer graphene is less well established. Detailed knowledge of the phonon spectra is, however, essential for understanding double-resonant Raman scattering experiments, offering a simple means for characterising multilayer graphene samples (number of layers and stacking sequence). Here we present a theoretical study of the phonon dispersions of AB- and ABC-stacked multilayers based on a phenomenological force-constants model. We find that the difference between the phonon spectra for the two variants is much less apparent than the difference between the respective electronic band structures; the main distinction concerns the low-energy phonon modes around the K-point. We argue that the observed difference in double-resonant Raman scattering signals for ABA and ABC trilayers mainly originates from the different electronic dispersions.

TT 60.8 Thu 17:00 H17

**Optical selection rules in graphene quantum dots** — •Eleftheria Kavousanaki and Keshav Dani — Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology, Graduate University, Okinawa, Japan

We theoretically study the optical absorption of graphene quantum dots for different shapes, sizes and edge types. We calculate the single particle energy spectrum using the tight-binding Hamiltonian and the Dirac-Weyl equation and show that dots with zigzag edges exhibit a degenerate shell of zero energy states, in agreement with previous results. Using standard group theoretical tools, we identify the optical selection rules for triangular and hexagonal quantum dots and discuss the role of light polarization on the absorption spectrum. Finally, we calculate the oscillator strengths and absorption spectra for different quantum dot sizes and identify the contribution of the zero energy states therein.

TT 60.9 Thu 17:15 H17

**Electronic reflection for a single layer graphene quantum well** — •Abir Mhamdi[1,2], Emna Ben Salem[1], and Sihem Jaziri[3] — [1]Laboratoire de Physique de la Matière Condensée, Faculté des Sciences de Tunis, Tunisia — [2]Institut für Theoretische Physik, Georg-August Universität Göttingen, Germany — [3]Laboratoire de Physique des Matériaux, Faculté des Sciences de Bizerte, Tunisia

We address the problem of Dirac fermions' graphene quantum well (GQW) and we focus on the low energy approximation for the Hamiltonian of the system where the former can be described by a Dirac-like Hamiltonian. Interesting relations are obtained and used to discuss the influence of the spin-orbit coupling, which induces an effective mass-like term, on the transport properties of single-layer graphene quantum well. It is found that the reflection probability of incident electrons is sensitive to the effective mass-like term. This can be explained by the dependence of reflection coefficient $R$ on the incident electrons' direction and their energies. Notably, we found that the re-

flection probability for massive fermions with a very small angle, i.e. the wave-vector along the transport direction is zero in the GQW, can be greatly suppressed.

## TT 61: Topological Insulators 4 (jointly with DS, HL, MA, and O)

Time: Thursday 15:00–18:00 Location: H18

**Topical Talk** TT 61.1 Thu 15:00 H18

**Correlation Effects in Quantum Spin Hall Insulators** — •Martin Hohenadler — Theoretische Physik I, Universität Würzburg, 97074 Würzburg, Germany

Time-reversal invariant insulating states with topological properties, including topological insulators, have been in the focus of research in recent years. On the theoretical side, electronic correlation effects are of particular interest, as they can both destroy and create topological phases. This talk gives an overview of research on two-dimensional, correlated topological insulators, with a focus on quantum Monte Carlo results for the Kane-Mele-Hubbard model.

TT 61.2 Thu 15:30 H18

**All in-ultra-high-vacuum study of thin film topological insulators: $Bi_2Te_3$** — •Katharina Hoefer, Diana Rata, Christoph Becker, and Liu Hao Tjeng — Max Planck Institute for Chemical Physics of Solids

Thin films of topological insulators offer the possibility for the experimental study of the expected spectacular phenomena occurring at the surface of or interface with these materials due to the increased surface to bulk ratio in comparison to bulk crystals. Bulk materials are always defective which leads to extra contributions in conductance.

High quality thin films of $Bi_2Te_3$ were grown on $\alpha$-$Al_2O_3$(0001) and $BaF_2$(111) using Molecular Beam Epitaxy. A two-step growth procedure provides high quality epitaxial films despite the large lattice mismatch of 9% to $Al_2O_3$; the mismatch to $BaF_2$ is less than 1%.

To protect the surface integrity an all in-ultra-high-vacuum study is crucial. This means not only the preparation and characterization by RHEED, LEED, XPS and ARPES, but especially the transport measurements are performed in-ultra-high-vacuum. The results of this study and ongoing work will be presented.

TT 61.3 Thu 15:45 H18

**Magnetotransport in MBE-grown topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ thin films** — •Christian Weyrich[1], Tobias Merzenich[1], Igor E. Batov[1,2], Gregor Mussler[1], Jörn Kampmeier[1], Yulieth Arango[1], Detlev Grützmacher[1], and Thomas Schäpers[1,3] — [1]Peter Grünberg Institute (PGI-9), Research Centre Jülich GmbH, 52425 Jülich, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432, Moscow Distr., Russia — [3]II. Physikalisches Institut, RWTH Aachen University, 52056 Aachen, Germany

We report on the magnetotransport study of topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ thin films. The films were grown on a silicon on insulator (SOI) substrate with a Si(111)-layer on top by molecular beam epitaxy. In $Bi_2Te_3$ samples, we observed a positive magnetoresistance at low magnetic fields with a cusplike minimum at $B = 0$ (weak antilocalization) as well as positive magnetoresistance in the entire magnetic field range (up to 12 T). The weak antilocalization effect disappears when an in-plane field is applied, showing the anisotropy between the transport parallel and perpendicular to the quintuple-layers. The estimated phase coherent lengths up to 250 nm at low temperatures are comparable to those previously obtained for $Bi_2Te_3$. The magnetotransport measurements were also performed on MBE-grown films of $Sb_2Te_3$ (p-doped) as well as on the ternary compound $(Bi_{1-x}Sb_x)_2Te_3$ ($0<x<1$). A transition from n- to p-doping depending on $x$ has been seen in the measurements.

TT 61.4 Thu 16:00 H18

**Surface state contribution to thermoelectric transport in $Bi_2Te_3$** — •Nicki F. Hinsche[1], Florian Rittweger[1], Peter Zahn[3] und Ingrid Mertig[1,2] — [1]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, DE-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, DE-06120 Halle — [3]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 51 01 19, DE-01314 Dresden

Bulk $Bi_2Te_3$ and related heterostructures are well known as efficient thermoelectric materials [1,2]. Recent research revealed $Bi_2Te_3$ to be a strong topological insulator, i.e. its bulk is insulating, while its surface is metallic due to the presence of robust gapless surface states [3]. While the spin structure and the low-temperature electrical transport gained much attention, the physics of the thermoelectric transport is still under debate. To contribute on this, we studied the electronic structure of the $Bi_2Te_3$ surface with a fully relativistic screened Korringa-Kohn-Rostoker Green's function method. The thermoelectric transport properties were calculated within the relaxation time approximation of the Boltzmann theory. The influence of temperature and doping on the thermoelectric properties of the surface state were analysed in detail.

[1] T. M. Tritt *et al.*, MRS bulletin **31**, 188 (2006)
[2] N. F. Hinsche *et al.*, Phys. Rev. B **86**, 085323 (2012)
[3] H. Zhang *et al.*, Nature Phys. **5**, 438 (2009)

TT 61.5 Thu 16:15 H18

**Quasi-ballistic transport of Dirac fermions in a $Bi_2Se_3$ nanowire** — •Joseph Dufouleur — IFW-Dresden, Dresden, Germany

Quantum coherent transport of Dirac fermions in a mesoscopic nanowire of the 3D topological insulator $Bi_2Se_3$ is studied in the weak-disorder limit. At very low temperatures, many harmonics are evidenced in the Fourier transform of Aharonov-Bohm oscillations, revealing the long phase coherence length of surface states. Remarkably, from their exponential temperature dependence, we infer an unusual 1/T power law for the phase coherence length. This decoherence is typical for quasi-ballistic fermions weakly coupled to the dynamics of their environment.

**15 min. break**

TT 61.6 Thu 16:45 H18

**Quasi-ballistic transport of Dirac fermions in a $Bi_2Se_3$ nanowire** — •Joseph Dufouleur[1], Louis Veyrat[1], Andreas Teichgräber[1], Stephan Neuhaus[1], Christian Nowka[1], Silke Hampel[1], J érôme Cayssol[2,3], Joachim Schumann[1], Barbara Eichler[1], Oliver Schmidt[1], Bernd Büchner[1], and Romain Giraud[1,4] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany — [2]LOMA, University Bordeaux 1, F-33045 Talence, France — [3]Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [4]CNRS - Laboratoire de Photonique et de Nanostructures, Route de Nozay, 91460 Marcoussis, France

Quantum coherent transport of Dirac fermions in a mesoscopic nanowire of the 3D topological insulator $Bi_2Se_3$ is studied in the weak-disorder limit. At very low temperatures, many harmonics are evidenced in the Fourier transform of Aharonov-Bohm oscillations, revealing the long phase-coherence length of surface states. Remarkably, from their exponential temperature dependence, we infer an unusual $1/T$ power law for the phase coherence length $L_\varphi(T)$. This decoherence is typical for quasi-ballistic fermions weakly coupled to the dynamics of their environment.

TT 61.7 Thu 17:00 H18

**Magnetotransport in disordered HgTe ribbons** — •Sven Essert and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

HgTe quantum wells allow the realization of 2D topological insulator structures. They feature edge states which are protected from backscattering by time-reversal symmetry leading to dissipationless transport in the presence of non-magnetic disorder. We perform transport calculations using the four-band BHZ model to investigate the lifting of this protection by an external magnetic field. We find that the edge state transport is very robust to the application of a perpendicular magnetic field as long as the transport is still in the quasi-one dimensional regime, i.e. as long as the system is far from a topological

phase transition to the topologically trivial insulating phase. However, by gating parts of the system to the metallic regime and thereby allowing for true 2d transport, the effect of the magnetic field can be drastically increased.

TT 61.8 Thu 17:15 H18

**Probing the Band Topology of Mercury Telluride through Weak Localization and Antilocalization** — •Viktor Krueckl and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg

We investigate the effect of weak localization (WL) and weak antilocalization (WAL) in the diffusive transport through HgTe/CdTe quantum wells. Our results reveal different transitions between WL and WAL depending on the Fermi energy as well as the band topology [1]. If spin-orbit interactions from bulk and structure inversion asymmetry can be neglected, the magnetoconductance of a system with inverted band ordering features a transition from WL to WAL and back. This is a signature of the Berry phase arising for inverted band ordering and not present in heterostructures with conventional ordering. In presence of strong spin-orbit interaction both band topologies exhibit WAL, which is distinctly energy dependent solely for quantum wells with inverted band ordering. This can be explained by an energy-dependent decomposition of the Hamiltonian into two blocks.

[1] V. Krueckl and K. Richter, Semicond. Sci. Technol. **27**, 124006 (2012)

TT 61.9 Thu 17:30 H18

**Robustness of edge states in non-centrosymmetric superconductors** — •Raquel Queiroz und Andreas P. Schnyder — Max Planck Institut für Festörperforschung, 70569 Stuttgart, Germany

Nodal superconductors without inversion symmetry have non-trivial topological properties, manifested by topologically protected flat-band edge states [1-3]. Since the bulk is not fully gapped, the edge states of nodal superconductors can in principle be susceptible to impurities, which break translational symmetries. Using recursive Green's function techniques we study the robustness of these edge states against both magnetic and non-magnetic disorder. We show that for weak and dilute non-magnetic impurities, a finite number of mid-gap edge states remains at zero-energy. We compute the zero bias conductance of a junction between a normal lead and a non-centrosymmetric superconductor as a function of disorder strength. It is found that the flat-band edge states give rise to a nearly quantized zero-bias conductance even in the presence of non-magnetic impurities.

[1] A. P. Schnyder and S. Ryu, Phys. Rev. B 84, 060504(R) (2011)
[2] P. M. R. Brydon, A. P. Schnyder, and C. Timm, Phys. Rev. B 84, 020501(R) (2011)
[3] A. P. Schnyder, P. M. R. Brydon, and C. Timm, Phys. Rev. B 85, 024522 (2012)

TT 61.10 Thu 17:45 H18

**The Kondo cloud in helical edge states** — •Thore Posske and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

The Kondo cloud is one of the last left unobserved phenomena of the Kondo effect. It stands for spatially extended spin-spin correlation between the electrons in the leads and the spin of the impurity in a Kondo system. Attempts to measure the Kondo cloud directly at the impurity usually perturb the system vastly and therefore modify the Kondo cloud. Helical edge states of topological insulators obey a unique coupling of the direction of motion and the spin degree of freedom. This, as we show, allows for the possibility to find signatures of the Kondo cloud far away from its origin by measuring current-current correlations.

## TT 62: Superconductivity: Properties, Electronic Structure, Order Parameter

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

TT 62.1 Thu 15:00 H19

**$Y_3Pt_4Ge_{13}$: a superconductor with non-centrosymmetric crystal structure** — •Roman Gumeniuk, Michael Nicklas, Lev Akselrud, Walter Schnelle, Ulrich Schwarz, Alexander Tsirlin, Ulrich Burkhardt, Yuri Grin, and Andreas Leithe-Jasper — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The intermetallic compound $Y_3Pt_4Ge_{13}$ has been synthesized by high-pressure and high-temperature technique ($p$ = 8 GPa, $T$ = 1070 K). It crystalizes with non-centrosymmetric type-of-structure in the monoclinic space group $Cc$ ($a$ = 12.8781(2) Å, $b$ = 12.8384(2) Å, $c$ = 9.1080(1) Å, $\beta$ = 90.042(2) °, $V$ = 1505.9(1) Å$^3$) and is stable in the temperature range 4 K - 380 K. At 383 K structural phase transition for $Y_3Pt_4Ge_{13}$ was observed. Above the transition temperature, the crystal structure becomes rhombohedral (space group $R3c$, $a$ = 12.7423(1) Å, $c$ = 15.6888(1) Å, $V$ = 2206.0(1) Å$^3$). The low-temperature monoclinic modification of $Y_3Pt_4Ge_{13}$ becomes superconducting below $T_c$ = 4.5 K. Thermodynamic properties as well as transport measurements were conducted down to 0.4 K. The upper critical field $\mu_0 H_{c2}$ is 3.8 T. The data are consistent with a single energy gap with $s$-wave symmetry for the superconducting phase.

TT 62.2 Thu 15:15 H19

**Superconducting properties of the filled skutterudite $LaPt_4Ge_{12}$ probed by thermal conductivity** — •Heike Pfau, Ulrike Stockert, Roman Gumeniuk, Walter Schnelle, Helge Rosner, Michael Nicklas, Andreas Leithe-Jasper, Yuri Grin, and Frank Steglich — MPI for Chemical Physics of Solids, 01187 Dresden, Germany

Filled skutterudites have attracted much interest due to a remarkable variety of physical properties and ground states. Particular interest has been paid to the superconductors, which range from conventional BCS over multiband to unconventional types.

In this contribution we present results on the filled skutterudite $LaPt_4Ge_{12}$, which becomes superconducting below $T_c$ = 8.3 K with a critical field of $H_{c2}^0$ = 1.6 T. While for its Pr-counterpart an unconventional and/or a multiband coupling mechanism is discussed, NMR and photoemission measurements on the La-compound suggest conventional s-wave superconductivity. However, results on the series $La_xPr_{1-x}Pt_4Ge_{12}$ indicate compatible order parameters for the two stoichiometric end-compounds. As a complementary and very sensitive probe of the order parameter, we performed temperature and field dependent thermal conductivity measurements on $LaPt_4Ge_{12}$ down to temperatures below 100 mK. Our results do not show a typical s-wave behaviour, but point towards a more complex gap structure, which will be discussed in the context of previous results on both, $LaPt_4Ge_{12}$ and $PrPt_4Ge_{12}$.

TT 62.3 Thu 15:30 H19

**Direct observation of the superconducting gap in thin films of titanium nitride using terahertz spectroscopy** — •Uwe Santiago Pracht[1], Marc Scheffler[1], Martin Dressel[1], Tatyana Baturina[2], David Kalok[3], and Christoph Strunk[3] — [1]1. Physikalisches Institut, University of Stuttgart, Germany — [2]A. V. Rzhanov Institute of Semiconductor Physics SB RAS, Russia — [3]Institute of Experimental and Applied Physics, University of Regensburg, Germany

Thin films of superconducting titantium nitride (TiN) have recently gained attention for both applications (such as single-photon detectors) and fundamental reseach (as model system for the superconductor-insulator transition which is accompanied by uncommon superconducting properties). TiN has been studied comprehensively with (magneto-)transport studies, but only little is known about it's electrodynamical properties.

We report on the charge carrier dynamics of TiN thin films with critical temperatures of 3.4 K and below, which we study with THz spectroscopy in the frequency range 90-510 GHz. Our analysis provides access to superconducting properties like the real and imaginary parts of the complex conductivity, energy gap and penetration depth. These findings as well as the normal-state properties strongly suggest conventional weak-coupling BCS superconductivity [1].

[1] U. S. Pracht et al. Phys. Rev. B 86, 184503 (2012)

TT 62.4 Thu 15:45 H19

**Soft-mode enhanced superconductivity in the antiperovskite $APt_3P$, A=Sr, Ca, La** — •Rolf Heid and Klaus-Peter Bohnen — Institut für Festkörperphysik, Karlsruher Institut für Technologie

The surprising discovery of superconductivity in iron pnictides initiated an increased search for superconductivity in other unconventional compounds. Recently, a new class of P-based antiperovskites was synthesized, and superconductivity with a $T_c$ of 8.4 K was observed for $SrPt_3P$ [1]. Specific heat measurements indicated a strong-coupling scenario and the presence of low-energy phonon modes. Replacing Sr by Ca or La resulted in lower $T_c$'s and a progressive loss of strong-coupling signatures.

Here we present results of a first principles study of lattice dynamics and electron-phonon coupling properties of $APt_3P$, A=Sr, Ca, La, with full consideration of spin-orbit interaction. For $SrPt_3P$, the coupling is carried almost totally by a single low-frequency branch consisting of planar Pt vibrations, which result in a coupling constant of $\lambda \approx 2$. In $CaPt_3P$ this mode stiffens significantly thereby reducing $\lambda$ to about 1, while in $LaPt_3P$ the coupling is further reduced to 0.5 because of a shift of the electronic bands. In contrast to previous work [2,3], our ab initio results provide a consistent quantitative description of the key features of superconductivity in this new class of materials within the framework of the strong-coupling Eliashberg theory.

[1] Takayama et al. PRL **108**, 27001 (2012)
[2] Chen et al., PRB **86**, 125116 (2012)
[3] Kang et al., arXiv:1207.6196

**Topical Talk** TT 62.5 Thu 16:00 H19

**Condensation Energy of $CeCu_2Si_2$ and Theoretical Implications** — •Stefan Kirchner — Max Planck Institute, Dresden, Germany

Unconventional superconductivity occurs in a broad range of strongly correlated electron systems. These systems are not only of varying effective dimensionality but their parent compounds out of which superconductivity emerges ranges from metals to bad metals and Mott insulators. The only unifying characteristic features seems that unconventional superconductivity occurs in close vicinity of zero-temperature instabilities which are most often magnetic in nature. Heavy fermion compounds represent prototype systems to address the interplay between quantum criticality and unconventional superconductivity. In $CeCu_2Si_2$, the magnetic quantum phase transition and superconductivity occur at ambient pressure which allows for a detailed study of the energetics across the superconducting transition. Based on an in-depth study of the magnetic excitation spectrum of $CeCu_2Si_2$ in the normal and superconducting state we obtain a lower bound for the change in exchange energy. The comparison with the superconducting condensation energy demonstrates that the built-up of magnetic correlations near the quantum critical point does drive superconductivity in $CeCu_2Si_2$. In addition, our comparison establishes a huge kinetic energy loss which we relate to the competition of Kondo screening and superconductivity as the opening of the gap weakens the Kondo effect. We discuss the relation between kinetic energy loss and the nature of the underlying quantum critical point.

**15 min. break**

TT 62.6 Thu 16:45 H19

**Magnetic and Superconducting Phases in RE-doped Chrysene** — •Franziska Hammerath, Pietro Carretta, Gianluca A. Artioli, and Lorenzo Malavasi — University of Pavia - CNISM, 27100 Pavia, Italy

We present the first magnetic susceptibility, nuclear magnetic resonance (NMR) and muon spin rotation ($\mu$SR) investigations of rare earth (RE) doped Chrysene, (RE = Sm, Eu and La), a promising candidate for a new superconducting (SC) hydrocarbon material. The magnetic susceptibility of pure Chrysene is only weakly temperature dependent, its zero-field $\mu$SR measurements indicate a high fraction of Muonium formation and its $^1$H-NMR spectra and relaxation rates are determined by the dominant nuclear dipolar interactions. The NMR, $\mu$SR and susceptibility measurements on the RE-doped compounds show different behaviors, thus confirming the formation of REChrysene phases. Indications of superconductivity are present in La- and Sm-doped Chrysene with SC transition temperatures of 6 K and 4-7 K, respectively. While LaChrysene exhibits a rather high SC volume fraction ($\approx$ 30 %), the one of SmChrysene is always very small. The pressure and magnetic field dependence of $T_c$ of LaChrysene is very similar to the one of LaPhenanthrene [1], but has to be discussed in the context of a possible spurious fcc La phase, which shows similar SC properties. Such an effect can be excluded for SmChrysene. Susceptibility, NMR and $\mu$SR measurements on EuChrysene on the other hand evidence the onset of a magnetic order involving Eu ions.

[1] X. F. Wang *et al.*, J. Phys. Condens. Matter **24**, 345701 (2012)

TT 62.7 Thu 17:00 H19

**Imaging the Anisotropic Nonlinear Meissner Effect in Unconventional Superconductors** — Alexander P. Zhuravel[1], Behnood G. Ghamsari[2], Cihan Kurter[2], •Philipp Jung[3], Stephen Remillard[4], John Abrahams[2], Alexander Lukashenko[3], Alexey V. Ustinov[3], and Steven M. Anlage[2,3] — [1]B. Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, 61103 Kharkov, Ukraine — [2]CNAM, Physics Department, University of Maryland, College Park, ML 20742-4111, USA — [3]Physikalisches Institut and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [4]Physics Department, 27 Graves Place, Hope College, Holland, MI 49422, USA

We present measurements on the anisotropic nonlinear Meissner effect (aNLME). Using a laser scanning microscope we have directly imaged this effect in a self-resonant spiral patterned from a thin film of the $d_{x^2-y^2}$ superconductor $YBa_2Cu_3O_{7-\delta}$. The spiral is excited at one of its resonant frequencies while a focused laser spot is scanned across its surface. The local illumination by the laser gives rise to a detectable change in the resonant properties. At low temperatures, the aNLME causes a direction dependent contribution to the critical current density. This makes it possible to image the directions of nodes and antinodes of the superconducting order parameter and the contribution of Andreev bound states associated with them. These two contributions to the photoresponse can be distinguished by their temperature dependence, which is consistent with theoretical predictions.

TT 62.8 Thu 17:15 H19

**Effect of photo-induced hole doping on the Meissner screening in underdoped $YBa_2Cu_3O_{7-\delta}$** — •Evelyn Stilp[1,2], Andreas Suter[2], Elvezio Morenzoni[2], Thomas Prokscha[2], Zaher Salman[2], Hugo Keller[1], Patrick Pahlke[3,4], Ruben Hühne[4], Jordan C. Baglo[5], Ruixing Liang[5], and Robert F. Kiefl[5] — [1]Physik-Institut, University of Zurich, CH-8057 Zurich, Switzerland — [2]Laboratory for Muonspin Spectroscopy, PSI, CH-5232 Villigen PSI, Switzerland — [3]Inst. für Festkörperphysik,TU Dresden, D-01069 Dresden, Germany — [4]IFW Dresden, D-01069 Dresden, Germany — [5]Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada, V6T

For classical superconductors the interaction with light results in a reduction of the energy gap due to excess of quasiparticles. Surprisingly, this is very different for cuprate superconductors where it was found that illumination with light increases the charge carrier density. Systematic investigations in $YBa_2Cu_3O_{7-\delta}$ showed that $T_c$ is increased by this effect which is most pronounced at the heavily underdoped side of the phase diagram. Up to now studies of photo-induced processes have been restricted to investigations of transport properties and critical temperatures. Using low energy $\mu$SR changes in the Meissner screening profile caused by illumination were directly investigated. We will show that the photo-persistent effect in underdoped $YBa_2Cu_3O_{7-\delta}$ is related to an increase of the superfluid density close to the surface. We are also able to show that the oxygen ordering is a crucial ingredient of the photo-induced effect.

TT 62.9 Thu 17:30 H19

**Is there a magnetic analogon of the isotope effect in HTSC?** — •Dirk Wulferding[1], Peter Lemmens[1], Gil Drachuck[2], Meni Shay[2], Galina Bazalitsky[2], Rinat Ofer[2], Zaher Salman[3], Alex Amato[3], Christof Niedermayer[3], and Amit Keren[2] — [1]IPKM, TU-BS, Braunschweig — [2]Technion, Haifa, Israel — [3]PSI, Villigen, Switzerland

The successful growth of large $(Ca_xLa_{1-x})(Ba_{1.75-x}La_{0.25+x})Cu_3O_y$ (CLBLCO) allows now a systematic investigation of correlations between material properties and $T_c$. In particular, the parameter $x$ varies the magnetic super-exchange coupling $J$ by controlling the Cu-O-Cu buckling angle. Using Raman scattering (and $\mu$SR) we determine $J$ for a series of samples, and show that $T_c$ monotonically increases with increasing $J$. Our results are in contrast to recent Raman data (B. Mallett, arXiv:1202.5078) showing the opposite behavior in other systems. The origin of the contradiction will be discussed. Work supported by

DFG, GIF and the ESF.

TT 62.10 Thu 17:45 H19

**Gold nanocrystals in high-temperature superconducting films: Creation of pinning patterns of choice** — •Christian Katzer[1], Claudia Stahl[2], Peter Michalowski[1], Sebastian Treiber[2], Georg Christiani[3], Frank Schmidl[1], Paul Seidel[1], Gisela Schütz[2], and Joachim Albrecht[4] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, 07743 Jena — [2]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart — [4]Hochschule Aalen, Beethovenstraße 1, 73430 Aalen

Many superconducting thin film devices require a spatially resolved current carrying capability due to different boundary conditions. On the one hand, the critical current density and the pinning of flux lines respectively should be high to reduce flux noise in the antenna regions of gradiometers; on the other hand, the critical current density of the Josephson junctions itself must not be too high to ensure a proper functionality. We report that adding gold nanoparticles during the preparation process of epitaxial $YBa_2Cu_3O_{7-\delta}$ thin films offers the possibility of creating spatially varying flux pinning properties, thus allowing to locally enhance the critical current density up to a factor of two. Magneto-optical investigations as well as transport measurements will be presented, indicating that an Au particle induced modification of the YBCO pinning properties allows the engineering of the critical current landscape on the sub-micrometre scale.

TT 62.11 Thu 18:00 H19

**Temperature dependence of band gaps in semiconductors: electron-phonon interaction** — •Reinhard K. Kremer[1], M. Cardona[1], R. Lauck[1], J. Bhosale[2], A. K. Ramdas[2], A. Burger[3], A. Muñoz[4], and A. H. Romero[5] — [1]MPI for Solid State Research, Stuttgart, Germany — [2]Physics Dep., Purdue University, West Lafayette, IN — [3]Fisk University, Dep. of Life and Physical Sciences, Nashville, TN, USA — [4]MALTA Consolider Team, Dep. de Física Fundamental II, and Instituto de Materiales y Nanotecnología, Universidad de La Laguna, La Laguna, Tenerife, Spain — [5]CINVESTAV, Dep. de Materiales, Unidad Querétaro, Querétaro, Mexico and MPI für Mikrostrukturphysik, Weinberg 2, Halle, Germany

We investigate the temperature dependence of the energy gap of several semiconductors with chalcopyrite structure and re-examine literature data and analyze own high-resolution reflectivity spectra in view of our new *ab initio* calculations of their phonon properties. This analysis leads us to distinguish between materials with *d*-electrons in the valence band (e.g. $CuGaS_2$, $AgGaS_2$) and those without *d*-electrons (e.g. $ZnSnAs_2$). The former exhibit a rather peculiar non-monotonic temperature dependence of the energy gap which, so far, has resisted cogent theoretical description. We demonstrate it can well be fitted by including two Bose-Einstein oscillators with weights of opposite sign leading to an increase at low-T and a decrease at higher T's. We find that the energy of the former correlates well with characteristic peaks in the phonon density of states associated with low-energy vibrations of the *d*-electron constituents.

## TT 63: Focused Session: Dynamical Mean-Field Approach to Correlated Electron Materials (jointly with MA)

During the last few years conventional band-structure calculations in the local density approximation (LDA) have been merged with a modern many-body approach, the dynamical mean-field theory (DMFT), into a novel computational method referred to as LDA+DMFT. This framework has proved to be a breakthrough for the realistic modeling of the electronic, magnetic, and structural properties of correlated electron materials. The Focused Session will review the significant recent progress made in this internationally active field of research.

Organizers: Ralph Claessen (University of Würzburg), Eva Pavarini (Forschungszentrum Jülich), Dieter Vollhardt (University of Augsburg)

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

**Invited Talk** TT 63.1 Thu 15:00 H20

**How Bad Metals Turn Good: Spectroscopic Signatures of Resilient Quasiparticles** — •Antoine Georges — College de France and Ecole Polytechnique, France

Many materials with strong electronic correlations display metallic-like resistivity up to very high temperature, with values exceeding the Ioffe-Regel-Mott (IRM) criterion. Yet, at low enough temperature, good metallic conductivity obeying Fermi liquid behaviour can be recovered. In this talk, I will explore how this crossover takes place. I will show that the Fermi liquid scale, which is strongly suppressed by strong correlations, should not be confused with the much higher Brinkman-Rice scale, at which incoherent transport sets in.

In between these two scales, an extended regime of metallic transport applies, in which the resistivity is smaller than the IRM value but does not follow a $T^2$ Fermi-liquid law. Well-defined quasiparticle excitations do exist in this regime, as manifested in the one-particle spectral function and optical conductivity, with properties distinct from Landau and Drude theories. For a hole-doped Mott insulator, a strong particle-hole asymmetry applies down to low-energy: electron-like excitations are much longer lived, placing these quasiparticle excitations on the 'dark side' for ARPES spectroscopy. This also has implications for the temperature dependence of the thermopower.

[1] X. Deng, J. Mravlje, R. Zitko, M. Ferrero, G. Kotliar, A. Georges, arXiv:1210.1769

**Topical Talk** TT 63.2 Thu 15:30 H20

**Correlation Effects in Organic Superconductors** — •Roser Valenti — Institut für Theoretische Physik, Goethe Universität Frankfurt, Frankfurt, Germany

Organic charge transfer salts are unique correlated systems with a complex phase diagram that can be finely tuned by chemical substitution or moderate pressures. Observed phases in these systems include metals, Fermi liquids, Mott insulators, antiferromagnets, spin liquids, and unconventional superconductors. A realistic description of these systems can be provided by a combination of density functional theory with dynamical mean field theory (LDA+DMFT). Such an approach has not been attempted in the past due to the complex crystal structures of these materials. Here we present recent LDA+DMFT calculations based on a new scheme to obtain molecular Wannier orbitals for a few families of organic layered conductors and discuss their spectral and optical conductivity properties.

[1] H. C. Kandpal, I. Opahle, Y.-Z. Zhang, H. O. Jeschke, and R. Valenti, Phys. Rev. Lett. **103**, 067004 (2009)
[2] J. Ferber, K. Foyevtsova, H.O. Jeschke, and R. Valenti, arXiv:1209.4466 (2012)

**Topical Talk** TT 63.3 Thu 16:00 H20

**Photoemission Study of Correlated Oxides at High Temperatures** — Jonas Weinen[1], Stefano Agrestini[1], Martin Rotter[1], Alexander Komarek[1], Yen-Fa Liao[2], Ku-Ding Tsuei[2], Chien-Te Chen[2], and •Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan

Strongly correlated oxides show often quite spectacular and intriguing properties which can be traced back to the presence of several competing interactions leading to various forms of ordered phases at low temperatures. In order to unravel which of the interactions are relevant, we have set out to study the excitation spectra of the several benchmark oxides as a function of temperature. By carrying out bulk-sensitive hard-x-ray photoemission experiments at high temperatures,

we can follow the changes in the spectra and thereby determine which and how local spin and orbital degrees of freedom as well as nearest neighbour spin-spin correlations influence the intricate and complex electronic structure of correlated oxides.

**15 min. break**

**Invited Talk** TT 63.4 Thu 16:45 H20

**Dynamical Mean Field Theory of Collective Excitations** — •Alexander Lichtenstein — University of Hamburg, Hamburg, Germany

Dynamical mean field theory (DMFT) in combination with the first-principle scheme is an optimal starting point to go beyond static density functional approximation and include effects of local spin, orbital and charge fluctuations. In order to investigate collective non-local excitations we formulate a general framework which start from the DMFT solution for strongly correlated materials within a numerically exact continuous-time Quantum Monte Carlo impurity solver[1] and use a dual-particle transformation in the path integral formalism to find an optimal diagrammatic series for the lattice Green functions.

[1] E. Gull, A.J. Millis, A.I. Lichtenstein, A.N. Rubtsov, M. Troyer, and Ph. Werner, Rev. Mod. Phys. **83**, 349 (2011)

**Topical Talk** TT 63.5 Thu 17:15 H20

**Electronic Correlations beyond Dynamical Mean Field Theory** — •Karsten Held — Institute for Solid State Physics, TU Wien

Dynamical mean field theory has been a big step forward for our understanding of electronic correlations. A major part of the electronic correlations, the local ones, are included. The arguably most fascinating physical phenomena of solid state physics, however, such as (quantum) criticality and the physics of high-T superconductors are based on non-local correlations.

To address these problems, recently diagrammatic extensions of the dynamical mean field theory have been developed, coined dynamical vertex approximation [1] and dual fermion approach [2]. Among others, these approaches allow for describing spin-fluctuation-mediated pseudogaps and for calculating critical exponents of the Hubbard model [3].

[1] A. Toschi, A. A. Katanin, and K. Held, Phys. Rev. B **75**, 045118 (2007)
[2] A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B **77**, 033101 (2008)
[3] G. Rohringer, A. Toschi, A. Katanin, and K. Held, Phys. Rev. Lett. **107**, 256402 (2011)

## TT 64: Superconductivity: Heterostructures, Andreev Scattering, Vortex Physics

Time: Thursday 15:00–18:15 Location: H21

TT 64.1 Thu 15:00 H21

**Spin injection from a normal metal into a mesoscopic superconductor** — •Michael J. Wolf[1], Florian Hübler[1,2,3], Stefan Kolenda[1], Hilbert v. Löhneysen[2,3,4], and Detlef Beckmann[1,2] — [1]Institut für Nanotechnologie, KIT, 76021 Karlsruhe, Germany — [2]Center for Functional Nanostructures, KIT, 76131 Karlsruhe, Germany — [3]Institut für Festkörperphysik, KIT, 76021 Karlsruhe, Germany — [4]Physikalisches Institut, KIT, 76128 Karlsruhe, Germany

We report on nonlocal transport in superconductor hybrid structures, with ferromagnetic as well as normal-metal tunnel junctions attached to the superconductor. In the presence of a strong Zeeman splitting of the density of states, both charge and spin imbalance is injected into the superconductor. While previous experiments [1,2] demonstrated spin injection from ferromagnetic electrodes, we show that spin imbalance is also created for normal-metal injector contacts. Using the combination of ferromagnetic and normal-metal detectors allows us to directly discriminate between charge and spin injection, and demonstrate a complete separation of charge and spin imbalance. The relaxation length of the spin imbalance is of the order of several $\mu$m and is found to increase with a magnetic field, but is independent of temperature. We further discuss possible relaxation mechanisms for the explanation of the spin relaxation length.

[1] F. Hübler *et al.*, Phys. Rev. Lett. **109**, 207001 (2012)
[2] C. H. L. Quay *et al.*, arXiv:1208.0500

TT 64.2 Thu 15:15 H21

**Subgap-anomalies in 3-terminal hybrid superconductor/normal metal nanostructures** — •Andreas H. Pfeffer[1,2], Hervé Courtois[3], and François Lefloch[1] — [1]CEA/INAC/SPSMS, Grenoble, France — [2]Nanoscience Foundation (RTRA), Grenoble, France — [3]CNRS/Néel Institute and UJF, Grenoble, France

We have studied the electronic transport properties of three terminal superconductor (S) - normal metal (N) - superconductor (S) nanodevices using a new SQUID-based experimental set-up working at very low temperature (30 mK) and dedicated for high sensitive conductance and current noise correlations measurements [1]. In a geometry where a T-shaped normal metal (Cu) is connected to three superconducting reservoirs (Al), new subgap anomalies appear in the differential conductance for specific values of the chemical potential applied to the superconductors. The most emphasized line appears when two superconductors (collectors) are biased at opposite voltage with respect to the third superconducting electrode (injector). This anomaly is consistent with the prediction of non-local quartets as the result of double crossed Andreev reflections (dCAR)[2]. In this particular process, a Cooper pair originating from the injector is split in two quasiparticles that recombine into Cooper pairs in each of the two collectors. Additional features appear for other integer voltage ratios and could be attributed to higher order processes of dCAR. The mechanism of non-local quartet opens perspectives toward a new generation of entanglers.

[1] PRL 107, 077005 (2011); RSI 83, 115107 (2012)
[2] PRL 106, 257005 (2011)

TT 64.3 Thu 15:30 H21

**Interaction of ultra soft magnetic materials with the high-$T_c$ superconductor YBCO** — •Claudia Stahl[1], Sebastian Treiber[1], Patrick Walker[1,2], Gisela Schütz[1], and Joachim Albrecht[2] — [1]Max Planck Institute for Intelligent Systems, Heisenbergstraße 3, 70569 Stuttgart — [2]Aalen University, Beethovenstraße 1, 73430 Aalen

We have grown bilayers of optimally doped $YBa_2Cu_3O_{7-\delta}$ (YBCO) and ferromagnetic CoFeB on single-crystalline substrates by pulsed laser deposition and sputtering. These heterostructures are typically composed of about 100 nm YBCO and several 10 nm of CoFeB. Regarding the superconductor, the properties of the YBCO film change as a consequence of the vicinity of the ferromagnet. In detail we investigated the critical current density as a function of temperature, applied field and time as well as the transition temperature by SQUID magnetization measurements and quantitative magneto-optical measurements. The amorphous material CoFeB exhibits an in plane anisotropy and a very low coercivity. From magneto-optical images we find that the flux line lattice of the superconductor is mapped into the magnet and still visible as significant magnetic out-of-plane contrast at room temperature. We discuss this phenomenon as a new route to high-resolution mapping of the flux line distribution on a nanometer scale.

TT 64.4 Thu 15:45 H21

**Proximity effect in ferromagnet-superconductor heterostructures with noncollinear magnetisation** — •Daniel Fritsch and James F. Annett — H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom

At the interface between a normal metal and a superconductor (SC) the proximity effect allows the (singlet pair) superconducting properties to leak into the normal metal side of the interface. Replacing the normal metal by a ferromagnet (FM) it has been found that unusual triplet pairs can form, which have been shown to decay much further into the metallic side compared to the singlet pairs [1]. This is called the long-range proximity effect.

To study the effects of triplet pair generation in the vicinity of a FM/SC interface we present results based on numerical solutions of the Bogoliubov - de Gennes equations, including spin-orbit coupling and noncollinear magnetisations. We use the calculated pairing amplitude and local density of states to obtain information about relevant

proximity length depending on system size and exchange fields.

[1] J. W. A. Robinson, J. D. S. Witt, and M. G. Blamire, Science **329**, 59 (2010).

TT 64.5 Thu 16:00 H21

**Nonlocal thermoelectric effects and nonlocal Onsager relations in a three-terminal proximity-coupled superconductor-ferromagnet device** — •Peter Machon[1], Matthias Eschrig[2], and Wolfgang Belzig[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]SEPnet and Hubbard Theory Consortium, Department of Physics, Royal Holloway, University of London, Egham, Surrey TW20 0EX, United Kingdom

We study thermal and charge transport in a three-terminal setup consisting of a superconducting and two ferromagnetic contacts. We predict that the simultaneous presence of spin-filtering and of spin-dependent scattering phase shifts at each of the two interfaces will lead to very large nonlocal thermoelectric effects both in clean and in disordered systems. The symmetries of thermal and electric transport coefficients are related to fundamental thermodynamic principles by the Onsager reciprocity. Our results show that a nonlocal version of the Onsager relations for thermoelectric currents holds in a three terminal quantum coherent ferromagnet-superconductor heterostructure including spin-dependent crossed Andreev reflection and coherent electron transfer processes.

TT 64.6 Thu 16:15 H21

**Josephson current through a quantum dot coupled to a molecular magnet** — •Pascal Stadler, Cecilia Holmqvist, and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Non-dissipative Josephson currents are carried by sharp Andreev states within the superconducting energy gap. We theoretically study the electronic transport of a magnetically tunable nanoscale junction consisting of a quantum dot connected to two superconducting leads and coupled to the spin of a molecular magnet. The exchange interaction between the molecular magnet and the quantum dot modifies the Andreev states due to a spin-dependent renormalization of the quantum dot's energy level and the induction of spin-flips. A magnetic field applied to the central region of the quantum dot and the molecular magnet further tunes the Josephson current and starts a precession of the molecular magnet's spin. We use a non-equilibrium Green's function approach to evaluate the transport properties of the junction. Our calculations reveal that the magnetic field and the exchange interaction between the molecular magnet and the electrons occupying the energy level of the quantum dot can trigger transitions from a 0 to a $\pi$ state of the Josephson junction. The redistribution of the occupied state induced by the magnetic field strongly modifies the current phase relation. The critical current exhibits a sharp increase as a function of the magnetic field.

**15 min. break**

TT 64.7 Thu 16:45 H21

**ac susceptibility investigation of vortex dynamics in nearly-optimally doped $ReFeAsO_{1-x}F_x$ (Re = La, Ce, Sm) and $Ba(Fe_{1-x}Co_x)_2As_2$ superconductors** — •Giacomo Prando[1], Romain Giraud[1], Saicharan Aswartham[1], Samuele Sanna[2], Mahmoud Abdel-Hafiez[1], Matteo Tropeano[3], Hans-Joachim Grafe[1], Marina Putti[3], Sabine Wurmehl[1], Anja Wolter-Giraud[1], Bernd Buechner[1], Roberto De Renzi[4], and Pietro Carretta[2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, Germany — [2]Dipartimento di Fisica, Universitá di Pavia and CNISM, Italy — [3]Dipartimento di Fisica, Universitá di Genova, Italy — [4]Dipartimento di Fisica, Universitá di Parma and CNISM, Italy

In this contribution we will report about the dynamical features of the flux lines in both optimally-doped $ReFeAsO_{1-x}F_x$ and $Ba(Fe_{1-x}Co_x)_2As_2$ superconductors as investigated by means of ac susceptometry. The features of pinning are derived in the case of $ReFeAsO_{1-x}F_x$ powder samples for several Re ions within the framework of the thermally-activated flux-creep model. In the case of the investigated $Ba(Fe_{1-x}Co_x)_2As_2$ single-crystal, the extremely high-quality and the associated low-degree of quenched disorder in the sample allow us to enlighten the emergence of a thermodynamical phase transition between the different configuration of vortices in the $H-T$ phase diagram. Insights will be provided into the features of this phase transition and into the nature of the glassy phase, being turned into a Bragg-like glass at low values of magnetic field.

TT 64.8 Thu 17:00 H21

**The relation between electrical fields and flux avalanches in $MgB_2$ films** — •Sebastian Treiber[1], Claudia Stahl[1], Soltan Soltan[2,4], and Joachim Albrecht[3] — [1]Max-Planck-Institut für Intelligente Systeme, Heisenbergstrasse 3, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Festkörperfoschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [3]Hochschule Aalen, Beethovenstrasse 1, 73430 Aalen, Germany — [4]Physics Department, Faculty of Science, Helwan University, 11792-Cairo, Egypt

The critical state in superconductors with strong pinning is inherently unstable. In most metallic materials, there is a threshold temperature below which large flux jump can destroy the critical state locally or even globally. The basic mechanism is a chain reaction due to local overheating. Thus, heat capacity and conductivity are important quantities in this process. Here, we want to focus on another important parameter, namely the electrical field. Large flux jumps, which are often referred to as flux avalanches, are triggered by a threshold value of the electrical field. Basically, one would expect the change of the external magnetic field $\dot{H}_{ext}$ as a direct source for electrical fields. Though a change of $H_{ext}$ is necessary to trigger an avalanche, the mechanism is more complex which is shown by means of magneto-optical, magnetization and transport measurements.

TT 64.9 Thu 17:15 H21

**Neutron dark field imaging of domain structures in superconductors** — •Tommy Reimann[1,2], Christian Grünzweig[3], Sebastian Mühlbauer[1], Michael Schulz[1,2], and Peter Böni[2] — [1]TU München, Forschungsneutronenquelle Heinz Maier Leibnitz (FRM II), 85747 Garching, Germany — [2]Physik Department E21, TU München, 85747 Garching, Germany — [3]Paul-Scherrer-Institut, CH-5232 Villigen, Switzerland

In the intermediate mixed state (IMS) of a type II superconductor (SC), the sample splits up into field-free Meissner domains and Shubnikov domains which carry the vortex lattice. The IMS is analog to the intermediate state (IS) of a type-I superconductor with normal and superconducting domains. Experiments on the topology of both states show a variety of different patterns including striped, dendritic and bubble phases, which represent typical domain morphologies also seen in various other physical contexts. A detailed investigation of domain patterns offers the possibility to study general characteristics of domain nucleation and morphology as well as the physical properties of vortex-vortex interactions. Domain structures in SC are typically investigated by surface sensitive techniques such as magneto optical imaging, but flux pinning as well as Landau branching can significantly hamper the deduction of bulk properties. In this talk we show how neutron grating interferometry (nGI) can be used as a tool for the unambiguous identification of bulk properties. The capability of this unique technique will be demonstrated on Pb and Nb single crystals, which are classical representatives of type I and type II SC respectively.

TT 64.10 Thu 17:30 H21

**Vortex dynamics in superconductor micro- and nanotubes: Interplay between the effects of curvature and pinning centers** — •V. M. Fomin[1], R. O. Rezaev[1,2], and O. G. Schmidt[1,3] — [1]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany — [2]National Research Nuclear University "Moscow Engineering Physics Institute", 115409 Moscow, Russia — [3]Material Systems for Nanoelectronics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Achievements in roll-up technique make it possible to fabricate cylindrical tubes of superconducting materials (e. g., Nb) of radius about 500 nm from a planar film of thickness about 50 nm, where the quasi-2-dimensionality of the film is combined with a curvature. The vortex dynamics in open tubes are significantly determined by the curvature of the superconductor at the nano- or microscale as well as by the impact of single and multiple pinning centers. The presence of the pinning centers allows for an efficient control over the threshold value of the transport current (for emergence of vortex dynamics) and the transition magnetic field (separating sparse- and many-vortex regimes).The detection of the tube curvature effects on vortex dynamics suggested in [1] stays feasible in the presence of pinning centers. This work was partly supported by the IEEE Council on Superconductivity.

[1] V. M. Fomin, R. O. Rezaev, and O. G. Schmidt, Nano Lett. 12,

1282 (2012).

TT 64.11 Thu 17:45 H21

**Electrical transport and pinning properties of Nb films with washboard-like nanostructures** — •Oleksandr V. Dobrovolskiy[1,2], Evgeniya Begun[1], Michael Huth[1], and Valerij A. Shklovskij[2,3] — [1]Physikalisches Institut Goethe-University, Frankfurt, Germany — [2]Department of Physics, Kharkiv National University, Ukraine — [3]Institute for Theoretical Physics NSC-KIPT, Kharkiv, Ukraine

A careful analysis of the magneto-transport properties of epitaxial nanostructured Nb thin films in the normal and the mixed state is performed. The nanopatterns were prepared by focused ion beam (FIB) milling. They provide a washboard-like pinning potential landscape for vortices in the mixed state and simultaneously cause a resistivity anisotropy in the normal state. Two matching magnetic fields for the vortex lattice with the underlying nanostructures have been observed. By applying these fields, the most likely pinning sites along which the flux lines move through the samples have been selected. By this, either the background isotropic pinning of the pristine film or the enhanced isotropic pinning originating from the nanoprocessing have been probed. Via an Arrhenius analysis of the resistivity data the pinning activation energies for three vortex lattice parameters have been quantified. The changes in the electrical transport and the pinning properties have been correlated with the results of the microstructural and topographical characterization of the FIB-patterned samples. The obtained results provide further insight into the pinning mechanisms at work in FIB-nanopatterned superconductors for fluxonic applications.

TT 64.12 Thu 18:00 H21

**Enhancement of critical current in mesoscopic superconducting strips by external magnetic field** — •Konstantin Ilin, Dagmar Henrich, Yannick Luck, Lea Fuchs, Johannes Maximilian Meckbach, and Michael Siegel — Institut für Mikro- und Nanoelektronische Systeme, Karlsruher Institut für Technologie, Hertzstraße 16, 76187 Karlsruhe, Germany

Current crowding in superconducting mesoscopic strips with bends results in decrease of critical current in these structures with respect to the strips without geometrical non-uniformities [1-3]. Recently it has been shown that Meissner currents induced by externally applied magnetic field of appropriate direction allow to suppress this effect so that $I_c(B)$ can exceed $I_c(0)$ [4]. Experimental dependencies of critical current in mesoscopic bended strips made from ultra-thin superconducting films on externally applied magnetic field and their comparison to the theoretical predictions will be presented and discussed.

[1] Phys. Rev. B 84, 174510 (2011)
[2] Phys. Rev. B 86, 144504 (2012)
[3] Appl. Phys. Lett. 100, 182602 (2012)
[4] Phys. Rev. B 85, 144511 (2012

## TT 65: Focused Session: Frontiers of Electronic Structure Theory 7 (jointly with HL and O)

Time: Thursday 16:00–19:00 Location: H36

TT 65.1 Thu 16:00 H36

**Determination of the one-body Green's function: freedom and constraints** — Giovanna Lani[1,4], •Pina Romaniello[2,4], and Lucia Reining[3,4] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Laboratoire de Physique Théorique-IRSAMC, CNRS, Université Paul Sabatier, Toulouse, France — [3]Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, Palaiseau, France — [4]European Theoretical Spectroscopy Facility (ETSF)

The one-particle Green's function $G$ plays a key role in many-body physics due to the wealth of physical information that it contains. In this work we go beyond the standard methods to calculate $G$, which are plagued by various shortcomings, and we use an approximate set of functional differential equations relating the one-particle Green's function to its functional derivative with respect to an external perturbing potential [1]. We show that this set of equations has, in principle, multiple solutions, but that only one is well behaved - this is the physical solution. We give the formally exact family of solutions, which depends on an auxiliary quantity $q$, for which we find stringent exact constraints. Our findings suggest that once $q$ is known, the physical solution is uniquely fixed by the vanishing Coulomb interaction limit [2-3].

[1] L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics (W.A. Benjamin Inc., New York, 1964)
[2] G. Lani, P. Romaniello, and L. Reining, New Journal of Physics, 14, 013056 (2012)
[3] G. Lani, P. Romaniello, and L. Reining, in preparation

TT 65.2 Thu 16:15 H36

**Restoring piecewise linearity in density-functional theory** — •Ismaila Dabo[1], Andrea Ferretti[2], Matteo Cococcioni[3], and Nicola Marzari[4] — [1]Ecole des Ponts ParisTech, Marne-la-Vallee, France — [2]CNR-Istituto Nanoscienze, Modena, Italy — [3]University of Minnesota, Minneapolis, USA — [4]EPFL, Lausanne, USA

Electronic-structure calculations based upon density-functional theory (DFT) have been fruitful in diverse areas of condensed matter physics. Despite their exceptional success, it can hardly be denied that a range of fundamental electronic properties fall beyond the scope of current DFT approximations. Many of the failures of DFT calculations take root in the lack of piecewise linearity of approximate functionals, which reverberates negatively on the electronic-structure description of systems involving fractionally occupied and spatially delocalized electronic states, including but not restricted to dissociated molecules, adsorbed species, charge-transfer complexes, and semiconducting compounds. In this talk, I will present a novel class of first-principles methods that restores the piecewise linearity of the total energy by imposing Koopmans' theorem to DFT approximations. The Koopmans-compliant approach is apt at describing full orbital spectra within a few tenths of an electron-volt relative to experimental direct and inverse photoemission data. This level of accuracy is comparable to the predictive performance of accurate many-body perturbation theory methods at a fraction of their computational cost, and with the additional benefit of providing accurate total energies for systems with fractional occupations.

TT 65.3 Thu 16:30 H36

**Self-interaction-corrected and Koopmans-compliant functionals: from molecules to solids** — •Giovanni Borghi[1], Linh Nguyen[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]Theory and Simulation of Materials, EPFL, Lausanne — [2]CNRNANO, University of Modena and Reggio Emilia — [3]Ecole des Ponts ParisTech, Université Paris-Est

We present an overview of the performance of self-interaction corrected, orbital-density dependent functionals as applied to the calculation of the electronic structure of atoms, molecules and solids.

In particular, we show how orbital-dependent corrections of Koopmans' compliant functionals are able to restore not only the correct ionization energies, but also the eigenvalues of low-lying single-particle states with an accuracy comparable or better to that of many-body perturbation theory, while retaining a variational principle which grants the possibility to optimize geometries and bond lengths.

The outcome of these orbital-density dependent calculation remain, even in the thermodynamic limit, Wannier-like orbitals, that localize thanks to a condition related to the Edmiston-Ruedenberg criterion. These localized functions can be used as Wannier interpolators of band structures, allowing to discuss the performance of the functionals in the solid-state limit.

TT 65.4 Thu 16:45 H36

**Lattice density functional theory at finite temperature with strongly density-dependent exchange-correlation potentials** — •Stefan Kurth[1], Gao Xianlong[2], A-Hai Chen[2], and Ilya Tokatly[1] — [1]Univ. of the Basque Country UPV/EHU, San Sebastian, Spain and IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [2]Zhejiang University, Jinhua, China

The derivative discontinuity of the exchange-correlation (xc) energy of density functional theory (DFT) at integer particle number is absent in many popular local and semilocal approximations. In lattice DFT, approximations exist which exhibit a discontinuity in the xc potential at half filling but due to convergence problems of the Kohn-

Sham (KS) self-consistency cycle, the use of these functionals is mostly restricted to situations where the local density is away from half filling. Here a numerical scheme for the self-consistent solution of the lattice KS Hamiltonian with a local xc potential with rapid (or quasi-discontinuous) density dependence is suggested. The problem is formulated in terms of finite-temperature DFT where the discontinuity in the xc potential emerges naturally in the limit of zero temperature. A simple parametrization is suggested for the xc potential of the uniform 1D Hubbard model at finite temperature obtained from the thermodynamic Bethe ansatz. The feasibility of the numerical scheme is demonstrated by application to a model of fermionic atoms in a harmonic trap. The corresponding density profile exhibits a plateau of integer occupation at low temperatures which melts away for higher temperatures.

TT 65.5 Thu 17:00 H36

**Kohn-Sham equations beyond the single-determinant approximation** — Nektarios N. Lathiotakis[1], •Nicole Helbig[2,3], Nikitas I. Gidopoulos[4], and Angel Rubio[3,5] — [1]Theoretical and Physical Chemistry Institute, NHRF, Athens, Greece — [2]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany — [3]Nano-Bio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC and DIPC, San Sebastián, Spain — [4]ISIS, STFC, Rutherford Appleton Laboratory, HSIC, Didcot, United Kingdom — [5]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We describe a new method for the optimization of the total energy in reduced density matrix functional theory (RDMFT) which reduces the computational costs to the costs of a density functional calculation within the optimized effective potential method. Within this method the natural orbitals are restricted to be solutions of a single-particle Schrödinger equation with a local effective potential which in addition to reducing the computational costs also provides an energy eigenvalue spectrum connected to the natural orbitals. This energy spectrum is shown to reproduce the ionization potentials of different atoms and molecules very well. In addition, the dissociation limit is well described without the need to break any spin symmetry, i.e. this attractive feature of RDMFT is preserved.

TT 65.6 Thu 17:15 H36

**Initial stages of time-evolution of excitations in Fermi liquids and finite systems** — •Yaroslav Pavlyukh[1], Jamal Berakdar[1], and Angel Rubio[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. de Física de Materiales, Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC and DIPC, Av. Tolosa 72, E-20018 San Sebastián, Spain

A particle-hole excitation in a many-body system is not an eigenstate and, thus, evolves in time. The evolution at short times after an excitation with the energy $\epsilon$ was created is the quadratic decay with the rate constant $\sigma^2(\epsilon)$. Later, after some set-in time $\tau(\epsilon)$, the exponential decay develops. It is governed by another rate constant $\gamma(\epsilon)$.

We study the electron-boson model for the homogenous electron gas and use the first order (in boson propagator) cumulant expansion of the electron Green's function. In addition to a quadratic decay in time upon triggering the excitation, we identify non-analytic terms in the time expansion similar to those found in the Fermi edge singularity phenomenon.

Finite systems (J. Chem. Phys., **135**, 201103 (2011)) give an opportunity to test the conjectured behavior numerically as an exact solution of a many-body problem is feasible. We propose a simple model for the electron spectral function that links together all three aforementioned parameters and give a prescription how the energy uncertainty $\sigma^2(\epsilon)$ can be computed within the many-body perturbation theory.

TT 65.7 Thu 17:30 H36

**Real-structure effects from *ab-initio* calculations** — •Andre Schleife — Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, Livermore, CA, USA

By harnessing the power of supercomputers, *computational materials science* is becoming a field that enables insight into fundamental materials physics. It is inevitable to further push *ab-initio* approaches, allowing them to account for effects that are important at the forefront of experimental research.

I will present the solution of the Bethe-Salpeter equation as a recent theoretical-spectroscopy technique and how it is extended and used to understand real-structure effects in oxide and nitride semiconductors. This talk will illustrate the success of our modification of this framework to describe the interplay of free electrons and excitonic effects in $n$-doped ZnO. Combining a cluster expansion scheme and electronic-structure calculations allows to explore the potential for band-gap tailoring in oxide and nitride alloys. These material systems are a driving force of current semiconductor technology, e.g. for solar cells and solid-state lighting; understanding fundamental effects will help to overcome performance limits.

In addition, computational materials science can *replace* dangerous experiments, e.g. in the context of radiation damage: I will present large-scale simulations of non-adiabatic electron-ion dynamics based on real-time time-dependent density functional theory that explain electronic stopping as an important mechanism responsible for radiation damage when fast H or He ions penetrate aluminum.

TT 65.8 Thu 17:45 H36

**Specwer: an efficient first-principle program for electronic structures and spectroscopic simulations of nanomaterials** — •Bin Gao — Center for Theoretical and Computational Chemistry, Department of Chemistry, University of Tromso, N-9037 Tromso, Norway

Although nanomaterials have been routinely synthesized and analyzed in various laboratories around the world, they still present great challenges for theoretical studies using the ab initio and/or first-principle methods due to the simple fact that they are too large to handle for the conventional theoretical approaches. Various linear-scaling methods have been proposed in recent decades to circumvent this difficulty. In this talk, I will present our recently developed program Specwer and its applications for electronic structures and spectroscopic simulations of different nanomaterials. For large-scale molecules, Specwer program employs the reduced single-electron density matrix and divide-and-conquer method. I will show its applications in the ground and excited states of nanomaterials at various density functional theory levels, in which the information of excited states is obtained via solving the so-called Liouville-von Neumann equation. I will also highlight the importance of including the spin-orbit coupling in some cases, for instance, the L-edge X-ray absorption spectroscopy, and the electron transport in double-stranded DNA molecules.

TT 65.9 Thu 18:00 H36

**Generalized incomplete-basis-set correction applied to EXX-OEP** — •Markus Betzinger, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We recently derived [1] an incomplete-basis-set correction (IBC) for all-electron response functions within the full-potential linearized augmented plane-wave (FLAPW) method as realized in the `FLEUR` code [2]. The IBC utilizes the potential dependence of the LAPW basis functions whose response is calculated explicitly by solving radial Sternheimer equations in the spheres. While in the original formulation of the IBC [1] only spherical perturbations of the potential have been taken into account, we show here an extension to non-spherical perturbations, replacing the single radial Sternheimer equation for each angular momentum $\ell$ by a set of equations coupling different angular momenta. Likewise, the response of the core electrons is computed. We demonstrate that this generalized IBC improves further the convergence in terms of basis-set size and number of unoccupied states. We apply the generalized IBC to the exact-exchange (EXX) optimized-effective-potential (OEP) approach. While for simple semiconductors and insulators the original IBC already leads to a physical and stable local EXX potential, we show that for more complex materials like NiO, whose band gap is formed by $d$ states, the generalization of the IBC is crucial to obtain a well-converged local optimized potential.

[1] M. Betzinger *et al.*, Phys. Rev. B **85**, 245124 (2012)
[2] http://www.flapw.de

TT 65.10 Thu 18:15 H36

**One particle spectral function and analytic continuation for many-body implementation in the exact muffin-tin orbitals method** — •Andreas Östlin[1], Liviu Chioncel[2,3], and Levente Vitos[1,4,5] — [1]Department of Materials Science and Engineering, Applied Materials Physics, KTH Royal Institute of Technology, Stockholm SE-100 44, Sweden — [2]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augs-

burg, Germany — [4]Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-751210, Uppsala, Sweden — [5]Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest H-1525, P.O. Box 49, Hungary

We investigate one of the most common analytic continuation techniques in condensed matter physics, namely the Padé approximant. Aspects concerning its implementation in the exact muffin-tin orbitals (EMTO) method are scrutinized with special regard towards making it stable and free of artificial defects. We discuss the difference between the **k**-integrated and **k**-resolved analytical continuations, as well as describing the use of random numbers and pole residues to analyze the approximant. It is found that the analytic properties of the approximant can be controlled by appropriate modifications. At the end, we propose a route to perform analytical continuation for the EMTO + dynamical mean field theory (DMFT) method.

TT 65.11 Thu 18:30 H36

**Core-electron forces within the FLAPW method** — •Daniel Aaron Klüppelberg, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

The full-potential linearized augmented-plane-wave method (FLAPW) is an all-electron electronic-structure method based on density functional theory (DFT). Characteristic to the method is that space is divided into spheres around the atoms, so called 'muffin-tins', and an interstitial region in between. Local orbitals can be used to describe semicore states within the valence-state formalism. It is established as an accurate tool for describing many properties of complex materials.

We address the occurrence of contributions to the forces due to core electrons described by wave functions having tails exceeding the muffin-tin boundary. Accurate forces are needed not only for relaxing the atomic structure to its ground state, but also in order to calculate precise phonon spectra via the finite-displacement method. We present a core-tail correction to the Pulay force term found by Yu *et al.* [1], implemented into the `FLEUR` code [2], which deals with the core electrons. This addition extends the known formula over the whole unit cell and therefore includes the complete force contribution coming from core states that extend beyond their muffin-tin. In this talk, we will present examples on the performance of this addition in comparison to the inclusion of local orbitals and the adjustment of the muffin-tin radii.

[1] R. Yu, D. Singh, and H. Krakauer, Phys. Rev. B **43**, 6411 (1991)
[2] www.flapw.de

TT 65.12 Thu 18:45 H36

**The linearized augmented lattice-adapted plane wave basis** — •Gregor Michalicek and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The full-potential linearized augmented plane wave method (FLAPW) is an all-electron electronic structure method that provides density functional results for complex solids with very high precision, irrespective of the chemical element of the solid. For this purpose the Kohn-Sham wavefunctions are expanded into LAPW basis functions. These are plane waves in an interstitial region (IR) that are augmented by atom-centered functions in non-overlapping spheres around each atom. The LAPW basis features many desirable properties that are a key component to the high precision of the FLAPW method.

In this talk we show that the capability of the FLAPW method can be kept with a modification of the basis-set that is numerically more efficient. We argue that the required plane-wave cut-off of the interstitial part of the LAPW basis results mostly from mathematical conditions and the efficiency of the LAPW description can be increased by incorporating more physics into the construction of this part of the basis. We propose a linearized augmented lattice-adapted plane wave basis ($(LA)^2PW$) that replaces the plane waves in the IR by smart linear combinations of plane waves, show how to realize an efficient implementation of such a basis, and provide a construction principle for the linear combination of plane waves. The so constructed basis is evaluated in terms of precision and calculation runtime performance.

## TT 66: Spintronics / Quantum Information: Vacancies in Diamond and SiC (jointly with HL)

Time: Friday 9:30–12:45 Location: H14

TT 66.1 Fri 9:30 H14

**Optical detection of coherent electron spin states of vacancy defects in silicon carbide** — •Sang-Yun Lee[1], Helmut Fedder[1], Torsten Rendler[1], Matthias Widmann[1], Nguyen Tien Son[2], Erik Janzén[2], and Jörg Wrachtrup[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Department of Physic, Chemistry and Biology, Linköping University, Linköping, Sweden

The diamond has been known as a hosting material in which an existing single spin system can be addressed optically at room temperature. A recent study has revealed that the individually detectible spin state can also exist in silicon carbide (SiC) [1]. However, the recent experimental finding has been done only on a newly found unknown defect in SiC. Among the other well known defects in SiC, the silicon vacancy ($V_{Si}$) can be another candidate because its coherent spin state has been successfully observed at room temperature with long life time by electron spin resonance [2], though the single spin detection is yet in question. While the conventional spin resonance method is suffered by the limited sensitivity, the optically detected magnetic resonance has been successfully used for the single spin detection. Thus the first step to elucidate whether this defect can be used as a room temperature solid state spin qubit, is to test the optical detection of its spin state at room temperature. We hereby report the optically detected spin coherence of the $V_{Si}$ spin ensemble at room temperature. Our efforts on single spin detection will be presented too.

[1] W. F. Koehl, *et al.*, Nature 479, 84 (2011)
[2] V. A. Soltamov, *et al.*, Physical Review Letters 108, 226402 (2012)

TT 66.2 Fri 9:45 H14

**Resonant addressing and manipulation of silicon vacancy spin qubits in silicon carbide** — •Daniel Riedel[1], Franziska Fuchs[1], Hannes Kraus[1], Andreas Sperlich[1], Vladimir Dyakonov[1,2], Alexandra Soltamova[3], Vladimir Ilyin[4], Pavel Baranov[3], and Georgy Astakhov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg — [3]Ioffe Physical-Technical Institute, St. Petersburg, RU-194021 Russia — [4]Saint Petersburg Electrotechnical University, St. Petersburg, RU-194021 Russia

Although several candidates have yielded feasible features for solid-state quantum information processing, there is a search for new systems with even higher potential [1].
We report that silicon vacancy ($V_{Si}$) defects in silicon carbide comprise the technological advantages of semiconductor quantum dots and the unique spin properties of nitrogen-vacancy defects in diamond.
Similar to atoms, the $V_{Si}$ qubits can be controlled under the double radio-optical resonance conditions, allowing for selective addressing and manipulation [2]. Magnetic resonance techniques are used to clarify the $V_{Si}$ spin multiplicity and reveal a long spin memory.
Our results pave the way for potential applications of the $V_{Si}$ defect in quantum information processing and spintronics.

References:
[1] D. DiVincenzo, Nature Materials 9, 468 (2010).
[2] D. Riedel et al., Physical Review Letters 109, 226402 (2012).

TT 66.3 Fri 10:00 H14

**Intrinsic defects in silicon carbide LEDs as a perspective single photon source** — •Franziska Fuchs[1], Victor Soltamov[2], Stefan Väth[1], Pavel Baranov[2], Eugeny Mokhov[2], Georgy Astakhov[1], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Ioffe Physical-Technical Institute, St. Petersburg, 194021 Russia — [3]ZAE Bayern, 97074 Würzburg

Single photon sources, reliably emitting on demand, are necessary for optical quantum computer architectures. Several systems seem suitable for this purpose, including atoms, molecules, quantum dots and colour centres in diamond. All these systems are difficult to implement, since they either only work at low temperatures, or do not emit

at typical wavelengths used in existing telecommunication infrastructure. We suggest another system - silicon vacancy defects in silicon carbide, emitting photons in the near infrared [1]. We fabricated light emitting diodes based on intrinsic defects in silicon carbide. The room temperature electroluminescence reveals two strong emission bands in visible and NIR, the latter assigned to silicon vacancy defects. Our approach can be used to realize an electrically driven single photon source for quantum telecommunication.

[1]Riedel et al.: Resonant Addressing and Manipulation of Silicon Vacancy Qubits in Silicon Carbide, Phys. Rev. Lett.109,226402(2012)

TT 66.4 Fri 10:15 H14

**A novel metastable spin triplet in diamond** — •Matthias Widmann[1], Sang-Yun Lee[1], Helmut Fedder[1], Torsten Rendler[1], Moritz Eyer[1], Sen Yang[1], Petr Siyushev[1], Marcus Doherty[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, University Stuttgart, Germany — [2]Laser Physics Center, National University, Canberra, Australia

In this talk a newly found, photo stable single spin center in a HTHP diamond nano-pillar, will be introduced. This new defect poses many properties, similar to those of the well-known NV-center in diamond. However, optically detected magnetic resonance showed positive contrast at room temperature in contrast to NV-centers. The photo physics and spin physics of this new defect have been studied to understand the enhancement of photon emission (contrast up to 45 %) at three different electron spin resonance frequencies. It will be shown that the defect contains a singlet ground-, and excited state, and a metastable spin 1 triplet state which act as a shelving state. The strong enhancement of photon emission by ESR can be attributed to the huge difference in the deshelving rates of each triplet states. It will be also shown that the coherent spin manipulation of the metastable triplet state is possible at room temperature. Even though the electron spin coherence time is limited by the life time of the triplet state (up to 2.5 $\mu$s), these findings suggest that the electron spin in this spin system can be used to read-out the coupled nuclear spin state because the nuclear spin can be protected during the initialization and storage processes thanks to the spin-less electron ground state.

TT 66.5 Fri 10:30 H14

**Nuclear spin control with a transient electron spin ancilla** — •Helmut Fedder[1], Sang-Yun Lee[1], Matthias Widman[1], Torsten Rendler[1], Moritz Eyer[1], Sen Yang[1], Petr Siyushev[1], Marcus Doherty[2], Neil Manson[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut and Research Center SCoPE, University Stuttgart, Germany — [2]Laser Physics Center, Research School of Physics and Engineering, Australian National University, Canberra, Australia

Electron spins associated with point defects in crystals are promising systems for solid state quantum technology [1-3]. In particular, defects with a spin-less ground state and an excited triplet state have been proposed as universal ancillae for addressing nuclear spins [2]. In here we demonstrate the control of an individual $^{13}$C lattice nuclear spin in diamond by exploiting a hitherto unknown electron spin defect that features an excited triplet state. Using optical and microwave control, we demonstrate coherent manipulation of the triplet electron spin and characterize its photo-physics. We then show coherent manipulation of the nuclear spin in the spin-less electronic ground state.

[1] J.J.L. Morton et al. Solid-state quantum memory using the 31P nuclear spin. Nature 455, 1085 (2008).
[2] V. Filidou et al. Ultrafast entangling gates between nuclear spins using photoexcited triplet states. Nature Phys. 8, 596 (2012).
[3] P.C. Maurer et al. Room-Temperature Quantum Bit Memory Exceeding One Second. Science 336, 1283 (2012).

TT 66.6 Fri 10:45 H14

**Entanglement by measurement and Bell inequality violation with spins in diamond** — •Wolfgang Pfaff[1], Tim H. Taminiau[1], Lucio Robledo[1], Hannes Bernien[1], Matthew Markham[2], Daniel J. Twitchen[2], and Ronald Hanson[1] — [1]Kavli Institute of Nanoscience Delft, Delft University of Technology, Netherlands — [2]Element Six, Ltd., Ascot, UK

Single spins in diamond have emerged as a promising platform for quantum information processing in the solid state. In particular, individual nuclear spins coupled to nitrogen-vacancy (NV) centers have been recognized as excellent candidates for solid state qubits, because they combine outstanding stability, excellent control by spin resonance techniques, and high-fidelity optical initialization and readout provided by the NV center.

Here we report the achievement of a milestone towards quantum computation with spins: The creation of high quality quantum entanglement between two nuclear spins in diamond. Entanglement is an important resource for quantum computation and lies at the heart of many key quantum protocols, such as teleportation and error correction. We show that we can produce entangled states of high fidelity using a projective quantum measurement. Our technique is non-destructive, and thus leaves the quantum information that is required for further computation unharmed. This enables us to demonstrate a violation of Bell's inequality for the first time with spins in the solid state.

Ref: Pfaff et al., Nature Phys., doi:10.1038/nphys2444 (2012).

**Coffee break**

TT 66.7 Fri 11:15 H14

**Spin polarisation mechanism in nitrogen-vacancy and related colour centres of diamond** — Lachlan Rogers[1], Neil Manson[2], and •Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm, Ulm, Deutschland — [2]Laser Physics Centre, Australian National University, Canberra, Australia

Optically induced spon polarisation of the negatively charged nitrogen vacancy centre in diamond ($NV^-$) has been known for a considerable time but there has not been a satisfactory account of how it arises. This lack of explanation is of concern because spin polarisation is the key unique property that allows the centre to function as a room temperature qubit. An optical emission band with ZPL at 1042 nm is understood to arise from a transition between spin-singlet levels which lie between the triplet ground and excited states. We report properties of the singlet levels obtained using spectroscopic techniques on the 1042 nm band. Importantly, we resolve the long-standing uncertainty over the order of these singlets. This improved understanding of the singlet system leads to a tentative description of the physical mechanism for spin polarisation in the $NV^-$ centre.

This raises the tantalising possibility of engineering "designer" colour centres for specific applications. For instance, the neutral $NV^0$ centre is known to have a metastable level between its ground and excited states. Manipulating it to open the intersystem crossing from this level back to the ground state would likely give rise to optically induced spin polarisation, opening a second solid-state optically-controlled qubit in diamond.

TT 66.8 Fri 11:30 H14

**Detecting and Polarizing Nuclear Spins in Diamond** — •Jochen Scheuer[1], Paz London[2], Jianming Cai[3], Ilai Schwarz[3], Alex Retzker[4], Martin B. Plenio[3], Masayuki Katagiri[5,6], Tokuyuki Teraji[6], Satoshi Koizumi[6], Junichi Isoya[5], Ran Fischer[2], Liam McGuinness[1], Boris Naydenov[1], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm, Ulm, Germany — [2]Department of Physics, Technion, Israel Institute of Technology, Haifa, Israel — [3]Institut für Theoretische Physik, Universität Ulm, Ulm, Germany — [4]Racah Institute of Physics, The Hebrew University of Jerusalem, Jerusalem, Israel — [5]Graduate School of Library, Information and Media Studies, University of Tsukuba, 1-2 Kasuga, Tsukuba, Ibaraki, Japan — [6]National Institute for Materials Science, Tsukuba, Ibaraki, Japan

Control and measurement of nuclear spins is essential for medicine, chemistry and physics, but the sensitivity of conventional measurement schemes is limited due to low thermal polarization of nuclei under ambient conditions. We use an electron-nuclear double resonance technique, known as Hartmann-Hahn double resonance, to demonstrate experimentally polarization of single and multiple nuclear spins in a room temperature solid. By transferring polarization from an optically cooled electron spin associated with the nitrogen-vacancy (NV) defect, to carbon nuclei we are able to control spin bath dynamics. This work opens new possibilities for different fields of science, from control over decoherence and use of mesoscopic ensemble of nuclear spins as qubits to enhancement of contrast in magnetic resonance imaging.

TT 66.9 Fri 11:45 H14

**Tailoring the Diamond: Microwave structures surrounding nano-fabricated solid immersion lenses registered to single emitters in diamond on demand** — •Luca Marseglia[1], Florian Striebel[1], Andreas Häussler[1], Boris Naydenov[1], Jan Meijer[2], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Universität Ulm,

Albert-Einstein-Allee 11, 89081 Ulm - Germany — [2]Ruhr-Universität Bochum, Universitätsstraße 150, 44801, Bochum, Germany.

The negatively charged Nitrogen Vacancy color center (NV) is a spin active defect with a long spin lifetime at room temperature. It is a three level system whose value of the ground state spin can be driven by applying a small microwave field making a NV centre a good candidate as qubit for quantum information purpose. To exploit the splitting of the ground state of the NV the control and the precision of a microwave field applied on a single NV is crucial. So we have successfully coupled the NV to a microwave structures, made of metal, lithographically deposited on the diamond, applying high intensity microwave field improving the addressing of the spin and the driving of the Rabi oscillation of the NV. Besides to directly improve the coupling efficiency from a planar surface we formerly developed a technique to fabricate solid immersion lenses (SILs), using Focus Ion Beam (FIB) system, who geometrically avoid any refraction at the diamond-air interface. Eventually we will create a microwave structure, placed precisely on the nanofabricated SIL coupled to the colour centre. These integrated structures will allow us to handle the spin of the NV centre with very high precision and microwave field intensity.

TT 66.10 Fri 12:00 H14

**Coherent Control of a $^{13}$C NV$^-$ center** — •Burkhard Scharfenberger[1], William J. Munro[2], and Kae Nemoto[1] — [1]National Institute of Informatics, 2-1-2 Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan — [2]NTT Basic Research Laboratories, NTT Corporation, 3-1 Morinosato Wakamiya, Atsugi, Kanagawa 243-0198, Japan

We investigate the theoretically achievable fidelities for coherently controlling an effective three qubit system consisting of a negatively charged NV center in diamond coupling via an hyperfine interaction to one nearby $^{13}$C nuclear spin using only micro- and radio wave pulses. With its long coherence times and comparatively simple optical accessibility, already the 'bare' NV$^-$ center has an interesting potential in quantum computing related applications. Although a number of experiments have already been conducted using NV centers with one or more $^{13}$C nearby, fidelities achieved are limited not only by experimental inaccuracies but a lack of theoretical understanding of the system dynamics. We seek to redress this by fully modelling the NVC systems behaviour in the ground state manifold, including all hyperfine interactions (between N and V as well as C and V) and dissipation where parameters are taken from previous experimental work as well as theoretical ab-initio studies. We show that for close-by carbons, the strong hyperfine interaction leads to unwanted mixing of levels which ultimately limits fidelities in single-qubit driving and entanglement generation to less than 99% in the experimentally interesting weak magnetic fields regime.

TT 66.11 Fri 12:15 H14

**Resolving individual spin defects in diamond beyond the diffraction limit by exploiting their charge state dynamics** — •Nabeel Aslam, Matthias Pfender, Gerald Waldherr, Philipp Neumann, and Jörg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart, Germany

The nitrogen-vacancy center in diamond is an electron and nuclear spin system that shows exceptionally good coherence properties at room temperature. This makes it a promising system for the implementation of quantum information processing. Furthermore the ability to sense magnetic and electric fields on the nanometer scale has been demonstrated for NV defects. Individual spin detection and initialization is performed optically by a confocal microscope which fails in resolving individual defects with a distance smaller than the diffraction limit. Here we demonstrate a novel microscopy method that is able to exploit the stochastically switching between different charge states achieving resolutions of 10 nm, well below the diffraction barrier. Compared with targeted switching based methods like STED this method applies at least five magnitudes lower laser power for a certain resolution. This is in fact a great improvement for the future use of nanodiamonds as biomarkers in cells with nanometer resolution. Even better resolutions can be achieved by combining this method with spin state manipulation.

TT 66.12 Fri 12:30 H14

**Investigations on nitrogen-vancancy center creation and its physical properties** — •Denis Antonov[1,2], Gabriel Bester[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

The negatively charged nitrogen-vacancy (NV$^-$) center embedded in extended and nanoscale diamond structures is a promising candidate for quantum information processing (QIP), magnetometry and even for biomarkers. A basic requirement for these applications is a precise prediction of the placement and a detailed understanding of the physical properties of the NV$^-$ center. Using a range of simulation techniques we consider the formation of NV$^-$ centers from the statistical standpoint, before performing accurate calculations for the optical properties of individual NV$^-$ centers. In particular, we investigate the channeling effect during shallow implantations in molecular dynamics and Monte Carlo simulations. Furthermore, a combination of a spin-polarized atomic effective pseudopotential and a configuration interaction approache is used to obtain many body effects in the excitonic spectra.

## TT 67: Topological Insulators 5 (jointly with DS, HL, MA, and O)

Time: Friday 9:30–13:00 Location: H18

TT 67.1 Fri 9:30 H18

**Structure factor of a weakly interacting helical liquid** — •Suhas Gangadharaiah[1,2], Thomas L. Schmidt[2], and Daniel Loss[2] — [1]Indian Institute of Science Education and Research, Bhopal, India — [2]Department of Physics, University of Basel, CH-4056 Basel, Switzerland

We calculate the density structure factor $S(q,\omega)$ of a weakly interacting helical liquid in the presence of a magnetic field $B$. The latter opens a gap of width $2B$ in the single-particle spectrum $\epsilon_\pm(k)$, and leads to a strongly nonlinear spectrum near $k = 0$. For chemical potentials $\mu > B$, the system then behaves as a nonlinear helical Luttinger liquid, and a mobile-impurity analysis reveals interaction-dependent power-law singularities in $S(q,\omega)$. For $\mu < B$, the low-energy excitations are gapped, and we determine $S(q,\omega)$ by using an analogy to exciton physics. We discuss the implications of the magnetic field induced non-linear spectrum on the Coulomb drag between the helical liquids.

TT 67.2 Fri 9:45 H18

**Strongly interacting Majorana modes in an array of Josephson junctions** — Fabian Hassler[1] and •Dirk Schuricht[2] — [1]Institute for Quantum Information, RWTH Aachen University — [2]Institute for Theory of Statistical Physics, RWTH Aachen University

An array of superconducting islands with semiconducting nanowires in the right regime provides a macroscopic implementation of Kitaev's toy model for Majorana wires. We show that a capacitive coupling between adjacent islands leads to an effective interaction between the Majorana modes. We demonstrate that even though strong repulsive interaction eventually drive the system into a Mott insulating state the competition between the (trivial) band-insulator and the (trivial) Mott insulator leads to an interjacent topological insulating state for arbitrary strong interactions.

TT 67.3 Fri 10:00 H18

**All-electrical measurement of crossed Andreev reflection in topological insulators** — •Rolf W. Reinthaler[1], Patrik Recher[2], and Ewelina M. Hankiewicz[1] — [1]Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Institute for Mathematical Physics, Technical University Braunschweig, Braunschweig, Germany

Using a generalized wave matching method we solve the full scattering problem for quantum spin Hall insulator (QSHI) - superconductor (SC) - QSHI junctions. We find that for systems narrow enough so

that the bulk states in the SC part couple both edges, the crossed Andreev reflection (CAR) is significant and the electron cotunneling (T) and CAR become spatially separated. We study the effectiveness of this separation as a function of the system geometry and the level of doping in the SC. Moreover, we show that the spatial separation of both effects allows for an all-electrical measurement of CAR and T separately in a 5-terminal setup or by using the spin selection of the quantum spin Hall effect in an H-bar structure [1].

We acknowledge financial support by the DFG grant HA 5893/3-1.

[1] R. W. Reinthaler, P. Recher, and E. M. Hankiewicz, arXiv:1209.5700 (2012)

TT 67.4 Fri 10:15 H18

**Zero-voltage conductance peak from weak antilocalization in a Majorana nanowire** — •Michael Wimmer[1], Dimitri Pikulin[1], Jan Dahlhaus[1], Henning Schomerus[2], and Carlo Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, The Netherlands — [2]Department of Physics, Lancaster University, United Kingdom

We show that weak antilocalization by disorder competes with resonant Andreev reflection from a Majorana zero-mode to produce a zero-voltage conductance peak of order $e^2/h$ in a superconducting nanowire. The phase conjugation needed for quantum interference to survive a disorder average is provided by particle-hole symmetry - in the absence of time-reversal symmetry and without requiring a topologically nontrivial phase. We identify methods to distinguish the Majorana resonance from the weak antilocalization effect.

TT 67.5 Fri 10:30 H18

**Spectral properties of disordered multi-channel Majorana wires** — •Patrick Neven, Dmitry Bagrets, and Alexander Altland — Institut für Theoretische Physik, Universität zu Köln, Köln, Germany

Proximity coupled multi-channel spin-orbit quantum wires may support midgap Majorana states at the ends. We study the fate of these Majorana fermions in the presence of disorder in such wires. Inspired by the widely established theoretical methods of mesoscopic superconductivity, we develop a quasiclassical approach which is valid in the limit of strong spin-orbit coupling. A numerical solution of the Eilenberger equation reveals that disordered topological wires are prone to the formation of a zero-energy anomaly (class D impurity spectral peak) in the local density of states which shares the key features of a Majorana peak. We also find that the $\mathbb{Z}_2$ topological invariant distinguishing between the state with and without Majorana fermions (symmetry class B and D, resp.) is related to the Pfaffians of quasiclassical Green's functions.

TT 67.6 Fri 10:45 H18

**Topological invariants and interacting one-dimensional fermionic systems** — •Salvatore R. Manmana[1,2,3], Andrew M. Essin[3], Reinhard M. Noack[4], and Victor Gurarie[3] — [1]Institut für Theoretische Physik, Universität Göttingen, Germany — [2]JILA, University of Colorado and NIST, Boulder (CO), USA — [3]Department of Physics, University of Colorado at Boulder, USA — [4]Fachbereich Physik, Philipps-Universität Marburg, Germany

We study one-dimensional, interacting, gapped fermionic systems described by variants of the Peierls-Hubbard model, and we characterize their phases via a topological invariant constructed out of their Green's functions. We demonstrate that the existence of topologically protected, zero-energy states at the boundaries of these systems can be tied to the value of the topological invariant, just like when working with the conventional, non-interacting topological insulators. We use a combination of analytical methods and the numerical density matrix renormalization group method to calculate the values of the topological invariant throughout the phase diagrams of these systems, thus deducing when topologically protected boundary states are present. We are also able to study topological states in spin systems because, deep in the Mott insulating regime, these fermionic systems reduce to spin chains. In this way, we associate the zero-energy states at the end of an antiferromagnetic spin-1 Heisenberg chain with a topological invariant equal to 2.

TT 67.7 Fri 11:00 H18

**Fluctuation driven topological Hund insulator** — •Jan Carl Budich[1], Bjoern Trauzettel[2], and Giorgio Sangiovanni[2] — [1]Department of Physics, Stockholm University, Se-106 91 Stockholm, Sweden — [2]Institute for theoretical physics and astrophysics, 97074 Würzburg, Germany

We investigate in the framework of dynamical mean field theory a two-band Hubbard model based on the Bernevig-Hughes-Zhang Hamiltonian describing the quantum spin Hall (QSH) effect in HgTe quantum wells. In the presence of interaction, we find that a system with topologically trivial non-interacting parameters can be driven into a QSH phase at finite interaction strength by virtue of local dynamical fluctuations. For very strong interaction, the system reenters a trivial insulating phase by going through a Mott transition. We obtain the phase diagram of our model by direct calculation of the bulk topological invariant of the interacting system in terms of its single particle Green's function.

**15 min. break**

TT 67.8 Fri 11:30 H18

**Floquet Topological Quantum Phase Transitions in the Wen-Plaquette Model** — •Victor Manuel Bastidas Valencia, Clive Emary, Gernot Schaller, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Our aim in this talk is to describe the nonequilibrium behavior of the topological quantum phase transition in the Ac-driven Wen-plaquette model. We show that under the effect of a nonadiabatic driving the system exhibits a novel topological phase. We define generalized topological order parameters by considering cycle-averaged expectation values of string operators in a Floquet state.

TT 67.9 Fri 11:45 H18

**Fermion-parity anomaly of the critical supercurrent in the quantum spin-Hall effect** — •Jan Dahlhaus[1], Dmitry Pikulin[1], Timo Hyart[1], Henning Schomerus[2], and Carlo Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, Niederlande — [2]Department of Physics, Lancaster University, United Kingdom

The helical edge state of a quantum spin-Hall insulator can carry a supercurrent in equilibrium between two superconducting electrodes (separation $L$, coherence length $\xi$). We calculate the maximum (critical) current $I_c$ that can flow without dissipation along a single edge, going beyond the short-junction restriction $L \ll \xi$ of earlier work, and find a dependence on the fermion parity of the ground state when $L$ becomes larger than $\xi$. Fermion-parity conservation doubles the critical current in the low-temperature, long-junction limit, while for a short junction $I_c$ is the same with or without parity constraints. This provides a phase-insensitive, dc signature of the $4\pi$-periodic Josephson effect.

TT 67.10 Fri 12:00 H18

**Topological kicked rotators** — •Jan Dahlhaus[1], Jonathan Edge[1], Jakub Tworzydlo[2], and Carlo Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, Niederlande — [2]Institute of Theoretical Physics, University of Warsaw, Poland

Topology is a nice mathematical concept that can have profound consequences on condensed matter systems. Maybe the most prominent examples are the quantum Hall effect, the quantum spin Hall effect and the 3D topological insulator. I will present a way to realize the ideas of band topology in a well-known and intensively-studied model - the quantum kicked rotator. This allows to study the Anderson localization properties of topological phase transitions numerically in a very efficient way, especially in higher dimensions. Furthermore it may open a way for experimental measurements of this transition behaviour with cold atomic gases in optical lattices.

TT 67.11 Fri 12:15 H18

**Theory of correlated topological insulators with broken axial spin symmetry** — •Stephan Rachel — TU Dresden, 01069 Dresden, Germany

The two-dimensional Hubbard model defined for topological band structures exhibiting a quantum spin Hall effect poses fundamental challenges in terms of phenomenological characterization and microscopic classification. We consider weak, moderate, and strong interactions and argue that the resulting phase diagrams depend on the microscopic details of the spin orbit interactions which give rise to the non-trivial topology. In particular, it turns out that there is a crucial difference between models with broken and with conserved axial spin symmetry. These results suggest that there is a general framework for

correlated 2D topological insulators with broken axial spin symmetry.

[1] Rachel, LeHur, PRB 82, 075106 (2010)
[2] Schmidt, Rachel, von Oppen, Glazman, PRL 108, 156402 (2012)
[3] Cocks, Orth, Rachel *et al.*, PRL 108, 205303 (2012)
[4] Reuther, Thomale, Rachel, PRB 86, 155127 (2012)

TT 67.12 Fri 12:30 H18

**Interaction effects on almost flat surface bands in topological insulators** — •Matthias Sitte, Lars Fritz, and Achim Rosch — Universität zu Köln, Institut für Theoretische Physik, Zülpicher Str. 77, 50937 Köln, Deutschland

We investigate ferromagnetic instabilities of the two-dimensional helical Dirac fermions hosted on the surface of three-dimensional topological insulators. We concentrate on ways to increase the role of interactions by means of modifying the bulk properties which in turn changes the surface Dirac theory characteristics. We discuss both long-ranged Coulomb interactions controlled by the dimensionless coupling constant $\alpha = e^2/(\hbar\epsilon v_F^{\rm surf})$ as well as short-ranged Hubbard-like interactions of strength $U$ which can induce spontaneous surface ferromagnetism, thereby gapping the surface Dirac metal. In both cases, we find that a prerequisite for observing this effect is to reduce the Fermi velocity $v_F^{\rm surf}$, and we consider different mechanisms to achieve this. While for long-ranged Coulomb interactions we find that screening hinders ferromagnetism, for short-ranged interactions screening is not that vital and the instability can prevail.

TT 67.13 Fri 12:45 H18

**Local spin susceptibility and surface states in doped three-dimensional topological insulators with odd-parity superconducting pairing symmetry** — •Björn Zocher[1,2] and Bernd Rosenow[1] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04103 Leipzig, Germany — [2]Max Planck Institut für Mathematik in den Naturwissenschaften, D-04103 Leipzig, Germany

We investigate characteristic features in the spin response of doped three-dimensional topological insulators with odd-parity unequal-spin superconducting pairing. To get insight into the nature of the superconducting pairing symmetry, we show that the odd-parity unequal-spin pairing can be mapped onto p-wave pairing and that these systems have gapless Majorana surface modes. The Majorana modes contribute to the local spin susceptibility, giving rise to a characteristic temperature behavior of the Knight shift and the spin-lattice relaxation time in magnetic resonance experiments. Because of their different decay lengths, the Majorana modes can be observed and clearly distinguished from the Dirac modes of the topological insulator by local probes which allow for a depth-controlled study of the electron spins on the nanometer length scale.

## TT 68: Transport: Spintronics, Magnetotransport 2 (jointly with HL and MA)

Time: Friday 9:30–10:30 Location: H20

TT 68.1 Fri 9:30 H20

**Bulk sensitive photoelectron spectroscopy on $CrO_2$ thin films** — •Jonas Weinen[1], Stefano Agrestini[1], Martin Rotter[1], Simone G. Altendorf[1], Zhiwei Hu[1], Chun-Fu Chang[1], Arun Gupta[2], Yen Fa Liao[3], Ku-Ding Tsuei[3], and Liu Hao Tjeng[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [2]The University of Alabama, Tuscaloosa, USA — [3]National Synchrotron Radiation Research Centre, Hsinchu, Taiwan

For transition metal compounds with a high oxidation state the so-called charge transfer energy can become negative, with the result that a spontaneous electron redistribution could occur in which oxygen holes are formed. Such seems to be the case for the ferromagnet $CrO_2$. Using the LDA+U method, Korotin et al. [PRL **80**, 4305 (1998)] calculated that the material is a metal and remains a metal even for very large values of U. This suggests that it is not so much the Cr 3*d* states that determine whether the system is metallic or insulating, but rather that it is the O 2*p* states which straddle the chemical potential.—Several photoelectron spectroscopy (PES) studies have been reported in the literature, but the results are not consistent, supposedly related to the fact that the surface of $CrO_2$ tends to decompose to $Cr_2O_3$ under vacuum conditions, so that surface sensitive PES may not have probed the true bulk spectrum of $CrO_2$.—We set out to perform bulk sensitive photoemission experiments below and above $T_C$ on $CrO_2$ thin films using our HAXPES system at SPring-8. Our results suggest that $CrO_2$ may be considered more like a bad metal rather than a normal metal.

This work is also supported by DFG through FOR1346.

TT 68.2 Fri 9:45 H20

**Initial stages of epitaxial growth of $Fe_3O_4$/MgO (001) thin films: atomic reconstruction at the polar interface** — •Chun-Fu Chang[1], Zhiwei Hu[1], Stefan Klein[2], Ronny Sutarto[2], Philipp Hansmann[2], Arata Tanaka[3], Julio Criginski Cesar[4], Nicholas Brookes[4], Hong-Ji Lin[5], Hui-Huang Hsieh[6], Chien-Te Chen[5], A. Diana Rata[1], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Köln, Germany — [3]Department of Quantum Matter, ADSM, Hiroshima University, Hiroshima, Japan — [4]ESRF, Grenoble Cédex, France — [5]NSRRC, Hsinchu, Taiwan — [6]Chung Cheng Institute of Technology, National Defense University, Taoyuan, Taiwan

By means of reflection high energy electron diffraction and Fe $L_{2,3}$ x-ray absorption spectroscopy we find evidence for an atomic structural reconstruction at the interface of polar $Fe_3O_4$/MgO (001) thin films. This reconstruction takes place over several monolayers, while each monolayer still preserves the $Fe_3O_4$ stoichiometery. Our findings for such a transition interface layer may have important implications especially in the field of spintronics, where ultrathin $Fe_3O_4$ films are widely used for various sensitive devices.

TT 68.3 Fri 10:00 H20

**Investigation of the Verwey transition in $Fe_3O_4$ thin films** — •Xionghua Liu, Akfiny Hasdi Aimon, A. Diana Rata, Chun-Fu Chang, and Liu Hao Tjeng — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

Magnetite $Fe_3O_4$ is one of the most investigated materials from the class of transition metal oxides. It shows a first-order anomaly in the temperature dependence of the electrical conductivity at $T_V$= 120 K, the famous Verwey transition. However, thin films of $Fe_3O_4$ show always a lower $T_V$ compared to the bulk material. In order to find out the reason for the decreased $T_V$ in magnetite thin films we have performed a systematic investigation of the transport properties in dependence of the oxygen pressure and thickness. Epitaxial $Fe_3O_4$ films were grown by Molecular Beam Epitaxy on MgO(100) and $MgAl_2O_4$ (100) substrates and the structural and spectroscopic characteristics were in-situ determined by RHEED and XPS, respectively. Resistivity measurements have been performed ex-situ by PPMS. Results of this study and ongoing work will be presented.

TT 68.4 Fri 10:15 H20

**Electronic Structure and Magnetic Properties of Sc doped EuO Thin Films** — •Andreas Reisner[1], Simone Altendorf[1], Chun-Fu Chang[1], Hong-Ji Lin[2], Chien-Te Chen[2], and Liu Hao Tjeng[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Str.40, 01187 Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsin-Ann Road, 30076 Hsinchu, Taiwan, R.O.C.

Europium monoxide is a ferromagnetic semiconductor with a Curie temperature $T_C$ of 69 K. Upon doping the material can show an increase of the Curie temperature, a metal-to-insulator transition and a high spin polarization of the charge carriers. Applying pressure can also enhance $T_C$. Mostly other trivalent rare earth metals are used as dopant. Here we set out to explore the possibility of using transition metals as dopants. As a start we focus on the non magnetic Sc ions. We are able to achieve excellent crystalline growth of Sc-doped EuO thin films on YSZ (001) substrates using molecular beam epitaxy. We will report our results on the crystal structure as characterized by RHEED and LEED, the electronic structure as determined by XPS and ARPES, and on the magnetic propertes as measured by SQUID.

# TT 69: Superconductivity: Fe-based Superconductors - Theory

Time: Friday 9:30–12:15 Location: H21

TT 69.1 Fri 9:30 H21

**Fermi surface topology of LaFePO, LiFeP and LiFeAs** — •Harald O. Jeschke, Johannes Ferber, and Roser Valenti — Institut für Theoretische Physik, Goethe-Unversität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany

We performed charge self-consistent LDA+DMFT (density functional theory combined with dynamical mean field theory) calculations to study correlation effects on the Fermi surfaces of the iron pnictide superconductors LaFePO, LiFeP and LiFeAs. We find a distinctive change in the topology of the Fermi surface in LaFePO and LiFeP where a hole pocket with Fe $3d_{z^2}$ orbital character changes its geometry from a closed shape in LDA to an open shape upon inclusion of correlations. In LiFeAs correlations influence mostly the shape of the hole pockets. We discuss our results in the context of angle-resolved photoemission spectroscopy and de Haas van Alphen observations.

TT 69.2 Fri 9:45 H21

**Finite temperature and pressure molecular dynamics for $BaFe_2As_2$** — •Steffen Backes and Harald Jeschke — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Germany

We investigate the temperature and pressure dependence of the structural and electronic properties of the iron pnictide superconductor $BaFe_2As_2$. We use density functional theory based Born-Oppenheimer molecular dynamics simulations to study the system at temperatures from $T = 5$ K to 150 K and pressures from $P = 0$ to 30 GPa. When increasing the pressure at low temperature, we find the two transitions from orthorhombic to tetragonal to collapsed tetragonal that are also observed in zero temperature structure relaxations and in experiment. However, the first of these transitions is considerably smeared out at finite temperature. We find a negative slope of the tetragonal to collapsed tetragonal transition in the T-P phase diagram in very good agreement with experiment. We also analyze the electronic structure of $BaFe_2As_2$ at finite temperature and work out differences between the time averaged band structure and Fermi surface at finite temperature compared to the known zero temperature results. Our results should be helpful for understanding some contradictions in experimental reports for $BaFe_2As_2$ under high pressure.

TT 69.3 Fri 10:00 H21

**Lattice dynamics of binary FeAs from first principles** — •Alexander Herbig[1,2], Rolf Heid[2], and Klaus-Peter Bohnen[2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie

Since the discovery of superconductivity in fluorine-doped LaFeAsO in 2008, the research on the so-called iron pnictides is rapidely developing. One of their building blocks, the FeAs layers, seem to play an important role for the physical properties of the iron pnictides. The rare theoretical work on binary FeAs motivated us to perform ab-initio calculations of electronic structure and lattice dynamics of this compound by means of density functional and linear response theory within the mixed-basis pseudopotential method.

We compared different collinear magnetic states with same crystal structure. Thereby an antiferromagnetic state, which is the best collinear approximation to the experimentally observed spin density wave [1], exhibits the lowest total energy in good agreement with previous calculations [2]. Without spin polarization, we found unstable phonon modes while magnetism stabilizes the phonon spectra.

Until now, no direct measurements of the phonon spectra are available. For the purpose of validating our phonon calculations we calculated the phononic heat-capacity and found good agreement with experiment.

[1] E. E. Rodriguez et al., Phys. Rev. B 83, 134520 (2011)
[2] D. Parker, I. I. Mazin, Phys. Rev. B 83, 180403 (2011)

**15 min. break**

TT 69.4 Fri 10:30 H21

**A1g phonon-induced electron dynamics of Fe pnictides at ultra-fast time scales** — •Bhaskar Kamble and Ilya Eremin — Theoretical Physics III, Ruhr Universität Bochum, 44801 Bochum

We employ the five-orbital tight-binding model to study the A1g phonon-induced electron dynamics of the Fe pnictides in the context of recent tr-ARPES experiments on BaFe2As2. By analyzing the experimental data we deduce the amplitude of the tetrahedra angle oscillation due to the A1g phonon and the modified band structure topology. We also find that in order to account for the experimental data in the coherent regime, the oscillations of the electronic structure should occur simultaneously with oscillations of the charge density on the iron site and we evaluate the amplitude of these oscillations from the five orbital model. Finally, we analyze the change in the magnetization as a function of the tetrahedral angle and find it is not symmetric around the mean value. This results in a higher value of the average magnetization within a cycle of the A1g phonon compared to the magnetization at the average value of the tetrahedral angle. This suggests that coherent oscillation of the A1g phonon mode may induce transient generation of the SDW state, and also suggests that the interaction strength in the Fe pnictides lies in the weak to the intermediately coupled regimes.

TT 69.5 Fri 10:45 H21

**Shedding light on the pairing mechanism in iron-based superconductors** — •Christoph Heil, Markus Aichhorn, Heinrich Sormann, Ewald Schachinger, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, University of Technology Graz, 8010 Graz, Austria

Whether superconductivity in iron-pnictides and -chalcogenides stems from local or itinerant effects is a question still debated on. In order to investigate the influence of Fermi surface nesting on the pairing mechanism, we calculate from first-principles calculations the static and dynamic susceptibility of various iron-based compounds. We show that the susceptibility depends sensitively on doping and pressure application and confront our theoretical results with conclusions drawn from experiments. For instance, our results give evidence that pairing through Fermi-nesting mechanisms alone is not sufficient to explain the evolution of the transition temperature with pressure in FeSe.

TT 69.6 Fri 11:00 H21

**The effect of weak disorder on the phase competition in unconventional superconductors** — •Mareike Hoyer and Jörg Schmalian — Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie

We investigate the phase competition between magnetism and superconductivity for iron pnictides in the presence of weak disorder. The competition of these two ordered states has been studied in detail by Fernandes and Schmalian [1] who came to the conclusion that in the case of unconventional $s^{+-}$ pairing, the superconducting and antiferromagnetic phase may coexist microscopically but are near to a parameter regime of mutual exclusion. Correspondingly, the multicritical point in the phase diagram is close to the transition from from a tetracritical to a bicritical point.

Close to the multicritical point, the free energy of the system can be expanded simultaneously in terms of magnetic and superconducting order parameters and the coefficients can be determined microscopically. We include the effect of impurity scattering in the model and investigate its influence on the phase diagram of iron pnictides.

[1] Rev. B **82**, 014521 (2010)

TT 69.7 Fri 11:15 H21

**Manifestations of impurity induced $s_{\pm} \rightarrow s_{++}$ transition: multiband model for dynamical response functions** — •Dmitri Efremov[1], Oleg Dolgov[2], and Alexander Golubov[3] — [1]IFW, Dresden — [2]FKF, Stuttgart — [3]University of Twente

We investigate effects of disorder on the density of states, the single particle response function and optical conductivity in multiband superconductors with $s_{\pm}$ symmetry of the order parameter, where $s_{+-} \rightarrow s_{++}$ transition may take place. In the vicinity of the transition the superconductive gapless regime is realized. It manifests itself in anomalies in the above mentioned properties. As a result, intrinsically phase-insensitive experimental methods like ARPES, tunneling and terahertz spectroscopy may be used for revealing of information about the underlying order parameter symmetry.

TT 69.8 Fri 11:30 H21

**Breaking of fourfold lattice symmetry in a model for pnictide superconductors** — Maria Daghofer and •Andre Fischer — IFW Dresden, Dresden, Germany

We investigate the interplay of onsite Coulomb repulsion and various mechanisms breaking the fourfold lattice symmetry in a three-band model for the iron planes of iron-based superconductors using cluster perturbation theory[1]. Previously investigated anisotropic magnetic couplings are compared to an orbital ordering field and anisotropic hoppings. We find that all three mechanisms lead to similar signatures once the onsite interactions are strong enough to bring the system close to a spin-density wave state.

[1] M. Daghofer and A. Fischer, Supercond. Sci. Technol. 25, 084003 (2012)

TT 69.9 Fri 11:45 H21

**Emergence of superconductivity in the presence of a metallic spin density wave** — •Jacob Schmiedt, Philip M. R. Brydon, and Carsten Timm — Institut für Theoretische Physik, TU Dresden, Germany

The coexistence of spin density wave (SDW) and superconducting (SC) order has gained significant attention in the field of iron pnictides since there is strong experimental evidence for microscopic coexistence in a number of compounds. Both types of order gap out the Fermi surface - at least partially. We study how the existence of a SDW gap influences the formation of the SC state and determines the preferred gap symmetry. In contrast to previous studies that use phenomenological pairing potentials, we take a more realistic approach of calculating the effective pairing interaction in the SDW background from the bare interactions using the random phase approximation. This scheme can also be applied to models with orbital degrees of freedom, which can lead to a deeper understanding of the coexistence and the interplay between SDW and SC order in multi-orbital systems such as the pnictides.

TT 69.10 Fri 12:00 H21

**Theoretical study of magneto-crystalline anisotropy in Fe pnictides** — •Alexander Yaresko — MPI FKF, Stuttgart, Germany

If spin-orbit coupling is taken into account, LSDA band structure calculations for parent Fe pnictides successfully reproduce the correct magnetic ground state with stripe antiferromagnetic (AFM) order and Fe moments aligned along $a$, i.e., along AFM Fe chains. They also predict that the out-of-plane ($ac$) magneto-crystalline anisotropy (MCA) in LaFeAsO and $BaFe_2As_2$ is stronger than the in-plane ($ab$) one. However, recent polarized inelastic neutron scattering experiment showed the opposite: the gap at zone center is larger for in-plane spin excitations than for out-of-plane ones, which means that it is easier to deviate Fe spins in the $ac$ plane. In this work it is shown that MCA in LaFeAsO, $BaFe_2As_2$, and NaFeAs is a non-monotonous function of the exchange splitting of Fe $d$ states. For large values of the splitting the out-of-plane MCA is stronger. However, for sufficiently small exchange splittings, which correspond to reduced Fe moments, the order of the MCA energies is reverted: in agreement with the experiment the in-plane $ab$ anisotropy becomes stronger. The microscopic origin of MCA in pnictides is also discussed.

## TT 70: Correlated Electrons: General Theory 2

Time: Friday 9:30–11:00 Location: H24

TT 70.1 Fri 9:30 H24

**Prethermalization and thermalization of weakly interacting quantum systems** — •Marcus Kollar and Michael Stark — Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg

When a quantum many-body system is suddenly forced out of equilibrium, it is expected to relax to the thermal state predicted by statistical mechanics, which depends only on energy and particle number. However, integrable systems usually relax instead to a nonthermal state, because a detailed memory on the initial conditions persists due to the many constants of motion. A special situation arises for weakly interacting systems: because of the nearby integrable, noninteracting Hamiltonian they are first trapped in a so-called prethermalized state, and can thermalize only at a later stage [1]. This prethermalization plateau is again due to a large number of – now only approximate – constants of motion and can be represented by a generalized Gibbs ensemble [2]. As the time evolution continues, we can describe the decay of this quasistationary state and the crossover to the thermal state by a kinetic integro-differential equation, with good quantitative agreement for quenches to small Hubbard interaction [3]. This approach provides a controlled and conceptually straightforward description of the thermalization dynamics and establishes that thermalization can occur even in the perturbative regime.

[1] M. Moeckel and S. Kehrein, PRL **100**, 175702 (2008).
[2] M. Kollar, F. A. Wolf, and M. Eckstein, PRB **84**, 054304 (2011).
[3] M. Eckstein, M. Kollar, and P. Werner, PRL **103**, 056403 (2009).

TT 70.2 Fri 9:45 H24

**Steady-State Nonequilibrium Dynamical Mean Field Theory: an auxiliary Master Equation approach** — •Enrico Arrigoni, Michael Knap, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics TU Graz, 8045 Graz, Austria

We present an approach to deal with nonequilibrium steady state properties of strongly correlated quantum many-body systems based on dynamical mean-field theory (DMFT). The impurity solver is based on the exact solution of an auxiliary system consisting of a finite number of bath sites coupled to the interacting impurity and to two Markovian reservoirs. The method can be seen as the extension of the DMFT impurity solver for the nonequilibrium case based on exact diagonalisation. We apply the method to study nonlinear quantum transport across correlated heterostructures.

TT 70.3 Fri 10:00 H24

**A variational cluster approach to strongly correlated quantum systems out of equilibrium** — •Martin Nuss, Enrico Arrigoni, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, Graz University of Technology, Petersgasse 16 8010 Graz , Austria

The theoretical understanding of the non-equilibrium behaviour of strongly correlated quantum many-body systems is a long standing challenge, which has become increasingly relevant with the progress made in the fields of molecular-and nano- electronics, spintronics, spectroscopy or quantum optics and simulation. We report on the development of non-equilibrium cluster perturbation theory, and its variational improvement, the non-equilibrium variational cluster approach for steady-state situations. Both methods are based on the Keldysh Green's function technique which allows accessing single particle dynamic quantities. These flexible and versatile techniques can in principle be applied to any fermionic / bosonic lattice Hamiltonian, including multi-band and multi-impurity systems. We present results for the steady-state of molecular / nanoscopic devices under bias including the effects of electron-electron interactions and magnetic fields.

TT 70.4 Fri 10:15 H24

**Dynamics in model systems of strongly interacting electrons** — •Malte Behrmann[1], Michele Fabrizio[2], and Frank Lechermann[1] — [1]I. Institut für Theoretische Physik, Jungiusstr. 9, 20355 Hamburg — [2]SISSA, via Bonomea 265, 34136 Trieste

Explicit time-dependent phenomena in strongly interacting quantum systems have recently become of great interest, especially in view of novel challenging experiments with time-dependent probing. Understanding the dynamic evolution of electronic correlations is a key issue in describing the non-equilibrium physics taking place in concrete material systems, e.g. after photo-excitation. This talk discusses work performed on the dynamics of strongly correlated model systems by means of a time-dependent slave-boson mean-field theory that allows for full rotational invariance in spin and orbital space. Therewith a generic time-dependent Mott scenario is accessible and the dynamics of quasiparticle and multiplet degrees of freedom may be monitored. Our approach is closely related to the time-dependent Gutzwiller framework by Fabrizio and coworkers [1].

[1] M. Schiró and M. Fabrizio, Phys. Rev. Lett. 105, 076401 (2010)

TT 70.5 Fri 10:30 H24

**Calculations of resonant x-ray emission spectra in compounds with localized f-electrons** — •Jindrich Kolorenc[1], Alexander B. Shick[1,2], and Roberto Caciuffo[2] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [2]European Commission, Joint Research Centre, Institute for Transuranium Elements, Karlsruhe, Germany

We discuss a theoretical description of the resonant x-ray emission spectroscopy (RXES) that is based on the Anderson impurity model. The theory builds on the ideas from [1-3] and extends them to take into account the f-electron multiplets. The parameters of the impurity model are taken from the LDA+DMFT calculations, and the coherent second-order optical process is calculated using the Lanczos method. The theory is applicable across the whole f series, not only in the limits of nearly empty (La, Ce) or nearly full (Yb) f shell. We illustrate the method on selected f-electron systems.

[1] O. Gunnarsson and K. Schönhammer, Phys. Rev. B **28**, 4315 (1983)
[2] S. Tanaka, H. Ogasawara, Y. Kayanuma, and A. Kotani, J. Phys. Soc. Jpn. **58**, 1087 (1989)
[3] M. Nakazawa, S. Tanaka, T. Uozumi, and A. Kotani, J. Phys. Soc. Jpn. **65**, 2303 (1996)

TT 70.6 Fri 10:45 H24

**Continuous Estimators for CT-HYB** — •Pavel Augustinský — University of Augsburg

We present an improved algorithm for measurement of the Green's function in the hybridization-expansion quantum Monte Carlo. The method is based on using continuous rather then discrete delta-function estimators. It fixes drawbacks of the standard approach at low perturbation orders and it can produce high-accuracy data for numerical analytical continuation of the selfenergy.

## TT 71: Graphene - Preparation and Characterization 2 (jointly with DS, HL, MA, and O)

Time: Friday 10:30–13:00 Location: H17

TT 71.1 Fri 10:30 H17

**Engineering of 2D-Nanomaterials by Swift Heavy Ion Irradiation** — •Oliver Ochedowski, Hanna Bukowska, Sevilay Akcöltekin, and Marika Schleberger — Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg

Two dimensional (2D) nanomaterials prepared from layered crystal materials have attracted a great amount of interest in multiple fields of science. These nanomaterials can be metallic (e.g. graphene), semiconducting (MoS2) or insulating (Mica) with properties often different from their bulk counterparts. Here, we will demonstrate how the morphology of several 2D-nanomaterials can be modified by swift heavy ion (SHI) irradiation in the MeV regime under glancing incidence angle. The induced modifications are investigated by means of atomic force microscopy. In the case of graphene we will show by Kelvin probe force microscopy how SHIs can be used to alter the electronic structure and induce doping of the graphene.

TT 71.2 Fri 10:45 H17

**Fabrication of laterally structured graphene/carbon nanomembrane hybrids** — •Andreas Winter[1], Stefan Wundrack[2], Rainer Stosch[2], and Andrey Turchanin[1] — [1]Universität Bielefeld, 33615 Bielefeld — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig

Laterally structured free-standing micro- and nanostructures of single-layer graphene (SLG) embedded into dielectric sheets with a thickness comparable to graphene are of great interest for applications in electronic or optoelectronic devices. However, their fabrication is not a trivial task at present. Here, we demonstrate how such hybrids can be engineered using electron-irradiation-induced crosslinking of graphene micro-/nanostructures with carbon nanomembranes (CNMs). CNMs are a dielectric 2D carbon material with the thickness of about 1 nm consisting of cross-linked randomly oriented benzene rings. We show scalable production of well-defined laterally patterned CNM-SLG hybrids of various architectures and characterize their structural, chemical and electronic quality by complementary spectroscopic and microscopic techniques including helium ion microscopy and Raman spectroscopy. Application areas of the generated hybrids will be discussed.

TT 71.3 Fri 11:00 H17

**Non-destructive chemical functionalization of single-layer graphene for electronic applications** — Mirosław Woszczyna[1], Miriam Grothe[1], Andreas Winter[2], Annika Willunat[1], Stefan Wundrack[1], Rainer Srosch[1], Franz Ahlers[1], Thomas Weimann[1], and •Andrey Turchanin[2] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [2]Faculty of Physics, University of Bielefeld, 33615 Bielefeld, Germany

Chemical functionalization of single-layer graphene (SLG) is of key importance for implementations of this material in functional electronic devices such as, e.g., field effect transistor (FET) based nanosensors. However, the electronic quality of graphene typically degrades after the functionalization with presently employed methods, significantly restricting the application areas. Here, we present a route to non-destructive chemical functionalization of graphene via engineering of carbon nanomembrane (CNM)/SLG hybrids. We employ SLG, grown by methane CVD on Cu foils, and amino-terminated 1 nm thick CNMs, generated by electron-beam-induced crosslinking of aromatic self-assembled monolayers, to fabricate hybrid CNM/SLG FETs on oxidized silicon wafers. Structural, chemical and electronic properties of these devices are characterized by Raman spectroscopy, X-ray photoelectron spectroscopy and electrical transport measurements. We unambiguously show that the intrinsically high electronic quality of pristine SLG is preserved in the amino-functionalized hybrids opening broad avenues for their use in graphene-based FETs.

TT 71.4 Fri 11:15 H17

**Etching Nanoscale tunnels into graphite- a new route to produce suspended graphene** — •Maya Lukas[1], Velimir Meded[1], Aravind Vijayaraghavan[1,2], Li Song[3,4], Pulickel M. Ajayan[4], Karin Fink[1], Wolfgang Wenzel[1], and Ralph Krupke[1,5] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, D-76021 Karlsruhe — [2]School of Computer Science, The University of Manchester, UK — [3]Research Center for Exotic Nanocarbons, Shinshu University, Nagano, Japan — [4]Department of Mechanical Engineering & Materials Science, Rice University, Houston, TX , USA — [5]Department of Materials and Earth Sciences, Technische Universität Darmstadt, D-64287 Darmstadt

Catalytic hydrogenation of graphite, although known since the 1970s, has recently attracted renewed attention, as a route for nanopatterning of graphene and to produce graphene nano-ribbons. These reports show that metallic nanoparticles etch surface layers of graphite or graphene anisotropically along the crystallographic zigzag <11-20> or armchair <1010> directions.

We report the sub-surface etching of highly oriented pyrolytic graphite (HOPG) by Ni nanoparticles, to form a network of tunnels, as seen by SEM and STM. The layers on top of tunnels which are only a few layers below the surface bend inward, while their local density of states remains fundamentally unchanged. Our work opens a new route to produce suspended graphene for the study of fundamental mechanical and electronic properties. M. Lukas, V. Meded *et al., Nat. Commun.* accepted for publication

TT 71.5 Fri 11:30 H17

**Direct e-beam writing of single-layer graphene nanostructures** — •Nils-Eike Weber[1], Henning Vieker[1], Stefan Wundrack[2], Rainer Stosch[2], and Andrey Turchanin[1] — [1]Fakultät für Physik, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig

We demonstrate direct writing of single-layer graphene nanostructures employing electron irradiation of aromatic self-assembled monolayers (SAM) and subsequent annealing. The process consists of the following technological steps: (i) formation of an aromatic SAM on a Cu substrate; (ii) electron-beam-irradiation of the SAM resulting in locally cross-linked SAM areas; (iii) conversion of these areas into single-layer graphene via annealing. In this way graphene nanostructures of various architectures are directly defined in the SAM by electron beam lithography reducing several manufacturing steps, which are typ-

ically applied for the patterning of two-dimensional sheets including graphene (baking and developing electron-beam resist, plasma etching, resist striping). The formed nanostructures were characterized by Raman spectroscopy, scanning electron and helium ion microscopy. We demonstrate their successful transfer from the original copper foils onto oxidized silicon wafers, where they can directly be integrated into electronic devices.

TT 71.6 Fri 11:45 H17

**Understanding of the imaging contrast in STM/NC-AFM of graphene on metals** — •Elena Voloshina[1], Edoardo Fertitta[1], Andreas Garhofer[2], Florian Mittendorfer[2], Mikhail Fonin[3], Torben Haenke[4], Oliver Schaff[4], Thorsten Kampen[4], Andreas Thissen[4], and Yuriy Dedkov[4] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institute of Applied Physics, Vienna University of Technology, Gusshausstr. 25/134, 1040 Vienna, Austria — [3]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [4]SPECS Surface Nano Analysis GmbH, Voltastraße 5, 13355 Berlin, Germany

Realization of graphene moiré superstructures on the surfaces of 4d and 5d transition metals offers templates with periodically modulated electron density, which is responsible for a number of fascinating effects, including the formation of quantum dots and the site selective adsorption of organic molecules or metal clusters on graphene. Here, applying the combination of scanning probe microscopy/spectroscopy and the density functional theory calculations, we gain a profound insight into the electronic and topographic contributions to the imaging contrast of the epitaxial graphene/Ir(111) system. We show directly that in STM imaging the electronic contribution is prevailing compared to the topographic one. In the force microscopy and spectroscopy experiments we observe a variation of the interaction strength between the tip and high-symmetry places within the graphene moiré supercell, which determine the adsorption sites for molecules or metal clusters on graphene/Ir(111).

TT 71.7 Fri 12:00 H17

**Precise imaging of graphene** — •Thomas Hofmann, Alfred J. Weymouth, Joachim Welker, and Franz J. Giessibl — Institut für Experimentelle und Angewandte Physik, Universität Regensburg

Atomic imaging of graphene with a scanning probe microscope is challenging due to its small atomic lattice. We show that metallic tips, which have been characterized prior to the measurement, cannot truthfully image the graphene surface due to their large, non-spherical electron density [1]. Calculations predict that the metal tip atom strongly interacts with the graphene surface [2]. Carbon oxide front atom identification (COFI) [2] shows that contact of a clean metal tip with graphene can lead to graphene flakes attaching to the tip apex. This results in blurred images and multi-valley force versus distance curves. As a solution we use a metal tip, functionalized with an inert carbon monoxide molecule as suggested by Gross et al. [3]. The closed-shell nature of the CO drastically reduces the attraction between tip and graphene. Additionally, the small size of the CO allows truthful imaging of the graphene surface.

[1] *J. Welker, and F. J. Giessibl, Science 336, 6080 (2012)

[2]*M. Ondráček, P. Pou, V. Rozsíval, C. González, P. Jelínek, and R. Pérez, PRL 106, 176101 (2011)

[3]*L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, Science 325, 5944 (2009)

TT 71.8 Fri 12:15 H17

**Role of substrate-molecular interactions in arrangement and collective motion of fullerene islands on graphene** — •Martin Svec[1], Pablo Merino[2], Yannick Dappe[3], Cesar Gonzalez[1], Enrique Abad[4], Pavel Jelinek[1], and Jose-Angel Martin-Gago[5] — [1]Institute of Physics, ASCR, Prague, CZ — [2]CAB INTA-CSIC, Madrid, ES — [3]CEA, IRAMIS, SPCSI, FR — [4]UAM, Madrid, ES — [5]ICMM-CSIC, Madrid, ES

Fullerenes interacting with graphene are a model system, that should be entirely driven by van der Waals (vdW) interactions. We concentrate on the interactions occurring between fullerenes and the single-layer graphene grown on SiC(0001) [1]. By using a VT-STM at 40K, regular islands of fullerenes were found. The particular orientation of the fullerenes in the islands, which occupy 4x4 graphene unit cells each, is critically evaluated by a comparison of STM measurements to extensive STM simulations with realistic fullerene-terminated tips. The determined orientation of fullerenes is independently confirmed by complex theoretical calculations of several adsorption configurations, taking into account the vdW interaction between the constituents of this system. Furthermore, islands of fullerenes were found collectively moving on the graphene. Surprisingly, according to the theory, the cohesion among the fullerenes is weaker than adhesion to the surface. Nevertheless, cohesion is a decisive factor in the collective motion, thanks to a low diffusion barrier of fullerenes on graphene.

[1] M. Švec et al., Phys. Rev. B 86 121407(R)(2012)

TT 71.9 Fri 12:30 H17

**XPS Analysis of Wet-Chemically Prepared Graphene Oxide** — •Ole Lytken, Michael Röckert, Jie Xiao, Christian Papp, Hans-Peter Steinrück, Siegfried Eigler, Michael Enzelberger, Stefan Grimm, Philipp Hofmann, Wolfgang Kroener, Christoph Dotzer, Paul Müller, and Andreas Hirsch — Universität Erlangen-Nürnberg

Graphene is one of the most studied materials of the last few years, but large scale production of high-quality graphene remains a challenge. One approach to a large scale production of graphene is the oxidation of graphite to graphite oxide, which can be exfoliated to graphene oxide and subsequently reduced to graphene. The challenge of this method is to keep the carbon structure intact during oxidation. We report on the XPS analysis of graphene oxide produced by a mild synthesis method that keeps the carbon structure intact and allows the reduction back to high-quality graphene. Only carbon with a single bond to one neighboring oxygen atom is observed (e.g. alcohols, expoxides or ethers), but no carbonyl (C=O) or carboxyl (-COOH) groups are found. Some common problems related to the interpretation of graphene oxide XPS spectra in the presence of charging and sulfur impurities will be touched upon.

Support by the SFB 953 and the Alexander-von-Humboldt Foundation is gratefully acknowledged.

TT 71.10 Fri 12:45 H17

**Morphological and Electronic Study of Moirê Patterns due to Dislocated Graphene on HOPG** — •Dilek Yildiz[1], Şener Şen[2], Oğuz Gülseren[2], and Oğuzhan Gürlü[1] — [1]Istanbul Technical University, Istanbul, Turkey — [2]Bilkent University, Ankara, Turkey

Highly oriented pyrolytic graphite (HOPG) is widely used as a calibration sample for scanning tunneling microscopy (STM) studies. It is also used as a substrate in surface science because of its smooth surface. HOPG is composed of stacked two dimensional hexagonal lattices formed by carbon atoms, popularly named as graphene layers. Because of the weak van der Waals bonding between the graphene layers, the topmost layer may be shifted or rotated on HOPG. Due to the rotation of the top layer, super-periodic structures called as Moiré patterns form on HOPG. These formations were investigated in numerous studies; however, they are rediscovered in graphene research and their origin is still not understood. In this study we used different solvents to see their effects on HOPG samples and the formation of super-periodic structures on these surfaces. We investigate the morphological and electronic properties by using scanning tunneling microscopy and spectroscopy (STM and STS) under ambient conditions. We compared electronic properties of Moiré patterns due to their periodicities. In order to shed light onto the observed electronic structures we also performed ab initio calculations on these super periodic structures. (Supported by TUBITAK 109T687 and ITU-BAP 33263).

## TT 72: Nanomechanics (jointly with BP, DF, and DY)

Time: Friday 10:45–11:45 Location: H20

TT 72.1 Fri 10:45 H20

**Two-tone experiments and time domain control in circuit nano-electromechanics** — •Hans Huebl[1], Fredrik Hocke[1], Xiaoqing Zhou[2,3], Albert Schliesser[2,3], Tobias J. Kippenberg[2,3], and Rudolf Gross[1,4] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland — [3]Max-Planck-Institut für Quantenoptik, Garching, Germany — [4]Physik-Department, TU München, Garching, Germany

In the field of optomechanics, a light field trapped in an optical resonator dynamically interacts with a mechanical degree of freedom, enabling cooling and amplification of mechanical motion. This concept of light matter interaction can be transferred to the microwave (MW) regime combining superconducting MW circuits with nanometer-sized mechanical beams, establishing the class of circuit nano-electromechanics. We discuss electromechanically induced transparency and electromechanically induced absorption employing continuous and pulsed excitation. With the latter technique, we access the dynamics of the hybrid system revealing that the switching dynamics of the transmitted light are not limited by the time constant imposed by the mechanical beam, the slowing of light pulses, and the phonon repopulation of a precooled mechanical mode due to thermal decoherence [1,2].

This work is supported by the Excellence Cluster "Nanosystems Initiative Munich (NIM)".

[1] X. Zhou et al., arXiv:1206.6052 (2012)
[2] F. Hocke et al., arXiv:1209.4470 (2012)

TT 72.2 Fri 11:00 H20

**Quantum Information Processing with Nanomechanical Qubits** — •Simon Rips and Michael Hartmann — Technische Universität München, James-Franck-Strasse, 85748 Garching, Germany

We introduce an approach to quantum information processing where the information is stored in the motional degrees of freedom of nanomechanical devices. The qubits of our approach are formed by the two lowest energy levels of mechanical resonators which are tuned to be strongly anharmonic by suitable electrostatic fields. Single qubit rotations are conducted by radio frequency voltage pulses that are applied to individual resonators. Two qubit entangling gates in turn are implemented via a coupling to a common optical resonance of a high finesse cavity. We explain the working principle of local and entangling operations and show that high gate fidelites can be obtained with realistic experimental parameters.

TT 72.3 Fri 11:15 H20

**Mechanical read-out of a single electron spin in a carbon nanotube** — •Philipp Struck, Heng Wang, and Guido Burkard — Universität Konstanz

The spin of a single electron in a suspended carbon nanotube can be read out by using its coupling to the nano-mechanical motion of the nanotube. To show this, we consider a single electron confined within a quantum dot formed by the suspended carbon nanotube. The spin-orbit interaction induces a coupling between the spin and one of the bending modes of the suspended part of the nanotube [1]. We simulate the response of the system to the external driving with a Jaynes-Cummings model by solving the quantum master equation. Using parameters comparable to those used in recent experiments, we calculate how information of the spin state of the system is imprinted on the mechanical motion. By measuring the current through a close-by charge sensor, the spin state can be read out. We show that the effect is measurable with current experimental expertise.

[1] A. Palyi, P. R. Struck, M. Rudner, K. Flensberg, and G. Burkard, Phys. Rev. Lett. **108**, 206811 (2012)

TT 72.4 Fri 11:30 H20

**Carbon nanotube nano-electromechanical resonators — driving, damping, detection** — Daniel Schmid, Peter Stiller, Sabine Kugler, Alois Dirnaichner, Christoph Strunk, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Single wall carbon nanotubes are not only excellent electrical conductors or semiconductors. Additionally, the carbon lattice causes large mechanical stability, with a Young's modulus significantly exceeding that of stainless steel. Recent research has shown the mechanical quality factor of a suspended carbon nanotube nano-electromechanical resonator to rise above $10^5$ at cryogenic temperatures. At these high values, mechanical motion can be excited by minute driving forces. At the same time, the electronically nonlinear behaviour of the quantum dot forming inside the carbon nanotube enables detection of the mechanical motion.

With this, we present a rich system where single-electron tunneling directly couples to and influences mechanical motion. A dc current alone is sufficient to excite vibration via feedback effects. In turn, the mechanical vibrations can be suppressed with a magnetic field by means of eddy current dissipation. The quantum dot provides a clean quantum-mechanical few-carrier system. As a perspective, future experiments may show a carbon nanotube as a system coherent in both electronic and mechanical aspects.

## TT 73: Fluctuations and Noise

Time: Friday 11:45–12:30 Location: H20

TT 73.1 Fri 11:45 H20

**Noise-induced Phase Transition in an Electronic Mach-Zehnder Interferometer: a Manifestation of Non-Gaussian Noise** — Andreas Helzel[1], Leonid V. Litvin[1], Ivan P. Levkivskyi[2,3], Eugene V. Sukhorukov[2], Werner Wegscheider[4], and •Christoph Strunk[1] — [1]Institut für experimentelle und angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland — [3]Bogolyubov Institute for Theoretical Physics, 03680 Kiev, Ukraine — [4]Laboratorium für Festkörperphysik, HPF E 7, ETH Zürich, 8093 Zürich, Switzerland

An electronic Mach-Zehnder interferometer is employed as a detector for the non-Gaussian current noise emitted from a quantum point contact (QPC). The visibility of Aharonov-Bohm interference in the interferometer constitutes a direct probe of the generator of the full counting statistics (FCS) of the current fluctuations. The visibility shows a lobe and node structure vs. the applied dc bias, which depends on the transmission $\mathcal{T}_0$ of the QPC, and changes qualitatively at $\mathcal{T}_0 = 1/2$. The analysis of the data provides direct experimental evidence for a singularity in the FCS. The noise is highly non-Gaussian and leads to an abrupt disappearance of the multiple side lobes for $\mathcal{T}_0 < 1/2$. Together with a singularity of the dephasing rate these observations constitute an experimental evidence of a recently predicted noise-induced phase transition occurring at $\mathcal{T}_0 = 1/2$.

TT 73.2 Fri 12:00 H20

**Finite-frequency noise properties of the nonequilibrium Anderson impurity model** — •Christoph P. Orth[1], Andreas Komnik[2], and Daniel F. Urban[3] — [1]University of Basel, Switzerland — [2]University of Heidelberg, Germany — [3]University of Freiburg, Germany

We analyze the spectrum of the electric-current autocorrelation function (noise power) in the Anderson impurity model biased by a finite transport voltage. Special emphasis is placed on the interplay of nonequilibrium effects and electron-electron interactions. Analytic results are presented for a perturbation expansion in the interaction strength U . Compared to the noninteracting setup we find a suppression of noise for finite frequencies in equilibrium and an amplification in nonequilibrium. Furthermore, we use a diagrammatic resummation scheme to obtain nonperturbative results in the regime of intermediate

U. At finite voltage, the noise spectrum shows sharp peaks at positions related to the Kondo temperature instead of the voltage.

TT 73.3 Fri 12:15 H20

**Detection of single-electron heat transfer statistics** — •Rafael Sánchez[1] and Markus Büttiker[2] — [1]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain — [2]Université de Genève, Genève, Switzerland

Capacitively coupled conductors permit separate directions of the heat and current flux. Energy is transferred between two conductors by means of electron-electron interaction. When one of systems is at a higher temperature, the transferred heat can be converted to electrical power. In quantum dot systems, the energy transfer is discrete, allowing for high conversion efficiencies[1]. Charge fluctuations of such a system can be monitored by quantum point contact. It allows us to extract the transferred heat statistics from the detection of state-resolved charge fluctuations. We investigate gate dependent deviations away from a charge fluctuation theorem in the presence of local temperature gradients (hot spots). Non universal relations are found for state dependent charge counting. A fluctuation theorem holds for coupled dot configurations with heat exchange and no net particle flow[2].

[1] R. Sánchez, and M. Büttiker, Phys. Rev. B 83, 085428 (2011)
[2] R. Sánchez, and M. Büttiker, Europhys. Lett. (in press); arXiv:1207.2587