Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(Lecture rooms: HSZ 01, HSZ 03, HSZ 201, HSZ 204, HSZ 304, BEY 81 and WIL C107; Posters: P2)

Invited and Topical Talks except for Focus Sessions

TT 7.8	Mon	11:30–12:00	HSZ 03	**Probing Decoherence in Atomic-Sized Defects Using a Superconducting Qubit** — •Jürgen Lisenfeld
TT 34.1	Tue	11:15–11:45	HSZ 201	**Giant Thermopower in the Emerging Field of Super-Spintronics** — •Matthias Eschrig
TT 37.1	Tue	9:30–10:00	HSZ 304	**Superfluidity and Collective Pairing in Polariton Microcavities** — •Francesca Maria Marchetti
TT 37.10	Tue	12:15–12:45	HSZ 304	**Mesoscopic Transport of Heat in Trapped-Ion Crystals** — •Martin Bruderer
TT 42.1	Tue	9:30–10:00	WIL C107	**A First-Principles Perspective on Two-Dimensional Transition-Metal Dichalcogenides** — •Udo Schwingenschlögl
TT 57.7	Wed	11:15–11:45	HSZ 304	**Quantum Transport at Molecular Scales** — •Ferdinand Evers
TT 68.1	Wed	15:00–15:30	HSZ 201	**Novel Effects of Disorder in Multiband Unconventional Superconductors** — •Peter J Hirschfeld
TT 71.6	Wed	16:30–17:00	HSZ 03	**Majorana Fermions in Chains of Magnetic Atoms on the Surface of a Superconductor** — •Ali Yazdani
TT 82.8	Thu	11:30–12:00	HSZ 204	**Density Matrix Renormalization Group: Probing the Topology of Quantum States** — •Frank Pollmann
TT 83.1	Thu	9:30–10:00	HSZ 03	**Kinetic Theory for the Relaxation of Quantum Many-Body Systems** — •Marcus Kollar
TT 98.6	Thu	16:30–17:00	BEY 81	**Real-Space Tailoring of the Electron-Phonon Coupling in Ultra-Clean Nanotube Mechanical Resonators** — •Shahal Ilani

Tutorial "Thermoelectricity - The Quest for a High Figure of Merit"

TT 1.1	Sun	16:00–16:45	HSZ 304	**Thermoelectric Effects: Basic Aspects, Boltzmann Theory, Onsager Relations** — •Arthur Ernst
TT 1.2	Sun	16:50–17:35	HSZ 304	**Thermal Transport Measurements at the Nanoscale** — •Saskia F. Fischer
TT 1.3	Sun	17:40–18:25	HSZ 304	**High Temperature Thermoelectric Power Generators: Materials and Devices** — •Anke Weidenkaff

Tutorial "Advanced Algorithms for Correlated Quantum Matter"

TT 2.1	Sun	16:00–16:45	HSZ 04	**DMRG and Entanglement Scaling** — •Fabian Heidrich-Meisner
TT 2.2	Sun	16:50–17:35	HSZ 04	**Introduction to Tensor Networks** — •Roman Orus
TT 2.3	Sun	17:40–18:25	HSZ 04	**Quantum Monte Carlo Methods** — •Stefan Wessel

Invited and Topical Talks of the Focus Session "Dynamics, Topology, and Fractionalisation"

TT 16.1	Mon	15:00–15:30	HSZ 01	**Dynamics in Heisenberg Chains: From Fractional Excitations to New Out-of-Equilibrium States of Matter** — •Jean-Sébastien Caux
TT 16.2	Mon	15:30–16:00	HSZ 01	**Inelastic Neutron Scattering on Candidate Kitaev Compounds** — •Radu Coldea
TT 16.3	Mon	16:00–16:30	HSZ 01	**Dynamics of Majorana Fermions in a Quantum Spin Liquid** — •John Chalker
TT 16.4	Mon	16:45–17:15	HSZ 01	**Molecular Quantum Magnetism in $LiZn_2Mo_3O_8$** — •Collin Broholm
TT 16.5	Mon	17:15–17:45	HSZ 01	**Unwinding a Skyrmion Lattice: Emergent Monopoles in Chiral Magnets** — •Achim Rosch

Invited and Topical Talks of the Focus Session "Advanced Algorithms for Strongly Correlated Quantum Matter"

TT 36.1	Tue	9:30–10:00	HSZ 03	**Quantum Computing and Strongly Correlated Materials** — •Matthias Troyer
TT 36.2	Tue	10:00–10:30	HSZ 03	**Quantum Monte Carlo Simulations of Deconfined Quantum-Criticality** — •Anders Sandvik
TT 36.3	Tue	10:30–11:00	HSZ 03	**Characterizing Entanglement Entropy with Quantum Monte Carlo** — •Roger Melko
TT 36.4	Tue	11:15–11:45	HSZ 03	**Field-Induced Superfluids and Bose Liquids in Projected Entangled Pair States** — •Didier Poilblanc
TT 36.5	Tue	11:45–12:15	HSZ 03	**Nature of the Spin Liquid Ground State of the Kagome Model** — •Uli Schollwoeck

Invited and Topical Talks of the Focus Session "Electronic Properties of Spin-Orbit Driven Oxides"

TT 56.1	Wed	9:30–10:00	HSZ 03	**Exotic Magnetism of J_{eff}=1/2 Iso-Spins in Complex Ir Oxides** — •Hidenori Takagi
TT 56.2	Wed	10:00–10:30	HSZ 03	**Isospin Dynamics in Sr_2IrO_4 Revealed by Resonant Inelastic X-Ray Scattering** — •Jungho Kim
TT 56.3	Wed	10:30–11:00	HSZ 03	**Honeycomb Lattice Iridates** — •Philipp Gegenwart
TT 56.4	Wed	11:15–11:45	HSZ 03	**Novel Magnetic States in Spin-Orbit Coupled Mott Insulators** — •Giniyat Khaliullin
TT 56.5	Wed	11:45–12:15	HSZ 03	**Electronic Structure of Honeycomb Iridates and Rhodates from a Density Functional Theory Perspective** — •Harald O. Jeschke

Invited and Topical Talks of the Focus Session "Theoretical Advances in Interacting Topological Phases"

TT 95.1	Thu	15:00–15:30	HSZ 03	**Fractional Topological Insulators** — •Andrei Bernevig
TT 95.2	Thu	15:30–16:00	HSZ 03	**Non-Fermi Liquid, Quantum Critical, and Topological States in Iridates** — •Leon Balents
TT 95.3	Thu	16:00–16:30	HSZ 03	**Collective Spin-Orbit Physics in $j = 1/2$ Mott Insulators** — •Simon Trebst
TT 95.4	Thu	16:45–17:15	HSZ 03	**Topological Kondo Insulators: An Example of Correlated Quantum Spin Hall States** — •Fakher Assaad
TT 95.5	Thu	17:15–17:45	HSZ 03	**Fractional Chern Insulators in Strongly Correlated Multiorbital Systems** — •Maria Daghofer

Invited talks of the joint symposium SYMO

See SYMO for the full program of the symposium.

SYMO 1.1	Mon	9:30–10:00	HSZ 02	**Molecular quantum spintronics with single-molecule magnets** — •Wolfgang Wernsdorfer
SYMO 1.2	Mon	10:00–10:30	HSZ 02	**EPR Studies of Rare-Earth Molecular Nanomagnets** — •Stephen Hill
SYMO 1.3	Mon	10:45–11:15	HSZ 02	**On-surface magnetochemistry of spin-bearing metalorganic molecules** — •Peter M. Oppeneer
SYMO 1.4	Mon	11:15–11:45	HSZ 02	**Interfacing single-molecule magnets with metals** — •Andrea Cornia
SYMO 1.5	Mon	11:45–12:15	HSZ 02	**Linking magnetic molecules to themselves, to others and to surfaces** — •Richard Winpenny

Invited talks of the joint symposium SYSG

See SYSG for the full program of the symposium.

SYSG 1.1	Tue	9:30–10:00	HSZ 02	**Intrinsic magnetism in graphene** — •Irina Grigorieva
SYSG 1.2	Tue	10:00–10:30	HSZ 02	**Defect Induced Magnetic Moments in Graphene** — •Roland Kawakami
SYSG 1.3	Tue	10:30–11:00	HSZ 02	**Role of MgO barriers for spin and charge transport in Co/MgO/graphene spin-valve devices** — •Bernd Beschoten
SYSG 1.4	Tue	11:15–11:45	HSZ 02	**Defect-Mediated Spin Relaxation and Dephasing in Graphene** — •Joshua Folk
SYSG 1.5	Tue	11:45–12:15	HSZ 02	**Electron spin relaxation in graphene: resonant scattering off local magnetic moments** — •Jaroslav Fabian

Invited talks of the joint symposium SYOM

See SYOM for the full program of the symposium.

SYOM 1.1	Fri	9:30–10:10	HSZ 02	**Atomic-scale dopant wires for quantum computer architectures** — •Michelle Y Simmons
SYOM 1.2	Fri	10:10–10:50	HSZ 02	**$1+\delta$: Tuning the Dimensionality of Organic Conductors** — •Martin Dressel
SYOM 1.3	Fri	11:10–11:50	HSZ 02	**Spectral and transport properties of one-dimensional correlated electrons** — •Volker Meden
SYOM 1.4	Fri	11:50–12:30	HSZ 02	**Atomic nanowires on surfaces: Spectroscopic reality versus theoretical fiction** — •Ralph Claessen

Sessions

TT 1.1–1.3	Sun	16:00–18:25	HSZ 304	**Tutorial: Thermoelectricity - The Quest for a High Figure of Merit**
TT 2.1–2.3	Sun	16:00–18:25	HSZ 04	**Tutorial: Advanced Algorithms for Correlated Quantum Matter**
TT 3.1–3.5	Mon	9:30–12:15	HSZ 02	**Magnetic/Organic Interfaces and Molecular Magnetism (organized by MA; with CPP, DS, HL, O, TT)**
TT 4.1–4.13	Mon	9:30–13:00	HSZ 201	**Low-Dimensional Systems: 1D - Theory**
TT 5.1–5.5	Mon	9:30–10:45	HSZ 204	**Transport: Quantum Coherence and Quantum Information Systems - Experiment**
TT 6.1–6.8	Mon	11:00–13:00	HSZ 204	**Transport: Quantum Coherence and Quantum Information Systems - Theory I**
TT 7.1–7.12	Mon	9:30–13:00	HSZ 03	**Superconductivity: Cryodetectors**
TT 8.1–8.13	Mon	9:30–13:00	HSZ 304	**Correlated Electrons: Spin Systems and Itinerant Magnets - Frustrated Magnets I**
TT 9.1–9.14	Mon	9:30–13:15	BEY 81	**Transport: Quantum Dots, Quantum Wires, Point Contacts I (organized by TT)**
TT 10.1–10.10	Mon	9:30–12:00	BEY 118	**Magnetic Heuslers, Half-Metals and Oxides I (organized by MA)**

TT 11.1–11.1	Mon	9:30–10:15	GER 37	**Invited Talk - Martin Fally (organized by DF; with CPP, KR, TT)**
TT 12.1–12.8	Mon	9:30–12:00	HÜL 186	**Quantum Dynamics, Decoherence and Quantum Information (organized by DY)**
TT 13.1–13.11	Mon	9:30–12:30	POT 051	**Topological Insulators: Mostly Structure and Electronic Structure (organized by HL)**
TT 14.1–14.4	Mon	9:30–11:30	POT 151	**Focus Session: Physics of Quantum Rings (organized by HL)**
TT 15.1–15.8	Mon	10:30–13:15	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale (organized by O)**
TT 16.1–16.5	Mon	15:00–17:45	HSZ 01	**Focus Session: Dynamics, Topology, and Fractionalisation**
TT 17.1–17.13	Mon	15:00–18:30	HSZ 201	**Superconductivity: Tunnelling, Josephson Junctions, SQUIDs**
TT 18.1–18.4	Mon	15:00–16:00	HSZ 204	**Transport: Fluctuations and Noise**
TT 19.1–19.9	Mon	16:00–18:30	HSZ 204	**Transport: Quantum Dots, Quantum Wires, Point Contacts II (organized by TT)**
TT 20.1–20.11	Mon	15:00–18:00	HSZ 304	**Correlated Electrons: Spin Systems and Itinerant Magnets - Frustrated Magnets II**
TT 21.1–21.5	Mon	15:00–17:30	HSZ 04	**Focus Session: New Trends in Molecular Magnetism (organized by MA)**
TT 22.1–22.6	Mon	15:00–16:30	BEY 81	**Low-Dimensional Systems: Charge Order**
TT 23.1–23.7	Mon	16:45–18:30	BEY 81	**Low-Dimensional Systems: Other Materials**
TT 24.1–24.12	Mon	15:00–18:45	BEY 118	**Magnetic Heuslers, Half-Metals and Oxides II (organized by MA)**
TT 25.1–25.11	Mon	15:00–18:45	POT 051	**Focus Session: Electron Spin Qubits in Semiconductor Quantum Dots (organized by HL)**
TT 26.1–26.7	Mon	16:00–17:45	POT 006	**Quantum Wires: Transport Properties (organized by HL)**
TT 27.1–27.8	Mon	15:45–17:45	POT 081	**Topological Insulators: Mostly Interaction with Magnetic Fields (organized by HL)**
TT 28.1–28.10	Mon	16:00–18:45	TRE Ma	**Focussed Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale II (organized by O)**
TT 29.1–29.12	Mon	16:00–19:00	WIL C107	**Graphene: Structural Properties (organized by O)**
TT 30.1–30.70	Mon	15:00–19:00	P2	**Superconductivity - Poster Session**
TT 31.1–31.5	Tue	9:30–12:15	HSZ 02	**Spin Properties of Graphene (organized by HL; with DS, MA, O, TT)**
TT 32.1–32.1	Tue	9:30– 9:45	HSZ 201	**Cryotechnique**
TT 33.1–33.5	Tue	9:45–11:00	HSZ 201	**Superconductivity: Vortex Physics**
TT 34.1–34.6	Tue	11:15–13:00	HSZ 201	**Superconductivity: Heterostructures**
TT 35.1–35.13	Tue	9:30–13:00	HSZ 204	**Correlated Electrons: Quantum-Critical Phenomena - Experiment I**
TT 36.1–36.5	Tue	9:30–12:15	HSZ 03	**Focus Session: Advanced Algorithms for Strongly Correlated Quantum Matter**
TT 37.1–37.10	Tue	9:30–12:45	HSZ 304	**Cold Atomic Gases**
TT 38.1–38.4	Tue	9:30–10:30	BEY 81	**Transport: Spintronics and Magnetotransport (organized by TT)**
TT 39.1–39.9	Tue	10:45–13:00	BEY 81	**Transport: Quantum Coherence and Quantum Information Systems - Theory II**
TT 40.1–40.12	Tue	9:30–12:45	BEY 118	**Multiferroics I (organized by MA)**
TT 41.1–41.5	Tue	9:30–11:15	POT 251	**Focus Session: Quantum Light Sources Based on Solid State Systems: Status and Visions I (organized by HL)**
TT 42.1–42.13	Tue	9:30–13:15	WIL C107	**Transport: Graphene (organized by TT)**
TT 43.1–43.11	Tue	10:30–13:15	GER 38	**Topological Insulators (organized by O)**
TT 44.1–44.9	Tue	10:30–13:15	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale III (organized by O)**
TT 45.1–45.8	Tue	14:00–16:00	HSZ 201	**Superconductivity: Fe-based Superconductors - 1111,111, FeSe**
TT 46.1–46.8	Tue	14:00–16:00	HSZ 204	**Low-Dimensional Systems: Molecular Conductors**

TT 47.1–47.8	Tue	14:00–16:00	HSZ 03	**Correlated Electrons: Spin Systems and Itinerant Magnets - Frustrated Magnets III**
TT 48.1–48.8	Tue	14:00–16:00	HSZ 304	**Transport: Topological Insulators I (organized by TT)**
TT 49.1–49.9	Tue	13:45–16:00	HSZ 401	**Spintronics (organized by MA)**
TT 50.1–50.8	Tue	14:00–16:00	BEY 81	**Correlated Electrons: Quantum-Critical Phenomena - Theory**
TT 51.1–51.7	Tue	14:30–16:15	POT 112	**Quantum Wires: Optical Properties (organized by HL)**
TT 52.1–52.6	Tue	14:00–15:45	POT 251	**Focus Session: Quantum Light Sources Based on Solid State Systems: Status and Visions II (organized by HL)**
TT 53.1–53.14	Wed	9:30–13:15	HSZ 201	**Superconductivity: Fe-based Superconductors - 122**
TT 54.1–54.6	Wed	9:30–11:00	HSZ 204	**Correlated Electrons: Heavy Fermions**
TT 55.1–55.5	Wed	11:15–12:30	HSZ 204	**Correlated Electrons: Quantum-Critical Phenomena - Experiment II**
TT 56.1–56.5	Wed	9:30–12:15	HSZ 03	**Focus Session: Electronic Properties of Spin-Orbit Driven Oxides**
TT 57.1–57.12	Wed	9:30–13:00	HSZ 304	**Transport: Molecular Electronics I**
TT 58.1–58.13	Wed	9:30–13:00	HSZ 04	**Multiferroics II (organized by MA)**
TT 59.1–59.13	Wed	9:30–13:00	BEY 81	**Low-Dimensional Systems: 2D - Theory (organized by TT)**
TT 60.1–60.5	Wed	9:30–12:15	BEY 118	**Focus Session: Chiral Domain Walls in Ultrathin Films (organized by MA)**
TT 61.1–61.10	Wed	9:30–12:15	POT 051	**Graphene: Transport (organized by HL)**
TT 62.1–62.7	Wed	10:15–12:00	POT 006	**Spintronics I (organized by HL)**
TT 63.1–63.7	Wed	9:30–11:15	POT 151	**Topological Insulators: Theory (organized by HL)**
TT 64.1–64.7	Wed	9:30–11:15	POT 251	**Quantum Dots: Optical Properties I (organized by HL)**
TT 65.1–65.6	Wed	11:30–13:00	POT 251	**Quantum Dots: Optical Properties II (organized by HL)**
TT 66.1–66.10	Wed	10:30–13:15	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale IV (organized by O)**
TT 67.1–67.1	Wed	12:30–13:00	HSZ 02	**Gaede Prize Talk (organized by VA; with DS, O, TT)**
TT 68.1–68.10	Wed	15:00–18:00	HSZ 201	**Superconductivity: Fe-based Superconductors - Theory I**
TT 69.1–69.5	Wed	15:00–16:15	HSZ 204	**Correlated Electrons: Spin Systems and Itinerant Magnets - Chiral Magnets**
TT 70.1–70.8	Wed	16:30–18:30	HSZ 204	**Transport: Topological Insulators II (organized by TT)**
TT 71.1–71.10	Wed	15:00–18:00	HSZ 03	**Transport: Majorana Fermions (organized by TT)**
TT 72.1–72.5	Wed	15:00–16:15	HSZ 304	**Transport: Molecular Electronics II**
TT 73.1–73.8	Wed	16:30–18:30	HSZ 304	**Transport: Carbon Nanotubes (organized by TT)**
TT 74.1–74.14	Wed	15:00–18:45	BEY 81	**Correlated Electrons: Quantum Impurities, Kondo Physics**
TT 75.1–75.5	Wed	15:00–17:45	BEY 118	**Focus Session: Spin-Orbit Torque at Surfaces and Interfaces (organized by MA)**
TT 76.1–76.6	Wed	15:00–16:30	POT 006	**Quantum Information Systems I (organized by HL)**
TT 77.1–77.11	Wed	16:00–19:15	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale V (organized by O)**
TT 78.1–78.13	Wed	16:00–19:15	WIL C107	**Graphene: Electronic Properties (organized by O)**
TT 79.1–79.75	Wed	15:00–19:00	P2	**Correlated Electrons - Poster Session**
TT 80.1–80.22	Wed	15:00–19:00	P2	**Low-Dimensional Systems - Poster Session**
TT 81.1–81.14	Thu	9:30–13:15	HSZ 201	**Superconductivity: Properties and Electronic Structure**
TT 82.1–82.13	Thu	9:30–13:15	HSZ 204	**Low-Dimensional Systems: Topological Order (organized by TT)**
TT 83.1–83.12	Thu	9:30–13:00	HSZ 03	**Correlated Electrons: Nonequilibrium Quantum Many-Body Systems I**
TT 84.1–84.14	Thu	9:30–13:15	HSZ 304	**Correlated Electrons: (General) Theory**
TT 85.1–85.10	Thu	9:30–12:15	HSZ 04	**Spincaloric Transport II (organized by MA)**
TT 86.1–86.12	Thu	9:30–12:45	BEY 81	**Correlated Electrons: Other Materials**
TT 87.1–87.6	Thu	9:30–12:45	BEY 118	**Focus Session: Unconventional Spin Structures (organized by MA)**
TT 88.1–88.1	Thu	9:30–10:00	POT 081	**Invited Talk - Tobias Korn (organized by HL)**
TT 89.1–89.9	Thu	10:00–12:30	POT 081	**Graphene-Like Materials: Silicene, MoS_2 and Relatives (organized by HL)**
TT 90.1–90.9	Thu	10:00–12:15	POT 151	**Spintronics II (organized by HL)**

TT 91.1–91.10	Thu	10:30–13:15	TRE Ma	**Focus Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale VI (organized by O)**
TT 92.1–92.5	Thu	15:00–16:15	HSZ 201	**Superconductivity: Fe-based Superconductors - Theory II**
TT 93.1–93.6	Thu	16:30–18:00	HSZ 201	**Superconductivity: (General) Theory**
TT 94.1–94.10	Thu	15:00–17:45	HSZ 204	**Low-Dimensional Systems: Oxide Hetero-Interfaces**
TT 95.1–95.7	Thu	15:00–18:25	HSZ 03	**Focus Session: Theoretical Advances in Interacting Topological Phases (organized by TT)**
TT 96.1–96.8	Thu	15:00–17:00	HSZ 304	**Correlated Electrons: Nonequilibrium Quantum Many-Body Systems II**
TT 97.1–97.8	Thu	16:45–18:45	HSZ 403	**Spincaloric Transport I (organized by MA)**
TT 98.1–98.10	Thu	15:00–18:00	BEY 81	**Transport: Nanomechanics**
TT 99.1–99.11	Thu	15:00–18:00	POT 081	**Graphene: Spintronics, Transistors, and Sensors (organized by HL)**
TT 100.1–100.11	Thu	16:00–18:45	WIL C107	**Graphene: Adsorption, Intercalation, Doping (organized by O)**
TT 101.1–101.45	Thu	15:00–19:00	P2	**Transport - Poster Session**
TT 102.1–102.6	Thu	15:00–19:00	P2	**Cold Atomic Gases - Poster Session**
TT 103.1–103.4	Fri	9:30–12:30	HSZ 02	**Symposium One-Dimensional Metals: Reality or Fiction (organized by DS; with HL, O, TT)**
TT 104.1–104.9	Fri	9:30–12:00	HSZ 04	**Topological Insulators (organized by MA)**
TT 105.1–105.6	Fri	9:30–11:00	POT 081	**Graphene: Bi- and Multi-Layers (organized by HL)**
TT 106.1–106.7	Fri	11:15–13:00	POT 081	**Graphene: Interaction with the Substrate (organized by HL)**
TT 107.1–107.5	Fri	9:30–10:45	POT 151	**Quantum Information Systems II (organized by HL)**
TT 108.1–108.7	Fri	11:30–13:15	CHE 89	**Graphene (joint session with TT, MA, HL, DY, O)**

Annual General Meeting of the Low Temperature Physics Division

Thursday 18:30 Room H304

TT 1: Tutorial: Thermoelectricity - The Quest for a High Figure of Merit

The search for and the investigation of novel materials with excellent thermoelectric properties, i.e., a high "figure of merit", has been a hot topic recently, in particular, in view of numerous technological applications. For example, a greater efficiency would generate brand new possibilities in the field of power engineering, by using directly the waste heat in combustion engines while lowering CO_2 emissions at the same time, or in energy self-sufficient sensors. In this Tutorial, after an introduction into the basic theoretical concepts, measurements at the nanoscale will be discussed, as well as applications in power generators.

Organizers: Ulrich Eckern (Uni Augsburg), Claudia Felser (MPI CPfS Dresden)

Time: Sunday 16:00–18:25 Location: HSZ 304

Tutorial TT 1.1 Sun 16:00 HSZ 304

Thermoelectric Effects: Basic Aspects, Boltzmann Theory, Onsager Relations — •Arthur Ernst — Max-Planck-Institut für Mikrostrukturphysik, Halle — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig

Thermoelectric phenomena which involve the conversion between thermal and electrical energy and provide a method of heating and cooling materials are expected to play an important role in meeting the energy challenge of the future. In my talk I shall present basic aspects of the microscopic theory for thermoelectricity. First, I discuss the basic definition of the thermoelectric heat. Then I present a short overview of non-equilibrium thermodynamics and the microscopic theory of the electronic transport. Further I review several approaches to describe thermoelectric properties, present the state of the art in the understanding the thermoelectric phenomena, and conclude my talk with some remarks on future prospects of the field.

5 min. break

Tutorial TT 1.2 Sun 16:50 HSZ 304

Thermal Transport Measurements at the Nanoscale — •Saskia F. Fischer — AG Neue Materialien, Humboldt-Universität zu Berlin, 10099 Berlin

In this tutorial first an introduction to measurements of the electrical conductivity, the thermopower and the thermal conductance will be given. All three material parameters are required to determine the thermoelectric figure of merit. However, the measurement techniques which are successfully applied to bulk materials often cannot be transferred to nanoscale materials such as individual ultra-thin films, flakes or nanowires. On behalf of particular examples, I will discuss measurement techniques for such nanomaterials. In particular, the application of a micro-machined platform for the full ZT-characterization allowing as well for the investigation of the crystal structure and chemical composition of a single nanowire will be demonstrated. If time allows, an outlook to thermal transport in low-dimensional charge carrier systems and the determination of the charge carrier temperature via noise thermometry will be given.

5 min. break

Tutorial TT 1.3 Sun 17:40 HSZ 304

High Temperature Thermoelectric Power Generators: Materials and Devices — •Anke Weidenkaff[1,2] and Wenjie Xie[2] — [1]Empa, 8600 Dübendorf, Switzerland — [2]Institut für Materialwissenschaft, Universität Stuttgart, 70174 Stuttgart, Germany

With a thermoelectric converter heat can be directly converted into electricity. A broad application of thermoelectric converters in future energy technologies requires the development of thermoelectric active, stable, low cost and sustainable materials. Suitable candidates are being selected among novel materials according to their temperature dependent ZT (thermoelectric figure of merit) values, and their compatibility factors to produce well performing thermoelectric converters, delivering a high power output. Theses converters are tested under ambient air at temperatures of $T > 900$ °C and applied in an exhaust gas stream of a custom made hybrid vehicle, concentrated solar thermal converters, metal casting furnaces and solid oxide fuel cells. The lectures will provide an overview on the development of novel perovskite-type and Heusler materials gaining importance for future energy technologies

TT 2: Tutorial: Advanced Algorithms for Correlated Quantum Matter

This Tutorial provides an introduction into a most important sub-field of computational physics, namely the investigation of strongly correlated quantum systems by modern numerical methods. Further details and recent scientific advancements will be presented in the corresponding TT Focus Session (Tuesday, starting at 9:30 in HSZ 03).

Organizers: Fakher Assaad (Uni Würzburg), Ulrich Eckern (Uni Augsburg)

Time: Sunday 16:00–18:25 Location: HSZ 04

Tutorial TT 2.1 Sun 16:00 HSZ 04

DMRG and Entanglement Scaling — •Fabian Heidrich-Meisner — Ludwig-Maximilians-University Munich, Germany

This talk will provide an introduction to the density matrix renormalization group method which provides numerical access to many-body wave functions of quantum lattice models such as the Hubbard, Heisenberg, or the t-J model. The main idea is to approximate wave-functions through finite-dimensional matrix product states (MPS). The performance of the technique is intimately related to the entanglement encoded in the target wave-function. For gapped Hamiltonians with short range interactions, the so-called area law states that their ground states are only mildly entangled, permitting an efficient representation of many-body states using MPS in one dimension. The more difficult case of two-dimensional systems, critical systems in one dimension, and time-evolution will also be discussed.

5 min. break

Tutorial TT 2.2 Sun 16:50 HSZ 04

Introduction to Tensor Networks — •Roman Orus — Institut für Physik, Johannes Gutenberg Universität, Staudingerweg 7, 55099 Mainz, Deutschland

In this tutorial I will give an introduction to Tensor Network methods for strongly correlated systems. Motivated by DMRG and the entanglement properties of 1d systems (see the related previous tutorial), I will extend the ideas to deal with other types of situations, such as 2d and scale-invariant systems. The PEPS and MERA tensor networks will be presented and discussed. After providing practical examples, I will explain some of the related numerical methods at an introductory level.

5 min. break

Tutorial TT 2.3 Sun 17:40 HSZ 04

Quantum Monte Carlo Methods — •Stefan Wessel — Institute for Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany

This tutorial will introduce the basic ideas behind modern quantum Monte Carlo simulation methods, focusing on world-line approaches for quantum spin systems. In particular, the cluster-based loop algorithm in the continuous-time formulation as well as the stochastic series expansion and the directed loop update approach will be presented. The advantages and limitations of these simulations methods will be discussed.

TT 3: Magnetic/Organic Interfaces and Molecular Magnetism (organized by MA; with CPP, DS, HL, O, TT)

Time: Monday 9:30–12:15 Location: HSZ 02

Invited Talk TT 3.1 Mon 9:30 HSZ 02

Molecular quantum spintronics with single-molecule magnets — •Wolfgang Wernsdorfer — Institut Néel, CNRS, BP 166, 38042 Grenoble, France

We will address the field called molecular quantum spintronics, combining the concepts of spintronics, molecular electronics and quantum computing. Various research groups are currently developing low-temperature scanning tunnelling microscopes to manipulate spins in single molecules, while others are working on molecular devices (such as molecular spin-transistors, spin valves and filters, and carbon-nanotube-based devices) to read and manipulate the spin state and perform basic quantum operations. For ex., we have built a novel spin-valve device in which a non-magnetic molecular quantum dot, consisting of a Single-Wall Carbon Nanotube, is laterally coupled to a TbPc2 molecular magnet. The localized magnetic moment of the SMM led to a magnetic field-dependent modulation of the conductance in the nanotube with magnetoresistance ratios of up to 300%. Using a molecular spin-transistor, we achieved the electronic read-out of the nuclear spin of an individual metal atom embedded in a single-molecule magnet (SMM). We could show very long spin lifetimes (several tens of seconds). Using the hyperfine Stark effect, which transforms electric fields into local effective magnetic fields, we could not only tune the resonant frequency by several MHz, but we also performed coherent quantum manipulations on a single nuclear qubit by means of electrical fields only.

Invited Talk TT 3.2 Mon 10:00 HSZ 02

EPR Studies of Rare-Earth Molecular Nanomagnets — •Stephen Hill[1], Sanhita Ghosh[1], Dorsa Komijani[1], Salvador Cardona-Serra[2], Jose-Jaime Baldovi[2], Yan Duan[2], Alejandro Gaita-Arino[2], and Eugenio Coronado[2] — [1]Department of Physics and NHMFL, Florida State University, Tallahassee, FL 32310, USA — [2]ICM, Universidad de Valencia, 46980 Paterna, Spain

I will discuss the application of multi-frequency EPR to study the static and dynamic properties of a family of mononuclear Ln(III) (Ln = Ho or Tb) nanomagnets encapsulated in polyoxometallate (POM) cages. The encapsulation offers the potential for spintronics applications on surfaces or in devices, as it preserves the intrinsic properties of the nanomagnet outside of a crystal. A large magnetic anisotropy arises due to a splitting of the Hund's coupled angular momentum ($J = L+S$) ground state in the POM ligand field. High-frequency EPR studies for the Ho(III) compound ($J = 8$) reveal an anisotropic eight line spectrum corresponding to transitions within the lowest $m_J = \pm 4$ doublet, split by a hyperfine interaction with the $I = 7/2$ Ho nucleus. Meanwhile, X-band studies reveal the presence of a large tunneling gap ($\Delta \sim 9$ GHz) within the $m_J = \pm 4$ doublet. Spin-echo measurements allow studies of the coherent spin dynamics, including Rabi oscillations. Remarkably long T_2 times are found, even for the most concentrated samples. It is postulated that this is due to the large gap, Δ, which provides an optimal operating point for coherent manipulations at X-band such that the quantum dynamics are relatively insensitive to dipolar fields.

15 min. break

Invited Talk TT 3.3 Mon 10:45 HSZ 02

On-surface magnetochemistry of spin-bearing metalorganic molecules — •Peter M. Oppeneer[1], Kartick Tarafder[1], Ehesan Ali[1], Nirmalya Ballav[2], Christian Wäckerlin[3], and Thomas A. Jung[3] — [1]Uppsala University, Uppsala, Sweden — [2]IISER, Pune, India — [3]PSI, Villigen, Switzerland

Planar spin-bearing metalorganic molecules such as metal-porphyrins and -phthalocyanines are paramagnetic in the gas phase, however an interface exchange coupling develops when these molecules are assembled on magnetic surfaces, which induces spontaneous molecular magnetic order at room temperature. To unveil fundamental origins of the exchange interaction leading to the metalorganic molecule/substrate spin-interface we use ab-initio DFT+U calculations with dispersion corrections added. Our calculations provide detailed, orbitally-resolved insight in the molecule-surface exchange interactions as well as the spin-switching induced by additional ligation in the free ligand position of the metal ion by small molecules such as NO and NH_3. We find that on-surface coordination chemistry of planar metalorganic complexes gives rise to novel magnetochemical effects, which challenge the notions of classical coordination chemistry. A key to these magnetochemical effects is the weak bonding to the surface, i.e. a "surface" trans effect. Our calculations further reveal that certain systems, as e.g. Cu-phthalocyanine on Co, are liable to formation of novel spin-polarized interface states that are expected to be particularly suited for spin-polarized electron injection in metalorganic layers.

Invited Talk TT 3.4 Mon 11:15 HSZ 02

Interfacing single-molecule magnets with metals — •Andrea Cornia[1], Valeria Lanzilotto[2], Luigi Malavolti[2], Matteo Mannini[2], Mauro Perfetti[2], Luca Rigamonti[1], and Roberta Sessoli[2] — [1]Dip. di Scienze Chimiche e Geologiche, Univ. di Modena e Reggio Emilia & INSTM, Modena, Italy — [2]Dip. di Chimica U. Schiff, Univ. di Firenze & INSTM, Sesto Fiorentino (FI), Italy

Encoding and manipulating information through the spin degrees of freedom of individual molecules are central challenges in molecular scale electronics. With their large magnetic moment and long spin relaxation time, single molecule magnets (SMMs) are of special importance in this field. The electrical addressing of individual SMMs is now well within reach using scanning probe methods, which require organizing molecules on electrically conductive surfaces [1,2]. Herein we present the latest achievements in the deposition of SMMs on metal substrates, like ultraflat surfaces [3] and nanoparticles [4]. Special emphasis is placed on the design of molecular structures that withstand processing by solution [3,4] or vapour-phase [5,6] methods as well as on chemical strategies for controlling molecular orientation. Rewardingly, these efforts have shown that the distinctive property of SMMs, i.e. slow spin relaxation, can persist in metal-wired molecules [3,4].

[1] S. Loth, et al. Science 2012, 335, 196. [2] A. A. Khajetoorians, et al. Science 2013, 339, 55. [3] M. Mannini, et al. Nature 2010, 468, 417. [4] M. Perfetti, et al. Small 2013, DOI: 10.1002/smll.201301617. [5] L. Rigamonti, et al. Inorg. Chem. 2013, 52, 5897. [6] L. Malavolti, et al. Chem. Commun. 2013, 49, 11506.

Invited Talk TT 3.5 Mon 11:45 HSZ 02

Linking magnetic molecules to themselves, to others and to surfaces — •Richard Winpenny — University of Manchester, United Kingdom

We are learning how to link together polymetallic compounds to give complex structures [1]. During this presentation recent work will be discussed in two distinct approaches. Firstly, we will describe recent work creating new hybrid inorganic-organic rotaxanes [2] and in the second approach we will discuss functionalising polymetallic rings so that they can act as ligands for other metal complexes and surfaces [3,4]. We will also describe the use of pulsed EPR spectroscopy to measure weak interactions between these molecular magnets.

1.G. A. Timco, T. B. Faust, F. Tuna and R. E. P. Winpenny, Chem. Soc. Rev., 2011, 40, 3067-3075. 2.C.- F. Lee, D. A. Leigh, R. G. Pritchard, D. Schultz, S. J. Teat, G. A. Timco and R. E. P. Winpenny, Nature, 2009, 458, 314-318. 3.G. A. Timco, S. Carretta, F. Troiani, F. Tuna, R. G. Pritchard, E. J. L. McInnes, A. Ghirri, A. Candini,

P. Santini, G. Amoretti, M. Affronte and R. E. P. Winpenny, Nature Nanotechnology, 2009, 4, 173-178. 4 G. F. S. Whitehead, F. Moro, G. A. Timco, W. Wernsdorfer, S. J. Teat and R. E. P. Winpenny, Angew. Chem. Int. Ed., 2013, 52, 9932-9935.

TT 4: Low-Dimensional Systems: 1D - Theory

Time: Monday 9:30–13:00 Location: HSZ 201

TT 4.1 Mon 9:30 HSZ 201

Diffusive and ballistic dynamics in local quenches in 1D spin-1/2 systems at finite temperatures — •Fabian Heidrich-Meisner[1], Christoph Karrasch[2], and Joel Moore[2] — [1]Ludwig-Maximilians-University Munich — [2]University of California, Berkeley

We study the spreading of local perturbations in the spin and energy density of spin-1/2 systems at finite temperatures [1], using the time-dependent density matrix renormalization group technique. In the integrable XXZ chain, we observe a ballistic dynamics of energy at all temperatures and for all exchange anisotropies. The spin dynamics, by contrast, is diffusive in the Ising phase at high temperatures. We extract the diffusion constant from these local quenches at infinite temperatures and show that the values are in quantitative agreement with the Einstein relation for sufficiently small local perturbations. We also study spin ladder systems, for which we observe examples of diffusive spin and energy dynamics at finite temperatures. The connection of our results to recent experiments with cold gases [2] and quantum magnets [3] is discussed.

[1] C. Karrasch, J. Moore, F. Heidrich-Meisner, in preparation.
[2] J.P. Ronzheimer et al., Phys. Rev. Lett. 110, 205301 (2013)
[3] M. Montagnese et al., Phys. Rev. Lett. 110, 147206 (2013)

TT 4.2 Mon 9:45 HSZ 201

Optimized tDMRG schemes for $T > 0$ response functions and application for quantum-critical bosons — •Thomas Barthel[1], Ulrich Schollwöck[2], and Subir Sachdev[3] — [1]Université Paris-Sud and CNRS — [2]LMU München — [3]Harvard University

I will present improved schemes for the precise and efficient evaluation of finite-temperature response functions of strongly correlated systems in the framework of the time-dependent density matrix renormalization group (tDMRG) [1,2]. The growth and scaling of entanglement in such simulations can be explained on the basis of quasi-locality. With the novel optimized schemes, the maximum times that can be reached are typically increased by at least a factor of two, when compared against the earlier approaches. These increased reachable times make many more physical applications accessible. I will show two applications: (a) the universal scaling form of the spectral function of 1D bosons in the quantum critical regime with dynamic critical exponent $z = 2$ [2], and (b) spin structure factors of the spin-1/2 XXZ chain in comparison to inelastic neutron scattering data for $KCuF_3$ [3].

[1] T. Barthel, NJP **15**, 073010 (2013)
[2] T. Barthel, U. Schollwöck, and S. Sachdev, arXiv:1212.3570
[3] B. Lake *et al.*, PRL **111**, 137205 (2013)

TT 4.3 Mon 10:00 HSZ 201

Finite temperature dynamics of Heisenberg spin chains with $S \geq 1/2$ — •Thomas Köhler[1], Salvatore R. Manmana[1], Christoph Karrasch[2], Thomas Pruschke[1], and Andreas Honecker[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [2]Department of Physics, University of California, Berkeley, CA 95720, United States

We present results for spectral functions of one-dimensional Heisenberg systems at finite temperatures obtained via a density-matrix renormalization group (DMRG) matrix product state implementation with real-time evolution. We show results for systems with $S = 1/2$ at zero and finite magnetic fields, as well as for systems with Dzyaloshinskii-Moriya anisotropy. At zero field, we discuss results for $S = 1$ and $S = 2$ and focus on the features realized in the dynamical structure factor at infinite temperature.

TT 4.4 Mon 10:15 HSZ 201

Matrix product state formulation of frequency-space dynamics at finite temperatures — •Alexander C. Tiegel, Salvatore R. Manmana, Thomas Pruschke, and Andreas Honecker — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

We use the density-matrix renormalization group (DMRG) to compute dynamical correlation functions of one-dimensional strongly correlated quantum systems at finite temperatures. The approach allows for the frequency-resolved evaluation of experimentally relevant quantities like line shapes in neutron or light scattering experiments. As a proof of principle, we study finite-temperature spectral functions of spin-1/2 XXZ Heisenberg chains with Dzyaloshinskii-Moriya interactions in magnetic fields. Based on our results, we provide an outlook for further improvements and developments of finite-temperature DMRG approaches to dynamical response functions.

TT 4.5 Mon 10:30 HSZ 201

Effective gauge field description for the bilinear-biquadratic spin-one chain — •Shijie Hu[1], Ari M. Turner[2], Karlo Penc[3,4], and Frank Pollmann[1] — [1]Max-Planck-Institut fuer Physik komplexer Systeme, 01187 Dresden, Germany — [2]University of Amsterdam, 1090 GL Amsterdam, The Netherlands — [3]Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, H-1525 Budapest, P.O.B. 49, Hungary — [4]Department of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary

We study the one-dimensional bilinear-biquadratic spin-one model. For this model, the possible existence of a nematic phase between a dimerized and a ferromagnetic phase has been debated. We present strong evidence for the absence of such an intermediate phase by comparing prediction of an effective gauge theory with the results of large scale density-matrix renormalization group (DMRG) simulations. In particular we compare the scaling of the correlations length and the dimerization strength obtained from the gauge theory with the DMRG results. It is found that quantum fluctuations melt the nematic order and stabilize a gapped, dimerized phase which persists all the way to the edge of the ferromagnetic phase. We furthermore discuss the multiplet structure found in the entanglement spectrum of the ground state wave functions.

TT 4.6 Mon 10:45 HSZ 201

The Cirac-Sierra construction and long range SU(N) spin models — Roberto Bondesan and •Thomas Quella — University of Cologne, Cologne, Germany

The Haldane-Shastry model for SU(2) is a paradigmatic example of a long range spin chain. The model is remarkable in that it allows for the analytic determination of the complete energy spectrum and explicit expressions for the associated wave functions. Besides being relevant in the context of fractional quantum Hall physics, it also provides a discretization of the critical SU(2) Wess-Zumino-Witten (WZW) conformal field theory.

Recently, Cirac and Sierra found a conceptually new and intriguing perspective on long range spin chains by reverting the previous idea. Now long range spin models arise as parent Hamiltonians of a given WZW correlator. This construction provides a generalization of the Haldane-Shastry model in the sense that the symmetry group, the representations and the positions of the spins may be freely chosen. It even permits the construction of 2D models with a specific groundstate wave function.

In this talk, we apply this construction to different types of SU(N) spin models and discuss the physical implications.

15 min. break.

TT 4.7 Mon 11:15 HSZ 201

The gl(1|1) Lie superalgebra as a basis for the Nielsen-Cirac-Sierra construction — Thomas Quella, Roberto Bondesan, and •Jochen Peschutter — University of Cologne, Cologne, Germany

By explicitly constructing quantum spin Hamiltonians and their groundstates for the SU(2)_k Wess-Zumino-Witten model, Nielsen, Cirac and Sierra have proposed a general blueprint for the construction

of quantum spin Hamiltonians with more general symmetries. The crucial ingredients in this pursuit are the so-called null vectors contained in the corresponding Verma module.

In this talk, we will present the status of our progress in specifically applying these ideas to the Lie superalgebra gl(1|1).

TT 4.8 Mon 11:30 HSZ 201

Self-assembling tensor networks and holography in disordered spin chains — •Andrew M. Goldsborough and Rudolf A. Römer — University of Warwick, Coventry, UK

We show that the numerical strong disorder renormalization group algorithm (SDRG) of Hikihara et al. for the disordered Heisenberg model [1] naturally describes a tree tensor network (TTN) with an irregular structure defined by the strength of the couplings. Using developments from TTNs [2] and the multi-scale entanglement renormalization ansatz (MERA) [3] we can efficiently calculate expectation values and entanglement entropy directly from the tensor network wavefunction. We also analyse the effect of the disordered geometry of the TTN on the two-point correlation functions and entanglement entropy. We show that disorder averaged correlation scales with the average path length through the tensor network, as suggested by Evenbly and Vidal [4] in the context of regular tensor network geometries and that entanglement entropy increases with both disorder and length, resulting in an area-law violation consistent with the results of [5].

[1] T. Hikihara, A. Furusaki, M. Sigrist, Phys. Rev. B 60, 12116 (1999)
[2] L. Tagliacozzo, G. Evenbly, G. Vidal, Phys. Rev. B 80, 235127 (2009)
[3] G. Evenbly and G. Vidal, Phys. Rev. B 79, 144108 (2009)
[4] G. Evenbly and G. Vidal, J. Stat. Phys. 145, 891 (2011)
[5] G. Refael and J. E. Moore, Phys. Rev. B 76, 024419 (2007)

TT 4.9 Mon 11:45 HSZ 201

Dynamical response functions in the 1D Hubbard model — •Imke Schneider[1], Rodrigo G. Pereira[2], and Fabian H. Essler[1] — [1]The Rudolf Peierls Centre for Theoretical Physics, Oxford University, Oxford OX1 3NP, United Kingdom — [2]Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, C.P. 369, Sao Carlos, SP, 13560-970, Brazil

Dynamical response functions are of particular interest in view of experimental applications such as momentum resolved tunneling in quantum wires. However, in recent works it was demonstrated that neglecting curvature in the generic dispersion in 1D - resulting in Luttinger liquid theory - leads to incorrect results for singularities in dynamical responses. Using a mapping to a Luttinger liquid with an additional high frequency mobile impurity and taking the leading irrelevant operators into account nonperturbatively it is possible to determine the exact threshold singularities.

We present a constructive derivation of such a mobile impurity model for the 1D Hubbard model. Crucially, the Luther-Emery point for both charge and spin fermions constitutes the good starting point for a weak coupling expansion. As an application we discuss the zero temperature optical conductivity of the 1D Hubbard model in the gapless phase.

TT 4.10 Mon 12:00 HSZ 201

Entanglement entropies for interacting many-fermion systems — •Peter Bröcker and Simon Trebst — Institute for Theoretical Physics, University of Cologne, Germany

The precise determination of the entanglement of an interacting quantum many-body systems is now appreciated as an indispensable tool to identify the fundamental character of the ground state of such systems. This is particularly true for unconventional ground states harboring non-local topological order or so-called quantum spin liquids that evade a standard description in terms of correlation functions.

With the entanglement entropy emerging as one of the central measures of entanglement, recent progress has focused on a precise characterization of its scaling behavior, in particular in the determination of (subleading) corrections to the prevalent boundary-law. While much progress has been made for spin and bosonic quantum many-body systems, fermion systems have proved to be more difficult.

For a large class of interacting fermionic systems, the numerical method of choice for unbiased, large-scale simulations is Determinantal Quantum Monte Carlo (DQMC) for which a generalization of the replica techniques developed to calculate entanglement entropies for spin and bosonic systems has remained an open question. Here we show one possibility how to construct the corresponding algorithm in DQMC and demonstrate its strength by studying the thermal crossover of the entanglement entropy in one-dimensional Hubbard systems. We also compare our results to another recent approach based on free fermion Green's functions.

TT 4.11 Mon 12:15 HSZ 201

Spin and charge dynamics of Hubbard chains with Rashba spin-orbit coupling — •Florian Goth and Fakher F. Assaad — Institut für theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

Interacting one-dimensional electrons have attracted considerable interest since the strong confinement marks the breakdown of the usual nearly free electron picture that is valid in higher dimensions. The experimental realization of these systems is often realized by considering adatoms on surfaces. Thereby, inversion symmetry is broken and a minimal model to capture the correlation physics is a Hubbard chain supplemented by a Rashba type spin-orbit interaction. We study this system using Quantum Monte Carlo methods as a function of doping and spin-orbit coupling strength. We present results on spin and charge dynamics as well as the single particle spectral functions.

TT 4.12 Mon 12:30 HSZ 201

Low-energy properties of fractional helical Luttinger liquids — •Tobias Meng[1], Lars Fritz[2], Dirk Schuricht[3], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA - Fundamentals of Future Information Technology, 52056 Aachen, Germany

We discuss how fractional helical Luttinger liquids, a one-dimensional state related to the fractional quantum Hall effect, can emerge as a consequence of an intricate mixing of charge and spin degrees of freedom in a quantum wire. We discuss their unusual low energy physics with an emphasis on their fractional conductance, the optical conductivity and density of states.

TT 4.13 Mon 12:45 HSZ 201

Quantum particles in periodically driven harmonic trap — •Eoin Quinn and Masudul Haque — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

We describe the effect of periodically modulating the strength of a confining trap on a one-dimensional trapped quantum system. We consider the driven dynamics of strongly interacting bosons (Tonks Giradeau gas) and free fermions. Having a discrete spectrum, the system exhibits a set of resonances. Our description combines an exact solution with a Floquet analysis.

TT 5: Transport: Quantum Coherence and Quantum Information Systems - Experiment

Time: Monday 9:30–10:45 Location: HSZ 204

TT 5.1 Mon 9:30 HSZ 204

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

The realization of a hybrid quantum system consisting of a superconducting on-chip microwave resonator and an ultracold paramagnetic atomic ensemble poses severe challenges regarding the design and optimization of the superconducting chip. The resonators have to be integrated with atom trapping wires nearby, they are not allowed to add strong perturbations to the magnetic trapping fields and extra resonator losses due to Abrikosov vortices must be avoided or minimized. Moreover, the resonators should be magnetic field insensitively tunable and optical access to the chip surface has to be granted. In the presentation, we will elucidate these experimental boundary conditions and present strategies to comply with them on the way towards strong coupling between ultracold atomic ensembles and on-chip microwave resonators.

TT 5.2 Mon 9:45 HSZ 204

Tunable coupling between two superconducting microwave resonators — •Friedrich Wulschner[1], Jan Goetz[1], Borja Peropadre[3], Alexander Baust[1], Elisabeth Hoffmann[1,2], David Zueco[4], Frank Deppe[1,2], Edwin P. Menzel[1], Achim Marx[1], Juan Jose Garcia-Ripoll[3], and Rudolf Gross[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, TU München, Garching, Germany — [3]IFF-CSIC, Madrid, Spain — [4]CSIC-Universidad de Zaragoza and Fundacion ARAID, Spain

In the field of superconducting quantum circuits, experiments with a small number of qubits and/or resonators have been successfully performed to realize proof-of-principle quantum information architectures. For scaling up such systems, it is desirable to achieve controllable couplings between individual circuit elements. In our experiment, we demonstrate a tunable coupling between two transmission line resonators via an RF-SQUID. The RF-SQUID can be considered as a tunable mutual inductance which can change both sign and magnitude. We show spectroscopic data of the tunable coupler and explain the magnetic flux dependence of the coupling with a theoretical model.

We acknowledge support from the DFG via SFB 631, the German excellence initiative via NIM, and the EU via PROMISCE.

TT 5.3 Mon 10:00 HSZ 204

Squeezing with a flux-driven Josephson parametric amplifier — •L. Zhong[1], E. P. Menzel[1], R. Di Candia[3], P. Eder[1,2], M. Ihmig[4], A. Baust[1], M. Haeberlein[1,2], K. Inomata[5], T. Yamamoto[5,6], Y. Nakamura[5,7], E. Solano[3], F. Deppe[1,2], A. Marx[1], and R. Gross[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, TU München, Garching, Germany — [3]University of the Basque Country UPV/EHU and IKERBASQUE Foundation, Bilbao, Spain — [4]TU München, Germany — [5]RIKEN Center for Emergent Matter Science, Japan — [6]NEC Smart Energy Research Laboratories, Japan — [7]The University of Tokyo, Japan

Josephson parametric amplifiers (JPA) are promising devices for continuous-variable quantum communication. In phase-sensitive mode, JPAs can beat the standard quantum limit for the added noise of phase-insensitive amplifiers. This property is a prerequisite for the generation of squeezed states. Here, we reconstruct the Wigner function of squeezed vacuum and thermal states with the dual-path method [1,2]. In addition, we illuminate the physics of propagating squeezed coherent microwave fields.

This work is supported by DFG via SFB 631, German Excellence Initiative via NIM, EU projects SOLID, CCQED, PROMISCE and SCALEQIT, MEXT Kakenhi "Quantum Cybernetics", JSPS FIRST Program, the NICT Commissioned Research, Basque Government IT472-10, Spanish MINECO FIS2012-36673-C03-02, and UPV/EHU UFI 11/55.

[1] L. Zhong *et al.*, arXiv:1307.7285 (2013)
[2] E. P. Menzel *et al.*, PRL **109** (2012) 250502

TT 5.4 Mon 10:15 HSZ 204

Interfacing rare earth spin ensembles with superconducting circuits — •Sebastian Probst[1], Andrej Tkalcec[1], Daniel Rieger[1], Hannes Rotzinger[1], Stefan Wünsch[2], Philipp Jung[1], Michael Siegel[2], Alexey V. Ustinov[1], and Pavel Bushev[3] — [1]Physikalisches Institut, KIT, 76128 Karlsruhe — [2]Institut für Mikro- und Nanoelektronische Systeme, KIT, 76189 Karlsruhe — [3]Institut für Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken

Interfacing photonic and solid-state qubits within a hybrid quantum architecture offers a promising route towards large scale distributed quantum computing. Ensembles of optically active rare earth spins embedded in a crystalline matrix are promising candidates for realizing such an interface. We report on single photon on-chip ESR spectroscopy of Er spin ensembles strongly coupled to superconducting and non superconducting microwave resonators [1,2]. The maximum coupling strength was measured to be 45 MHz at 200 ppm, and the minimum linewidth was 4 MHz at 50 ppm Er concentration, respectively. The strong anisotropy of Er:YSO prevents us from reaching the strong coupling regime at low field transitions. However, with crystals of higher symmetry such as YAP, strong coupling can be reached at relatively small magnetic fields of 30 mT at 5 GHz. In addition, we measured T_2 of the spins at millikelvins of about 40 μs. The experiments demonstrate the potential of rare earth ion doped crystals for their application in quantum information processing and communication. [1] Phys. Rev. B 84, 06051 (R) (2011), [2] Phys. Rev. Lett. 110, 157001 (2013)

TT 5.5 Mon 10:30 HSZ 204

Nuclear Spin Polarization in Bulk ZnSe:F — •Fabian Heisterkamp[1], Eugeny A. Zhukov[1], Vladimir L. Korenev[2], Alex Greilich[1], Alexander Pawlis[3], Dmitri R. Yakovlev[1,2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Department Physik, Universität Paderborn, 33098 Paderborn, Germany

Fluorine donor in ZnSe has been considered as a promising candidate for a quantum bit [1]. It is therefore crucial to study the influence of the environment on the spin coherence. In particular, we perform a study of interaction between electron and nuclei spins. Using the time-resolved optical pump-probe spectroscopy in the regime of resonant spin amplification we are able to resolve nuclear magnetic resonances (NMR) of ^{77}Zn and ^{67}Se isotopes with non-zero spin. The effective nuclei fields show a dispersive form of its strength around NMR as a function of magnetic field. Dependences of that signal are measured as a function of external parameters, like: pump power, polarization modulation frequency and temperature. Theoretical considerations support our findings.

[1] Sanaka et al., Phys. Rev. Lett. **103**, 053601 (2009).

TT 6: Transport: Quantum Coherence and Quantum Information Systems - Theory I

Time: Monday 11:00–13:00 Location: HSZ 204

TT 6.1 Mon 11:00 HSZ 204

Efficient Qubit Readout Using Josephson Photomultipliers — •Luke C. G. Govia[1], Emily J. Pritchett[1,2], Canran Xu[3], Maxim G. Vavilov[3], Britton L. T. Plourde[4], Robert McDermott[3], and Frank K. Wilhelm[1] — [1]Universität des Saarlandes, Saarbrücken, Germany. — [2]HRL Laboratories, Malibu, California, USA. — [3]University of Wisconsin-Madison, Wisconsin, USA. — [4]Syracuse University, New York, USA.

A Josephson Photomultplier (JPM) - a current-biased Josephson junction operated near its critical bias - can absorb and detect weak microwave signals with high sensitivity (PRL 107, 217401 (2011)). When strongly coupled to a high-Q transmission line "cavity", the JPM can detect single microwave photons with large bandwidth and with near unit efficiency (PRB 86, 174506 (2012)). The switching of a JPM into its voltage state acts on the adjacent cavity via the back action of photon subtraction (PRA 86, 032311 (2012)). While a destructive measurement of the microwave cavity, this switching can perform a binary non-demolition measurement of a quantum system coupled to the cavity. We present a protocol by which the presence and subsequent detection of a cavity photon by a JPM conveys information about the state of a superconducting qubit without destroying it, thus performing a quantum non-demolition measurement of the qubit's state. Multi-qubit generalizations of this protocol are discussed.

TT 6.2 Mon 11:15 HSZ 204

Controlling qubits with tight frequency separation — Daniel Egger[1], Visa Vesterinen[2], Ron Schutjens[1,2], Fadi Abu Dagga[1], Olli-Pentti Saira[2], Alessandro Bruno[2], Leo DiCarlo[2], and •Frank Wilhelm[1] — [1]Theoretical Physics, Saarland University, Saarbrücken, Germany — [2]Quantum Transport, Kavli Institute for Nanoscience, TU Delft, The Netherlands

As quantum computer architectures are scaled up, addressing multiple qubits by their individual frequencies becomes increasingly difficult. This is in particular true for superconducting transmon qubits which in themselves are anharmonic oscillators. We present a strategy to combat closeness of wanted and unwanted transitions in multiple qubits that allows to significantly reduce this problem. This Weak AnHarmonicity With Average Hamiltonian (WAHWAH)]1] technique can handle cases that go beyond the familiar DRAG method [2].This technique is based on sideband modulation. We show experimentally that this technique allows two-transmon settings with significant frequency overlap to reach fidelities, as measured by interleaved randomized benchmarking, limited by decoherence alone.

[1] R. Schutjens et al., Phys. Rev. A 88, 052330 (2013)
[2] F. Motzoi et al., Phys. Rev. Lett. 103, 110501 (2009)

TT 6.3 Mon 11:30 HSZ 204

Parity switching and decoherence by quasiparticles in single-junction transmons — •Gianluigi Catelani — Forschungszentrum Jülich, PGI-2, Jülich, Germany

Transmons are at present among the most coherent superconducting qubits, reaching quality factors of order 10^6 both in 3D and 2D architectures. These high quality factors enable detailed investigations of decoherence mechanisms. An intrinsic decoherence process originates from the coupling between the qubit degree of freedom and the quasiparticles that tunnel across Josephson junctions. In a transmon, tunneling of a single quasiparticle is associated with a change in parity. I will discuss the theory of the parity switching rate in single-junction transmons, compare it with recent measurements, and consider the role of parity switching in limiting the coherence time.

Partial support by the EU under REA grant agreement CIG-618258 is acknowledged.

TT 6.4 Mon 11:45 HSZ 204

Hybrid quantum magnetism in the strong and ultrastrong coupling regime — •Andreas Kurcz, Alejandro Bermudez, and Juan Jose Garcia-Ripoll — Instituto de Fisica Fundamental (IFF-CSIC), Calle Serrano 113bis, Madrid E-28006, Spain

We study a quantum setup that consist of superconducting qubit mediated resonators, where quantum magnetism arises non-perturbatively and can be understood both analytically and numerically (A. Kurcz et. al., arXiv:1310.8173). The setup exhibits a set of interspersed spin-boson lattice models [1,2] and reveals a phase transition of the Ising type [3], where both qubits and cavities spontaneously polarise and where the cavity-qubit detuning acts as the equivalent of a magnetic field. We develop a many-body correlated mean field theory that accurately predicts the nature of the ground state and that captures this phenomenon all the way, from a perturbative dispersive regime where photons can be traced out, to the non-perturbative ultrastrong coupling regime where photons must be treated on the same footing as qubits. Our ansatz also reproduces the low-energy excitations, which are described by hybridised spin-photon quasiparticles, and can be probed spectroscopically from transmission experiments in circuit-QED, as shown by Matrix-Product-State methods. Our model offers an ideal playground in order to simulate the existing many-body machinery from spin-photon waves to many body-spectroscopy.

[1] D. Porras et. al., Phys. Rev. Lett. 108, 235701 (2012)
[2] M. Schiro et. al., Phys. Rev. Lett. 109, 053601 (2012)
[3] P. Pfeuty, Ann. Phys. 57, 79 (1970).

TT 6.5 Mon 12:00 HSZ 204

Optimizing quantum measurements in circuit QED — •Daniel Egger and Frank Wilhelm — Universität des Saarlandes, Saarbrücken, Deutschland

Manipulating quantum systems requires knowing the shape of the control pulses to achieve a desired state or specified time evolution. Optimal control is the framework in which the pulses are designed. Typically such pulses are optimal with respect to time and can be found through a gradient search [1]. In superconducting qubits these methods have been applied to gate design , usually in an idealised unitary process [2,3]. In this work we instead focus on optimizing the time evolution of systems where non-unitary processes are the source for the desired time evolution. As example we consider a measurement process in circuit QED where a "click" of the detector corresponds to a tunneling event and find control pulses that optimize a contrast. We first analyze the standard phase qubit readout, we then evaluate its generalization to the JBA.

[1] N. Khaneja *et al.*, J. Magn. Reson. **172**, 296
[2] R. Schutjens *et al.*, Phys. Rev. A **88**, 052330
[3] D. J. Egger & F. K. Wilhelm, Supercond. Sci. Technol. **27**, 014001

TT 6.6 Mon 12:15 HSZ 204

Metamaterials for circuit QED: Quantum simulations and other applications — •Bruno G. Taketani and Frank K. Wilhelm — Saarland University, Saarbrücken, Germany

The ability to design periodically structured materials not present in nature provides scientists with new tools, ranging from sub-wavelength imaging to well controlled band structures for wave propagation in photonic crystals. Superconducting metamaterials have been recently proposed to manipulate the density-of-modes of transmission lines [1]. We further build on these ideas and develop a toolbox for environment manipulation based on nano-structured, periodic, lossless, superconducting circuits. In particular we show that high density of low energy states can be achieved using a superlattice arrangement of left-handed circuit elements. Multimode, ultra-strong coupling of superconducing qubits to such engineered environments thus allow for experimental implementation of quantum simulation of interesting new phenomena as well as for complex quantum state engineering.

[1] D. J. Egger and F. K. Wilhelm, Phys. Rev. Lett. **111**, 163601 (2013)

TT 6.7 Mon 12:30 HSZ 204

Resonant versus dispersive gates in circuit quantum electrodynamics — •Per Liebermann and Frank Wilhelm — Universität des Saarlandes, Saarbrücken, Germany

Implementation of accurate two-qubit gates in the presence of decoherence is one of the main tasks of building a quantum computer. In this work we describe two superconducting qubits coupled via a resonator and perform a controlled-Z operation on them. Being able to control the qubits' transition frequencies, we compare the resonant and dispersive gate implementation of CZ [1,2], where in the latter case qubit-qubit interaction is mediated by virtual photons. We make use of the Lindblad master equation to study different regimes of resonator relaxation and qubit decoherence and their impact on gate fidelity. Fi-

nally, we discuss the tradeoff between the higher speed of the resonant gate versus the protection from the Purcell effect in the dispersive gate, which we show to usually be in favor of resonant gates.
[1] A. Blais et al., Phys. Rev. A 75, 032329 (2007)
[2] D.J. Egger and F.K. Wilhelm, Supercond. Sci. Technol. 27 (2014)

TT 6.8 Mon 12:45 HSZ 204

From Coulomb-Blockade to Nonlinear Quantum Dynamics in a Superconducting Circuit with a Resonator — Vera Gramich, •Björn Kubala, Selina Rohrer, and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Motivated by recent experiments [1] on superconducting circuits consisting of a dc-voltage-biased Josephson junction in series with a resonator, quantum properties of these devices far from equilibrium are studied [2]. This includes a crossover from a domain of incoherent to a domain of coherent Cooper pair tunneling, where the circuit realizes a driven nonlinear oscillator. Equivalently, weak photon-charge coupling turns into strong correlations captured by a single degree of freedom. Radiated photons offer a new tool to monitor charge flow and current noise gives access to nonlinear dynamics, which allows us to analyze quantum-classical boundaries. Higher order resonances are discussed as well and provide new avenues for future experiments.
[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] V. Gramich, B. Kubala, S. Rohrer, and J. Ankerhold, accepted for publication in Phys. Rev. Lett., arXiv:1307.2495.

TT 7: Superconductivity: Cryodetectors

Time: Monday 9:30–13:00 Location: HSZ 03

TT 7.1 Mon 9:30 HSZ 03

First demonstration of a TES with High-Frequency Readout at 0.65 THz — •Artem Kuzmin[1], Michael Merker[1], Sergey Shitov[2,3], Nikolay Abramov[2], Mathias Arndt[1], Stefan Wuensch[1], Konstantin Ilin[1], Alexey Ustinov[2,4], and Michael Siegel[1] — [1]Institut für Mikro- und Nanoelektronische Systeme, Karlsruher Institut für Technology — [2]National University of Science and Technology MISIS — [3]Kotel'nikov Institute of Radio Engineering and Electronics RAS — [4]Institute of Physics and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology

We suggested an antenna-coupled TES bolometer embedded in a high-Q GHz resonator as a load to isolate the sensitive element from excess noise and disturbances. The resonator is weakly coupled to the readout transmission line. This approach allows for biasing the TES with RF power at their individual resonance frequencies and readout incident THz signal as modulation of this RF biasing signal with "conversion gain" ¿ 1, thus it is possible to use a single broadband low-noise HEMT amplifier for a relatively large number of TES bolometers in array. This approach could be used down to 300 mK without a SQUID amplifier [1-2]. To proof the concept of the new device we fabricated sub-micron sized prototypes of single-pixel RF-TES from Nb for operation temperature of 5.0 K. Results of DC and RF characterization of the TES devices along with measurement of the optical sensitivity at 0.65 THz and NEP will be presented and discussed.
[1] Technical Physics Letters **37** (2011) 932
[2] IEEE Trans. Terahertz Sci. and Tech.**3** (2013) 25

TT 7.2 Mon 9:45 HSZ 03

Detecting single infrared photons with a Transition Edge Sensor for ALPS-II — •Friederike Januschek[1], Noemie Bastidon[2], Jan Dreyling-Eschweiler[1,2], Dieter Horns[2], and Axel Lindner[1] — [1]Deutsches Elektronen-Synchrotron, Hamburg — [2]Institut für Experimentalphysik, Universität Hamburg

For the ALPS-II experiment at DESY, which will be looking for ultralight fundamental bosons, a detector with the ability to measure rates below 10^{-3} s^{-1} of single NIR photons with a wavelength of 1064 nm is necessary. Therefore, the ALPS-II detection system is required to have even lower dark count and background rates, while keeping a reasonable efficiency for photons with an energy of about 1.165 eV. For this purpose, a detector system with a superconducting Transition Edge Sensor chip from NIST, being read out by SQUIDs, was set up inside an Adiabatic Demagnetisation Refrigerator and operated at 80 mK. In this talk, results of the characterisation of this system will be presented. The focus will be on the achievable and achieved background rates of intrinsic background and background from black body radiation.

TT 7.3 Mon 10:00 HSZ 03

Design and commissioning of a X-ray spectroscopy detector setup at storage rings — •Pascal Scholz and Saskia Kraft-Bermuth — Justus-Liebig-Universität, Gießen, Germany

X-ray spectroscopy of highly-charged heavy ions in the X-ray regime, commonly performed at storage ring facilities, provides a sensitive test of quantum electrodynamics. Silicon microcalorimeters have already demonstrated their potential for such experiments. To improve performance, a cryogen-free cryostat has been commissioned, which is equipped with a side arm with the detector mounted on a cold finger centered in the front of this side arm. For inherent correction of Doppler shifts, a new detector array with improved design and pixels for high as well as low x-ray energies will be equipped. This upgrade will improve the lateral sensitivity and detector resolution in the further analysis. The design serves also as a benchmark for a larger array with approximately 100 pixels. The design and performance results will be presented with this talk.

TT 7.4 Mon 10:15 HSZ 03

High-precision X-ray spectroscopy of highly-charged ions with silicon microcalorimeters — •Saskia Kraft-Bermuth[1], Victor Andrianov[2,3], Alexander Bleile[2], Artur Echler[1,2], Peter Egelhof[2], Patrick Grabitz[2], Caroline Kilbourne[4], Oleg Kisselev[2], Dan McCammon[5], and Pascal Scholz[1] — [1]Institut f. Atomphysik, Justus-Liebig-Universität, Gießen, Germany — [2]Helmholtzzentrum f. Schwerionenforschung, Darmstadt, Germany — [3]Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia — [4]NASA/Goddard SFC, Greenbelt, USA — [5]Dept, Physics, University of Wisconsin, Madison, USA

High-precision X-ray spectroscopy of highly-charged ions provides a sensitive test of quantum electrodynamics in very strong Coulomb fields. Silicon microcalorimeters with absorbers of lead and tin have been applied in two experiments for the determination of the 1s Lamb shift in hydrogen-like lead and gold at the Experimental Storage Ring (ESR) at GSI. The experimental results agree well with theoretical predictions. The obtained uncertainty is comparable to conventional detection techniques. Further improvement may be obtained, in addition to an improved detector setup, by using decelerated beams at the socalled CRYRING and HITRAP facilities currently under construction at GSI. This talk will present the results of the ESR experiments and discuss perspectives for experiments at CRYRING and HITRAP as well as for experiments at the future FAIR facility, with a focus on detector development and technical challenges.

TT 7.5 Mon 10:30 HSZ 03

Application of Calorimetric Low Temperature Detectors (CLTD's) for Precise Stopping Power Measurements of Heavy Ions in Matter — •Artur Echler[1,2,3], Peter Egelhof[2,3], Patrick Grabitz[2,3], Heikki Kettunen[4], Saskia Kraft-Bermuth[1], Mikko Laitinen[4], Katrin Müller[1], Mikko Rossi[4], Wladyslaw Trzaska[4], and Ari Virtanen[4] — [1]Justus-Liebig-Universität, Gießen — [2]GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt — [3]Johannes Gutenberg Universität, Mainz — [4]University of Jyväskylä

Precise data on stopping powers (i.e. specific energy loss dE/dx) of heavy ions in matter are needed in many fields of basic and applied science, and for our understanding of the interaction of energetic ions with matter. As the available datasets are still scarce, in particular for heavy projectiles at energies below the Bragg-peak, and discrepancies between measured and theoretical values are often significant, CLTD's have been recently applied in combination with a time-of-flight detector to perform transition-type energy loss measurements at the accelerator facility of the University of Jyväskylä. As compared to conventional ionization detectors, CLTD's provide substantially better energy resolution and linearity (with the absence of any pulse height

defect) for heavy ion detection, which leads to a higher sensitivity and accuracy for dE/dx measurements using the E-TOF method, and allows to extend the accessible energy range towards lower energies. The new experimental technique was used to determine precise stopping power data for 0.05 - 1 MeV/u ^{131}Xe ions in Carbon, Nickel and Gold.

TT 7.6 Mon 10:45 HSZ 03

Solid state physics and engineering to push resolving power of magnetic calorimeters beyond 10000 — •Daniel Hengstler, Anna Ferring, Lisa Gamer, Jeshua Geist, Mathäus Krantz, Andreas Pabinger, Christian Pies, Christian Schötz, Sebastian Kempf, Loredana Gastaldo, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg

Metallic magnetic calorimeters are energy dispersive particle detectors, operated at temperatures below 50 mK that make use of a paramagnetic temperature sensor to convert the energy deposited by an absorbed particle into a magnetic flux change in a SQUID, which can be read-out as a voltage signal with low noise and large bandwidth. During the last decade we've been optimizing the signal size of MMCs by numerical optimizations and the consequent use of micro-fabrication techniques, while lowering the readout noise close to quantum limit. The combination of both rewarded us recently with an instrumental linewidth of 1.6 eV (FWHM) for 6 keV x-rays, which on the one hand is a world record, on the other hand is much less than expected from the signal-to-noise-ratio in those measurements. Such discrepancies can easily arise from instabilities of the total gain, or — more interestingly — from a-thermal phonon loss or position dependencies.

In this talk we summerize the physics of MMCs, highlighting the presently done homework in solid state physics and engineering to reach resolving powers beyond 10000, and show recent results of MMCs in various applications.

TT 7.7 Mon 11:00 HSZ 03

Current sensing SQUIDs for the readout of low impedance cryogenic particle detectors — •S. Kempf, A. Ferring, M. Wegner, A. Fleischmann, L. Gastaldo, and C. Enss — Kirchhoff-Institute for Physics, Heidelberg University.

Superconducting quantum interference devices (SQUIDs) are presently the most sensitive wideband devices for measuring various physical quantities that can be converted in magnetic flux. They are commonly used in measurement systems in which a very sensitive sensor or an ultra low noise wideband amplifier is required. A prominent example for the use of SQUIDs is the readout of low impedance cryogenic particle detectors (LTDs). Here, the SQUIDs are used as very fast current sensors that are compatible with the very low operation temperature of LTDs. Driven by the need for devices that are matched to state-of-the-art LTDs, we have recently started the development of low-T_c current sensing SQUIDs. In particular, we are developing cryogenic frequency-domain multiplexers that are based on non-hysteretic rf-SQUIDs as well as single channel dc-SQUIDs.

After a presentation of our multiplexer and dc-SQUID designs as well as our fabrication process that is based on selective Niobium etching, we will discuss the measured performance of both types of devices. We will show that the devices are operational and that their performance can be numerically predicted with confidence, thus allowing for a design optimization with respect to the readout requirements of low impedance LTDs. Finally, we outline future developments that are forseen to improve the noise performance of our devices.

15 min. break.

Topical Talk TT 7.8 Mon 11:30 HSZ 03

Probing Decoherence in Atomic-Sized Defects Using a Superconducting Qubit — •Jürgen Lisenfeld, Georg Weiss, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institute for Technology (KIT), Karlsruhe, Germany

Advances in nanotechnology lay the ground for a thriving variety of novel devices suitable to explore new realms of quantum phenomena on the mesoscopic scale. Superconducting quantum bits, as an example, have reached very long coherence times by designs that weaken their undesired coupling to environmental degrees of freedom. One particular problem are parasitic Two-level systems (TLS), reported to cause noise in single-photon detectors, SETs, SQUIDs, and microwave- as well as nano-mechanical resonators, although their physical origin remains in dispute.

A particular strong coupling between superconducting qubits and TLS occurs when they reside in the tunnel barrier of Josephson junctions, and this renders qubits ideal tools for the study of single material defects in the coherent regime. Here, we use a phase qubit to directly manipulate and readout the TLS quantum state. We tune TLS properties by the applied mechanical strain and perform high-resolution defect spectroscopy to obtain their distribution and to reveal mutual TLS coupling. By analyzing their coherent dynamics, we utilize single microscopic defects as quantum spectrum analyzers that provide a view into their environment. These new techniques grant multifaceted insights into the TLS nature, which is a prerequisite for avoiding their detrimental effects in nanoscale devices.

TT 7.9 Mon 12:00 HSZ 03

Dc SQUIDs for the detection of Bose-Einstein-Condensates — •Matthias Rudolph[1], Michael Merker[2], Johannes Maximilian Meckbach[2], Martin Knufinke[1], Petra Vergien[1], Florian Jessen[1], Simon Bell[1], Patrizia Weiss[1], Helge Hattermann[1], Konstantin Ilin[2], Michael Siegel[2], József Fortágh[1], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut 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

One example of an exciting quantum hybrid system is created by coupling a SQUID with an ensemble of ultra cold atoms. Here we suggest using a gradiometric dc SQUID to non-destructively detect the center of mass motion of Bose-Einstein Condensates (BECs) which are confined in a magnetic trap. The Gradiometer, fabricated using a self-aligning Nb/AlO$_x$/Nb process, has been characterized with respect to its transport and noise properties at a temperature of $T = 4.2$ K, revealing an equivalent density of flux noise $S_\Phi^{1/2} \approx 350\,\mathrm{n}\Phi_0/\mathrm{Hz}^{1/2}$ in a magnetically unshielded environment. Numerical simulations based on the London equations suggest that with these noise properties we can expect to detect a rubidium BEC with 10^5 atoms at a distance of $10\,\mu$m from the SQUID with a signal-to-noise ratio SNR ≈ 10.

TT 7.10 Mon 12:15 HSZ 03

Magnetic Johnson noise thermometry for μK temperatures — Daniel Rothfuss, •Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Noise thermometry instrinsically is a non-driven method. When minimal heat input is required this method is highly advantageous. Our noise thermometer is a magnetic Johnson noise thermometer. The noise source is a cold-worked high purity copper cylinder with a diameter of 5 mm and a length of 20 mm. The magnetic flux fluctuations caused by the brownian motion of the electrons are measured inductively by two dc-SQUID magnetometers simultaneously. The signals from these two channels are cross-correlated. This leads to a reduction of parasitic noise by more than one order of magnitude. Applying this technique together with the highly sensitive SQUID preamplifiers allows the measurement of the tiny noise powers at microkelvin temperatures. Experimentally we characterized the thermometer for temperatures between $43\,\mu$K and $0.8\,$K. The measuring time is approximately 400 seconds for one temperature, the extremely low heat input to the thermometer allows a continuous measurements without heating effects.

TT 7.11 Mon 12:30 HSZ 03

Manipulation of a two-photon pump in superconductor – semiconductor heterostructures — •Peter P. Orth[1], Paul Baireuther[2], Ilya Vekhter[3], and Jörg Schmalian[1] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), , 76131 Karlsruhe, Germany — [2]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [3]Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana, 70803, USA

We investigate the photon statistics, entanglement and squeezing of a pn-junction sandwiched between two superconducting leads, and show that such an electrically-driven photon pump generates correlated and entangled pairs of photons. In particular, we demonstrate that the squeezing of the fluctuations in the quadrature amplitudes of the emitted light can be manipulated by changing the relative phase of the order parameters of the superconductors. This reveals how macro-

scopic coherence of the superconducting state can be used to tailor the properties of a two-photon state.

TT 7.12 Mon 12:45 HSZ 03

Luminescence and photon coherence in superconducting pn-heterostructures — •Patrik Hlobil, Peter Orth, and Jörg Schmalian — Karlsruhe Institute of Technology, Germany

Semiconducting pn-heterostructures coupled to superconducting leads appear to be promising candidates as a source of entangled and squeezed light. Due to an applied bias voltage V, we have to use a non-equilibrium field theory approach to study the electron-photon system. Particular emphasis is placed on the consequence of the superconducting coherence for the photon statistics, the luminescence and possible feedback on the electronic system.

TT 8: Correlated Electrons: Spin Systems and Itinerant Magnets - Frustrated Magnets I

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

TT 8.1 Mon 9:30 HSZ 304

Critical speeding-up near the monopole liquid-gas transition in magnetoelectric spin-ice — •Christoph P. Grams[1], Martin Valldor[1,2], Markus Garst[3], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Institut für Theoretische Physik, Universität zu Köln, Cologne, Germany

Competing interactions in the so-called spin-ice compounds stabilize a frustrated ground-state with finite zero-point entropy and, interestingly, emergent magnetic monopole excitations[1]. The properties of these monopoles are at the focus of recent research with particular emphasis on their quantum dynamics. It is predicted[2] that each monopole also possesses an electric dipole moment, which allows to investigate their dynamics via the dielectric function $\varepsilon(\nu)$.

In this talk I report on broadband spectroscopic measurements of $\varepsilon(\nu)$ in $Dy_2Ti_2O_7$ down to temperatures of 200 mK with a specific focus on the critical endpoint present for a magnetic field along the crystallographic [111] direction[3].

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

[1] C. Castelnovo et al., Nature 451 (2008) 42
[2] D. I. Khomskii, Nature Comm. 3 (2012) 1
[3] C. P. Grams et al., arXiv:1307.8287

TT 8.2 Mon 9:45 HSZ 304

Vibrating coil magnetometry in $Dy_2Ti_2O_7$ at milli-Kelvin temperatures — •Christopher Duvinage[1], Dharmalingam Prabhakaran[2], Christian Pfleiderer[1], and Andrew T. Boothroyd[2] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, United Kingdom

Spin ice attracts great interest as a state in which emergent fractionalized excitations and magnetic-field induced topological forms of order may occur. 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 [1,2]. We report vibrating coil magnetometry down to mK temperatures of $Dy_2Ti_2O_7$, addressing the evidence for field-induced phase transitions. Of particular interest is the observation of putative magnetisation avalanches in the spin-frozen state which depend sensitively in number and size on the sweep rate of the applied magnetic field. These avalanches have been interpreted in terms of monopole excitations [3].

[1] Krey *et al.*, PRL **108** (2012) 257204
[2] Legl *et al.*, PRL **109** (2012) 047201
[3] Slobinsky *et al.*, PRL **105** (2010) 267205

TT 8.3 Mon 10:00 HSZ 304

Hysteresis and Relaxation Effects in the Spin-Ice Compound $Dy_2Ti_2O_7$ studied by Heat Transport — •Simon Scharffe, Gerhard Kolland, Martin Hiertz, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

The magnetic Dy^{3+} ions in the spin ice $Dy_2Ti_2O_7$ form a pyrochlore lattice consisting of corner-sharing tetrahedra. Due to strong crystal field effects an Ising anisotropy arises which aligns the spins along its local easy axis, pointing into or out of a tetrahedra. Possible ground-states at temperatures below 1 K are given by the "ice rule": two spins point into and two out of a tetrahedron. Excited states can be created by flipping one spin and are discussed as magnetic monopoles[1]. We measured the low-temperature thermal conductivity κ and found experimental evidence for heat transport by magnetic monopoles[2,3]. In addition we observe pronounced hysteresis effects which depend on temperature, the magnetic-field direction, the rate of magnetic-field change, and on the direction of the heat current. Moreover the time-dependent relaxation of the heat conductivity is investigated. These data yield information about possible equilibrium states and reveal that in the low-field and low-temperature region extremely slow relaxation processes occur[4].

This work was supported by DFG through SFB 608 and LO 818/2-1.

[1] Castelnovo *et al.*, Nature **451** (2008) 42
[2] Kolland *et al.*, Phys. Rev. B, **86** (2012) 060402(R)
[3] Kolland *et al.*, Phys. Rev. B, **88** (2013) 054406
[4] Scharffe *et al.*, J. Phys. Soc. Jpn. Suppl. (in press), arXiv:1311.1139

TT 8.4 Mon 10:15 HSZ 304

Wien Effect on a Lattice — •Vojtech Kaiser[1,2], Steven Bramwell[3], Peter Holdsworth[1], and Roderich Moessner[2] — [1]ENS Lyon — [2]MPI PKS Dresden — [3]London Centre for Nanotechnology, UCL

The Second Wien Effect is an increase of conductivity of Coulomb gas in an external field, driven by enhanced dissociation of Coulombically bound pairs. The importance of the Wien effect for spin ice was suggested previously since spin ice maps to a Coulomb gas of magnetic monopoles. We present simulations of lattice Coulomb gas and spin ice. The results confirm Onsager's theory of the Wien effect and reveal additional corrections, while allowing access to microscopic dynamics underlying the increase in the charge carrier density. Main extensions of the original theory involve the Debye screening, field dependent mobility and the character of the association constant. We discuss further corrections specific to spin ice due its emergent topological charge and Dirac string network.

TT 8.5 Mon 10:30 HSZ 304

Magnetic and dielectric Properties of the cubic pyrochlore $Nd_2Hf_2O_7$ — •J.-H. Chun[1], P. G. Reuvekamp[1], R. K. Kremer[1], C. T. Lin[1], R. Glaum[2], and A. Bronova[2] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Rheinische Friedrich-Wilhelms-Universität, Institut für Anorganische Chemie, D-53121 Bonn, Germany

The magnetic properties of rare-earth (R) pyrochlores (PC) of $R_2M_2O_7$, where M is a 3d or 4d transition metal, have attracted broad attention because geometrical frustration gives rise to unusual magnetic ground states and excitations like spin-ice or magnetic monopoles.[1,2] In contrast the properties and especially the magnetism of the rare-earth PCs with 5d cations are considerably less well investigated. Reasons are the close proximity of the cubic PCs to the fluorite structure and that oxides of the PC family tend to exhibit disorder involving a statistical redistribution of the metal atom cations accompanied by a redistribution of the oxygen vacancy sites. We have prepared polycrystalline samples and single-crystal of $Nd_2Hf_2O_7$ and investigated their structural, magnetic, thermal, lattice and dielectric properties. We report low-temperature magnetic ordering determined by heat capacity and magnetic susceptibility measurements and investigations of the dielectric properties. Measurements of the thermal expansion gave no indication of a structural phase transition down to 5 K.

[1] J. S. Gardner, M. J. P. Gingras, and J. E. Greedan, Rev. Mod. Phys. 82 (2010) 53
[2] A. P. Ramirez, Annu. Rev. Mater. Sci. 24 (1994) 453

TT 8.6 Mon 10:45 HSZ 304

Novel magnetism in the spin-orbit driven Mott insulator Ba_2YIrO_6 — •Tusharkanti Dey[1], Andrey Maljuk[1], Olga Kataeva[1,2], Frank Steckel[1], Daniel Gruner[1], Tobias Ritschel[1], Christian G. F. Blum[1], Anja U. B. Wolter[1], Jochen Geck[1], Christian Hess[1,3], Sabine Wurmehl[1,4], and Bernd Büchner[1,4] — [1]Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany — [2]Kazan Federal University, Kremlevskaya str. 18, 420008, Kazan, Russia — [3]Center for Transport and Devices of Emergent Materials, TU Dresden, 01069 Dresden, Germany — [4]Institute for Solid State Physics, Dresden Technical University, TU-Dresden, 01062 Dresden, Germany

Single crystals of Ba_2YIrO_6 were synthesized for the first time. The material crystalizes in cubic double perovskite structure. Here the only magnetic ion Ir is expected to be in +5 oxidation state with $5d^4$ electronic configuration. Instead of the expected weak Van Vleck-type magnetism [1], we found Ba_2YIrO_6 is paramagnetic in the temperature range 2-300K. Curie-Weiss fitting (30-300K) of susceptibility data gives a Weiss constant θ_{CW}=-15K (AF) but no magnetic ordering is found down to 1.8K. Our study suggests that Ba_2YIrO_6 is a spin-orbit driven Mott insulator with highly frustrated magnetic interactions originating from the face centered cubic (FCC) lattice formed by the Ir moments. In this presentation, details of crystal growth along with structural, magnetic, thermal and electrical transport measurement results will be discussed.

[1] G. Khaliullin, Phys. Rev. Lett. 111 (2013) 197201

TT 8.7 Mon 11:00 HSZ 304

Spiral order in Li_2IrO_3 — •Stephan Rachel[1], Johannes Reuther[2], and Ronny Thomale[3] — [1]Institut für Theoretische Physik, TU Dresden — [2]California Institute of Technology — [3]Institut für Theoretische Physik, Universität Würzburg

Iridates are amongst the most interesting complex oxide materials. The non-interacting band structure of the honeycomb Iridates has been claimed to feature the quantum spin Hall effect due to large spin orbit coupling. The true materials exhibit considerable Coulomb interactions leading to different types of magnetic order (e.g., zig-zag or spiral order). Here we show how one can obtain such magnetic phases by considering the strong-coupling limit of a topological Hubbard model. In particular, we find an incommensurate phase with spiral order which is consistent with the recent experimental findings for Li_2IrO_3.

15 min. break.

TT 8.8 Mon 11:30 HSZ 304

Theoretical investigation of isoelectronic Li doping in sodium iridate $(Na_{1-x}Li_x)_2IrO_3$ — •Michaela Altmeyer[1], S. Manni[2], S. K. Choi[3], I. I. Mazin[4], R. Coldea[3], Harald O. Jeschke[1], Roser Valenti[1], and P. Gegenwart[2] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, D-37077, Göttingen, Germany — [3]Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom — [4]Code 6393, Naval Research Laboratory, Washington, DC 20375, USA

In the recent years honeycomb iridates have been intensively debated as promising candidates for the realization of the Heisenberg-Kitaev-model. Due to the different magnetic ground states of Na_2IrO_3 and Li_2IrO_3 (zigzag for the former and possibly incommensurate for the latter), it is interesting to investigate the series $(Na_{1-x}Li_x)_2IrO_3$. Synthesis of the Li doped Na_2IrO_3 was successful at least up to 20% Li, but there are indications of phase separation at higher concentrations. We investigated the $(Na_{1-x}Li_x)_2IrO_3$ series by full relaxation within density functional theory (DFT). At each doping level, we investigated all possible Na/Li distributions in a supercell containing four formula units and found the substitution of Na by Li in the honeycomb plane Ir_2Na to be most stable for small dopings in the area $0 < x <= 0.25$. Total energies yield a tendency for phase separation above a doping level of $x = 0.25$ in agreement with experiment.

TT 8.9 Mon 11:45 HSZ 304

Band structure and optical properties of $Na_3Ir_3O_8$ — •Alexander Yaresko — MPI FKF, Stuttgart, Germany

$Na_4Ir_3O_8$ attracted much attention due to its fascinating magnetic properties. It is a weak Mott insulator in which magnetic Ir^{4+} ions form a frustrated non-centrosymmetric hyper-kagome lattice. Because of geometrical frustrations Ir spins do not order down to lowest temperature but instead remain in a 3D spin-liquid state. Recently, monocrystals of another hyper-kagome Ir compound $Na_3Ir_3O_8$ have been synthesized, In contrast to $Na_4Ir_3O_8$, $Na_3Ir_3O_8$ is a semi-metal with a low carrier density and weak paramagnetism of valence electrons. If spin-orbit interaction (SOI) is neglected, LDA calculations for $Na_3Ir_3O_8$ give an insulating solution despite of noninteger $Ir^{4.33+}$ valence. SOI, however, closes the band gap and $Na_3Ir_3O_8$ becomes a compensated metal. In this presentation it is shown that the gap appears because of formation of quasi-molecular orbitals on Ir triangles which become partially delocalized due to SOI. The semi-metallic band structure together with the lack of inversion symmetry lead to unusual optical properties which seem to suggest anomalously strong electron-phonon coupling.

TT 8.10 Mon 12:00 HSZ 304

Magnetism in spin models for depleted honeycomb-lattice iridates: Spin-glass order towards percolation — •Matthias Vojta and Eric C. Andrade — Technische Universität Dresden, 01062 Dresden, Germany

Iridates are characterized by a fascinating interplay of spin-orbit and electron-electron interactions. The honeycomb-lattice materials A_2IrO_3 (A=Na,Li) have been proposed to realize pseudospin-1/2 Mott insulating states with strongly anisotropic exchange interactions, described by the Heisenberg-Kitaev model, but other scenarios involving longer-range exchange interactions or more delocalized electrons have been put forward as well.

Here we study the influence of non-magnetic doping, i.e., depleted moments, on the magnetic properties of experimentally relevant variants of the Heisenberg-Kitaev and Heisenberg J_1-J_2-J_3 models. We generically find that the zigzag order of the clean system is replaced, upon doping, by a spin-glass state with short-ranged zigzag correlations. We determine the spin-glass temperature as function of the doping level and argue that this quantity allows to experimentally distinguish the different proposed spin models when the doping is driven across the site percolation threshold of the honeycomb lattice.

TT 8.11 Mon 12:15 HSZ 304

Analysis of the electronic and magnetic properties of honeycomb and triangular lattice iridates — •Ying Li[1], Harald O. Jeschke[1], Igor I. Mazin[2], and Roser Valentí[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Code 6393, Naval Research Laboratory, Washington, DC 20375, USA

Honeycomb lattice iridates have been recently discussed as a possible realization of the Heisenberg-Kitaev model in which the electronic structure is dominated by the spin-orbit (SO) interaction. This picture is still under debate. We present calculations on the electronic structure and optical conductivity of Na_2IrO_3 within the density functional theory (DFT) method. Our results show that the measured insulator gap and optical conductivity can be reproduced by GGA+SO+U with a magnetic zigzag configuration. Besides, we analyze the optical conductivity on different directions and the contribution due to different states. Further, we also discuss the electronic structure and underlying microscopic model of a few triangular lattice iridates and compare their properties with the behavior of the honeycomb iridates.

TT 8.12 Mon 12:30 HSZ 304

Spin-orbit physics of j=1/2 Mott insulators on the triangular lattice — •Michael Becker[1], Maria Hermanns[1], Bela Bauer[2], Markus Garst[1], and Simon Trebst[1] — [1]Cologne University, Cologne, Germany — [2]Microsoft Research Station Q, Santa Barbara, USA

We investigate the Heisenberg-Kitaev model on the triangular lattice which is thought to capture the essential physics of the spin-orbital entanglement in a broad class of effective $j = 1/2$ Mott insulators such as certain Iridate compounds – one potential candidate material being the recently synthesized $Ba_3IrTi_2O_9$. While first results have recently been reported for the classical limit of this model, our focus is on its quantum version. Using a combination of numerical techniques, such as exact diagonalization and the density matrix renormalization group, which we complement with various analytical approaches, we can identify its entire phase diagram. The most interesting features of this phase diagram resemble what has already been found in the classical limit – a Z_2 vortex lattice phase in the vicinity of the Heisenberg limit and a "nematic" phase around the antiferromagnetic Kitaev point.

TT 8.13 Mon 12:45 HSZ 304

Discriminating antiferromagnetic signatures in ultracold fermions by tunable geometric frustration — Chia-Chen Chang[1], Richard T. Scalettar[1], •Elena V. Gorelik[2], and Nils Blümer[2] — [1]Department of Physics, University of California, Davis, USA — [2]Institute of Physics, Johannes Gutenberg University, Mainz, Germany

Recently, it has become possible to tune optical lattices continuously between square and triangular geometries. We compute thermodynamics and spin correlations in the corresponding Hubbard model using determinant quantum Monte Carlo and show that the frustration effects induced by the variable hopping terms can be clearly separated from concomitant bandwidth changes by a proper rescaling of the interaction. An enhancement of the double occupancy by geometric frustration signals the destruction of nontrivial antiferromagnetic correlations at weak coupling and entropy $s \lesssim \ln(2)$ (and restores Pomeranchuk cooling at strong frustration), paving the way to the long-sought experimental detection of antiferromagnetism in ultracold fermions on optical lattices.

[1] C.-C. Chang, R. T. Scalettar, E. V. Gorelik, and N. Blümer, Phys. Rev. B **88** (2013) 195121.

TT 9: Transport: Quantum Dots, Quantum Wires, Point Contacts I (organized by TT)

Time: Monday 9:30–13:15 Location: BEY 81

TT 9.1 Mon 9:30 BEY 81

Transport through nanostructures: Finite time vs. finite size — •Peter Schmitteckert[1], Sam Carr[2], and Hubert Saleur[3,4] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]School of Physical Sciences, University of Kent, Canterbury CT2 7NH, UK — [3]Institut de Physique Théorique, CEA, IPhT and CNRS, URA2306, 91191 Gif Sur Yvette, France — [4]Department of Physics, University of Southern California, Los Angeles, CA 90089-0484

Numerical simulations and experiments on nanostructures out of equilibrium usually exhibit strong finite size and finite measuring time t_{m} effects. We discuss how these affect the determination of the full counting statistics for a general quantum impurity problem [1]. We find that, while there are many methods available to improve upon finite-size effects, any real-time simulation or experiment will still be subject to finite time effects: in short **size matters**, but **time is limiting**. We show that the leading correction to the cumulant generating function (CGF) at zero temperature for single-channel quantum impurity problems goes as $\ln t_{\mathrm{m}}$ and is universally related to the steady state CGF itself for non-interacting systems. We then give detailed numerical evidence for the case of the self-dual interacting resonant level model that this relation survives the addition of interactions. This allows the extrapolation of finite measuring time in our numerics to the long-time limit, to excellent agreement with Bethe-ansatz results.

[1] P. Schmitteckert, S. C. Carr, H. Saleur, arXiv:1307.7506

TT 9.2 Mon 9:45 BEY 81

Towards steady state currents on finite systems — •Tim Collet[1] and Peter Schmitteckert[2] — [1]Theoretical Condensed Matter physics, KIT — [2]Institute for Nanotechnology, KIT

The determination of transport properties of strongly correlated quantum systems by quenches in the charge imbalance is a well established technique. However, the achievable time scales are limited by the system size inducing a finite transit time. Here we present a technique in the spirit of absorbing boundary conditions. This allows to obtain steady states on a finite system and to overcome said limitation from finite transit times. We discuss the application of this concept in the context of transport through quantum impurities.

TT 9.3 Mon 10:00 BEY 81

Kwant - a software package for quantum transport — •Michael Wimmer[1], Christoph Groth[2], Anton Akhmerov[1], and Xavier Waintal[2] — [1]TU Delft, The Netherlands — [2]CEA Grenoble, France

Computing transport properties numerically is a problem that appears in many different areas of physics. I will present a wave-function based approach to computing transport properties in non-interacting tight-binding systems that scales more favourably than standard algorithms such as the recursive Green's function algorithm.

We have implemented this method in an open-source software package Kwant based on the python language. It allows for an easy definition of arbitrary tight-binding problems using intuitive concepts ("like writing the problem on the blackboard"), and allows to compute transport properties such as the conductance, but also local properties such as electron densities. The software package itself together with extensive documentation, tutorials and examples of research where Kwant has already been used can be found at www.kwant-project.org.

[1] C. W. Groth, M. Wimmer, A. R. Akhmerov, X. Waintal. arXiv:1309.2926 (2013)

TT 9.4 Mon 10:15 BEY 81

Non perturbative approach to transport through Anderson quantum dot: the influence of charge fluctuations — •Davide Mantelli and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Deutschland

Transport through a strongly interacting Anderson quantum dot is analyzed for tunneling couplings Γ comparable or larger than the thermal energy $k_{\mathrm{B}}T$. In this regime the commonly used sequential tunneling approximation, where tunneling rates are calculated to the lowest order in Γ, breaks down. By accounting for charge fluctuations accompanying the transfer of one electron onto the dot, "dressed" tunneling rates and the associated current across the dot can be calculated [1]. The difference between the standard lowest order theory and the "dressed" one is carefully analyzed in the weak ($\Gamma \ll k_{\mathrm{B}}T$), intermediate ($\Gamma \simeq k_{\mathrm{B}}T$) and strong ($\Gamma \gg k_{\mathrm{B}}T$) coupling regimes. At low temperatures features typical of the Kondo resonance are recovered.

[1] J. Kern and M. Grifoni, Eur. Phys. J. B **86**, (2013) 384

TT 9.5 Mon 10:30 BEY 81

Energy current cotunnelling features for the Anderson quantum dot — •Niklas M. Gergs[1], Christoph B. M. Hörig[1], Dirk Schuricht[1], and Maarten R. Wegewijs[2,3,4] — [1]Institute for Theoretical Physics, Utrecht University, Netherlands — [2]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [3]JARA–Fundamentals of Future Information Technology — [4]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

We discuss the particle and energy current through an Anderson quantum dot with a strong Coulomb interaction U subject to both voltage and temperature bias. A diagrammatic perturbation theory up to second order in the tunnel rates Γ is set up in Liouville space. We find that pair tunnelling features show up in the particle and energy current, while pure inelastic cotunnelling spinflip features are absent in the energy current. The latter cotunnelling processes do appear however when assisted by sequential tunnelling (COSET). Therefore, the energy current contains more distinctive features than the particle current. Thus one can use the energy current for enhanced spectroscopy of quantum dot systems.

TT 9.6 Mon 10:45 BEY 81

Non-equilibrium transport through a Josephson quantum dot — •Jan Frederik Rentrop[1,2], Severin Jakobs[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 investigate a quantum dot featuring Hubbard interaction coupled to superconducting leads. Applying a bias voltage across the system leads to a time-dependent periodic Hamiltonian. This implies that the observable, namely the current through the system, aquires a periodic time-dependence (AC Josephson effect). The non-equilibrium feature of so called Multiple Andreev Reflections (MAR), known from the non-interacting case, is observed in the static component of the current.

The self-energy on the dot is calculated with the functional renormalization group method. The derived first and second order truncation schemes allow for a "quasi-static" (i.e. allowing for the periodic time-dependence but not more) approximation of the self-energy. Model and method allow for asymmetric choices of the super-conducting gaps, the lead temperatures, the lead-dot couplings, tuning of the Hubbard interaction, shifting of on-site energy and applying a magnetic field.

Numerical results are presented for symmetric choices at zero magnetic field and zero temperature, while lead-dot coupling, on-site energy and Hubbard interaction are tuned. Also, first order self-consistent perturbation theory results are presented as a benchmark.

We discuss limitations that the MAR physics impose on any perturbative scheme that expands in small orders of the interaction.

TT 9.7 Mon 11:00 BEY 81

Magneto-electric spectroscopy of Andreev bound states in Josephson quantum dots — •Nils Wentzell[1], Tobias Meng[2], Volker Meden[3], Sabine Andergassen[1], and Serge Florens[4] — [1]University of Vienna — [2]University of Basel — [3]RWTH Aachen University — [4]CNRS Grenoble

We theoretically investigate the behavior of Andreev levels in a single-orbital interacting quantum dot in contact to superconducting leads, focusing on the effect of electrostatic gating and applied magnetic field, as relevant for recent experimental spectroscopic studies. In order to account reliably for spin-polarization effects in presence of strong correlations, we further extend here two simple and complementary approaches that are tailored to capture effective Andreev levels: the static functional renormalization group and the self-consistent Andreev bound states theory. We provide a systematic analysis of the Andreev level spectroscopy for the full electric and magnetic tuning available in quantum dot devices.

15 min. break.

TT 9.8 Mon 11:30 BEY 81

In gap and out of gap features in the cotunneling spectroscopy of a superconductor coupled quantum dot — •Sascha Ratz and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We present a nonequilibrium real-time diagrammatic theory for the systematic investigation of low temperature quantum transport properties of a superconductor contacted quantum dot in an individual single wall carbon nanotube. In the low temperature regime particle transport is dominated by cotunneling and Andreev reflection processes. As recent experiments show, elastic/inelastic cotunneling features are clearly visible inside the Coulomb blockade regime, sharpened by the superconducting leads. The proximity induced higher order Andreev reflection processes result in subgap features, however. Temperature dependent measurements show in addition rich features inside the superconducting gap which can be attribute to thermally excited quasiparticles. More detailed experimental investigations and theoretical calculations are in progress to understand the experimental findings.

TT 9.9 Mon 11:45 BEY 81

Unconventional superconductivity in quantum dot systems — Björn Sothmann[1], •Stephan Weiss[2], Michele Governale[3], and Jürgen König[1] — [1]Departement de Physique Theorique, Universite de Geneve, Switzerland — [2]Theoretische Physik, Universität Duisburg-Essen and CENIDE, Germany — [3]School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand

Conventional superconductivity of electrons is well described in terms of the BCS theory. Fermi statistics dictates the overall symmetry of e.g. the order parameter. The single ingredients could take either symmetric or antisymmetric properties, hence spin as well as spatial degrees of freedom and time might independently change sign and unconventional pairing amplitudes emerge [1]. We show how quantum dot setups may be used to create unconventional pairing between electrons. Brought into proximity to a conventional SC, Cooper pairs tunnel into the double (quadrupel)-quantum dot (DQD/QDD) system [2,3]. Locally, manipulations of the electronic state is possible by tuning electric and/or magnetic fields. An inhomogeneous magnetic field between the dots breaks the SU(2) symmetry of the spin. This results in nonzero unconventional order parameters. We study the emergence and decay of even/odd singlet and triplet order parameters in different geometries. For DQD and QDD setups spectroscopic properties and signatures of unconventional correlations in the Andreev current are studied.

[1] F. S. Bergeret, et al., Rev. Mod. Phys. 77, 1321 (2005).
[2] M. Governale, et al., Phys. Rev. B 77, 134513 (2008).
[3] J. Eldridge, et al., Phys. Rev. B 82, 184507 (2010).

TT 9.10 Mon 12:00 BEY 81

The interplay of the proximity and Kondo effects in spin-resolved transport through quantum dots — •Krzysztof P. Wójcik and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

Transport properties of hybrid quantum dots coupled to ferromagnetic (FM) and superconducting (SC) leads are studied by means of the numerical renormalization group method [1,2]. By constructing the full density matrix of the system [3], the linear conductance and respective spectral functions are calculated. Aiming to emphasize the role of Andreev processes in transport, we model the quantum dot coupled to the superconductor by an effective Hamiltonian in the limit of large superconducting gap [4]. First, a three-terminal setup is considered, for which we study the proximity effect on the spin-dependent current flowing between the two FM leads. Then, the transport properties in a two-terminal setup, with one FM and one SC lead, are analyzed. In this case we focus on the interplay of the exchange field induced by FM lead, the Kondo effect and the Andreev processes. We show that the conductance generally depends on the ratio of these three quantities, leading to nontrivial transport behavior.

[1] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[2] We use the open-access Budapest NRG code, O. Legeza, C. P. Moca, A. I. Toth, I. Weymann, G. Zarand, arXiv:0809.3143 (2008).
[3] A. Weichselbaum, J. von Delft, Phys. Rev. Lett. **99**, 076402 (2007).
[4] Y. Tanaka, N. Kawakami, A. Oguri, J. Phys. Soc. Jap. **76**, 074701 (2007).

TT 9.11 Mon 12:15 BEY 81

The electroluminescence of the transmission line driven by a biased quantum point contact — •Jinshuang Jin[1,2,3], Michael Marthaler[2,4], Andreas Heimes[2,4], and Gerd Schön[2,4] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Karlsruhe, Germany — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology(KIT), Karlsruhe, Germany — [3]Department of Physics, Hangzhou Normal University, Hangzhou, China — [4]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, Karlsruhe, Germany

A transmission line resonator driven by a biased quantum point contact is investigated. The quantum point contact (QPC) is not only an efficient detector but also a light emission device. We find that the excited photon number in the resonator is monotonically increased with the bias voltage for $eV > \hbar\omega_r$ with V the applied bias voltage and $\hbar\omega_r$ the frequency of the resonator. The linewidth and the height of the emission spectrum are sensitive to the parameters of the QPC, such as the tunneling rate, the applied bias voltage, and the coupling strength between the QPC and resonator. Moreover, we demonstrate that the noise spectrum of the current through QPC has characteristic features showing peak and dip, which is closely related to the excited photon dynamics of the resonator.

TT 9.12 Mon 12:30 BEY 81

Accumulation of spin anisotropy in a nanoparticle in the mesoscopic Stoner regime — •Philipp Stegmann[1], Björn Sothmann[2], and Jürgen König[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

We theoretically discuss the accumulation of spin-quadrupole moment [1, 2] in an isotropic system giving rise to a large spin anisotropy although the spin-dipole moment remains strongly suppressed. Our system is a nanoparticle weakly tunnel coupled to two ferromagnetic leads. For such system, it has been demonstrated that the spin fluctuations give rise to enhanced shot noise [3]. Here, large positive spin-quadrupole moments are generated by abruptly switching off the bias voltage for parallel leads‘ polarizations. Moreover, applying an oscillating bias voltage results in large negative spin-quadrupole moments for parallel or antiparallel polarizations.

[1] B. Sothmann, and J. König, Phys. Rev. B **82**, 245319 (2010).
[2] M. M. E. Baumgärtel, M. Hell, S. Das, and M. R. Wegewijs, Phys. Rev. Lett **107**, 087202 (2011).
[3] B. Sothmann, J. König, and Y. Gefen, Phys. Rev. Lett. **108**, 166603 (2012).

TT 9.13 Mon 12:45 BEY 81

Overhauser effect in spin blockaded double quantum dots-the case of dual hysteresis — •Bhaskaran Muralidharan and Siddharth Buddhiraju — Electrical Engineering Department, Indian

Institute of Technology Bombay, Mumbai, India

In the spin blockade transport regime through GaAs double quantum dots (DQD), experiments [1] revealed that the hyperfine interaction with host nuclei can have profound consequences on the electron-spin dynamics. One of which, is the observation of bistablity and flat-topped behavior in the current versus applied DC magnetic-field characteristics. In this talk, we will first explain the essence of this flat-topped hysteretic behavior using a simple six-state model that captures the multiple-feedback mechanisms that are involved. We will then consider a more detailed model that elucidates the role of the physical parameter space of the DQD set up and a feedback mechanism involving the difference Overhauser field caused by the two separate nuclear spin baths of the DQD set up.

[1] K. Ono and S. Tarucha, Phys Rev Lett., 92, 256803 (2004).

TT 9.14 Mon 13:00 BEY 81

Fixing the Energy Scale in Scanning Tunneling Microscopy on Semiconductor Surfaces — Gerhard Münnich[1], •Andrea Donarini[2], Jascha Repp[1], and Martin Wenderoth[3] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany — [3]IV. Physikalisches Institut der Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In scanning tunneling experiments on semiconductor surfaces, the energy scale within the tunneling junction is usually unknown due to tip-induced band bending. Here, we experimentally recover the zero point of the energy scale by combining scanning tunneling microscopy with Kelvin probe force spectroscopy. With this technique, we revisit shallow acceptors buried in GaAs [1]. Enhanced acceptor-related conductance is observed in negative, zero, and positive band-bending regimes. An Anderson-Hubbard model is used to rationalize our findings, capturing the crossover between the acceptor state being part of an impurity band for zero band bending and the acceptor state being split off and localized for strong negative or positive band bending, respectively.

[1] G. Münnich, A. Donarini, J. Repp, and M. Wenderoth, Phys. Rev. Lett. 111, 216802 (2013)

TT 10: Magnetic Heuslers, Half-Metals and Oxides I (organized by MA)

Time: Monday 9:30–12:00 Location: BEY 118

TT 10.1 Mon 9:30 BEY 118

Explaining magnetism in Manganese-based Heusler compounds — •Lukas Wollmann, Gerhard H. Fecher, and Claudia Felser — Max Planck Insitute for Chemical Physics of Solids, Dresden, Germany

From the onset of research in the field of half-metallic ferromagnets, Manganese containing Heusler compounds were the most promising, and most intensely studied trailblazing materials. Accompanying the field of half-metallicity, spintronics emerges as a natural consequence. Focusing on the measurable quantities as Curie temperatures, spin-polarized currents and Hall conductance the field has been, from the beginning on, supported by theoretical methods.

In contrast to purely ferromagnetic Co_2-based Heusler compounds, Manganese containing Heusler alloys (Mn_2YZ and X_2MnZ) exhibit different types of magnetic ordering. The peculiar role of the Manganese atoms and their related magnetic contribution to the quantities of interest shall be elucidated. The main focus lies on the local magnetic structures of the aforementioned material. Following this local perspective, the influence of the magnetic moments on the atomic interplay in form of the Heisenberg exchange interactions is monitored. The computations have been carried out employing the FLAPW DFT code Wien2k and the relativistic Munich SPR-KKR package for the calculation of the exchange constants.

TT 10.2 Mon 9:45 BEY 118

Structural and magnetic properties of the Heusler system Mn-Fe-Ga — •Ajaya Kumar Nayak, Adel Kalache, Michael Nicklas, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

In recent time Mn based Heusler alloys received significant research interest as they show several interesting fundamental as well as functional properties. In particular, Mn_2YZ based materials are considered to be promising candidates for spintronics and spin-torque transfer (STT) applications due to a large spin polarization of the conduction electrons and a large anisotropy in tetragonal phase. The tetragonal ferrimagnetic (FI) compound Mn_3Ga is the center of attraction due to its low saturation magnetization, high Curie temperature (T_C), and high spin polarization. To further tune the magnetic properties of the system we substitute Mn by Fe to obtain Mn_2FeGa up to Fe_2MnGa. All samples crystallize in a pseudo-cubic structure when annealed at 1073 K. Mn_2FeGa undergoes second order paramagnetic (PM) to antiferromagnetic (AFM) ordering around 350 K. In contrast, Fe_2MnGa shows The sample shows a PM to ferromagnetic (FM) ordering around 800 K followed by a first-order FM-AFM transition around 300 K. Here, we present a complete study of the magnetic properties of the Mn-Fe-Ga system with help of various magnetization measurements.

TT 10.3 Mon 10:00 BEY 118

Neutron diffraction study of $Ni_{45}Co_5Mn_{38}Sb_{12}$ Heusler system — •Roshnee Sahoo[1], Amitabh Das[2], KG Suresh[1], Daniel Ebke[3], and Claudia Felser[3] — [1]Department of Physics, Indian Institute of Technology Bombay, Mumbai-400076, India — [2]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai- 400085, India — [3]Max Planck Institute of Chemical Physics of Solids, Dresden-01187, Germany

Considerably large martensitic transition temperature has been observed after substituting Co for Ni site in $Ni_{45}Co_5Mn_{38}Sb_{12}$ system. This system exhibits austenite $L2_1$ cubic structure with a=5.96 $\AA$ at high temperatures, while it has orthorhombic structure in the martensitic phase. We have carried out a detailed neutron diffraction study in order to establish the magnetic structure and the nature of magnetic coupling in this system. In $Ni_{45}Co_5Mn_{38}Sb_{12}$ system, from temperature variation of neutron diffraction data has shown that with increase in temperature the moments of 2a and 2f site decrease up to 250 K and after that both decrease. At 300 K, the material is in the austenite phase, which gives a moment of $1.1\mu_B$ at 4a site and $0.8\mu_B$ at 4b site. The fact that the spontaneous magnetization of $2\mu_B$ is obtained from magnetization measurement suggests that the Mn moment at 4a and 4b sites are coupled ferromagnetically in austenite phase. It is also noticed that with increase in temperature the cell volume increases. However, near the martensitic transition there is a decrease of 0.3% of cell volume. Detailed structural and magnetic results, as obtained from the neutron data, will be discussed in the full paper.

TT 10.4 Mon 10:15 BEY 118

Large non-collinearity and spin reorientation in the Mn2YSn Heusler family — •O. Meshcheriakova[1,2], S. Chadov[1], A. Nayak[1], J. Kübler[3], J. Kiss[1], G. Andé[4], A. Tsirlin[1], W. Schnelle[1], M. Nicklas[1], and C. Felser[1,2] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden Germany — [2]Graduate School of Excellence "Materials Science in Mainz", 55128 Mainz, Germany — [3]Institut für Festkörperphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [4]Laboratoire Léon Brillouin, CEA-CNRS Saclay, Gif-sur-Yvette Cedex, France

Non-collinear magnets provide essential ingredients for next generation memory technology. Recent discoveries have demonstrated the possibility to move certain non-collinear spin structures (skyrmions) at significantly low current densities. To establish such magnetic arrangement, the corresponding materials should possess a non-centrosymmetric crystal structure together with high spin-orbit coupling. Heusler compounds show diverse fundamental properties but in the context of non-collinearity they were not considered so far. Here we present a novel non-collinear tetragonal Mn2RhSn Heusler material exhibiting unusually strong canting of its magnetic sublattices. It undergoes a spin-reorientation transition, induced by a temperature change and suppressed by the external magnetic field. In addition, because of the non-centrosymmetric structure, Dzyaloshinskii-Moriya exchange and magnetic anisotropy, Mn2RhSn is supposed to be a promising candidate for realizing the skyrmion state in the Heusler family.

TT 10.5 Mon 10:30 BEY 118

Design of compensated ferrimagnets based on Mn-rich Heusler compounds — •Stanislav Chadov, Olga Meshcheriakova, Ajaya Nayak, and Claudia Felser — Max-Planck-Institut für Chemische Physik fester Stoffe Nöthnitzer Straße 40 01187 Dresden

Recent developments in the field of MRAM technologies such as ultrafast optical spin-switching has stimulated the search for materials which provide efficient mechanisms of exchange relaxation. The best candidate materials can be provided within the class of the compensated ferrimagnets. Here we propose the design scheme of compensated ferrimagnets based on tetragonal Mn-rich Heusler alloys. Together with the properties typical for antiferromagnets (e.g. exchange bias) we analyze the phenomena (e.g. anomalous Hall effect or MOKE) which are absent in the systems with zero net magnetization.

TT 10.6 Mon 10:45 BEY 118

Atom Probe Tomography of Thin Film Magnetic Heusler Alloy Interfaces — •Torben Boll[1], Niclas Teichert[2], Andreas Hütten[2], and Talaat Al-Kassab[1] — [1]King Abdullah University of Science and Technology (KAUST), Division of Physical Sciences and Engineering, Thuwal 23955-6900, Saudi Arabia — [2]Bielefeld University, Thin Film and Physics of Nanostructures, Universitätsstr. 25, 33615 Bielefeld, Germany

NiMn-X ferromagnetic shape memory alloys have been gaining interest for various applications. For microelectronic devices these alloys have to be made available as thin films. The properties of these films are dominated by the microstructure and especially the interfaces between different layers.

For this study thin film samples of NiMnGa-NiMnSn grown on MgO or Si substrates were prepared by magnetron sputtering. The system was covered with an additional layer of Ag or Ni for protection. Then needle shaped specimens, as required for atom probe tomography, were cut out by means of focused ion beam preparation. The NiMnGa-NiMnSn interface and the MgO-metal interface were characterized with a Local Electrode Atom Probe (LEAP) 4000 HR and a Laser Assisted Wide Angle Tomographic Atom Probe (LAWATAP).

TT 10.7 Mon 11:00 BEY 118

Growth and physical properties of off-stoichiometric Co2Cr0.4Fe0.4Al1.2 Heusler compound — •Ahmad Omar, Marcel Haft, Jan Trinckauf, Christian G.F. Blum, Wolfgang Löser, Silke Hampel, Jochen Geck, Bernd Büchner, and Sabine Wurmehl — Leibniz Institute for Solid State and Materials Research IFW Dresden, Germany

Many Heusler compounds are predicted to be half-metallic ferromagnets and find extensive interest as materials for spintronic applications. Co2Cr0.6Fe0.4Al has been predicted to be 100% spin polarized, but so far, bulk samples as well as thin films do not verify those predictions and various results are fraught with anomalies. Recently, it has been shown that the underlying thermodynamic instability leads to phase transformation via spinodal decomposition in the material. The evolving secondary phase strongly affects the physical properties including spin polarization. One possible way to avoid the spinodal decomposition is to move in the phase diagram and thus avoid the immiscibility gap. We have grown off-stoichiometric Co2Cr0.4Fe0.4Al1.2 composition using optical Floating Zone (FZ) technique, which is known to be the technique of choice for incongruent melting systems such as materials in the Co-Cr- Fe-Al system. We do not observe any spinodal decomposition in our sample. The physical property measurements also match nicely with the theory, which has so far not been possible for Co2Cr1-xFexAl series. We have also performed X-ray Magnetic Circular Dichroism (XMCD) measurements on the sample which are promising compared to the band structure calculations.

TT 10.8 Mon 11:15 BEY 118

Growth of perovskite manganites via MAD Atomic Layer Epitaxy (ALE) — •Markus Jungbauer, Sebastian Hühn, Felix Massel, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August-Universität, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Interfacial effects between transition metal perovskites lead to many unexpected phenomena due to charge, spin and orbital rearrangements. Recently it was pointed out that reconstructions at the scale of half a perovskite layer can take place to reduce Coulomb energy due to the polarization catastrophe [1]. So deposition techniques which are able to build up perovskites ABO_3 by alternating deposition of AO and BO_2 layers are highly desirable. Utilizing this scheme we grow $La_{1-x}MnO_3$ and $La_{2/3}Sr_{1/3}MnO_3$ on $SrTiO_3$ (100) substrates by metalorganic aerosol deposition (MAD) [2]. We monitor the growth by in situ ellipsometry which enables us to distinguish between a layer by layer and block by block growth mode. Modifications of the stoichiometry of the first two layers SrO and MnO_2 result in profound changes of the structural, electrical and magnetic properties of the films. We explain this by an interplay of interfacial intermixing and electrostatic driving forces which can be reduced by excess MnO_2 in the first layer. Financial support of EU via FP7 (IFOX) is acknowledged.

[1] S. Turner et al, Phys. Rev. B 87, 035418 (2013)
[2] Moshnyaga et.al. Appl. Phys. Lett. 74, 2842 (1999)

TT 10.9 Mon 11:30 BEY 118

Observation of magnetization processes in manganite thin films using the planar Hall effect — •Camillo Ballani, Eduard Unger, Markus Jungbauer, Markus Michelmann, Sebastian Hühn, Danny Schwarzbach, and Vasily Moshnyaga — I.Physikalisches Institut, Universität Göttingen

We present a technique for monitoring magnetization processes in thin magnetic films by a simple voltage measurement. The planar Hall effect (PHE) in ferromagnetic materials, which is a direct consequence of the anisotropic magnetoresistance (AMR), is highly sensitive to changes in the magnetization induced by an in-plane external magnetic field. Therefore, rotation of magnetization as well as flops of single magnetic domains can be investigated by measuring the transverse voltage in a Hall bar structure. This method was applied to manganite thin films ($La_{0.7}Sr_{0.3}MnO_3$ and $La_{0.6}Ba_{0.4}MnO_3$) with thicknesses from 5 nm to 30 nm that were grown by metalorganic aerosol deposition (MAD) technique on $SrTiO_3$ substrates with orientations (100), (110) and (111) and hence with different magnetocrystalline anisotropy. Structures with a Hall bar geometry of various sizes (bar width: 10–300 μm) were processed by electron beam lithography. The films showed AMR ratios up to 1% at temperatures slightly below T_C. The results for the transverse voltage measurements for magnetic hysteresis loops driven by an applied external field are consistent with simultaneously conducted measurements of magneto-optical Kerr effect (MOKE) and fit well to a Stoner-Wohlfarth model. Financial support from EU FP 7 Project IFOX (interfacing oxides) is acknowledged.

TT 10.10 Mon 11:45 BEY 118

Magnetic and electronic properties of $La_{2/3}Sr_{1/3}MnO_3$ with planar order along (100) and (111) — •Sebastian Hühn[1], Markus Jungbauer[1], Ricardo Egoavil[2], Jo Verbeeck[2], and Vasily Moshnyaga[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Electron Microscopy for Materials Science (EMAT), Groenenborgerlaan 171, 2020 Antwerp, Belgium

Cation ordering has a large impact on the physical properties of strongly correlated materials. In $AA'BB'O_3$ perovskites A- and B-site ordering can lead to stabilization of the bulk properties, i.e. higher transition temperatures and saturation magnetization. Furthermore interface related properties different from those of bulk materials can emerge. We present an approach of A-site ordering in ferromagnetic-half-metallic $La_{2/3}Sr_{1/3}MnO_3$ by the growth of $(La_{1/2}Sr_{1/2}MnO_3)2n/(LaMnO_3)n$ and $(LaMnO_3)2n/(SrMnO_3)n$ (with n=1...4) superlattices on $SrTiO_3$ (100) and $SrTiO_3$ (111) substrates by metalorganic-aerosol deposition (MAD) with in situ ellipsometric growth control. Structural properties were investigated by STM/AFM, XRD, XRR and TEM-EELS. The resistivity and magnetization were measured between 5-400K by PPMS and MPMS, respectively. Our observation of the Curie point T_C as a function of the parameter n shows a huge difference for the planar order directions (100) and (111). Financial support from EU FP 7, IFOX (interfacing oxides) project is acknowledged.

TT 11: Invited Talk - Martin Fally (organized by DF; with CPP, KR, TT)

Time: Monday 9:30–10:15 Location: GER 37

Invited Talk TT 11.1 Mon 9:30 GER 37

Optics with neutrons using holographic gratings — •Martin Fally[1], Jürgen Klepp[1], Christian Pruner[2], and Yasuo Tomita[3] — [1]Faculty of Physics, Uni Wien, Austria — [2]Department of Materials Science and Physics, Uni Salzburg, Austria — [3]University of Electro-Communications, Tokyo, Japan

All neutron-optical phenomena are governed by the neutron-optical potential or, equivalently, the neutron refractive-index. Thus, an important task in the design of neutron-optical elements is to efficiently pattern the neutron refractive-index of materials. For this purpose we use light-sensitive materials and employ holographic techniques to produce diffraction gratings for neutrons.

After an introduction to the basics of neutron optics and the challenges as compared to light optics I will discuss our recent experiments, where we successfully demonstrated the power of this approach. Two- and three-port beam-splitters as well as free-standing film mirrors for cold and very-cold neutrons were set up by exploiting the Pendellösung interference effect. Another intriguing possibility is offered by holographic gratings containing superparamagnetic nanoparticles to produce business card-size neutron polarizers working in comparably low external magnetic induction. Such devices are being developed at present. Finally, I will give an outlook on novel neutron-scattering instrumentation and techniques which are expected from those advancements.

In collaboration with: I. Drevensek-Olenik, S. Gyergyek, J. Kohlbrecher, P. Geltenbort, R. A. Rupp

TT 12: Quantum Dynamics, Decoherence and Quantum Information (organized by DY)

Time: Monday 9:30–12:00 Location: HÜL 186

Invited Talk TT 12.1 Mon 9:30 HÜL 186

Welcome to Twin Peaks: momentum-space signatures of Anderson localization — •Cord A. Müller — Fachbereich Physik, Universität Konstanz

Quantum Systems with structural disorder present unusual challenges when is comes to understanding long-time limits of their phase-space dynamics. In particular, Anderson localization is well known to suppress classical diffusion of (matter) waves in real space—but much less is known about its momentum-space signatures.

Recently, a new signature of strong Anderson localization has been discovered for ultracold atoms following a quantum quench: a twin-peak signal in the particles' momentum distribution. This structure combines the familiar back-scattering peak with a coherent forward-scattering peak [1]. The forward peak appears to be a genuine signal for the onset of strong localization, surviving in the presence of weak magnetic fields. Recent non-perturbative calculations in a quasi-1D setting [2] have confirmed that the forward peak can serve as a reliable signature of Anderson localization. This theory describes the peak's temporal genesis as well as its aymptotic features such as width and height, and arguably presents the only instance where the temporal evolution of a strong localization phenomenon can be described analytically at all times.

[1] T. Karpiuk et al., PRL 109, 190601 (2012)
[2] T. Micklitz et al., arXiv:1311.2268

TT 12.2 Mon 10:00 HÜL 186

Adiabatic-Markovian Dynamics at Avoided Crossings — •Peter Nalbach — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstr. 9, 20355 Hamburg

In order to study Landau-Zener transitions at avoided crossings under the influence of environmental fluctuations we derive effective nonequilibrium Bloch equations. Thereby, we employ an adiabatic-Markovian approximation which results in effectively time-dependent relaxation and dephasing rates and a time-dependent quasi-equilibrium statistical operator to which the system is driven. At weak coupling, where in a static case a Markovian approximation is valid, we observe very good agreement for the full driving speed range between the nonequilibrium Bloch equations predictions and numerical exact data for the Landau-Zener transition and the excitation survival probability [1]. The nonequilibrium Bloch equations, thus, allow for an efficient tool to analyze and model the dynamics in driven double quantum dot [2] and other qubit realizations.

[1] P. Nalbach and M. Thorwart, Phys. Rev. Lett. 103, 220401 (2009) & Chem. Phys. 375, 234 (2010).

[2] P. Nalbach, J. Knörzer and S. Ludwig, Phys. Rev. B 87, 165425 (2013).

TT 12.3 Mon 10:15 HÜL 186

A generalized quantum regression theorem for non-Markovian two-time correlation functions of system operators — •Jinshuang Jin[1,2,3], Michael Marthaler[3,4], and Gerd Schön[3,4] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Karlsruhe, Germany — [2]Department of Physics, Hangzhou Normal University, Hangzhou, China — [3]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology(KIT), Karlsruhe, Germany — [4]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, Karlsruhe, Germany

We present an efficient scheme for the calculation of two-time correlation functions for open quantum systems with memory effect. This scheme is the generalization of the quantum regression theorem with the consideration of non-Markovian effects. We further apply the present method to both Ferminonic and Bosonic systems. The former is to study the charge fluctuation spectrum of the interacting quantum dots in the sequential tunneling regime. The latter is to investigate the non-Markovian effect of the phonon bath on the emission spectrum of a cavity. The characteristic non-Markovian features in the spectra are explored.

TT 12.4 Mon 10:30 HÜL 186

Coherence phase diagram and a quench dynamics of a spin-boson model. — •Oleksiy Kashuba[1], D.M. Kennes[2], M. Pletyukhov[2], V. Meden[2], and H. Schoeller[2] — [1]Institut für Theoretischen Physik, Technische Universität Dresden — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen

We study the non-Markovian dynamics of the small dissipative quantum system coupled to an thermodynamically equilibrated environment. The memory effects probed by the quenching of the coupling strength. We discovered the contra-intuinive tendency of the system to the enhancement of the coherence in response to stronger memory of the incoherent behaviour before the quench. Studying the dynamics of the system at different coupling and temperatures we revealed several distinct "phases" by discriminating between the dynamics on intermediate and long time scales. Surprisingly, elevated temperature can render the system "more coherent" by inducing a transition from the partially coherent to the coherent regime.

15 min break

TT 12.5 Mon 11:00 HÜL 186

Beyond Born-Markov: validity, dependencies and the initial state problem — •Christian Karlewski, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, KIT, 76128 Karlsruhe

We expand the master equation for an open quantum system in terms of the Born and the Markov approximation. This makes it possible to calculate higher order-terms in the coupling strength to the bath beyond the famous Born-Markov approximation. Additionally, we are able to compare and distinguish between the terms belonging to Born or Markov approximation. The first issue we address with this approach is the initial state problem. Our method allows to quantify initial correlations and thus the error made by neglecting them. Secondly, we investigate the behaviour of a specific system, the spin boson

model with an Ohmic noise with Drude-Lorentz cutoff, and we compare our computations with the Born-Markov approximation.

TT 12.6 Mon 11:15 HÜL 186

Dissipative dynamics and energy transfer of a harmonic oscillator coupled to nonthermal baths — •Daniel Pagel[1], Andreas Alvermann[1], Holger Fehske[1], Peter Nalbach[2], and Michael Thorwart[2] — [1]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald — [2]I. Institut für Theoretische Physik, Universität Hamburg

The dissipative dynamics of a quantum-mechanical system can be studied in a microscopic setting if one includes an explicit coupling to one or more baths of harmonic oscillators. Allowing for general nonequilibrium bath preparations instead of the usually employed thermal ones, we look at the long-time behavior of the dissipative harmonic oscillator coupled to one bath and prove that it equilibrates in the absence of isolated modes. The stationary density matrix in the long-time limit then depends on the initial bath state only. We discuss the requirements for full thermalization of the central oscillator. In the case of multiple baths, where stationary nonequilibrium states of the central oscillator become possible, we show that the fluctuations of the central oscillator follow an exact generalized nonequilibrium fluctuation relation. Finally, we discuss the generalization of the cumulant generating function for the energy transfer through the oscillator to the nonthermal situation.

TT 12.7 Mon 11:30 HÜL 186

Optimal control of non-interacting (quantum) harmonic oscillators and qubits — •Frank Boldt and Karl Heinz Hoffmann — Professur Theoretische Physik, insbesondere Computerphysik, Technische Universität Chemnitz

In this talk the time-optimal and decoherence free control of an ensemble of non-interacting (quantum) harmonic oscillators is given, using an geometrical approach based on the Casimir companion [1]. These time-optimal decoherence free passages are shortcuts to adiabaticity. Therefore fast optimal cooling processes are possible and maximum cooling rates will be given [2]. Further, time-optimal and decoherence free controls of an ensemble of non-interacting qubits will be deduced as a second example [3].
The optimal controls presented are piece-wise continuous functions (Bang-Bang controls) and thus hard to realize experimentally. As an outline, bounds for continuous controls with finite switching times were calculated to give experimenters hard limits for instance to adjust their experimental realized version of the control by a feedback loop.

[1] F. Boldt et al., PRA 87, 022116 (2013)

[2] P. Salamon et al., Phys. Chem. Chem. Phys., 2009, 11, 1027-1032

[3] F. Boldt et al., EPL 99, 40002 (2012)

TT 12.8 Mon 11:45 HÜL 186

Dynamics of entanglement entropy and entanglement spectrum crossing a quantum phase transition — •Elena Canovi[1], Elisa Ercolessi[2], Piero Naldesi[2], Luca Taddia[2], and Davide Vodola[2,3] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Dipartimento di Fisica e Astronomia dell'Università di Bologna and INFN, Sezione di Bologna, Via Irnerio 46, 40127 Bologna, Italy — [3]PCMS (UMR 7504) and ISIS (UMR 7006), Université de Strasbourg and CNRS, Strasbourg, France

We study the time evolution of entanglement entropy and entanglement spectrum in a finite-size system which crosses a quantum phase transition at different speeds. We focus on the Ising model with a time-dependent magnetic field, which is linearly tuned on a time scale τ. The time evolution of the entanglement entropy displays different regimes depending on the value of τ, showing also oscillations which depend on the instantaneous energy spectrum. The entanglement spectrum is characterized by a rich dynamics where multiple crossings take place with a gap-dependent frequency. Moreover, we investigate the Kibble-Zurek scaling of entanglement entropy and Schmidt gap.

TT 13: Topological Insulators: Mostly Structure and Electronic Structure (organized by HL)

Time: Monday 9:30–12:30 Location: POT 051

TT 13.1 Mon 9:30 POT 051

InAs/GaSb compound quantum wells for electrically tunable topological insulator devices — •Georg Knebl[1], Matthias Dallner[1], Robert Weih[1], Sven Höfling[1,2], and Martin Kamp[1] — [1]Universität Würzburg, Deutschland — [2]University of St Andrews, Scotland

InAs/GaSb compound quantum wells (CQW) sandwiched between two AlSb layers and a front/back gate were proposed by Liu et al. [1] to show a topological insulator phase. The advantage of this structure is the possibility to tune the phase transition from a normal to a topological insulator via the front and back gate voltage. In addition, this material combination allows the use of established III/V semiconductor technology for epitaxy and device processing.

We present results on the growth of InAs/GaSb CQWs via molecular beam epitaxy on GaSb and GaAs substrates using different buffers. Furthermore, we will discuss device fabrication on InAs/GaSb layer structures, which requires special care since oxidation or process induced damage can lead to the formation of conducting surface channels. Electrical characterization of Hall bars and the tunability of the transport properties via gates will be reported.

[1] C. Liu, et al., Phys. Rev. Lett. 100, pp. 1-4, (2008)

TT 13.2 Mon 9:45 POT 051

Resolving the linear dispersion relation of topological insulator nanowires — •Johannes Gooth, Bacel Hamdou, August Dorn, Robert Zierold, and Kornelius Nielsch — Institute of Applied Physics, Universität Hamburg, Hamburg, Germany

Due to the linear dispersion relation, charge carriers in the surface states of a topological insulator (TI) behave like relativistic particles described by the Dirac equation for spin-1/2 particles leading to exotic new physics and applications. In bulk topological insulators the linear dispersion relation at the surface has been resolved by angle-resolved photoemission spectroscopy (ARPES). On nanostructures ARPES measurements have not been successful, due to the limited sample size. Instead magnetoelectrical transport measurements became the most common way to indicate the existance of surface states in nanomaterials. However, the linear dispersion relation has not been directly resolved in nanostructures to date.

Here, we show that the linear dispersion relation on the surface of a Bi_2Te_3 nanowire can directly be deduced from gate dependend magnetototransport measurements. Further carrier concentration, mobility and effective mass of the dirac fermions are determined as a function of gate voltage. It can be shown that at 2K the transport in the surface states is dominated by electron-electron interaction.

TT 13.3 Mon 10:00 POT 051

Temperature-dependent surface band gap of Dirac fermions observed at the (111) surface of the crystalline topological insulator Pb-Sn-Se — •Partha S. Mandal[1], Gunther Springholz[2], Günther Bauer[2], Valentine V. Volobuev[2], Andrei Varykhalov[1], Oliver Rader[1], and Jaime Sánchez-Barriga[1] — [1]Helmholtz-Zentrum Berlin — [2]Johannes-Kepler-Universität Linz

Using angle-resolved photoemission, we studied (111)-oriented epitaxial films of Pb-Sn-Se grown by molecular beam epitaxy. The topological-to-trivial-insulator phase transition [1] is monitored probing the bulk valence band as a function of Sn concentration and temperature between 30 K and room temperature. In the topological phase, the topological surface state opens a band gap indicating a mass aquisition that is not caused by broken time reversal symmetry. We discuss this phenomenon in comparison to conventional topological insulators [2] protected by time-reversal symmetry.

[1] P. Dziawa, B. J. Kowalski, K. Dybko, R. Buczko, A. Szczerbakow, M. Szot, E. Łusakowska, T. Balasubramanian, B. M. Wojek, M. H. Berntsen, O. Tjernberg, T. Story, Nature Mat. 11, 1023 (2012).

[2] T. Sato, K. Segawa, K. Kosaka, S. Souma, K. Nakayama, K. Eto,

T. Minami, Y. Ando, and T. Takahashi, Nature Phys. 7, 840 (2011).

TT 13.4 Mon 10:15 POT 051

Surface-Dominated Transport on a Bulk Topological Insulator — •Lisa Kühnemund[1], Lucas Barreto[2], Frederik Edler[1], Christoph Tegenkamp[1], Jianli Mi[3], Martin Bremholm[3], Bo Brummerstedt Iversen[3], Christian Frydendahl[2], Marco Bianchi[2], and Philip Hofmann[2] — [1]Leibniz Universität Hannover, Inst. f. Festkörperphysik — [2]Aarhus University, Dep. of Physics and Astronomy, iNANO — [3]Aarhus University, Center for Materials Crystallography, iNANO

Topological insulators are guaranteed to support metallic surface states on an insulating bulk, and one should thus expect that the electronic transport in these materials is dominated by the surfaces states. Alas, due to the high remaining bulk conductivity, surface contributions to transport have so-far only been singled out indirectly via quantum oscillations, or for devices based on gated and doped topological insulator thin films, a situation in which the surface carrier mobility could be limited by defect and interface scattering. Here we present a direct measurement of surface-dominated conduction on an atomically clean surface of Bi_2Te_2Se. Using nano-scale four point setups with variable contact distance, we show that the transport at 30 K is two-dimensional rather than three-dimensional and by combining these measurements with angle-resolved photoemission results from the same crystals, we find a surface state mobility of 390(30) $cm^2V^{-1}s^{-1}$ at 30 K at a carrier concentration of $8.71(7)\times10^{12}$ cm^{-2}.

TT 13.5 Mon 10:30 POT 051

Room temperature high frequency transport of Dirac fermions in MBE grown Sb_2Te_3 based topological insulators — •T. Herrmann[1], P. Olbrich[1], S.N. Danilov[1], Ch. Weyrich[3], J. Kampmeier[3], G. Mussler[3], D. Grützmacher[3], L. Plucinski[3], C.M. Schneider[3], M. Eschbach[3], L.E. Golub[2], V.V. Bel'kov[2], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Peter Grünberg Institute (PGI) & Jülich Aachen Research Alliance (JARA-FIT), Research Center Jülich, Jülich, Germany

We report on the observation of terahertz (THz) laser radiation induced currents in epitaxially grown Sb_2Te_3 based topological insulators (TI) [1]. We demonstrate that the excitation of the sample with linearly polarized THz radiation results in a photoresponse solely stemming from the surface states of the 3D TI. Our analysis shows that the photocurrent is caused by the photogalvanic effect [2], which emerges in the surface states but is forbidden in the centrosymmetric bulk material. As an important result our measurements demonstrate that the high frequency transport can be obtained in the Dirac fermion system even at room temperature.

[1] Plucinski et al.; J. Appl. Phys. **113**, 053706 (2013)
[2] Weber et al.; Phys. Rev. B **77**, 245304 (2008)

TT 13.6 Mon 10:45 POT 051

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

Topological insulators (TIs) are a new state of quantum matter which insulates in the bulk and conducts on the surface. The study of bulk TIs has been hindered by high conductivity in the bulk, arising from crystalline defects. Such problems can be tackled through compositional engineering or the synthesis of TI nanomaterials. We combined both approaches in a systematic study of various growth parameters to achieve uniform, high purity nanowires with high substrate coverage.

The highlight of this study is the development of a new growth route for nanowires, based on a TiO_2 catalyst rather than the conventional Au. Comparative studies demonstrate that Au significantly contaminates the nanowires, whereas TiO_2 stays well separated. Details of the Au and TiO_2-catalysed growth mechanism were investigated. For Au it was found that the growth mechanism is vapour-liquid-solid. For TiO_2 nanoparticles, in contrast, the growth mechanism can be described in the vapour-solid scheme.

Nanowires of the doped compound $(Bi_{0.78}Sb_{0.22})_2Se_3$ were studied using synchrotron radiation. It was discovered that the material mainly adopts an orthorhombic phase known from Sb_2Se_3. The Raman spectrum is reported and matched with the structural information for the first time. Furthermore, a method to control the length and diameter of Bi_2Se_3 nanowires through laser-cutting was developed.

Coffee break (15 min.)

TT 13.7 Mon 11:15 POT 051

Optoelectronic flow trajectories in topological insulators — •Paul Seifert[1], Christoph Kastl[1], Tong Guan[2], Kehui Wu[2], X. Y. He[2], Yongqing Li[2], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München — [2]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

We report on the optoelectronic properties of thin films of the topological insulator $(Bi_xSb_{1-x})_2Te_3$ grown by molecular beam epitaxy. In spatially resolved experiments, we observe photocurrent patterns with positive and negative amplitude [1]. We interpret the patterns to originate from a local photocurrent generation due to potential fluctuations [1]. Exploiting the local photocurrent generation in combination with a sub 100-nm lithography, we visualize the current flow in nanoscale circuits based on topological insulators [2].

[1] C. Kastl, T. Guan, X. Y. He, K. H. Wu, Y. Q. Li, and A. W. Holleitner, Appl. Phys. Lett. 101, 251110 (2012). [2] C. Kastl et al., (2014).

We gratefully acknowledge financial support from the DFG-project HO3324/8 within the SPP 1666 on topological insulators.

TT 13.8 Mon 11:30 POT 051

Polarization-controlled picosecond spin currents in topological insulators — •Christoph Kastl[1], Christoph Karnetzky[1], Helmut Karl[2], and Alexander W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, 85748 Garching, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Controlling spin currents in topological insulators may lead to applications in future spintronic devices [1]. Here, we show that surface currents in Bi2Se3 can be controlled by circularly polarized light on a time-scale of a picosecond with a fidelity near unity even at room temperature. We reveal the temporal interplay of such ultrafast spin currents with photo-induced thermoelectric and drift currents in optoelectronic circuits [2].

[1] C. Kastl, T. Guan, X. Y. He, K. H. Wu, Y. Q. Li, and A. W. Holleitner, Appl. Phys. Lett. 101, 251110 (2012).
[2] C. Kastl et al., (2014).

We gratefully acknowledge financial support from the DFG-project HO3324/8 within the SPP 1666 on topological insulators.

TT 13.9 Mon 11:45 POT 051

Scanning Tunneling Microscopy of Ultrathin Topological Insulator Sb_2Te_3 Films on Si(111) grown by Molecular Beam Epitaxy — •Martin Lanius, Jörn Kampmeier, Gregor Mussler, and Detlev Grützmacher — Peter Grünberg Institut, Forschungszentrum Jülich, Germany

Topological insulators (TIs) are a class of materials in the field of condensed matter physics. In addition to the fascinating electronic properties, the Van der Waals growth mode of TIs, i.e. the TI epilayer is only weakly bonded to the substrate, which allows the use of substrates with high lattice mismatch, is of high interest. In this case we have studied the nucleation and growth process of the TI Sb_2Te_3 on Si(111) substrates by STM (Scanning Tunneling Microscopy) and AFM (Atomic Force Microscopy). The thin films from several nanometers thickness down to one quintuple layer thickness have been grown by molecular beam epitaxy. To determine the thickness and composition of the films we used x-ray reflectivity and x-ray diffraction. Further investigations of $Ge_2Sb_2Te_3$, which is a phase-changing material and a topological insulator, and the comparison to the growth mode of Sb_2Te_3 will be presented.

TT 13.10 Mon 12:00 POT 051

Transport of Dirac fermions in the presence of spin-orbit impurities — •Pierre Adroguer[1], Dimitri Culcer[2], and Ewelina Hankiewicz[1] — [1]Institute for Theoretical Physics and Astronomy, Würzburg University, Würzburg, Germany — [2]School of Physics, University of New South Wales, Sidney, Australia

The recent exprimental realizations of three dimensional topological insulators (3DTI) have provided a new tool to investigate Dirac physics.

Indeed, these materials exhibit an insulating bulk and a single metallic surface state described by Dirac fermion physics.

In the regime of weak scalar disorder, Dirac fermions do not backscatter because of time-reversal symmetry. Further, this absence

of backscattering leads to a weak antilocalization correction (an increase in conductivity in the absence of magnetic field, due to quantum interference of conjugated paths) [1,2].

In this presentation, we will review these phenomena, and show how these features are modified when there are spin-orbit impurities in the Dirac fermion systems.

We acknowledge financial support via grant HA 5893/4-1 within SPP 1666.

[1] G. Tkachov and E. M. Hankiewicz, Phys. Rev. B 84, 035444 (2011)

[2] P. Adroguer, D. Carpentier, J. Cayssol, and E. Orignac, New Journal of Physics 14, 103027 (2012)

TT 13.11 Mon 12:15 POT 051

Oscillatory surface dichroism of the insulating topological insulator Bi_2Te_2Se — •Susmita Basak[1], Madhab Neupane[2], Hsin Lin[1], N. Alidoust[2], S.-Y. Xu[2], Chang Liu[2], I. Belopolski[2], G. Bian[2], J. Xiong[2], H. Ji[3], S. Jia[3], S.-K. Mo[4], M. Bissen[5], M. Severson[5], N. P. Ong[2], T. Durakiewicz[6], R. J. Cava[3], A. Bansil[1], and M. Z. Hasan[2] — [1]Department of Physics, Northeastern University, Boston, Massachusetts, USA — [2]Joseph Henry Laboratory and Department of Physics, Princeton University, Princeton, New Jersey, USA — [3]Department of Chemistry, Princeton University, Princeton, New Jersey, USA — [4]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, USA — [5]Synchrotron Radiation Center, Stoughton, Wisconsin, USA — [6]Condensed Matter and Magnet Science Group, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

We present a study of the effect of angular momentum transfer between polarized photons and topological surface states of the insulating topological insulator Bi_2Te_2Se using circular dichroism-angle resolved photoemission spectroscopy. The photoelectron dichroism demonstrate a dramatic sign flip with the change of photon frequency and we show that this is a consequence of a strong coupling between the photon field and the spin-orbit nature of the initial Dirac states on the surface. Our studies reveal the intrinsic dichroic behavior of topological surface states and point toward the potential utility of bulk insulating topological insulators in opto-spintronics device applications.

TT 14: Focus Session: Physics of Quantum Rings (organized by HL)

Innovative recent findings in both experimental and theoretical physics of quantum rings and ring-like atom systems based on the most advanced state-of-the-art fabrication and characterization techniques as well as theoretical methods will be discussed. The experimental efforts allow for obtaining new classes of semiconductor quantum rings and quantum-ring-based metamaterials. An adequate characterization of quantum rings is realized using scanning tunneling microscopy methods. Dedicated theoretical models allow for interpretation of the novel topology-driven physical properties of quantum rings.

Organizer: Axel Lorke, Universität Duisburg-Essen.

Time: Monday 9:30–11:30 Location: POT 151

Topical Talk TT 14.1 Mon 9:30 POT 151

Impact of topology on physical properties of quantum rings — •Vladimir M. Fomin — Institute for Integrative Nanosciences, IFW-Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Advanced micro- and nanostructure fabrication techniques can be exploited to generate non-trivially shaped objects possessing man-designed topological features, such as doubly-connectedness (quantum rings) and one-sidedness (Möbius strips) [1]. Even though self-assembled semiconductor quantum rings ('quantum volcanos') are singly-connected and anisotropic, they exhibit the Aharonov-Bohm effect on the persistent current because the electron wave functions are exponentially decaying towards the center and are topologically identical to those in doubly-connected quantum rings. Theoretically predicted Aharonov-Bohm effect in 'quantum volcanos' was experimentally detected by torsion magnetometry. Symbiosis of a geometric potential and an inhomogeneous twist renders an observation of the topology effect on the electron ground-state energy in microscale Möbius strips into the realm of experimental verification. A 'delocalization-to-localization' transition for the electron ground state is unveiled in inhomogeneous Möbius strips [2]. This transition can be quantified through the Aharonov-Bohm effect on the persistent current. Recent findings suggest perspectives of topological control over electronic, spin, optical, magnetic and transport properties of micro- and nanostructures.

[1] V. M. Fomin (Ed.), Physics of Quantum Rings, Springer, Berlin–Heidelberg, 2014, 487 p. [2] V. M. Fomin, S. Kiravittaya, O. G. Schmidt, Phys. Rev. B 86, 195421 (2012).

Topical Talk TT 14.2 Mon 10:00 POT 151

Fabrication of ordered quantum rings — •Zhiming Wang — School of Microelectronics and Solid-State Electronics, University of Electronic Science and Technology of China, Chengdu, 610054 , P. R. China

Quantum rings possess unique properties and have attracted extensive theoretical and experimental attention. Up to now, various effects have been devoted to fabrication of quantum rings via both top-down techniques and self-assembly. Epitaxy has been demonstrated as an effective method to fabricate self-assembled quantum rings. Despite the well-controlled morphology of self-assembled quantum rings produced by using both Stranski-Krastanov growth and droplet epitaxy, the lateral ordering of quantum rings remains challenging[1]. In this presentation, both vertically and laterally aligned quantum rings are described. The fabrication of laterally aligned quantum rings is based on the transformation of ordered quantum dots using the self-organized anisotropic strain engineering technique. The vertically aligned quantum rings are fabricated by multi-step droplet epitaxy. The growth mechanisms of both vertically aligned and laterally ordered quantum rings are discussed. Fabrication of ordered quantum rings is of high priority for practical applications, in particular, as photovoltaic devices and photodetectors.

References

[1] J. Wu and Z. Wang, in: V. M. Fomin (Ed.), Physics of Quantum Rings, Springer, Berlin-Heidelberg, 2014, pp. 143-159.

Coffee break (15 min.)

Topical Talk TT 14.3 Mon 10:45 POT 151

Self-organized formation and XSTM characterization of GaSb/GaAs quantum rings — •Andrea Lenz — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

In the GaSb/GaAs material system, quantum rings (QRs) can occur already after the material deposition on GaAs(001), sometimes even without capping. Upon capping almost all quantum dots are transformed into QRs [1].

This presentation gives an overview of the structural parameters and the formation process of the GaSb/GaAs QRs using cross-sectional scanning tunneling microscopy (XSTM). Furthermore, information on the electronic structure of the QRs is shown, which is gained using scanning tunneling spectroscopy mode (XSTS). XSTS reveals the type-II alignment for GaSb/GaAs QRs [2], which makes them very promising for charge storage devices and in photovoltaics. Furthermore, the GaSb/GaAs system exhibits a strong Aharonov-Bohm effect since the central opening of the QRs is much more pronounced as compared with other material systems, like e.g. the InGaAs/GaP system, for which QRs have been observed quite recently [3].

This work was supported by the EC through the SANDiE NoE and by projects Da 408/13 and Sfb 787 of the DFG.

[1] A. Lenz and H. Eisele, in: V. M. Fomin (Ed.), Physics of Quantum Rings, Springer, Berlin-Heidelberg, 2014, pp. 123-142. [2] R. Timm et al., Nano Lett. 10, 3972 (2010). [3] C. Prohl et al., Appl. Phys. Lett. 102, 123102 (2013).

TT 14.4 Mon 11:15 POT 151

Current-induced spin dynamics in ring-like atom clusters on surfaces — •Benjamin Baxevanis, Christoph Hübner, Lars-Hendrik Frahm, and Daniela Pfannkuche — I. Institut für Theoretische Physik, Universität Hamburg, Germany

Recently, much attention has been devoted to artificially assembled magnetic structures made of iron atoms on non-magnetic substrates using a scanning tunneling microscope [1,2,3]. Some of these structures show unique dynamics and switching of magnetism under the influence of a spin-polarized current and the interaction with the substrate [2,3]. We theoretically consider the spin dynamics in a ring-like cluster of Fe atoms on a substrate tunnel-coupled to a magnetic tip. Employing a master equation approach, the effects of the spin-polarized current, anisotropy field and symmetry of the ring-like cluster [4] on the spin dynamics are studied.

[1] A. A. Khajetoorians, J. Wiebe et al., Nature Physics 8, 497 (2012)
[2] S. Loth, S. Baumann, C. P. Lutz et al., Science 335, 196 (2012)
[3] A. A. Khajetoorians, B. Baxevanis et al., Science 339, 55 (2013)
[4] B. Baxevanis and D. Pfannkuche, in: V. M. Fomin (Ed.), Physics of Quantum Rings, Springer, Berlin-Heidelberg, 2014, pp. 381-408.

TT 15: Focus Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale (organized by O)

Non-equilibrium processes such as charge and heat transport are central to electronic and thermoelectric applications. Understanding these phenomena at the nanoscale challenges both theory and experiment. Basic theoretical issues are related to the role of quantum mechanics, the interplay of ballistic, diffusion and hopping processes, the importance of dissipation, the effect of electronic correlation, and the signatures of unusual quantum states. On the experimental side devising measurements to unravel these phenomena in a controlled way poses severe difficulties. In this regard, optical lattices of cold atoms are emerging as a powerful laboratory to test theoretical models and discover unforeseen phenomena.

This symposium will cover current issues in the field by bringing together scientists working in different specific areas with the aim of fostering interdisciplinary discussion, assessing current theoretical understanding, and indicating future goals with emphasis on electronic structure theory.

Organizers: Roberto Car (Princeton), Kristian S. Thygesen (Lyngby) and Matthias Scheffler (Berlin)

Time: Monday 10:30–13:15 Location: TRE Ma

Topical Talk TT 15.1 Mon 10:30 TRE Ma

Molecular junction transport: some theoretical and computational considerations — •Mark Ratner[1] and Matthew Reuter[2] — [1]Chemistry, Northwestern University, Evanston Illinois 60208 USA — [2]Chemistry, Northwestern University, Evanston Illinois 60208 USA

Following the development of break junction techniques, and very elegant measurements by many labs worldwide, the understanding of the community for single molecule transport junctions on the experimental side has been very nicely unified. While there are still challenges, interpretations of the transport (and indeed of some second-order response properties) is now quite sophisticated.

There have been major advances in the computational approaches also, and in many cases, computations and measurements can be compared quantitatively. But there are some remaining difficulties in the computational and theoretical approaches, and this talk will discuss a few of them.

The topics addressed will be: single molecule aspects, histograms and their usage, time-dependence of the transport, and ghost transmission and computational accuracy.

TT 15.2 Mon 11:00 TRE Ma

On the description of biased nanocontacts from ab initio — •Steven Achilles[1], Jürgen Henk[1], Michael Czerner[2], Christian Heiliger[2], and Ingrid Mertig[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — [2]I. Physikalisches Institut, Justus Liebig University, D-35392 Giessen, Germany

A suitable description of arbitrary shaped and biased nanocontacts is very important for investigating and predicting physical effects of materials on the nanometer scale. In particular, the electronic transport properties under finite bias voltages are of great interest.

To account for systems under finite bias we extended our Korringa-Kohn-Rostoker Green's function method [1] to the Keldysh formalism [2]. The method was developed for different types of geometries, i.e. planar junctions [3] and embedded real-space clusters [4]. Both implementations include a self-consistent treatment of the electronic structure under external bias using the nonequilibrium density.

We present ab initio results of voltage drops, the charge relaxation under finite bias voltage and current-voltage characteristics for different types of geometries.

[1] R. Zeller, P.H. Dederichs, B. Ujfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B 52, 8807 (1995).; P. Zahn, I. Mertig, R. Zeller, and P.H. Dederichs, Mat. Res. Soc. Symp. Proc. 475, 525 (1997).
[2] L.V. Keldysh, Sov. Phys. JETP 20 (4), 1018-1026 (1965).
[3] S. Achilles et al., Phys. Rev. B 88 (12), 125411 (2013).
[4] S. Achilles et al., to be published

TT 15.3 Mon 11:15 TRE Ma

Elasticity changes in molecular junctions under bias: an ab-initio study — •Clotilde S. Cucinotta[1], Meilin Bai[1,2], Ivan Rungger[1], Shmin Hou[2], and Stefano Sanvito[1] — [1]School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Ireland — [2]2Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Non-conservative current induced forces are at the origin of a rich variety of dynamical processes, including vibrations, rotations, phonon energy flow, desorption and reactions. The ability to simulate these phenomena paves the way for crucial advances in interface physics and in molecular electronics. New insights into how the presence of non-conservative forces can affect the vibrational spectrum of prototypic Au-H2-Au nano-junctions are obtained by the Non Equilibrium Green Functions approach combined with Density Functional Theory as implemented in the Smeagol code [1]. The modification of the phonon spectrum of the junction in the presence of an external bias is for the first time analysed, in terms of charge redistribution caused by the electron flow, potential drop and differences in an average distance collective variable. Phonon modes changes are related to a change in bias of some of the elastic constants.The importance of electric field vs. current effects is compared. The elasticity changes of the molecular junction with bias are interpreted in terms of the current flowing through the system. [1] http://www.smeagol.tcd.ie/SmeagolDownloads.htm.

TT 15.4 Mon 11:30 TRE Ma

Carbon nanotubes decorated with magnetic clusters: magnetism, electron transport and gas sensing — •Zeila Zanolli[1] and Jean-Christophe Charlier[2] — [1]Forschungszentrum Juelich, PGI and IAS, Juelich, Germany — [2]IMCN, Université catholique de Louvain (UCL), Belgium

In this work, first-principles techniques and non-equilibrium Green's function approaches are used to investigate magnetism and spin-polarized quantum transport in carbon nanotubes (CNTs) decorated with transition metal magnetic nanoclusters (NC).

For small cluster sizes (< 1 nm), *ab initio* calculations predict a considerable local magnetic moment that induces spin polarization in the host CNT due to a strong mutual interaction with the magnetic NC.

Such a huge local magnetic perturbation can be tailored by molecular adsorption on the metallic NC, thus modifying both the magnetization and the spin-dependent conductance of the hybrid CNT-NC system. The adsorption of benzene on Ni- or Pt-decorated metallic CNTs has been investigated as a test case. The ab initio simulations demonstrate that the magnetization change due to the absorption of a single C_6H_6 molecule should be large enough to be detected experimentally using either magnetic-AFM or SQUID magnetometer. Consequently, the present research suggests a novel approach for single molecule gas detection, based on local magnetic moment measurements in CNT-NC hybrid systems [1].

[1] Z. Zanolli, J.-C. Charlier, ACSnano **6** (2012) 10786-10791.

15 min. break

Topical Talk TT 15.5 Mon 12:00 TRE Ma

Insight into Charge Transport in Molecular Junctions from Ab Initio Theories of Level Alignment — •Jeffrey B. Neaton — Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — Department of Physics, University of California, Berkeley, Berkeley, CA — Kavli Energy Nanosciences Institute, Berkeley, CA

Recent scanning tunneling microscope-based break-junction experiments of molecular junctions – devices formed by trapping organic molecules between macroscopic metallic electrodes – have reported robust conductance, thermopower, switching behavior, quantum interference effects, spin-filtering phenomena, and even nonlinear effects such as rectification, establishing such junctions as unique and revealing windows into the physics of charge transport at the molecular scale. In this talk, I will summarize a predictive approach to compute and understand the transport properties of molecular junctions with good accuracy. Our approach includes important exchange and correlation effects missing in standard DFT Kohn-Sham junction level alignment, building on self-energy corrections within a GW approximation. Advantages and limitations of our approach will be discussed quantitatively in the context of a direct comparison with recent photoemission and transport measurements. I will also describe applications of this approach to select junctions exhibiting novel trends in conductance, thermopower, and nonlinear IV characteristics, where new physical insight is obtained by relating computed transport phenomena to junction structure and chemistry.

TT 15.6 Mon 12:30 TRE Ma

Towards First-Principles Modeling of Solvent Effects in Photo-Catalytic Water Splitting — •Stefan Ringe, Harald Oberhofer, Sebastian Matera, and Karsten Reuter — Technische Universität München, Germany

In the context of solar energy conversion the search for new materials for photo-catalytic water splitting has received new impetus. While in general powerful, computational screening approaches are struggling with the complexity of the underlying physical processes at the solid-liquid interface. Recent work points in particular at the necessity to include at least an efficient description of solvent screening effects to compute meaningful descriptors even in simple computational hydrogen electrode approaches. To this end, we present an implementation of the modified Poisson-Boltzmann (MPB) implicit solvation model in the highly parallel and numerically efficient all-electron DFT code FHI-aims. Optimally integrating into this code environment, we solve the MPB equation in a novel approach based on an expansion of the electrostatic potential in the localized basis functions of FHI-aims. In contrast to common numerical multi-grid solvers this approach can directly make use of the optimized integration schemes used to reach self-consistency and removes the need for numerical interpolation between different grids. We demonstrate the approach and its efficiency for a range of molecular test systems, and show first results for catalytic water splitting on gold nano-clusters.

TT 15.7 Mon 12:45 TRE Ma

Towards a combined QM/MM and implicit solvent description of photoelectrochemical processes — •Markus Sinstein[1], Daniel Berger[1], Ran Jia[2], Volker Blum[3], Harald Oberhofer[1], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Jilin University, P.R. China — [3]Duke University, USA

Photoelectrochemical systems are widely explored to drive energy-relevant redox reactions like water splitting or CO_2 reduction. The detailed analysis of the involved elementary processes via first-principles calculations is challenged by the necessity to simultaneously account for the extended semiconductor photocatalyst and the liquid electrolyte. Especially for charge (proton and/or electron) transfer steps traditionally employed periodic boundary condition approaches involve charged supercells with difficult to control finite size errors. To this end, we present a solid state QM/MM embedding approach, in which only a finite cluster model of the photocatalyst surface is treated quantum mechanically and the correct Madelung potential of the periodic system is obtained by embedding into a charge field. For the efficient modeling of photoelectrochemical processes we combine this approach with an implicit solvation scheme within the DFT package FHI-aims. Finally, we also show early test results of the combined QM/MM implicit solvent model.

TT 15.8 Mon 13:00 TRE Ma

Ab-initio Simulation of Molecular Networks on the Surface of Water — •Ralph Koitz, Marcella Iannuzzi, Ari P Seitsonen, and Jürg Hutter — University of Zurich, Zurich, Switzerland

Molecules adsorbed on surfaces play an important role in catalysis, surface science, and nanotechnology. Traditionally, research has focused on various adsorbates atop metals and metal oxides using computational and surface-science techniques. More recently, however, it was demonstrated that ordered monolayer networks can also be formed on the surface of liquid water by using metal ions to bind together multidentate precursor molecules. As these assemblies are difficult to characterize, computational methods can provide valuable insight into their formation and structure.

In this contribution we present large-scale DFT-based molecular dynamics simulations of the formation of a network of *tris*-terpyridine-derived molecules (TTPB) on a water slab. In particular, we focus on the structure of the molecule on the surface, the mechanism of Zn^{2+} ion insertion from the solution and the subsequent linking of molecules into aggregates. We employ the metadynamics method to quantify the free energy surface of the involved processes. Our results provide detailed insight into on-surface and subsurface diffusion in this system and chemical reactions of TTPB on the surface of water.

TT 16: Focus Session: Dynamics, Topology, and Fractionalisation

The "breaking-up" of electronic excitations into fractionalised quasiparticles such as spinons and holons is one of the most surprising phenomena in the quantum physics of solids. It represents one of the core concepts of topological and stronlgy correlated electron physics that features even exotic particles such as magnetic monopoles, Majorana fermions, anyons or emergent gauge fluxes.

Very recently, a number of important theoretical and experimental advances in studying fractionalisation have been reported. Experimentally a series of model systems has been identified, predominantly by advanced neutron scattering techniques that offer direct access to the investigation of fractionalised quasiparticles. On the theoretical side, it has become possible to describe the real-time dynamics of such systems in sufficient detail to be predictive for experiment. The dynamical properties provide thereby information on the entire spectrum of excited states, probing in particular also the fractionalised quasiparticles. This Focus Session summarizes important recent developments in this field.

Organizers: Roderich Moessner (MPI PKS Dresden), Christian Pfleiderer (TU München)

Time: Monday 15:00–17:45 Location: HSZ 01

Topical Talk TT 16.1 Mon 15:00 HSZ 01
Dynamics in Heisenberg Chains: From Fractional Excitations to New Out-of-Equilibrium States of Matter — •Jean-Sébastien Caux — Institute for Theoretical Physics, University of Amsterdam, Science Park 904, Postbus 94485, 1090 GL Amsterdam, The Netherlands

The Heisenberg chain has long been a fertile laboratory for the investigation of strongly-correlated many-body quantum physics. The spin-1/2 Heisenberg model has been the theoretical paradigm of exactly-solvable (integrable) systems since Bethe wrote down its wavefunctions in 1931, but recent years have witnessed much progress on the theoretical understanding and experimental observation of its dynamical properties. This talk will review a number of recent results, focusing on the characterization and observation of fractional excitations in the vicinity of the ground state, and on the exotic situations which can occur when one puts the system strongly out of equilibrium, for example after a quantum quench.

Topical Talk TT 16.2 Mon 15:30 HSZ 01
Inelastic Neutron Scattering on Candidate Kitaev Compounds — •Radu Coldea — Clarendon Laboratory, University of Oxford Physics Department, United Kindom

We explore the spin dynamics in the frustrated honeycomb magnets Na_2IrO_3 [1] and Li_2IrO_3 , candidates to display novel magnetic states stabilized by the strong spin-orbit coupling at the 5d Ir ions. Theory [2] predicts composite spin-orbital J=1/2 moments at the Ir ions coupled by strongly-anisotropic and bond-directional exchanges, the so-called Kitaev honeycomb model, which has in its phase diagram novel magnetically-ordered ordered phases and a quantum spin liquid with exotic excitations. To search for such physics the experimental technique of choice is inelastic neutron scattering to probe the spin dynamics, however this is technically very challenging due to the large absorption cross-section of neutrons by the Ir nuclei. Using an optimised setup to minimise neutron absorption we have been successful in observing strongly dispersive spin-wave excitations of the Ir moments in both compounds and results are compared with predictions for a Kitaev-Heisenberg model as well as a Heisenberg model with further neighbour couplings.
[1] S. K. Choi, R. Coldea, A. N. Kolmogorov, T. Lancaster, I. I. Mazin, S. J. Blundell, P. G. Radaelli, Yogesh Singh, P. Gegenwart, K. R. Choi, S.-W. Cheong, P. J. Baker, C. Stock, and J. Taylor, Phys. Rev. Lett. 108, 127204 (2012)
[2] J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev. Lett. 105, 027204 (2010).

Invited Talk TT 16.3 Mon 16:00 HSZ 01
Dynamics of Majorana Fermions in a Quantum Spin Liquid — •John Chalker[1], Johannes Knolle[2], Dmitry Kovrizhin[3], and Roderich Moessner[2] — [1]Physics Department, Oxford University, Oxford, U.K. — [2]Max Planck Institute for Physics of Complex Systems, Dresden — [3]Cavendish Laboratory, Cambridge University, U.K.

The study of spin liquids has been central to advancing our understanding of correlated phases of quantum matter ever since Anderson's 1973 proposal of the resonating valence bond liquid state. However, detailed theoretical investigations of dynamics in spin liquids are hampered by the lack of suitable approaches, with analytical descriptions restricted to general features and numerical methods limited to small systems sizes, to models with a robust excitation gap, or ones that avoid the sign problem in quantum Monte Carlo. In this setting the Kitaev honeycomb model provides a benchmark: it gives an exactly solvable model in which spins dissolve into new degrees of freedom – fluxes of a Z_2 gauge field and Majorana fermions moving in this field – and is representative of a broad class of systems. I will present results from a numerically exact calculation of the dynamical structure factor for this system. These include counter-intuitive manifestations of quantum number fractionalisation, such as a neutron scattering response with a gap even in the presence of gapless excitations, and a sharp component despite the fractionalisation of electron spin.
[1] J. Knolle, D. L. Kovrizhin, J. T. Chalker, and R. Moessner, arXiv:1308.4336

15 min. break.

Invited Talk TT 16.4 Mon 16:45 HSZ 01
Molecular Quantum Magnetism in $LiZn_2Mo_3O_8$ — •Collin Broholm — Johns Hopkins University, Baltimore, USA

I shall discuss the unusual quantum magnetism of $LiZn_2Mo_3O_8$ where Mo_3O_{13} molecules realize spin-1/2 degrees of freedom on a triangular lattice and the spin system remains in a quantum fluctuating state deep into the low temperature regime [1]. Neutron scattering experiments on a powder sample show apparently gapless ($\Delta < 0.2$ meV) magnetic excitations extending at least to 2.5 meV [2]. The data are consistent with a disordered valence bond solid or a resonating valence bond state involving nearest-neighbor and next-nearest-neighbor spins.
[1] J. P. Sheckelton, J. R. Neilson, D. G. Soltan, and T. M. McQueen, Nature Mater. **11**, 493496 (2012)
[2] M. Mourigal, W. T. Fuhrman, J. P. Sheckelton, A. Wartelle, J. A. Rodriguez-Rivera, T. M. McQueen, C. L. Broholm, arXiv:1309.1165 (2013).

Topical Talk TT 16.5 Mon 17:15 HSZ 01
Unwinding a Skyrmion Lattice: Emergent Monopoles in Chiral Magnets — •Achim Rosch — University of Cologne, Cologne, Germany

Small magnetic fields and thermal fluctuations stabilize lattices of magnetic whirls, so-called skyrmions, in chiral magnets. These skyrmions are characterized by a topological winding number and couple very efficiently to electric currents by Berry phases. The effect of these Berry phases can be described by emergent electromagnetic fields [1].

The skyrmion lattice can be destroyed by a change of magnetic field [2]. The associated change of the topology of the magnetic structure has to occur by singular magnetic configurations which act as sources and sinks of the emergent magnetic flux. Thereby they can be viewed as emergent magnetic monopols. Combining numerical simulations, magnetic force microscopy and neutron scattering [2], we investigate the signatures and the dynamics of a topological first-order phase transition driven by the creation of monopoles and antimonopoles.
[1] T. Schulz, R. Ritz, A. Bauer, M. Halder, M. Wagner, C. Franz, and C. Pfleiderer, K. Everschor, M. Garst, and A. Rosch, Nature Physics, 8, 301 (2012).
[2] P. Milde, D. Köhler, J. Seidel, L. M. Eng, A. Bauer, A. Chacon, J. Kindervater, S. Mühlbauer, C. Pfleiderer, S. Buhrandt, C. Schütte, A. Rosch, Science 340, 1076 (2013).

TT 17: Superconductivity: Tunnelling, Josephson Junctions, SQUIDs

Time: Monday 15:00–18:30 Location: HSZ 201

TT 17.1 Mon 15:00 HSZ 201

Fabrication of a transparent NbAl interface in hybrid Josephson junctions and flux qubits with π-shifters and their low-temperature measurements. — •Anastasia Shcherbakova[1], Kirill Fedorov[2], Kirill Shulga[3], Valery Ryazanov[4], Vitaly Bol'ginov[4], Detlef Beckman[5], and Alexey V. Ustinov[1,2,5] — [1]Physikalisches Institut, Karlsruhe Institut fuer Technologie, D-76131, Karlsruhe, Germany — [2]Walther-Meißner-Institut, D-85748, Garching, Germany — [3]National University of Science and Technology MISIS, 119049 Moscow, Russian Federation — [4]Institute of Solid State Physics, Chernogolovka, 142432 Russian Federation — [5]RQC, BC "Ural", Skolkovo, Moscow region, 143025 Russian Federation

Aluminum-based superconducting flux qubits can be made very compact and employ high-quality Josephson junctions. An external magnetic flux need to be applied in order to set the flux qubit to a working point at minimal frequency. Adding a π-junction to the qubit loop makes applying the magnetic flux unnecessary, thus removing possible source of external fluctuations. The conventional fabrication of π-junctions requires depositing of niobium layers separated by a ferromagnet. We report fabrication of composite Al/Nb flux qubits with Nb/CuNi/Nb junctions embedded in the loop. The π-biased qubits show the characteristic microwave spectrum shifted by a half of a magnetic flux quantum. The reported technological approach opens way to a variety of quantum circuits employing Nb and Al elements.

TT 17.2 Mon 15:15 HSZ 201

φ-Josephson junctions based on current injectors — •rosina menditto[1], hanna sickinger[1], johannes maximilian meckbach[2], michael merker[2], konstantin ilin[2], michael siegel[2], dieter kölle[1], and reinhold kleiner[1] — [1]Physikalisches Institut and Center vor Collective Quantum Phenomena in LISA+, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [2]Institut für Mikro- und Nanoelektronische Systeme, Karlsruher Institut für Technologie, Hertzstrasse 16, D-76187 Karlsruhe, Germany

We propose and implement φ-Josephson junctions with high critical current density fabricated using Nb/AlO_x/Nb technology. In previous works we showed that in conventional junctions a π, or more general a κ, phase discontinuity can be realized by means of a pair of tiny current injectors placed in the middle of the junction. Currently, we introduced two additional pairs of injectors in asymmetric positions, in order to obtain a φ-junction completely tunable electronically. By controlling the external magnetic field and the current flowing in the secondary injectors, we are able to investigate several effects: preparation and readout of the initial state, rearrangements of fractional vortices, thermal/resonant escape and retrapping of the phase.

TT 17.3 Mon 15:30 HSZ 201

Tuning the ground state of a φ-Josephson junction with current injectors — •Matthias Zimmermann, Karl Vogel, and Wolfgang Schleich — Institut für Quantenphysik, Universität Ulm, D-89069 Ulm

We propose to use a pair of tiny current injectors to control the ground states of a φ-Josephson junction. The system is based on a $0-\pi$-Josephson junction with different lengths of the 0- and π-regions. To describe this asymmetric system, we use analytic solutions of the Sine-Gordon equation and apply an external magnetic field as additional control parameter. As a result we are able to calculate the energy of the stationary states as a function of the injected current and the external magnetic field. Furthermore, we show that the injected current can be used to prepare the Josephson junction in one of its doubly degenerate ground states.

TT 17.4 Mon 15:45 HSZ 201

Hybrid superconducting magnetic tunnel junctions: Coexistence of TMR and Josephson effects — •Ondrej Vavra[1,2], Rohit Soni[2], Nico Ruppelt[2], Adrian Petraru[2], Hermann Kohlstedt[2], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Nanoelektronik, Technical Faculty, University of Kiel, D-24143 Kiel, Germany

We report on the latest results observed on hybrid superconducting SFIFS Josephson junctions with ferromagnet thickness-wedge (F). The Nb-Fe-Al_2O_3-Fe-Nb junctions were deposited by means of dc-magnetron sputtering technique. Junctions exhibit both Josephson effect and tunneling magnetoresistance (TMR) effect. Fraunhofer magnetic field dependence of the critical current I_C(B) proves the homogeneity of the barrier over the 4 inch wafer. The properties of the junctions such as I_C, normal conductance G_n and the tunneling magnetoresistance (TMR), respectively, strongly dependent on the oxidation parameters of the barrier (Al2O3). The different thickness of intermediate Al gives rise to the over- or under-oxidation, resulting in the Nb-Fe-Fe*-Al_2O_3-Fe-Nb or the Nb-Fe-Al-Al_2O_3-Fe-Nb, respectively. The layers denoted as Fe* (by oxygen affected Fe) and Al (residual Al layer underlying the Al_2O_3) are considered as parasitic since they suppress TMR. The impact of different thickness of both ferromagnetic layers d_F on density of states, TMR and Josephson effect will be presented too.

TT 17.5 Mon 16:00 HSZ 201

Bicrystal Grain Boundary Junctions of P-doped and Co doped Ba-122 Thin Films — •Stefan Schmidt[1], Sebastian Döring[1], Frank Schmidl[1], Volker Tympel[1], Fritz Kurth[2], Kazumasa Iida[2], Bernhard Holzapfel[2], Takahiko Kawaguchi[3], Yasuhiro Mori[3], Hiroshi Ikuta[3], and Paul Seidel[1] — [1]Friedrich-Schiller-University Jena, Institute of Solid State Physics, Jena, Germany — [2]IFW Dresden, Institute for Metallic Materials, Dresden, Germany — [3]Nagoya University, Department of Crystalline Materials Science, Nagoya, Japan

We prepared grain boundary (GB) junctions of $BaFe_2(As_{0.66}P_{0.34})_2$ thin films on bicrystal [001]-tilt LSAT and MgO substrates with GB angles of $\theta = 45°$. The junctions show clear Josephson effects and distinct Shapiro steps under microwave irradiation. Electrical characterization shows symmetric I-V characteristics which can be described with a combination of flux-flow behavior and the resistively shunted junction (RSJ) model. A large excess current I_{ex} is observed. Their formal I_CR_N product is up to 50 μV at 4.2 K, which is decreased to 11 μV when taking I_{ex} into account. Additionally, measurements on GB junctions of Fe-buffered $Ba(Fe_{0.9}Co_{0.1})_2As_2$ thin films on STO bicrystal substrates ($\theta = 30°$) are shown for comparison. Their asymmetric RSJ behavior exhibits a formal I_CR_N product of 20 μV, whereas the excess corrected value is 6.5 μV.

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

TT 17.6 Mon 16:15 HSZ 201

Planar hybrid Josephson junctions with $BaFe_{2-x}Co_xAs_2$ base electrode and a conventional Pb counter electrode using barriers from Au and TiO_x — •Sebastian Döring[1], Stefan Schmidt[1], Manuel Monecke[1], Volker Tympel[1], Frank Schmidl[1], Fritz Kurth[2], Kazumasa Iida[2], Ingolf Mönch[3], Bernhard Holzapfel[2,4], 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, Institut für Integrative Nanowissenschaften, Helmholtzstraße 20, 01069 Dresden — [4]Karlsruhe Institute of Technology, Institut für Technische Physik, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

We prepared Josephson junctions from $BaFe_{2-x}Co_xAs_2$ thin films using photolithography and ion beam etching to pattern the base electrode and sputtering of SiO_2 for the preparation of insulation frameworks. The counter electrode was made from thermally evaporated lead in-situ covered by indium to avoid degradation. As barriers we use sputtered gold layers or additional layers from sputtered and subsequently oxidized titanium, respectively. While for the pure gold barrier we reached an I_cR_n-product of about 18 μV it could be increased to 90 μV using the additional TiO_x layer. The current noise behavior and microwave response of the Josephson junctions could be improved, too.

15 min. break.

TT 17.7 Mon 16:45 HSZ 201

Coherent terahertz emission from $Bi_2Sr_2CaCu_2O_8$ intrinsic Josephson junction stacks — •Fabian Rudau[1], Boris Gross[1],

Deyue An[2,3], Nickolay Kinev[4], Xianjing Zhou[2], Min Ji[2,3], Ya Huang[2], Takeshi Hatano[3], Roman Mints[5], Peiheng Wu[2], Valery Koshelets[4], Huabing Wang[2,3], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut, Universität Tübingen — [2]Institute of Superconductor Electronics, Nanjing University — [3]National Institute for Materials Science, Tsukuba — [4]Kotel'nikov Institute of Radio Engineering and Electronics, Moscow — [5]School of Physics and Astronomy, Tel Aviv University

Josephson Junctions (JJs) offer a natural way to convert a dc voltage into high-frequency electromagnetic radiation. In the high-transition temperature superconductor $Bi_2Sr_2CaCu_2O_8$ JJs form intrinsically, allowing to fabricate stacks of hundreds of junctions easily. Such arrays are promising candidates to be used as generators of electromagnetic waves in the terahertz regime. Ranging from 0.4 to 1 THz, coherent radiation has been detected from large, rectangular $Bi_2Sr_2CaCu_2O_8$ mesa structures, producing several tens of microwatt in power. The mesas are believed to work as a cavity for electromagnetic standing waves, synchronizing all the junctions in the stack. We report on the investigation of the heat distribution and electromagnetic standing waves in such mesa structures, as well as the generation of terahertz radiation, using a combination of transport measurements, direct radiation detection, low temperature scanning laser microscopy and computer assisted modelling.

TT 17.8 Mon 17:00 HSZ 201

Quantum Brownian motion in an oscillating tilted periodic potential: application to a Josephson junction under microwave irradiation in the dual regime — •Angelo Di Marco[1], Gianluca Rastelli[2], and Frank W. J. Hekking[1] — [1]LPMMC-CNRS, Université Joseph Fourier, 25 Avenue des Martyrs BP166 38042, Grenoble Cedex, France — [2]Zukunftskolleg, Fachbereich Physik, Universität Konstanz, D-78457, Konstanz, Germany

We study a current-biased Josephson junction in the presence of an applied microwave field and influenced by an external electromagnetic environment. This problem can be mapped onto the one of a quantum Brownian particle moving in a tilted periodic potential under the effect of an oscillating force. We focus on the regime where the junction's Josephson energy E_J dominates its charging energy E_C. In this case, it is the dynamics of the so-called quasi-charge that accounts for the current-voltage characteristic of the junction. Using a full quantum approach, we study numerically and analytically the I-V curve at low temperature. In particular, we analyze the role of the quantum fluctuations on the theoretically expected Shapiro steps for current. We compare our results with the one based on a classical approach for the dynamics of the quasi-charge.

TT 17.9 Mon 17:15 HSZ 201

Coherent radiation from the fractional Josephson effect — •Christoph Ohm and Fabian Hassler — Institut für Quanteninformation, RWTH Aachen

At a Josephson junction between two topological superconductors single electrons are transported coherently between the two superconducting reservoirs. This effect is known as the fractional Josephson effect. It has been shown that a voltage-biased fractional Josephson junction produces radiation at a frequency that is half of the ordinary Josephson frequency. We study the coherence properties of this unconventional Josephson radiation including phase- and frequency-fluctuations. We show that the coherence time of the emitted radiation is dominated by quasi-particle poisoning. In addition, we discuss the fermionic parity constraint as well as pinning of the Josephson frequency in terms of second order correlation functions between radiation fields from different emitters.

TT 17.10 Mon 17:30 HSZ 201

Long Range Triplet Josephson Current and $0-\pi$ Transition in Tunable Domain Walls — Thomas E. Baker[1,2], Adam C. Richie-Halford[1,3], and •Andreas Bill[1] — [1]Dept. of Physics & Astronomy, California State University, Long Beach, CA 90840, USA — [2]Dept. of Physics & Astronomy, University of California, Irvine, CA 92697, USA — [3]Department of Physics, University of Washington, Seattle, WA 98195, USA

The order parameter of superconducting pairs penetrating an inhomogeneous magnetic material can acquire a long range triplet component (LRTC) with non-zero spin projection of the pairs ($S_z = \pm 1$). This state has been predicted and generated recently in proximity systems and Josephson junctions. We show using an analytically derived domain wall of an exchange spring how the LRTC emerges and can be tuned with the twisting of the magnetization [1]. We also introduce a new kind of Josephson current reversal, the triplet $0-\pi$ transition, that can be observed in one and the same system either by tuning the domain wall or by varying temperature. Finally, we show how the LRTC may be manipulated to produce a singlet current and how it can be observed in a superconducting-magnetic multilayer.

We gratefully acknowledge the support of the National Science Foundation (DMR-0907242), the Army Research Laboratory and the Research Corporation.

[1] T.E. Baker, A. Richie-Halford, and A. Bill, arXiv:1310.6632

TT 17.11 Mon 17:45 HSZ 201

Quantum transport signatures of chiral edge states in Sr_2RuO_4 — •Rakesh Tiwari[1], W Belzig[2], M Sigrist[3], and C Bruder[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [3]Theoretical Physics, ETH Zurich, CH-8093 Zurich, Switzerland

We investigate transport properties of a double quantum dot based Cooper pair splitter, where the superconducting lead consists of Sr_2RuO_4. The proposed device can be used to explore the symmetry of the superconducting order parameter in Sr_2RuO_4 by testing the presence of gapless chiral edge states, which are predicted to exist if the bulk superconductor is described by a chiral p–wave state. The odd orbital symmetry of the bulk order parameter ensures that we can realize a regime where the electrons tunneling into the double dot system come from the chiral edge states and thereby leave their signature in the conductance. The proposed Cooper pair splitter has the potential to probe order parameters in unconventional superconductors.

TT 17.12 Mon 18:00 HSZ 201

Quasiperiodicity and revivals in dynamics of quantum phase slips in Josephson junction chains and superconducting nanowires — •Gianluca Rastelli[1,3], Mihajlo Vanević[2], and Wolfgang Belzig[3] — [1]Zukunftskolleg, Universität Konstanz, Germany — [2]Department of Physics, University of Belgrade, Serbia — [3]Fachbereich Physik, Universität Konstanz, Germany

Quantum phase slips in superconducting loops threaded by an external magnetic field provide a coupling between macroscopic quantum states with supercurrents circulating in opposite directions. We analyze dynamics of the phase slips as a function of the superconducting loop length, from fully coherent dynamics for short loops to dissipative dynamics for the long ones. For intermediate lengths of the superconducting loop, we find that the phase slips are coupled to a discrete bath of oscillators with frequencies comparable to the phase-slip amplitude. This gives rise to a quasi-periodic dynamics of the phase slips which manifests itself as a decay of oscillations between the two counterpropagating current states at short times, followed by oscillation revivals at later times. We analyze possible experimental implications of this non-adiabatic regime in Josephson junction chains and superconducting nanowires.

TT 17.13 Mon 18:15 HSZ 201

Correlated transport through junction arrays in the small Josephson energy limit: incoherent Cooper-pairs and hot electrons — Jared Cole[1], Juha Leppäkangas[2], and •Michael Marthaler[3] — [1]Chemical and Quantum Physics, RMIT University, Melbourne — [2]Department of Microtechnology and Nanoscience, Chalmers University of Technology — [3]Institut für Theoretische Festkörperphysik, KIT, Karlsruhe

We study correlated transport in a Josephson junction array for small Josephson energies. In this regime transport is dominated by Cooper-pair hopping, although we observe that quasiparticles can not be neglected. We assume that the energy dissipated by a Cooper-pair is absorbed by the intrinsic impedance of the array. This allows us to formulate explicit Cooper-pair hopping rates without adding any parameters to the system. We show that the current is correlated and crucially, these correlations rely fundamentally on the interplay between the Cooper-pairs and equilibrium quasiparticles.

TT 18: Transport: Fluctuations and Noise

Time: Monday 15:00–16:00 Location: HSZ 204

TT 18.1 Mon 15:00 HSZ 204

Energy noise in a voltage-driven quantum point contact — •Federica Haupt, Francesca Battista, and Janine Splettstösser — Institut für Theorie der Statistischen Physik, RWTH Aachen, Germany

Single electron sources are of key importance in research fields such as metrology and quantum electron optics [1]. Ideally, these time-periodically driven devices emit a controlled number of particles in each driving period. This is predicted to be reached when applying a series of Lorentzian-shaped pulses to the conductor [2]. In experimental realisations, the shot noise provides a tool to measure the precision with which particles are emitted. In particular, it is sensitive to extra electron-hole excitations induced by the driving itself [3,4].

In order to complement the investigations on the electron-hole pair creation based on the study of charge transport [5,6], we address the energy transport properties of a quantum point contact subject to a periodic driving. In particular, we discuss features of the driving in the energy current and the low-frequency energy noise, and show that the latter carries detailed informations on the energetics of the particle-like excitations transmitted through the conductor [7].

[1] J. P. Pekola et al., arxiv:1208.4030 (2012)
[2] J. Keeling et al., Phys. Rev. Lett. 97, 116403 (2006)
[3] J. Gabelli and B. Reulet, Phys. Rev. B 87, 075403 (2013)
[4]J. Dubois et al., Nature 502, 659 (2013)
[5] M. Vanevic Y. V. Nazarov, and W. Belzig, Phys. Rev. Lett. 99, 076601 (2007)
[6] M. Vanevic and W. Belzig, Phys. Rev. B 86, 241306 (2012)
[7] F. Battista, F. Haupt, J. Splesttoesser, in preparation.

TT 18.2 Mon 15:15 HSZ 204

Non-Gaussian noise- and plasmon-assisted over-bias light emission from tunnel contacts — •Fei Xu, Cecilia Holmqvist, and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Understanding tunneling from an atomically sharp tip to a metallic surface requires to account for interactions on a nanoscopic scale. Inelastic tunneling of electrons gives rise to the emission of photons, whose energies should intuitively be limited by the applied bias voltage eV. However, experiments [1,2] indicate that more complex processes involving the interaction of electrons with plasmons lead to photon emission with over-bias energies. We propose a model of this observation in analogy to the dynamical Coulomb blockade, originally developed to treat the electronic environment in mesoscopic circuits. We explain the experimental finding quantitatively by correlated tunneling of two electrons interacting with an RCL circuit to model the local plasmon mode. We show that the non-Gaussian statistics of the tunneling dynamics of the electrons is essential to describe the over bias emission .

[1] G. Schull et al., PRL 102, 057401 (2009)
[2] N. L. Schneider et al., PRL 105, 026601 (2010)

TT 18.3 Mon 15:30 HSZ 204

Inverse counting statistics for stochastic and open quantum systems: the characteristic polynomial approach — •Martin Bruderer[1], Debora Contreras-Pulido[1], Maximilian Thaller[2], Lucia Sironi[3], Danail Obreschkow[4], and Martin B. Plenio[1] — [1]Institut für Theoretische Physik, Universität Ulm, Germany — [2]Fachbereich Physik, Universität Konstanz, Germany — [3]Department of Biology, Universität Konstanz, Germany — [4]University of Western Australia, ICRAR, Crawley, Australia

We consider stochastic and open quantum systems with a finite number of states, where a stochastic transition between two specific states is monitored by a detector. The long-time counting statistics of the observed realizations of the transition, parametrized by cumulants, is the only available information about the system. We present an analytical method for reconstructing generators of the time evolution of the system compatible with the observations. Moreover, we propose cumulant-based criteria for testing the non-classicality and non-Markovianity of the time evolution, and lower bounds for the system dimension. Our analytical results rely on the close connection between the cumulants of the counting statistics and the characteristic polynomial of the generator, which takes the role of the cumulant generating function.

[1] M. Bruderer et *al.*, arXiv:1311.2673

TT 18.4 Mon 15:45 HSZ 204

Floquet Theory of Electron Waiting Times in Quantum-Coherent Conductors — •David Dasenbrook, Christian Flindt, and Markus Büttiker — Département de Physique Théorique, Université de Genève, 1211 Genève, Switzerland

The distribution of waiting times between charge detection events has recently gained some interest in theoretical mesoscopic physics. As an alternative to full counting statistics (FCS), which is typically evaluated in the long time limit, it allows for a complementary characterization of electron transport on short and intermediate time scales. Waiting time distributions (WTD) can be used as a tool to investigate the interplay between extrinsic and intrinsic time scales in periodically driven systems.

However, while there have been results on waiting times in classical driven systems, a formalism for WTDs in phase coherent systems with an external time-dependence has so far been lacking. We present such a formalism for one-dimensional non-interacting systems based on a Floquet scattering approach.

We demonstrate the usefulness of our formalism by means of two examples: a quantum point contact (QPC) whose transmission is weakly and slowly modulated and the application of Lorentzian voltage pulses of integer charge to an ideal conductor.

TT 19: Transport: Quantum Dots, Quantum Wires, Point Contacts II (organized by TT)

Time: Monday 16:00–18:30 Location: HSZ 204

TT 19.1 Mon 16:00 HSZ 204

A two-atom electron pump — Benoit Roche[1], Roman-Pascal Riwar[1], Benoit Voisin[1], Eva Dupont-Ferrier[1], Romain Waquez[3], Maud Vinet[3], Marc Sanquer[1], •Janine Splettstoesser[2], and Xavier Jehl[1] — [1]SPSMS, UMR-E, CEA Grenoble, INAC, Grenoble, France — [2]MC2, Chalmers University of Technology, Göteborg, Sweden — [3]CEA, LETI, MINATEC, Grenoble, France

In recent years there has been a lot of interest in time-dependently driven quantum systems, such as quantum-dot pumps, both in the adiabatic regime of slow driving as well as in the high-frequency regime. However, all experiments so far were carried out in either one of these regimes, but were not subsequently tuned to both. I will present an experimental realization [1] of electron pumping through two phosphorus donors in series implanted in a silicon nanowire. While quantized pumping is achieved in the low-frequency adiabatic regime, remarkable features are observed at higher frequency, when the charge transfer is limited either by the tunnelling rates to the electrodes or between the two donors. We model the transitions between quantum states involving a Landau-Zener transition, allowing to reproduce in detail the characteristic signatures observed in the non-adiabatic regime. Interestingly, the breakdown of the adiabatic limit can thus accurately be associated to the relation of the respective time-scales of tunneling to the electrodes or between the donors, compared to the time-scales of the driving. Consequently, information on the time-scales can be extracted from a detailed inspection of the pumping signal.

[1] B. Roche, *et al.*, Nat. Commun. 4, 1581 (2013)

TT 19.2 Mon 16:15 HSZ 204

Functional renormalization group in Floquet space and its application to periodically driven quantum dots — •Katharina Eissing[1,2], Stefan Göttel[1,2], Dante Marvin Kennes[1,2], and Volker Meden[1,2] — [1]Institut für Theorie der Statistischen Physik,

RWTH Aachen University, 52074 Aachen, Germany — [2]JARA Fundamentals of Future Information Technology, 52056 Aachen, Germany

The functional renormalization group (RG) was recently extended to study interacting, low-dimensional systems out of equilibrium. This includes correlated quantum dot setups with explicitly time-dependent Hamiltonians as e.g. realized in quantum quenches or in the presence of time-dependent bias voltages [Phys. Rev. B 85, 085113 (2012), Phys. Rev. B 85, 245101 (2012)]. However, following this route periodic pumping processes, which are of particular interest in e.g. nanoelectronics and quantum information science, can only be described in an inefficient way. Taking advantage of the periodicity, we combine the Floquet theorem with the functional RG. This allows us to transform the double-time self-energy and Green functions in the Floquet basis [J. Phys.: Condens. Matter 20 085224] and the functional RG treatment resembles the stationary formalism. This makes it feasible to study transport in periodically driven systems. In my talk, I will shortly introduce this Floquet theorem based functional RG and present first results on transport through a quantum dot described by the interacting resonant level model.

TT 19.3 Mon 16:30 HSZ 204

Interplay of edge state polarization and a Zeeman split quantum dot — •Benedikt Probst[1], Pauli Virtanen[2], and Patrik Recher[1] — [1]Institute for Mathematical Physics, TU Braunschweig, Braunschweig, Germany — [2]O.V. Lounasmaa Laboratory, Aalto University, Finland

Topological insulators are a novel state of matter showing interesting physics. One of the effects realized in these materials is the quantum spin Hall effect in which electrons with different spin propagate in different directions on the edge of the system. Applying a bias to the system therefore leads to a spin bias for the edge state. We consider a system in which a quantum dot in the Coulomb blockade regime is attached to a helical Luttinger liquid. This quantum dot is treated as a localized spin, which can be manipulated by a magnetic field. The dynamics of the dots are described by setting up a general master equation. From the steady state of the system the polarization of the dot and the differential edge conductance is calculated. We discuss a regime in which the dot polarization exhibits a strong bias dependence and a regime in which the transport shows a characteristic bias asymmetry which allows to identify the relative orientation of the spin polarization in the edge state with respect to the magnetic field.

15 min. break.

TT 19.4 Mon 17:00 HSZ 204

Entanglement detection in an interacting beam-splitter device — •Alexander Schroer[1], Bernd Braunecker[2], Alfredo Levy Yeyati[3], and Patrik Recher[1] — [1]Institute for Mathematical Physics, TU Braunschweig, Germany — [2]Department of Theoretical Condensed Matter Physics, Universidad Autónoma de Madrid, Spain — [3]School of Physics & Astronomy, University of St Andrews, UK

We investigate a tunnel contact between two Luttinger liquids, e.g. realized as two crossed one-dimensional nanowires. When injecting one of two electrons with opposite spin in each wire, the current measured behind the crossing differs for singlet, triplet or product states. This is an apparent non-Fermi liquid feature because the current has been shown to be independent of spin-entanglement for Fermi liquid beam-splitters before. It can be understood in terms of collective excitations and by taking spin-charge separation into account. This behavior may offer an easier alternative to traditional entanglement detection schemes based on current noise, which turns out to be suppressed by the electron-electron interaction.

TT 19.5 Mon 17:15 HSZ 204

Hierarchical Equation of Motion Investigation of Decoherence and Relaxation Dynamics in Nonequilibrium Transport through Interacting Quantum Dots — •Rainer Härtle[1,2], Guy Cohen[3], David R. Reichman[3], and Andrew J. Millis[2] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Physics, Columbia Universtiy, New York, USA — [3]Department of Chemistry, Columbia Universtiy, New York, USA

A recently developed hierarchical quantum master equation approach [1,2] is used to investigate nonequilibrium electron transport through an interacting double quantum dot system in the regime where the inter-dot coupling is weaker than the coupling to the electrodes. The corresponding eigenstates provide tunneling paths that may interfere constructively or destructively, depending on the energy of the tunneling electrons [3]. Electron-electron interactions are shown to quench these interference effects in bias-voltage dependent ways, leading, in particular, to negative differential resistance, population inversion and an enhanced broadening of resonances in the respective transport characteristics [2]. Relaxation times are found to be very long, and to be correlated with very slow dynamics of the inter-dot coherences. The ability of the hierarchical quantum master equation approach to access very long time scales is crucial for the study of this physics.

[1] J. Jin *et al.*, J. Chem. Phys. 128, 234703 (2008).
[2] R. Härtle *et al.*, arXiv:1309.1170 (2013)
[3] R. Härtle *et al.*, Phys. Rev. B 87, 085422 (2013)

TT 19.6 Mon 17:30 HSZ 204

Detection of the decay rates in interacting quantum dots — •Jens Schulenborg[1,2], L. Debora Contreras- Pulido[3], Michele Governale[4], and Janine Splettstoesser[1,2] — [1]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Göteborg, Sweden — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [3]Institut für Theoretische Physik, Universität Ulm, Germany — [4]School of Physical and Chemical Sciences, Victoria University of Wellington, New Zealand

Over the past years, potential applications in nanoelectronics, metrology and quantum information sparked great interest in studying the *dynamics* of time-dependently driven quantum dots. Recently, the relaxation rates in the dynamical response of an interacting single-level quantum dot, weakly tunnel coupled to an electronic reservoir and brought out of equilibrium by a step pulse, have been investigated [1].

This theoretical work focuses on the readout of these relaxation rates with a capacitively coupled sensor quantum dot (SQD). Using a generalized master equation approach for the combined system of dot and SQD, we investigate the measurability of the dot relaxation behavior via the SQD current, especially accounting for back-action effects.

Our results reveal parameter regimes in which back-action leads to a decrease of the dot decay rates and to a mixing of relaxation modes that decay independently in the absence of a measurement. However, avoiding these regimes, we show that the original dot rates can still be extracted from the SQD current.

[1] L. D. Contreras-Pulido et al., Phys. Rev. B **85**, 075301 (2012).

TT 19.7 Mon 17:45 HSZ 204

Hybrid Microwave Cavity Heat Engine — Christian Bergenfeldt[1], Peter Samuelsson[1], •Björn Sothmann[2], Christian Flindt[2], and Markus Büttiker[2] — [1]Physics Department, Lund University, Box 118, SE-22100 Lund, Sweden — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

We propose and analyze the use of hybrid microwave cavities as quantum heat engines. A possible realization consists of two macroscopically separated quantum dot conductors coupled capacitively to the fundamental mode of a microwave cavity. We demonstrate that an electrical current can be induced in one conductor through cavity-mediated processes by heating up the other conductor. The heat engine can reach Carnot efficiency with optimal conversion of heat to work. When the system delivers the maximum power, the efficiency can be a large fraction of the Carnot efficiency. The heat engine functions even with moderate electronic relaxation and dephasing in the quantum dots. We provide detailed estimates for the electrical current and output power using realistic parameters.

[1] C. Bergenfeldt, P. Samuelsson, B. Sothmann, C. Flindt and M. Büttiker, arXiv:1307.4833v1 (2013).

TT 19.8 Mon 18:00 HSZ 204

Vibration-induced thermoelectric effects in quantum dots — •Matti Laakso and Volker Meden — Institut für Theorie der Statistischen Physik, RWTH Aachen, Aachen, Germany

We study the thermoelectric transport through a quantum dot coupled to a single vibrational mode described by the Anderson-Holstein model. We use analytical methods in the linear response regime as well as the functional renormalization group (FRG) in the non-linear regime. We predict relatively large thermoelectric effects in the parameter regime where the phonon-mediated electron-electron interaction dominates over the bare Coulomb repulsion.

TT 19.9 Mon 18:15 HSZ 204

Superexchange transport and blockade in triple quan-

tum dots — •Rafael Sánchez[1], Ghislain Granger[2], Fernando Gallego-Marcos[1], Sergei A. Studenikin[2], Andrew S. Sachrajda[2], and Gloria Platero[1] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049 Madrid, Spain — [2]National Research Council Canada, Ottawa, ON K1A 0R6 Canada

We present recent experimental evidence of long range transport in triple quantum dots. Superexchange is responsible for the spin-dependent indirect coupling of the two outer quantum dots, mediated by virtual transitions through the middle one. They are manifested in the form of sharp current resonances at the degeneracy points of states with left-right symmetric charge distributions [1,2]. The transition can take two paths: two electrons in different dots tunnel simultaneously [1] or a single electron tunnels twice [2].

We analyze a configuration where the two paths with different virtual intermediate states are possible and lead to quantum interference. Remarkably, we find conditions where the destructive interference of these transitions completely cancels the transport, what we call superexchange blockade [3]. Spin correlations play an essential role by avoiding certain transitions. This effect, known as spin blockade, leads to the suppression of certain resonances whose observation gives a measure of spin decoherence times.

[1] M. Busl et al., Nature Nanotech. 8, 261 (2013).
[2] R. Sánchez et al., submitted.
[3] R. Sánchez, F. Gallego-Marcos and G. Platero, submitted.

TT 20: Correlated Electrons: Spin Systems and Itinerant Magnets - Frustrated Magnets II

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

TT 20.1 Mon 15:00 HSZ 304

Magnetic properties of $VOMoO_4$ and Li_2VOSiO_4: an LDA+DMFT study — •Amin Kiani and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

By using the local density approximation+dynamical mean field theory and local vertex approximation we calculate the static magnetic response function overall the Brillouin zone for the two highly correlated materials $VOMoO_4$ and Li_2VOSiO_4. We show that the vertex function is crucial to understand the magnetic properties. From the $\mathbf{q}-$dependent spin susceptibility we identify the magnetic instabilities related to anti-ferromagnetic and collinear order for $VOMoO_4$ and Li_2VOSiO_4, respectively. Furthermore we determine the local magnetic moment and the Neel temperature from the high temperature uniform magnetic susceptibility. We also investigate the role of the magnetic coupling in the third dimension.

TT 20.2 Mon 15:15 HSZ 304

Magnetic anisotropies in the Ising spin-chain compound $BaCo_2V_2O_8$ and the effect of substitution — •Sandra Niesen[1], Gerhard Kolland[1], Michael Seher[1], Oliver Breunig[1], Martin Valldor[1], Markus Braden[1], Beatrice Grenier[2], and Thomas Lorenz[1] — [1]II. Phys. Institut, Universität zu Köln — [2]SPSMS, CEA-INAC/UJF-Grenoble, France

The effective Ising spin-1/2 system $BaCo_2V_2O_8$ consists of CoO_6 octahedra that form screw chains along the c axis. Long-range antiferromagnetic order is observed below $T_N = 5.5$ K in zero magnetic field with the spins aligned along c. Within the ab plane the spin arrangement is known to be frustrated with a ferromagnetic alignment of neighbouring spins along [100] and an antiferromagnetic one along [010]. Our zero field thermal expansion data show that the Néel order is accompanied by a structural transition from tetragonal to orthorhombic, which lifts the magnetic frustration [1]. Consequently, the magnetic-field influence is anisotropic within the ab plane as seen in, *e.g.* measurements of the magnetization, thermal expansion, specific heat, and thermal conductivity. A detailed study of this anisotropy and the resulting magnetic phase diagrams will be presented. In addition, we will discuss the influence of partial substitution of Ba by Sr and of Co by either magnetic or nonmagnetic ions.

This work has been supported by the DFG via SFB 608 and through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

[1] S. Niesen *et al.*, PRB **87**, 224413 (2013)

TT 20.3 Mon 15:30 HSZ 304

Spin-lattice coupling in the frustrated S=1/2 compound $Cu_7Te_6O_{18}F_2$ — Vladimir Gnezdilov[1,2], •Peter Lemmens[1], Azat Sharafeev[1], Angela Möller[3], Shichao Hu[4] und Mats Johnsson[4] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE NAS, Ukraine — [3]Dept. Chem., Univ., Houston, USA — [4]DMEC, Stockholm, Sweden

We present a Raman scattering study of the novel spin-frustrated S=1/2 compound $Cu_7Te_6O_{18}F_2$. The phonons of this compound display evidence for strong spin-lattice coupling. Furthermore, there exists a broad magnetic scattering continuum that markedly changes with the onset of long-range ordering. Work supported by DFG and B-IGSM.

TT 20.4 Mon 15:45 HSZ 304

The 2D Shastry-Sutherland model and $SrCu_2(BO_3)_2$ in Magnetic Fields up to 118T — •Andreas Honecker[1], Philippe Corboz[2], Frédéric Mila[3], HongYu Yang[3], Salvatore R. Manmana[1], Kai P. Schmidt[4], Gregor R. Foltin[4], Hiroshi Kageyama[5], Nozomu Abe[6], Shojiro Takeyama[6], and Yasuhiro Matsuda[6] — [1]Georg-August-Universität Göttingen, Germany — [2]ETH Zürich, Switzerland — [3]Ecole Polytechnique Fédérale de Lausanne, Switzerland — [4]TU Dortmund, Germany — [5]Kyoto University, Japan — [6]ISSP, University of Tokyo, Japan

The magnetization process of the orthogonal-dimer antiferromagnet $SrCu_2(BO_3)_2$ is investigated in high magnetic fields of up to 118T. A 1/2 plateau is clearly observed in the field range 84 to 108T in addition to 1/3, 1/4, and 1/8 plateaux at lower fields. Using a combination of state-of-the-art numerical simulations, the main features of the high-field magnetization curve are shown to agree quantitatively with the Shastry-Sutherland model for a ratio of inter- to intra-dimer exchange interactions $J'/J = 0.63$. It is further predicted that the intermediate phase between the 1/3 and 1/2 plateau consists of a 1/3 supersolid followed by a non-plateau 2/5 supersolid. As a byproduct, we obtain estimates for the boundaries of a zero-field plaquette phase based on exact diagonalization with up to $N = 40$ sites.

TT 20.5 Mon 16:00 HSZ 304

NMR on the Frustrated Spin-chain Compound $PbCuSO_4(OH)_2$ - Linarite — •M. Schäpers[1], A. U. B. Wolter[1], B. Willenberg[2,4], S.-L. Drechsler[1], H. Rosner[3], S. Süllow[4], and B. Büchner[1] — [1]Leibniz-Institut IFW Dresden, Dresden, Germany — [2]HZB, Berlin, Germany — [3]MPI CPfS, Dresden, Germany — [4]IPKM, TU Braunschweig, Braunschweig, Germany

We present an extensive microscopic magnetic study of the quasi-one-dimensional frustrated $s = \frac{1}{2}$ spin-chain compound linarite. Angular dependent susceptibility and ^{1}H-NMR measurements were performed at various temperatures in the paramagnetic state. All relevant NMR parameters, viz., the chemical, dipolar, and Fermi-contact contribution, were extracted to analytically calculate the local magnetic fields at the ^{1}H sites. From this analysis, a significant total spin transfer of $\sim$10.5 % from the magnetic copper ions onto the two oxygen ligands was derived. The magnetically ordered spin-spiral ground state below $T_N = 2.8$ K was investigated by ^{1}H-NMR for fields $\mu_0 H = 2.0$ T along the three crystallographic main directions. With the derived NMR parameters in the paramagnetic regime it is possible to model the NMR spectrum for $H \parallel c$, which is in agreement with previous neutron studies [1]. Furthermore, we compare our results with density functional band structure calculations and subsequent cluster calculations applying a *pd* model.

This work has partially been supported by the DFG under Contracts No. WO 1532/3-1 and No. SU229/10-1.

[1] B. Willenberg *et al.*, Phys. Rev. Lett. **108,** 117202 (2012).

TT 20.6 Mon 16:15 HSZ 304

Multipolar states in coupled frustrated spin-1/2 chains with exchange anisotropy — •Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], Roman Kuzian[1,2], Johannes Richter[3], and Jeroen van den Brink[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Institute for Problems of Materials Science NASU, 03180 Kiev, Ukraine — [3]Universität Magdeburg, Institut für Theoretische Physik, Germany

We studied coupled frustrated spin-1/2 Heisenberg chains at high magnetic field. The effects of inter-chain couplings and easy-axis exchange anisotropy on the multipolar states were considered using the spin-wave theory and density-matrix renormalization group method. We quantified the instability towards the formation of multipolar states against various kinds of antiferromagnetic and ferromagnetic inter-chain couplings, and also found that an easy-axis anisotropy of the ferromagnetic in-chain nearest-neighbor exchange significantly enhances the multipolar stability region [1]. We will discuss the relevance to edge-shared cuprate spin-chain compounds such as $LiVCuO_4$, $PbCuSO_4(OH)_2$ [2], etc, which are found to be possible candidates for multipolar physics.

[1] S. Nishimoto, S.-L. Drechsler, R.O. Kuzian, J. Richter, J. van den Brink, arXiv:1303.1933v1.

[2] M. Schäpers, A.U.B. Wolter, S.-L. Drechsler, S. Nishimoto, R. Vogel, W. Schottenhamel, B. Büchner, J. Richter, B. Ouladdiaf, M. Uhlarz, R. Beyer, Y. Skourski, J. Wosnitza, K.C. Rule, M. Reehuis, B. Willenberg, S. Süllow, Phys. Rev. B **88**, 195138 (2013).

15 min. break.

TT 20.7 Mon 16:45 HSZ 304

Electronic structure and magnetism of libethenite - Cu_2PO_4OH — Miriam Schmitt[1], Oleg Janson[2], Stefan Lebernegg[2], and •Helge Rosner[2] — [1]Universität Kaiserslautern, 67663 Kaiserslautern — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden

The spin 1/2 compound Cu_2PO_4OH attracted interest not only by its unusual crystal structure containing a combination of edge shared CuO_4 chains linked by Cu_2O_8 dimers, but also by the formation of a spin gap at low temperatures. Recently, a tetramer model was suggested in a combined experimental and theoretical study [1]. Based on density functional band structure calculations we suggest that the simple tetramer model should be refined by additional intra- and inter-tetramer exchange couplings for an accurate description of the magnetic properties of libethenite.

TT 20.8 Mon 17:00 HSZ 304

Hindered magnetic order from multiple dimensionalities in CuP_2O_6 — •Alexander A. Tsirlin[1], Ramesh Nath[2], Jörg Sichelschmidt[3], Fabien Alet[4], and Ioannis Rousochatzakis[5] — [1]NICPB, Tallinn, Estonia — [2]Indian Institute of Science Education and Research, Trivandrum, India — [3]MPI CPfS, Dresden, Germany — [4]Universite de Toulouse, France — [5]IFW Dresden, Germany

We report magnetic properties of CuP_2O_6, where spin systems of different dimensionalities coexist and lead to a strong suppression of the magnetic ordering transition. This compound features spin planes formed by the Cu1 sites (2D) and spin chains formed by the Cu2 sites (1D), with the antiferromagnetic couplings $J_{2D} \simeq 40$ K and $J_{1D} \simeq 3$ K, respectively. The estimates obtained from density-functional band structure calculations are verified by quantum Monte-Carlo fits to the experimental magnetization data. The magnetic ordering transition at $T_N \simeq 8$ K results in the formation of a very weak net moment arising from Dzyaloshinsky-Moriya anisotropy in the Cu1 planes. However, the ESR signal does not vanish below T_N. We ascribe this peculiar effect to the drastic difference between the two sublattices: in the weakly coupled 1D sublattice, the ordered moment grows very slowly, hence the behavior of this sublattice is largely paramagnetic even below T_N. This physics is captured by a mean-field theory showing that the Néel temperature of CuP_2O_6 is determined by the geometrical mean value of staggered susceptibilities in the 1D and 2D sublattices.

Financial support of the Mobilitas program is acknowledged.

TT 20.9 Mon 17:15 HSZ 304

The interplay of crystal structure, electronic structure and magnetism in $SrCo_2P_2$ — •Helge Rosner, Deepa Kasinathan, Inga Kraft, Vivien Lorenz, Christoph Bergmann, and Christoph Geibel — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden

Since the discovery of high temperature superconductivity in doped iron pniktides, in particular AFe_2As_2 systems of the $ThCr_2Si_2$ structure type, the intricate interplay of crystal structure, magnetism and superconductivity in these compounds has attracted broad attention. It is widely believed that the superconductivity of this compound family is closely related tho spin fluctuations. A clear picture of the coupling scenario, however, has not yet emerged. $SrCo_2P_2$ is a structural homologue of the AFe_2As_2 compound series. Experimental investigations indicate a paramagnetic ground state of the system, but a closed vicinity to a (quantum) critical point. We studied the electronic structure and magnetic properties of this compound applying DFT calculations in different approximations. In all setups, we find a pronounced peak in the electronic density of states close to the Fermi level originating from Co-3d states, indicating an instability towards magnetic order. However, structural details have a surprisingly strong influence on details of the band structure and the topology of the Fermi surface. Our calculational results are compared with thermodynamic measurements and de-Haas-van-Alphen data.

TT 20.10 Mon 17:30 HSZ 304

Hour-glass magnetic spectrum in a stripeless insulating transition metal oxide — •Jan Yvo Drees[1], Daniel Lamago[2], Andrea Piovano[3], and Alexander C. Komarek[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Physics of Correlated Matter, Nöthnitzer Street 40, D-01187 Dresden, Germany — [2]Laboratoire Léon Brillouin, CEA/CNRS, F-91191 Gif-sur Yvette, France — [3]Institut Laue-Langevin (ILL), 6 Rue Jules Horowitz, F-38043 Grenoble, France

An hour-glass-shaped magnetic excitation spectrum appears to be a universal characteristic of the high-temperature superconducting cuprates. Fluctuating charge stripes or alternative band structure approaches are able to explain the origin of these spectra. Recently, an hour-glass spectrum has been observed in an insulating cobaltate, thus favouring the charge stripe scenario. Here we show that neither charge stripes nor band structure effects are responsible for the hour-glass dispersion in a cobaltate within the checkerboard charge-ordered regime of $La_{2-x}Sr_xCoO_4$. The search for charge stripe ordering reflections yields no evidence for charge stripes in $La_{1.6}Sr9.4CoO_4$, which is supported by our phonon studies. With the observation of an hour-glass-shaped excitation spectrum in this stripeless insulating cobaltate, we provide experimental evidence that the hour-glass spectrum is neither necessarily connected to charge stripes nor to band structure effects, but instead, probably intimately coupled to frustration and arising chiral or non-collinear magnetic correlations.

TT 20.11 Mon 17:45 HSZ 304

Magnetic properties of intermetallic AT_4X_2 compounds — •Vivien Lorenz, Inga Kraft, Christoph Bergmann, Katharina Weber, Nandang Mufti, Christoph Geibel, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Magnetic systems with reduced dimensionality or frustration attract strong interest because these features lead to an increase of quantum fluctuations and often result in unusual properties. The vicinity of magnetic and non magnetic states can further increase the fluctuations. Here, we present a detailed density-functional-based study of the electronic, magnetic and structural properties of the intermetallic AT_4X_2 compounds (A=Sc,Y,Lu,Zr,Hf; T=Fe,Ni,Re; X=Si,Ge,P,As) crystallizing in the $ZrFe_4Si_2$ structure type. Magnetic and structural transitions were previously reported for YFe_4Ge_2 and closely related compounds with trivalent A-site occupation. However, transition temperatures, nature of the transition as well as the relation between structural and magnetic transitions change significantly with the A element. Our calculational results evidence that: (i) all investigated T=Fe compounds have a magnetic ground state; (ii) all investigated T=Ni systems are non magnetic, but several of them are very close to magnetism; (iii) the magnetic properties of these compounds can be "tuned" by partial substitution on the T and X site. We also study the instability towards a structural distortion related to strong magneto-elastic coupling. Our findings will be compared to recent experimental results.

TT 21: Focus Session: New Trends in Molecular Magnetism (organized by MA)

Organizers: J. Schnack (U. Bielefeld), O. Waldmann (U. Freiburg)

During the past 25 years molecular magnetism has developed into a broad field. Today's major research directions include applications in quantum computing or as quantum simulators as well as the use as sub-Kelvin magnetic refrigerants. For direct manipulation as part of spintronic systems molecules are deposited and manipulated on surfaces. The progress of this interdisciplinary field is intimately related to the ability of coordination chemists to synthesize unprecedented molecules, to the ability of experimental physicists to characterize them as well as to the ability of theorists to model their properties.

Time: Monday 15:00–17:30 Location: HSZ 04

Topical Talk TT 21.1 Mon 15:00 HSZ 04

Spin dynamics in Molecular Nanomagnets — •Stefano Carretta — Dipartimento di Fisica e Scienze della Terra, Universita' di Parma, I-43124 Parma, Italy

Molecular nanomagnets (MNMs) have been test beds for addressing several quantum phenomena. In particular, one of the major current objectives is to exploit their coherent spin dynamics for quantum information processing (QIP). We show that recently developed instrumentation yields the four-dimensional inelastic-neutron scattering function and enables the direct determination of the spin dynamics [1]. We use the Cr8 antiferromagnetic ring as a benchmark to demonstrate the potential of this approach, which allows us, for instance, to examine how quantum fluctuations propagate along the ring. We show that parameters of the spin Hamiltonian can be reliably calculated ab-initio. In particular, we present a flexible and effective ab-initio scheme to build many-body models for MNMs, and to calculate magnetic exchange couplings and zero-field splittings [2]. We have applied this scheme to three paradigmatic systems, the antiferromagnetic rings Cr8 and Cr7Ni and the single molecule magnet Fe4 and have found excellent agreement with experimental results. At last, we discuss the dynamics of ensembles of spin systems coherently coupled to microwave photons in coplanar waveguide resonators. We introduce a scheme to perform QIP that is based on a hybrid spin-photon qubit encoding [3].

[1] M. Baker et al, Nature Physics 8, 906 (2012); [2] A. Chiesa et al, Phys. Rev. Lett. 110, 157204 (2013); [3] S. Carretta, et al, Phys. Rev. Lett. 111, 110501 (2013).

Topical Talk TT 21.2 Mon 15:30 HSZ 04

Exchange interaction in lanthanides — •Liviu Chibotaru, Liviu Ungur, Naoya Iwahara, and Veaceslav Vieru — Theory of Nanomaterials Group, KU Leuven, Heverlee, Belgium

Using ab initio, DFT and model calculations we analyze the main features of exchange interactions in lanthanide complexes.

Andersons superexchange model is applied for analytical derivation of exchange interaction between total magnetic moments $\mathbf{J}_1$ and $\mathbf{J}_2$ corresponding to ground atomic multiplets of two exchange-coupled lanthanide ions. Despite the common belief that the exchange interaction is of $\sim \mathbf{J}_1 \cdot \mathbf{J}_2$ form, we find it strongly anisotropic. If the crystal field (CF) on Ln sites exceeds significantly the exchange splitting, the exchange interaction between low-lying CF doublet states generally becomes of non-collinear Ising type.

In the case of exchange-coupled lanthanide ion ($\mathbf{J}$) and isotropic magnetic center ($\mathbf{S}$) the exchange interaction is found not to be of the form $\sim \mathbf{J} \cdot \mathbf{S}$, as supposed before, but again very anisotropic. When the CF splitting on Ln exceeds the exchange splitting, the exchange interaction between the low-lying CF doublet on Ln and the isotropic spin generally becomes of collinear Ising type.

Finally, we give arguments why the mixed Ln-TM complexes are more efficient SMMs than pure Ln ones despite less anisotropic magnetic ions involved.

Topical Talk TT 21.3 Mon 16:00 HSZ 04

Cool molecules — •Marco Evangelisti — Instituto de Ciencia de Materiales de Aragón, CSIC - Universidad de Zaragoza, Departamento de Física de la Materia Condensada, 50009 Zaragoza, Spain

The recent progress in molecule-based magnetic materials exhibiting a large magnetocaloric effect at liquid-helium temperatures is reviewed. Advanced applications and future perspectives in cryogenic magnetic refrigeration are also discussed.

Topical Talk TT 21.4 Mon 16:30 HSZ 04

Bulk and submonolayer studies of novel single-ion molecular magnets — •Jan Dreiser — Ecole Polytechnique Federale de Lausanne, Institute of Condensed Matter Physics, 1015 Lausanne, Switzerland — Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Single-ion magnets (SIMs) [1,2] contain a single transition-metal or rare-earth ion embedded in an organic ligand. In contrast to many other mononuclear molecular magnets, SIMs exhibit long magnetization relaxation times at low temperatures ranging from milliseconds to more than hours. In order to exploit their properties in possible applications they should be organized and addressable one-by-one [3]. A promising path to achieve this goal is the deposition of submonolayers of SIMs on to surfaces.

In this talk I will report on our recent studies of the Er(trensal) SIM [2] in which the Er(III) ion is seven-fold coordinated to the very robust tripodal ligand. In addition to the investigations of the bulk phase I will present first results obtained on (sub)monolayer deposits on metallic surfaces using X-ray magnetic circular dichroism and scanning tunneling microscopy.

[1] N. Ishikawa, M. Sugita, T. Ishikawa, S.-y. Koshihara, Y. Kaizu, J. Am. Chem. Soc. 2003, 125, 8694; [2] K. S. Pedersen, L. Ungur, M. Sigrist, A. Sundt, M. Schau-Magnussen, V. Vieru, H. Mutka, S. Rols, H. Weihe, O. Waldmann, L. F. Chibotaru, J. Bendix, J. Dreiser, submitted; [3] D. Gatteschi, A. Cornia, M. Mannini, R. Sessoli, Inorg. Chem. 2009, 48, 3408.

Topical Talk TT 21.5 Mon 17:00 HSZ 04

When Organic Materials Interact with Ferromagnetic Surfaces: A First-Principles Perspective — •Nicolae Atodiresei — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The adsorption of π-conjugated organic materials on ferromagnetic surfaces offers the possibility to merge the concepts of molecular electronics with spintronics to build future nanoscale data storage, sensing and computing multifunctional devices. Based on the density functional theory, we performed theoretical studies to understand how to tailor the magnetic properties of organic-ferromagnetic interfaces. For such hybrid systems, the magnetic properties like molecular magnetic moments and their spatial orientation, the spin-polarization and the magnetic exchange coupling can be specifically tuned by an appropriate choice of the organic material and ferromagnetic surface. [1] N. Atodiresei et al., Phys. Rev. Lett. 105, 066601 (2010); [2] N. Atodiresei et al., Phys. Rev. B 84, 172402 (2011); [3] K. V. Raman et al., Nature 493, 509 (2013); [4] M. Callsen et al., Phys. Rev. Lett. 111, 106805 (2013).

TT 22: Low-Dimensional Systems: Charge Order

Time: Monday 15:00–16:30 Location: BEY 81

TT 22.1 Mon 15:00 BEY 81

Competing soft phonon modes in charge-density-wave rare-earth tritellurides — •Michael Maschek[1], Sven Krannich[1], Frank Weber[1], Rolf Heid[1], Stephan Rosenkranz[2], Ayman Said[2], Ian Fisher[3], Paula Giraldo-Gallo[3], and Ahmet Alatas[2] — [1]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 competing soft phonon modes close to the charge-density-wave (CDW) transition in the rare-earth tritelluride $DyTe_3$ obtained by high energy resolution inelastic x-ray measurements. We investigated transverse polarized modes dispersing along the reciprocal (100) and (001) directions corresponding the two CDW orders lying in the basal plane of the nearly tetragonal unit cell. $DyTe_3$ has two CDW-transitions ($T_{CDW,1} = 50K, T_{CDW,2} = 310K$), but for technical reasons we could only investigate the transition at $T_{CDW,2}$. We found a full softening at $q_{CDW,2} = (0, 0, 0.3)$ and a strong but not complete softening of the orthogonal mode at $q_{CDW,1} = (0.3, 0, 0)$ at the same temperature which is reminiscent of previous measurements on $TbTe_3$. Our results are corroborated by lattice dynamical calculations demonstrating the near degeneracy between the two crystallographic axes with respect to the formation of CDW order.

TT 22.2 Mon 15:15 BEY 81

Electronic band structure of 1*T*-TaS_2 and new implications for the Mott-phase — •Tobias Ritschel[1,5], Jan Trinckauf[1], Gaston Garbarino[2], Alexei Bosak[2], Martin von Zimmermann[3], Klaus Koepernik[1], 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 1*T*-TaS_2 exhibits a multitude of distinct charge density wave (CDW) phases as a function of temperature and pressure. A unique feature of 1*T*-TaS_2 among the CDW systems is the occurrence of a commensurate (C)-CDW phase which is commonly described as a Mott-phase due to electron-electron interactions and which is extremely sensitive upon applying external pressure. We studied the electronic band structure of the C-CDW phase in terms of density functional theory (DFT) as a function of the amplitude of the lattice modulation. Surprisingly we found that the experimental electronic band structure of the so-called Mott-phase, can already be very well described by conventional DFT calculations in the local density approximation (LDA). Moreover slight changes of the amplitude of the lattice modulation have dramatic effects on the calculated band structure, which agrees very well with the strong pressure dependence of the C-CDW phase. We will discuss our results with respect to Mott-physics associated with the C-CDW phase and its pronounced sensitivity to pressure.

TT 22.3 Mon 15:30 BEY 81

Influence of Doping on the 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], and Dmitry Reznik[1,3] — [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 Physics, University of Colorado at Boulder, Boulder, Colorado, 80309, USA

We studied the influence of doping on the soft-mode behaviour of phonons in the Charge Density Wave (CDW) systems $NbSe_2$ and $TiSe_2$ both experimentally by means of high resolution Inelastic X-ray Scattering (IXS) and theoretically in Density Functional Theory (DFT) based ab-initio phonon calculations. In agreement with our experiments on Cu-doped $TiSe_2$ and Co-doped $NbSe_2$ our calculations show that doping weakens the tendency towards the CDW instability.

[1] F. Weber et al., Phys. Rev. B 87 (2013) 245111
[2] F. Weber et al., Phys. Rev. Lett. 107 (2011) 266401.

TT 22.4 Mon 15:45 BEY 81

Interplay of covalency and correlations in the edge shared spin 1/2 $A_3T_2O_4$ chain compounds (A = Na, K; T = Cu, Ni) — •Deepa Kasinathan[1], Klaus Koepernik[2], and Helge Rosner[1] — [1]MPI CPfS, Dresden, Germany — [2]IFW Dresden, Germany

$Na_3Cu_2O_4$, $K_3Cu_2O_4$ and $K_3Ni_2O_4$ belong to a new class of quasi-1D insulating cuprates which feature strongly buckled, one-dimensional $^1_\infty CuO_2$ ribbon-like chains consisting of edge-sharing CuO_4 plaquettes. Structural analysis of the metal-oxygen bond lengths and thermodynamic measurements[1,2,3] imply that these systems are intrinsically charge ordered (... $(Ni/Cu)^{2+}$-$(Ni/Cu)^{3+}$-$(Ni/Cu)^{2+}$-$(Ni/Cu)^{3+}$ ...) and show dominant antiferromagnetic interactions. No electronic structure analysis of these systems exist to date. Using density functional theory based calculations (LDA, Wannier functions, LDA+U), we analyze the microscopic origin of the magentic interactions in these systems. The main interaction along the chains are the second neighbor superexchanges. Nonetheless, a careful analysis of the first neighbor interaction between the mangnetic (Cu^{2+}/Ni^{3+}) cation and the non-magnetic cation (Cu^{3+}/Ni^{2+}) is necessary. We report on the interplay of covalency, crystal field splitting and correlations in these systems.

[1] H. Zentgraf, K. Claes, and R. Hoppe, Z. Anorg. Allg.Chem. **462**, 92 (1980)
[2] M. Sofin, Eva-Maria Peters, and M. Jansen, J. Solid State Chem. **178**, 3708 (2005)
[3] K. Duris, R. K. Kremer, and M. Jansen, Z. Anorg. Allg. Chem. **637**, 1101 (2011)

TT 22.5 Mon 16:00 BEY 81

Doping dependence of charge order in single-layered manganites $R_{1-x}A_{1+x}MnO_4$ — •Johannes Engelmayer, 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 half-doped ($x = 0.5$) $La_{1-x}Sr_{1+x}MnO_4$ and $Pr_{1-x}Ca_{1+x}MnO_4$ the so-called Goodenough model is well established. This model proposes a site-centered charge order with a checkerboard pattern of Mn^{3+} and Mn^{4+} ions 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 $x > 0.5$ zig-zag chains with larger step size have been reported in $Pr_{1-x}Ca_{1+x}MnO_4$ and $Nd_{1-x}Sr_{1+x}MnO_4$, *e.g.* four-spin zig-zag chains arise for $x = 2/3$ due to a 2:1 ratio of Mn^{4+} and Mn^{3+} [1]. In order to study the effect of different dopants on the ordering temperature, single crystals of $Pr_{1-x}Sr_{1+x}MnO_4$, $Nd_{1-x}Ca_{1+x}MnO_4$ and $Nd_{1-x}Sr_{1+x}MnO_4$ 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 features associated with charge order. The dependence of the ordering temperature on the dopants and the doping level is discussed.

Supported by the DFG through SFB 608

[1] H. Ulbrich, M. Braden, Physica C **481**, 31 (2012)

TT 22.6 Mon 16:15 BEY 81

Charge ordered metals on the triangular extended Hubbard model — •Luca Fausto Tocchio[1,2], Claudius Gros[1], Xue-Feng Zhang[3], and Sebastian Eggert[3] — [1]University of Frankfurt, Germany — [2]SISSA, Trieste, Italy — [3]University of Kaiserslautern, Germany

We study the extended Hubbard model on the triangular lattice as a function of filling and interaction strength. The complex interplay of kinetic frustration and strong interactions on the triangular lattice leads to exotic phases where long range charge order and a finite metallic conductivity coexist. Variational Monte Carlo simulations show that two kinds of ordered metallic states are stable as function of nearest neighbor interaction and filling; in one of the two phases we observe separation into two classes of particles: one of them contributes to stable order, while the other one forms a partially filled band on the remaining substructure. The relation to charge ordering in charge transfer salts is discussed.

TT 23: Low-Dimensional Systems: Other Materials

Time: Monday 16:45–18:30 Location: BEY 81

TT 23.1 Mon 16:45 BEY 81

Huge magneto-elastic coupling and negative Poisson ratio in low-dimensional spin systems — •Bernd Wolf, Pham Thanh Cong, Rudra Sekhar Manna, Ulrich Tutsch, and Michael Lang — Physikalisches Institut, J.W. Goethe-Universität, SFB/TR49, D-60438 Frankfurt (Main), Germany

Azurite $Cu_3(CO_3)_2(OH)_2$, a model system for the distorted diamond-chain, exhibits pronounced elastic anomalies in the temperature - and magnetic field dependence of the longitudinal elastic mode c_{22}. These features are assigned to the relevant magnetic interactions in the material and their couplings to the lattice degrees of freedom. From a quantitative analysis of the magnetic contribution to c_{22}, the magneto-elastic coupling $G = \partial J_2/\partial\epsilon_b$ is determined, with ϵ_b denoting the strain along the chain b-axis. We find an exceptionally large value highlighting an extraordinarily strong sensitivity of J_2 against changes of the b-axis lattice parameter. These results are complemented by measurements of the hydrostatic pressure dependence of J_2 by means of thermal expansion and magnetic susceptibility measurements performed both at ambient and finite hydrostatic pressure. We discuss the results in light of an anomalous negative Poisson effect at low temperatures. We compare the results with the magneto-elastic coupling constants determined for other low-D quantum spin systems, such as the antiferromagnetic S = 1/2 Heisenberg spin chain based on a Cu-coordination polymer [1], the dimerized spin chain and $SrCu_2(BO_3)_2$ as a coupled quasi-2D system [2].

[1] B. Wolf, et al., Phys. Rev. B **69**, 092403 (2004)
[2] S. Zherlitsyn, et al., Phys. Rev. B **62**, R6097 (2000)

TT 23.2 Mon 17:00 BEY 81

Nuclear Magnetic Resonance on S=1/2 Heisenberg Spin Chains under the Impact of Different Impurities — •Yannic Utz[1], Franziska Hammerath[1], Hans-Joachim Grafe[1], Ashwin Mohan[1], Neela Sekhar Beesetty[2], Romuald Saint-Martin[2], Alexandre Revcolevschi[2], Christian Hess[1], and Bernd Büchner[1] — [1]IFW Dresden, Germany — [2]ILPCES - ICMMO, Université Paris-Sud, France

We present ^{63}Cu NMR measurements on single crystals of undoped, Ni doped and Zn doped $SrCuO_2$ and of Ni doped Sr_2CuO_3. While $SrCuO_2$ forms a double chain structure, the copper ions of Sr_2CuO_3 are arranged as single chains. Despite these structural differences, both are known to be good realizations of the antiferromagnetic S=1/2 Heisenberg chain. The measurements show that Ni doping (S=1) has a major impact on the magnetic properties of both spin chain systems. An unusual line broadening in the low temperature NMR spectra reveals the existence of an impurity-induced local alternating magnetization (LAM), and exponentially decaying spin-lattice relaxation rates T_1^{-1} towards low temperatures indicate the opening of a spin gap similar to Ca-doped $SrCuO_2$ [1]. Zn doping (S=0), however, shows a similar impact on the NMR spectra, but the opening of a spin gap could not be observed. While the different impact of Ni and Zn 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 23.3 Mon 17:15 BEY 81

Hydrogen positions and their effect on exchange couplings of Cu-minerals — •Stefan Lebernegg[1], Alexander Tsirlin[2], Oleg Janson[1,2], and Helge Rosner[1] — [1]MPI Chemical Physics of Solids, Dresden — [2]National Institute of Chemical Physics and Biophysics, Tallinn

Exotic magnetic properties and the possibility of challenging our understanding of collective quantum phenomena are the reasons why low-dimensional spin-1/2 quantum magnets attract so much attention. Cu(2+) minerals belong to this class of compounds where several hundredths of them are provided by nature. However, only very few of them have ever been investigated with respect to their magnetic properties. Thus, the Cu-minerals keep a high potential for the discovery of new effects and materials. However, many of these compounds contain crystal water or OH groups where the position of hydrogen in the crystal structure crucially affects the magnetic behavior. Since the experimental determination of H-positions is highly elaborating if possible at all, these positions are usually not available in the structural data of minerals. We will, thus, present a valuable DFT-based alternative for determining the hydrogen positions. Then, the importance of the hydrogen positions for the magnetic properties and the computation of microscopic magnetic models will be discussed for selected Cu-minerals which have been investigated by combining several experimental and computational techniques.

TT 23.4 Mon 17:30 BEY 81

Magnetic excitation spectra of the 4-leg ladder $La_2Cu_2O_5$ — •Ignacio Vergara[1], Kris Cöster[2], Luis Fels[1], Martin Valldor[1,3], Stefan Wessel[4], Kai Philip Schimdt[2], and Markus Grüninger[1] — [1]II. Physicalisches Institut, Universität zu Köln — [2]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund — [3]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University

In low-dimensional spin-1/2 cuprates, optical spectroscopy has been established as a powerful tool for the study of magnetic excitations with total S=0. The simultaneous excitation of a symmetry-breaking phonon allows us to study the magnetic excitations at high energies ($\sim$ 0.1 - 1 eV) throughout the entire Brillouin zone, since the phonon ensures momentum conservation. The line shape of the optical conductivity provides important information on the kinetics and on the interactions of the magnetic excitations.

The magnetism of n-leg S=1/2 cuprate ladders is particularly interesting due to the dimensional crossover between 1D and 2D and the possible relevance for high T_c superconductivity. We present optical conductivity data of the 4-leg ladder $La_2Cu_2O_5$ for polarization of the electric field parallel to the legs and to the rungs, respectively. Comparison with theory (CUT, QMC) and with the results for a 2-leg ladder suggests the existence of two-triplon bound states below the continuum also for n=4.

TT 23.5 Mon 17:45 BEY 81

Electronic instabilities of the AA-honeycomb bilayer — •David Sanchez de la Peña[1], Michael M Scherer[2], and Carsten Honerkamp[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]Institute for Theoretical Physics, Heidelberg University, Germany

We use a functional renormalization group approach to study the instabilities due to electron-electron interactions in a bilayer honeycomb lattice model with AA stacking, as it might be relevant for layered graphene. Starting with a tight-binding description for the four π-bands, we integrate out the modes of the dispersion by successively lowering an infrared cutoff and determine the leading tendencies in the effective interactions. The antiferromagnetic spin-density wave is an expected instability for dominant local repulsions among the electrons, but for nonlocal interaction terms also other instabilities occur. We discuss the phase diagrams depending on the model parameters. We compare our results to single-layer graphene and the more common AB-stacked bilayer, both qualitatively and quantitatively.

TT 23.6 Mon 18:00 BEY 81

Susceptibility measurements on a weakly coupled spin-dimer system consisting of nitronyl-nitroxid stable biradicals — •L. Postulka[1], B. Wolf[1], U. Tutsch[1], P.T. Cong[1], M. Baumgarten[2], Y. Borozdina[2], D. Strassel[3], S. Eggert[3], and M. Lang[1] — [1]Physics Institute, Uni Frankfurt SFB/TR 49, D-60438 Frankfurt, Germany — [2]MPI for Polymer Research SFB/TR 49, D-55128 Mainz, Germany — [3]Physics Department and Research Center OPTIMA SFB/TR 49, Uni Kaiserslautern, D-67663 Kaiserslautern, Germany

We present low-temperature susceptibility data on a spin $S = \frac{1}{2}$ dimer system consisting of nitronyl-nitroxid radicals which are bridged via tolan molecules. The material, exhibiting a double-layer structure, can be regarded as a quasi- 2D system. From SQUID magnetisation measurements on high-quality single crystals, an intra-dimer coupling constant of $J_{intra}/k_B \approx 9.6\,\mathrm{K}$ can be determined. In addition, the data reveal indications for an inter-dimer coupling of the order of 1 K. In order to look for magnetic field-induced ordering phenomena, AC-susceptibility measurements were performed down to temperatures as low as $T = 34\,\mathrm{mK}$ and magnetic fields up to $B = 10.5\,\mathrm{T}$. For tem-

peratures below $T = 250\,\mathrm{mK}$, a double-peak structure was observed at fields between 8 T and 9.5 T consistent with the expectation based on the above-mentioned coupling constants. Furthermore, in the same temperature range another anomaly around $B = 4.5\,\mathrm{T}$ appears. For a detailed understanding especially with regard to the dimensionality of the interactions and the implications for the type of order that is realized here, Quantum Monte Carlo simulations are underway.

TT 23.7 Mon 18:15 BEY 81

Orbital contribution to spin-Peierls transition in $TiPO_4$ — Dirk Wulferding[1], Angela Moeller[2], Kwang-Yong Choi[3], Yurii Pashkevich[4], Roman Babkin[4], Karina Lamonova[4], •Peter Lemmens[1], Joseph Law[5], Reinhardt Kremer[6], and Robert Glaum[7] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]Dept. Chem., Univ., Houston, USA — [3]Dept. Phys., CA Univ., Seoul, Korea — [4]DonFTI, Donetsk, Ukraine — [5]Dresden HMFL, Dresden, Germany — [6]MPI-FKF, Stuttgart, Germany — [7]IAC, Bonn, Germany

We observe unusual lattice dynamics as well as evidence for an orbital instability preceding the spin-Peierls transition in $TiPO_4$. Furthermore, there exist high energy excitations of mixed electronic and lattice origin that suggest an exotic dimerization process, different from other spin-Peierls materials. Therefore, the energy gain is related to magnetoelastic and orbital contributions.

TT 24: Magnetic Heuslers, Half-Metals and Oxides II (organized by MA)

Time: Monday 15:00–18:45 Location: BEY 118

Invited Talk TT 24.1 Mon 15:00 BEY 118

Design principles of Dirac fermions and Mott insulating states in (111) oriented perovskite superlattices — •Rossitza Pentcheva — Ludwig Maximilians University, Munich, Germany

Oxide interfaces exhibit a broad spectrum of functional properties that are not available in the respective bulk compounds, such as two-dimensional conductivity, superconductivity and magnetism. With their distinct topology, (111) perovskite superlattices promise to host even more exotic electronic states compared to the much studied (001)-oriented systems. Material-specific density functional theory calculations with an on-site Coulomb repulsion term are used to explore the role of confinement, symmetry breaking, polarity mismatch and strain in the emergence of novel phases. The results illuminate a rich set of competing ground states in $(LaAlO_3)_M/(SrTiO_3)_N(111)$ [1] and $(LaNiO_3)_N/\,(LaAlO_3)_M(111)$ superlattices, ranging from spin-polarized, Dirac-point Fermi surfaces to charge-ordered Mott or Peierls insulating phases. Orbital reconstructions and metal-to-insulator transitions depend critically on the thickness of the quantum well N and in-plane strain, thus opening avenues for engineering properties at the nanoscale. Research in collaboration with D. Doennig and W.E. Pickett, supported by the DFG, SFB/TR80. [1] D. Doennig, W. E. Pickett, and R. Pentcheva, Phys. Rev. Lett. **111** 126804 (2013).

15 min. break

TT 24.2 Mon 15:45 BEY 118

Giant Verwey transition in magnetite thin films — Mehrdad Baghaie Yazdi and •Lambert Alff — Institut für Materialwissenschaft, TU Darmstadt

The Verwey transition in magnetite is an enigmatic challenge of solid state physics since several decades. It is generally believed that the change in magnetic moment at the Verwey transition is due to a change in magnetocrystalline anisotropy and spin reorientation. In thin films of magnetite with extraordinary high Verwey transition at 128 K, we have observed a giant change of magnetic moment above 1000%. Using several methods including neutron reflectometry we rule out spin reorientation as the origin of our observation. In addition, Raman scattering experiments show that the structural phase transition occurs at temperatures above the magnetic Verwey transition while, in contrast, newly emerging modes indicating additional charge and orbital order appear only at the Verwey transition. This result suggests that the structural phase transition in magnetite is a necessary precursor triggering a transition into a complex charge and orbitally ordered state.

TT 24.3 Mon 16:00 BEY 118

$NiFe_2O_4$: a candidate for efficient spin filtering at room temperature? — •Michael Hoppe[1], Sven Döring[1], Mihaela Gorgoi[3], Felix Gunkel[4], Claus M. Schneider[1,2], and Martina Müller[1,2] — [1]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen — [3]BESSY II, Helmholtz-Zentrum Berlin für Materialien und Energie — [4]Peter-Grünberg-Institut (PGI-7), Forschungszentrum Jülich

For the optimized performance of spintronic devices, one major challenge is to create highly spin-polarized electron currents. One promising approach is the usage of both insulating and magnetic tunnel barriers, with a highly spin-dependent tunneling probability. For this purpose, the spinel ferrite $NiFe_2O_4$ (NFO) is a very auspicious material since it shows both features even at room temperature.

To realize magnetic tunnel junctions, it is necessary to grow NFO films (d < 5 nm) which maintain quasi bulk-like properties down to this ultrathin film limit. Therefore, NFO films with varying thickness between 2 and 20 nm are deposited on Nb-doped $SrTiO_3$ substrates via pulsed laser deposition. HAXPES, XRD and XANES measurements reveal them to be chemically and structurally comparable to the bulk material. XMCD studies of the Ni- and Fe-L-edges in those films show that the alignment of the magnetic moments carried by these elements is preserved for all thicknesses. The insulating behavior is confirmed by CFM measurements. On this basis, we fabricated Nb:STO/NFO/Au tunnel junctions by means of optical lithography and characterized their electrical transport properties.

TT 24.4 Mon 16:15 BEY 118

Combined theoretical and optical band gap determination of NiFe2O4 and CoFe2O4 — •Markus Meinert and Günter Reiss — Center for Spinelectronic Materials and Devices, Bielefeld University, Germany

In a theoretical study we investigate the electronic structure and the band gap of the inverse spinel ferrites $NiFe_2O_4$ (NFO) and $CoFe_2O_4$ (CFO). The experimental optical absorption spectrum of NFO is well reproduced by fitting the Tran-Blaha parameter in the modified Becke-Johnson (mBJLDA) potential. For CFO, the agreement is less satisfying. The accuracy of the commonly applied Tauc plot to find the optical gap is assessed based on the computed spectra and we find that this approach can lead to a misinterpretation of the experimental data.

The minimum gap of $NiFe_2O_4$ is found to be a 1.53 eV wide indirect gap, which is located in the minority spin channel. In $CoFe_2O_4$, the band gap is about 0.9 eV wide and is also located in the minority spin channel.

TT 24.5 Mon 16:30 BEY 118

Exploring spin-filter tunneling in single-crystalline magnetic oxide heterostructures — •Bernardus Zijlstra[1], Patrick Lömker[1], Christian Caspers[1], Michael Hoppe[1], Jürgen Schubert[2], Willi Zander[2], Mihaela Gorgoi[3], Claus M. Schneider[1], and Martina Müller[1] — [1]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich — [3]BESSY II, Helmholtz-Zentrum Berlin

Magnetic insulators, like Europium Oxide (EuO) are of tremendous interest for spintronic research, since they can generate highly spin-polarized currents. In contrast to conventional tunneling, spin-filter tunneling through single-crystalline magnetic insulator barriers is not yet fully understood.

In order to realize fully epitaxial magnetic oxide tunnel barriers, ultrathin EuO films were grown directly on conductive Sn-doped In_2O_3 (001) (ITO), Nb-doped $SrTiO_3$ (001) (STO) and As-doped Si (001).

The EuO heteroepitaxy was characterized by LEED, RHEED and XRD, whereas the magnetic and chemical properties were analyzed by SQUID and hard x-ray photoelectron spectroscopy. We find EuO/Si(001) and EuO/STO(001) to be epitaxial, stoichiometric and to display bulk-like magnetic properties, however, EuO/ITO(001) is strongly affected by oxygen diffusion at elevated T_S. Electrical transport experiments reveal the respective spin filter tunneling properties.

TT 24.6 Mon 16:45 BEY 118

Direct observation of half metallicity in the Heusler compound Co2MnSi — •Martin Jourdan[1], Alexander Kronenberg[1], Jan Minar[2], Michaela Kolbe[1], Andrey Gloskovskij[3], Gerd Schönhense[1], Hans Joachim Elmers[1], Stanislav Chadov[4], Claudia Felser[4], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]Department Chemie und Biochemie, Ludwig-Maximilians-Universität München — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Heusler compounds are in the focus of interest due to their predicted half-metallic properties, which makes them highly interesting for spintronics. Apart from applications those materials are a test for modern band structure calculations for materials with electronic correlations of medium strength. Although a large body of those calculations is available, their experimental verification remains a major task. Here epitaxial thin films of the compound Co2MnSi are investigated in-situ by UV-photoemission spectroscopy (UPS) taking advantage of a novel multi-channel spin filter. An exceptionally large spin polarization of 93% is obtained at room temperature, providing strong direct evidence for half-metallicity. The energy dependencies of the measured spin polarization as well as of spin integrated UPS essentially agree with bulk band structure calculations. Additional ex-situ spin integrated hard x-ray photoemission spectroscopy experiments (HAXPES) corroborate that indeed bulk states are observed by SRUPS.

15 min. break

TT 24.7 Mon 17:15 BEY 118

Spin dependent lifetimes and non-degenerate spin hot spots in Heusler compounds — •Steffen Kaltenborn and Hans Christian Schneider — Physics Department and Research Center OPTIMAS, University of Kaiserslautern

We present results of an accurate ab-initio calculation of the dielectric function of the half-metallic Heusler compounds Co_2MnSi and Co_2FeSi. The numerical method is based on density functional theory [1,2] in combination with a wave-vector dependent linear tetrahedron method [3]. The dielectric function is used study optical, acoustic and intraband plasmon dispersions in these half metals. As in the case of simple metals, a negative intraband plasmon dispersion [3] is found. Furthermore, we use the dielectric function to analyze the **k** and spin-resolved electronic lifetimes in these materials. Qualitatively, the lifetimes reflect the lineup of electron and hole bands. We determine the spin-flip and spin-conserving contributions to the lifetimes and predict that different excitation conditions may lead to different spin-flip dynamics of excited electrons and may even give rise to an enhancement of the non-equilibrium spin polarization. Finally, we study in detail the behavior of the lifetimes around states that are strongly spin mixed by spin-orbit coupling. We find that, for non-degenerate bands, the spin mixing alone does not determine the energy dependence of the (spin-flip) lifetimes.
[1] DFT-Program The Elk FP-LAPW Code, http://elk.sourceforge.net. [2] C. Ambrosch-Draxl et al., Comp. Phys. Commun. **175**, 1-14, (2006). [3] S. Kaltenborn and H. C. Schneider, Phys. Rev. B **88**, 045124 (2013).

TT 24.8 Mon 17:30 BEY 118

NMR Investigation of Optimal Mn Content in $Co_2Mn_xSi_{0.88}$ Thin Films for High Tunneling Magneto-Resistance — •Steven Rodan[1], Tomoyuki Taira[2], Masafumi Yamamoto[2], Bernd Büchner[1,3], and Sabine Wurmehl[1,3] — [1]Leibniz Institute for Solid State and Materials Research, 01171 Dresden, Germany — [2]Division of Electronics for Informatics, Hokkaido University, Sapporo 060-0814, Japan — [3]Institute für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany

Half-metallic ferromagnets (HMFs), with 100% spin-polarized conduction electrons, are prime candidates for developing spintronics devices. Many Heusler compounds, such as Co_2MnSi, are predicted to be HMFs. A technique for probing local structure such as nuclear magnetic resonance (NMR) is essential for understanding the microscopic origin of manifested physical properties. Local atomic disorder was investigated using both ^{59}Co and ^{55}Mn NMR on epitaxial films of $Co_2Mn_xSi_{0.88}$, with varying Mn content (x = 0.72, 1.12, 1.32). NMR spectra confirmed that the high tunneling magneto-resistance ratio values for magnetic tunnel junctions with electrodes made from highest Mn excess (x=0.32), can be attributed mainly to the reduction of Co antisites (Co on Mn and/or Si sites), which are expected to strongly decrease the half-metallicity.

TT 24.9 Mon 17:45 BEY 118

Evolution of the coercive field of Co_2FeGa Heusler nanocrystals and related oxide nanoparticles inside carbon nanotubes — •Markus Gellesch[1], Usue Palomares Iñiguez de Ciriano[1], Changhai Wang[2], Sabine Wurmehl[1], Silke Hampel[1], and Bernd Büchner[1] — [1]Leibniz Institut für Festkörper- und Werkstoffforschung Dresden — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Magnetic properties of nanoscale systems may differ largely from the magnetism in the respective bulk phase and thus can lead to the emergence of interesting and also novel physical properties. Here we present results of investigations of magnetic properties of Heusler nanoparticles and related oxide materials prepared inside multi-walled carbon nanotubes via a wet-chemical approach. While previous studies[1] already showed, that the coercive field of the Heusler nanocrystals inside carbon nanotubes is enhanced by a factor of at least 30, we now report of an enhancement factor of approximately 100 in Co_2FeGa nanoparticles and of coercive fields as large as 6000 Oe in related oxide materials. Further we present results of the diameter dependence of the coercive field in the later material. The results of our work open the door for the exploration of Heusler and related magnetic materials at the nanoscale and also guide the way to the synthesis of nanomaterials with tailored physical properties.
[1] Gellesch et al., Cryst. Growth Des., 2013, 13 (7), pp 2707–2710

TT 24.10 Mon 18:00 BEY 118

The influence of p- and n-doping on the intrinsic properties of the Heusler compound Fe_2VAl — •Franziska Seifert[1,2], Christian G.F. Blum[1], Frank Steckel[1], Christian Hess[1], Hans-Joachim Grafe[1], Bernd Büchner[1], Sabine Wurmehl[1], Stefan Martin[2], Volker Klemm[2], and David Rafaja[2] — [1]Leibniz-Institute for Solid State and Materials Research, Dresden, Germany — [2]TU Bergakademie Freiberg, Germany

In this work, we studied the intrinsic properties of the Heusler compound Fe_2VAl and the influence of p (V substituted by Ti)- and n-doping (Al substituted by Si) on the intrinsic materials properties using single crystals. Electron back scattering diffraction reveals the presence of a V-rich secondary ferromagnetic phase in particular in crystals with Si and in the parent compound, which could be further confirmed by TEM investigations. The depletion of V from the Fe_2VAl matrix apparently leads to localized Fe moments and also to magnetic order in the corresponding samples. The evolution of magnetic order and thermoelectric key parameters were further analysed by means of nuclear magnetic resonance, transport and magnetization measurements. Interestingly, the sample with Ti and less V depletion shows a significant enhancement of the figure of merit compared to the other samples.

TT 24.11 Mon 18:15 BEY 118

Effect of high pressures synthesis on $Ba_3YIr_2O_9$ — •Hannes Stummer, Tusharkanti Dey, Sabine Wurmehl, and Bernd Büchner — Leibniz-Institute for Solid State and Materials Research Dresden, Germany

The emergent field of Iridium oxide based materials recently came into focus due to their variety of interesting physical properties, specifically the new and unknown combinations of magnetic properties with interesting ground states [1]. These fascinating phenomena are induced by interaction of large Spin-Orbit-Coupling of the 5d transition metal and the onsite Coulomb energy U. Recent investigations of the Iridate $Ba_3YIr_2O_9$ show that sample grown under normal pressure crystallize in a hexagonal structure and exhibit magnetic ordering below 4 K [2]. The crystal structure is transformed to a cubic double perovskite configuration (stable at ambient pressure), when treated at 8 GPa pressure. In this cubic double perovskite phase the magnetic ordering is suppressed. A possible spin-orbit driven spin liquid ground state is proposed for the high pressure perovskite structure [3]. We will present recent results about the systematic high pressure synthesis of $Ba_3YIr_2O_9$ samples grown under different growth pressure in a Multi-Anvil assembly.The main focus will be on the measurements of structural and magnetic properties depending on the applied pressure during the synthesis process. [1] B. J. Kim et al., Phys. Rev. Lett. 101, 076402 (2008) [2] Y. Doi et al., J. Phys.: Condens. Matter 16, 2849 (2004) [3] T. Dey et al., Phys. Rev. B 88, 134425 (2013)

TT 24.12 Mon 18:30 BEY 118

Pressure-tuning of the magnetic properties of the zero-field cooled exchange-bias Heusler compound Mn_2PtGa — •Catalina Salazar, Ajaya K. Nayak, Claudia Felser, and Michael Nicklas — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

The Heusler compound Mn_2PtGa crystallizes in a tetragonal structure at room temperature. It undergoes a paramagnetic to ferrimagnetic (FI) transition around T_c=230 K followed by a first-order ferrimagnetic to antiferromagnetic (AFM) transition at lower temperature. The most intriguing feature observed in Mn_2PtGa is, however, a large zero-field cooled exchange bias. Here, we present a study of the pressure evolution of the magnetic properties of the Mn_2PtGa Heusler alloy by magnetization measurements under hydrostatic pressures up to 1.2 GPa.

TT 25: Focus Session: Electron Spin Qubits in Semiconductor Quantum Dots (organized by HL)

There have been remarkable new developments in the physics of electron spins confined in semiconductor quantum dots. In articular, silicon quantum dots have come to prominence, following in steps developments in GaAs dots. Spin hot spots — parametric regions with drastically reduced spin relaxation time — have been experimentally observed in both silicon and GaAs, in accord with theoretical investigations. Furthermore, novel ways of controlling and manipulating coherent dynamics of electron and nuclear spins in quantum dots by optics have been developed. This focused session will highlight those recent developments.

Organizer: Jaroslav Fabian, Universität Regensburg, and Jonathan Finley, Walter Schottky Institut, TU München.

Time: Monday 15:00–18:45 Location: POT 051

Topical Talk TT 25.1 Mon 15:00 POT 051

Single Charge Relaxation in a Silicon Double Quantum Dot — •Jason Petta — Department of Physics, Princeton University

Silicon has a weak spin-orbit interaction and can be isotopically purified resulting in an ultra-coherent environment for semiconductor qubits. I will describe recent measurements of single electron double quantum dots formed from undoped Si/SiGe quantum wells. Photon assisted tunneling is used to probe the energy level structure of the charge qubit, revealing the presence of low lying excited states. We measure the interdot charge relaxation time T_1 of a single electron as a function of detuning and interdot tunnel coupling and show that it is tunable over four orders of magnitude, with a maximum of 45 μs.

TT 25.2 Mon 15:30 POT 051

Entanglement Purification with the Exchange Interaction — •Adrian Auer and Guido Burkard — Department of Physics, University of Konstanz, Germany

Entanglement purification techniques provide means to create qubit pairs of arbitrary high fidelity with respect to a maximally entangled state, starting from a larger number of low fidelity pairs. So-called recurrence protocols act iteratively on two or more qubit pairs to produce one pair with higher fidelity, using local unitary operations, measurements, and communication of the measurement results. In this talk, we present a purification protocol that solely uses a single pulsed Heisenberg-type exchange interaction between two qubit pairs, therefore being especially suitable for spin qubits in tunnel-coupled quantum dots. In contrast to previously known protocols, we allow for asymmetric bilateral operations where the two communication parties operate differently on their qubits. In the most efficient version of our protocol, the local two-qubit interactions correspond to the $\sqrt{\text{SWAP}}$ gate and its inverse, which are the natural entangling gates generated from a Heisenberg-type interaction. Furthermore, we show how the same fidelity gain can be reached using XY-type interactions.

TT 25.3 Mon 15:45 POT 051

Reservoir-assisted coherent control of a quantum-dot spin — •Carsten H. H. Schulte[1], Jack Hansom[1], Claire Le Gall[1], Clemens Matthiesen[1], Jacob M. Taylor[2,3], and Mete Atatüre[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [2]Joint Quantum Institute, University of Maryland, College Park, Maryland 20742, USA — [3]National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

The interaction of a quantum-dot electron spin with the nuclear spins of its environment has attracted a lot of attention recently [1]. In equilibrium, the stochastic polarisation of the unperturbed nuclear spin bath leads to a splitting of the electron spin states. Here, we show that this effective Zeeman splitting is smaller than the linewidth of the charged exciton transition. The transitions in the unperturbed regime represent dynamically evolving Λ-systems. Harnessing these level schemes with sub-linewidth spin splittings, we implement spin-bath enabled coherent population trapping in the absence of an external magnetic field. We verify the coherence of the created spin state by coherent dark- and bright-state basis rotation through phase control of the laser fields, yielding arbitrary spin state initialisation and spin rotation with only hyperfine-induced spin orientation. The shown sub-linewidth level splitting advantageously reduces the influence of Larmor precession in spin manipulation schemes and facilitates photonic cluster state generation by triggered photon emission [2].

[1] Urbaszek et al., Rev. Mod. Phys. 85, 79-133 (2013).
[2] Lindner et al., Phys. Rev. Lett. 103, 113602 (2009).

Topical Talk TT 25.4 Mon 16:00 POT 051

Spin Qubits in Silicon — •Andrew Dzurak — University of New South Wales, Sydney 2052, Australia

Spin qubits in silicon are excellent candidates for scalable quantum information processing [1] due to their long coherence and the enormous investment in Si-MOS technology. Projective readout had proved challenging until single-shot measurement of a single donor electron spin was demonstrated [2] using a Si-SET and spin-to-charge conversion. The high readout fidelities > 90% and spin lifetimes T1 > 6 seconds [2] observed opened a path to electron and nuclear spin qubits in Si.

On-chip ESR of the P donor electron enables Rabi oscillations of the electron spin qubit, while Hahn echo reveals coherence T2 > 0.2 ms [3]. We also achieve single-shot readout of the 31P nuclear spin with fidelity > 99.8% and apply (local) NMR pulses to demonstrate coherent control of the nuclear spin qubit, with T2 > 60 ms [4].

Finally, I discuss recent experiments on both single-atom and Si-MOS quantum dot qubits in isotopically enriched 28Si devices, with even longer spin coherence exceeding 30 seconds.

[1] D.D. Awschalom et al., Quantum Spintronics, Science 339, 1174 (2013).
[2] A. Morello et al., Single-shot readout of an electron spin in silicon, Nature 467, 687 (2010).
[3] J.J. Pla et al., A single-atom electron spin qubit in silicon, Nature 489, 541 (2012).
[4] J.J. Pla et al., High-fidelity readout and control of a nuclear spin qubit in Si, Nature 496, 334 (2013).

TT 25.5 Mon 16:30 POT 051

Combining spin and valley singlet-triplet qubits for universal quantum computing — •Niklas Rohling, Maximilian Russ, and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

The valley degree of freedom in silicon or other materials is often considered to be an obstacle for quantum computing based on electron spins in quantum dots. Nevertheless, controlling the valley states opens new possibilities for quantum information processing. Combining qubits encoded in the single-triplet subspace of spin and of valley

states allows for universal quantum computing because the exchange interaction directly provides a universal two-qubit gate between those qubits if they are stored in the same two-electron double quantum dot [1]. We show how spin and valley qubits can be separated in order to enable single-qubit rotations. Finally we propose explicit sequences for quantum gates in two kinds of spin-valley quantum registers.

[1] N. Rohling and G. Burkard, New Journal of Physics **14**, 083008 (2012).

TT 25.6 Mon 16:45 POT 051

Optical detection of coherent electron spin states of silicon vacancy defects in silicon carbide — •Matthias Widmann[1], Sang-Yun Lee[1], Nguyen Tien-Son[2], Helmut Fedder[1], Torsten Rendler[1], Adam Gali[3], Erik Janzén[2], and Jörg Wrachtrup[1,4] — [1]3. Physikalisches Institut, Universität Stuttgart — [2]Department of Physics, Chemistry and Biology, Linköping University — [3]Institute for Solid State Physics and Optics, Budapest — [4]Max-Planck Institute for Solid State Research, Stuttgart

Deep defects in wide band gap materials are promising candidates for realizing quantum information processing [QIP]. One candidate is the negatively charged nitrogen-vacancy (NV) center in diamond. NV centers can be used for realization of QIP[1] and nano-scale magnetic field sensing[2]. The diamond serving as a host material, however, is rather hard to be implemented in existing silicon based semiconducting materials and devices. In order to circumvent this challenge, we focus on 4H silicon carbide (4H-SiC) which houses missing silicon atoms, forming the negatively charged silicon vacancies (T_V centers). Unlike the visible light emissions from NV centers in diamond, T_V centers in SiC also have the advantage of the infrared emissions around 900 nm, in which the optical attenuation is weaker in silica based fibers. We will present that single T_V emissions can be observed and coherent spin manipulation of both ensemble and single T_V centers are possible at room temperature.

[1] Neumann et al, Science, 2010, 329, 542
[2] J. R. Maze et al, Nature 455, 644-647

Coffee break (15 min.)

Topical Talk TT 25.7 Mon 17:15 POT 051

Spin Hot Spots in Quantum Dots — •Peter Stano — RIKEN Center for Emergent Matter Science, 2-1 Hirosawa, Wako, Saitama 351-0198 Japan — Institute of Physics, Slovak Academy of Sciences, 845 11 Bratislava, Slovakia

Spin hot spots are points in parameter space which dominate spin relaxation in quantum dots. The relaxation proceeds through spin-orbit interactions and a phonon emission. In a spin hot spot the otherwise weak spin-orbit effects become non-perturbative and thus unusually strong.

The hot-spot dominance leads to a pronounced anisotropy of the relaxation rate as a function of the quantum dot and/or magnetic field orientation with respect to crystallographic axes. This behavior is very general, occurring for different electron occupations, quantum dot geometry and material composition. Of practical interest is the possibility to individually identify different types of spin-orbit interactions (e.g. Rashba vs Dresselhaus), and obtain their relative strengths in a given sample, from the relaxation rate anisotropy.[1]

The important influence that the spin hot-spots might imply on spin relaxation was first recognized in bulk metals and later in quantum dots. The theoretically predicted spin hot-spots were recently established experimentally in gated Si [2] and GaAs [3] quantum dots.

[1] P. Stano and J. Fabian, Phys. Rev. B 74, 045320 (2006).
[2] C. H. Yang, et al., Nature Comm. 4, 2069 (2013).
[3] V. Srinivasa, et al., Phys. Rev. Lett. 110, 196803 (2013).

TT 25.8 Mon 17:45 POT 051

ESR Spin manipulation in spin light emitting diodes — •Andreas Merz, Jan Siller, Heinz Kalt, and Michael Hetterich — Inst. für angew. Physik KIT, Karlsruhe, Germany

Electron spin resonance is one of the most promising mechanisms to enable coherent quantum information processing. In spin light emitting diodes (spin-LEDs) we are able to initialize single electron spins all electrically by injecting them through a ZnMnSe spin-aligner layer into single self-assembled InGaAs quantum dots (QDs) with up to 100% fidelity. In a 53GHz microwave (MW) cavity we are able to manipulate the 3d Mn spin system of the spin aligner resonantly and detect the spin manipulation after the injection of band electrons into the QDs. We can optically observe the effect by analyzing the circular polarization of the recombination radiation during electrical excitation of the spin-LED for the magnetic field tuned such that the MW is resonant with the spin splitting in the Mn system. Furthermore we are able to differentiate between the resonant spin heating and non-resonant lattice heating of an amplified MW pulse for longer pulse lengths and pure spin heating for sub-microsecond MW pulses. The understanding of these mechanisms plays an important role for MW spin manipulation of single electron spins in semiconductor QDs on a ns timescale.

TT 25.9 Mon 18:00 POT 051

Optical Spin Noise of a Single Hole in a Quantum Dot — •Ramin Dahbashi[1], Jens Hübner[1], Fabian Berski[1], Klaus Pierz[2], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany

We present spin noise spectroscopy (SNS) [1] at the extreme limit of single spin detection, i.e., measurements of the spin dynamics of a single heavy hole localized in a self-assembled (InGa)As quantum dot (QD) [2]. Magnetic field dependent measurements reveal a strong dependence of the heavy hole spin relaxation rate T_1^{-1} on the longitudinal external magnetic field ($\propto B_z^{-3/2}$) even for very low magnetic fields up to 31 mT. At very low probe light intensities we detect an extremely long T_1 of > 180 μs at 31 mT and 5 K. The inhomogeneously broadening of a single QD SN spectrum is unveiled by the probe energy dependence of the SN power for finite light intensities. This feature is explained by charge fluctuations in the QD vicinity leading to distinct charge configurations. The corresponding fluctuations of the QD resonance energy are corroborated by a distinct probe intensity dependence of the spin lifetime. We further investigate time correlation effects of single QD SN spectra to gain insight into charging dynamics in the surrounding.

[1] Müller et al., Physica E **43**, 569 (2010).
[2] Dahbashi et al., arXiv:1306.3183 (2013).
[3] Dahbashi et al., Appl. Phys. Lett. **100**, 031906 (2012).

TT 25.10 Mon 18:15 POT 051

Spin-orbit effects on nuclear state preparation at the $S - T_+$ anti-crossing in double quantum dots — •Marko J. Rančić and Guido Burkard — University of Konstanz

We explore the interplay of spin-orbit and hyperfine effects on the nuclear preparation schemes in two-electron double quantum dots, e.g. in GaAs. The quantity of utmost interest is the electron spin decoherence time T_2^* in dependence of the number of sweeps through the electron spin singlet S triplet T_+ anti-crossing. Decoherence of the electron spin is caused by the difference field induced by the nuclear spins. We study the case where a singlet $S(2,0)$ is initialized, in which both electrons are in the left dot. Subsequently, the system is driven repeatedly through the anti-crossing and back using linear electrical bias sweeps. Our model describes the passage through the anti-crossing with a large number of equally spaced, step-like parameter increments. We develop a numerical method describing the nuclear spins fully quantum mechanically, which allows us to track their dynamics. Both Rashba and Dresselhaus spin-orbit terms do depend on the angle θ between the [110] crystallographic and the inter-dot axis. Our results show that the suppression of decoherence (and therefore the enhancement of T_2^*) is inversely proportional to the strength of the spin-orbit interaction, which is tuned by varying the angle θ.

TT 25.11 Mon 18:30 POT 051

Addressing ionized ^{75}As nuclear spin qubits in silicon using nuclear quadrupole interaction — •Florian M. Hrubesch, David P. Franke, Markus Künzl, Andrej Voss, Felix Hoehne, Lukas Dreher, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching

Electrically detected electron nuclear double resonance (EDENDOR) studies have shown coherence times of $^{31}P^+$ nuclear spins in crystalline ^{nat}Si of 18 ms [1]. In isotopically enriched ^{28}Si these T_2 times can reach up to 3 hours [2], making these nuclear spins promising candidates for quantum information storage. However, these long coherence times are caused by the nearly perfect isolation of the ionized donor nuclear spins from their environment, which hampers selective addressing with e.g. electric fields. We present EDENDOR measurements on $^{75}As^+$ nuclear spins in ^{nat}Si which exhibit similarly long decoherence times as $^{31}P^+$ nuclear spins in ^{nat}Si. By applying elastic strain, the transition

frequencies involving the $|m_I| = \frac{3}{2}$ states can be shifted by about 25 kHz, while the transitions between the $|m_I| = \frac{1}{2}$ states remain virtually unaffected. This allows the selective manipulation of the nuclear spin state via magnetic resonance, which could enable the addressing of single $^{75}As^{+}$ qubits with the help of nanoscale piezoactuators positioned on top of the donors [3]. [1] L. Dreher *et al.*, Phys. Rev. Lett. 108, 027602 (2012) [2] K. Saeedi *et al.*, Science 342, 830 (2013) [3] L. Dreher *et al*, Phys. Rev. Lett. 106, 037601 (2011)

TT 26: Quantum Wires: Transport Properties (organized by HL)

Time: Monday 16:00–17:45 Location: POT 006

TT 26.1 Mon 16:00 POT 006

Strongly interacting holes in Ge/Si core/shell nanowires — •Franziska Maier, Tobias Meng, and Daniel Loss — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

We consider holes confined to the core of Ge/Si core/shell nanowires subject to strong Rashba spin-orbit coupling and screened Coulomb interactions. We find that both, spin-orbit coupling and Coulomb interactions, are largely dependent on wire radius, shell-induced strain and the magnitude of applied electric fields. This tunability allows to drive the system from a Luttinger liquid phase towards a Wentzel-Bardeen singularity.

TT 26.2 Mon 16:15 POT 006

***In-situ* x-ray diffraction during MBE growth of InAs nanowires on Si** — •Andreas Biermanns[1], Anton Davydok[1], Emmanouil Dimakis[2,3], Masamitu Takahasi[4], Takuo Sasaki[4], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Festkörperphysik, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [4]Quantum Beam Science Directorate, Japan Atomic Energy Agency, Hyogo, Japan

Compared to the vapor-liquid-solid growth modes of group III-V semiconductor nanowires (NWs), e.g. Au-assisted growth or the self-assisted growth of GaAs NWs, it is a matter of intense debate whether or not liquid Indium is involved during the self-assisted growth of InAs NWs. Here, we present the results of an *in-situ* study of the nucleation phase of InAs NW growth on Si (111). X-ray scattering and diffraction methods have been employed during NW-growth at the synchrotron beamline 11XU at SPring-8 using a MBE chamber integrated with a surface diffractometer. The characteristic scattering signals from liquid In as well as the diffracted intensity of the crystalline NWs growing in the wurtzite (WZ) phase have been monitored during growth. We find that liquid In is present during the initial stage of growth, associated with the formation of extended WZ segments in the NWs. After the nucleation phase of the NWs, the liquid In vanishes, accompanied by a more defective crystal structure with a large number of stacking faults. The results are in accordance with a growth model, predicting a transition from locally In-rich to locally As rich conditions.

TT 26.3 Mon 16:30 POT 006

Ga droplet templates: Density control of self-assisted GaAs nanowires — •Hanno Küpers, Faebian Bastiman, Claudio Somaschini, and Lutz Geelhaar — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin

The self-assisted growth of GaAs nanowires (NWs) on Si is a popular approach for integrating III-V materials on Si. However, growth on unpatterned Si substrates suffers from a lack of control over nanowire density and a high degree of parasitic growth. We report on a new two-step NW density control technique for self-assisted GaAs nanowires grown on Si(111) by molecular beam epitaxy. The first step involves pre-depositing Ga on the substrate utilising a relatively high Ga flux at elevated temperatures. The Ga droplet density can be controlled by changing the magnitude of the Ga flux and the duration of the Ga pre-deposition time. The resulting Ga droplet template provides selective density control for ensuing NW growth. In this second step a maximum of 50% of the Ga droplets can be successfully converted into vertical NWs. The magnitude of the As flux and the size distribution of the Ga droplets underpins both the observed NW yield and the type of parasitic growth. A 10% improvement in the vertical yield can be gained by including a droplet ripening step before As flux exposure in order to narrow the droplet size distribution, but the Gaussian nature of the distribution prevents access to a 100% vertical yield.

TT 26.4 Mon 16:45 POT 006

Transport measurements of ballistic quantum wires exposed to two magnetic spikes. — •Bernd Schüler[1], Mihai Cerchez[1], Hengyi Xu[1], Thomas Heinzel[1], and Andreas Wieck[2] — [1]Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [2]Ruhr-Universität, 44780 Bochum, Germany

Quantum point contacts (QPC) are still fascinating elementary structures, which can lead in combination with localized magnetic fields to quite interesting effects [A. Tarasov et al., Phys. Rev. Lett. 104, 186801 (2010)]. We have designed a ferromagnet/semiconductor hybrid structure device which consists of a combination of an AFM-defined QPC and localized magnetic fields in the form of two magnetic spikes (magnetic barriers) at sub-micron distances inside the channel. The transport measurements are performed in the open regime of the QPC as function of a superimposed, homogeneous perpendicular magnetic field and as function of the barrier height. On top of the mode depopulation we found transmission resonances which could be explained with theoretically predicted signatures of zero-dimensional states weakly bound by the magnetic field [H. Xu et al. Phys. Rev. B 84, 035319 (2011)].

TT 26.5 Mon 17:00 POT 006

Resistance profiling of freestanding GaAs nanowires by multitip STM — •Stefan Korte[1], Matthias Steidl[2], Hubertus Junker[1], Weihong Zhao[2], Werner Prost[3], Vasily Cherepanov[1], Bert Voigtländer[1], Peter Kleinschmidt[2], and Thomas Hannappel[2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology — [2]Photovoltaics Group, Institute for Physics, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [3]CeNIDE and Center for Semiconductor Technology and Optoelectronics, University of Duisburg-Essen, 47057 Duisburg, Germany

Due to their specific one-dimensional geometry, III-V semiconductor nanowires are promising candidates for future optoelectronic devices. However, for the fabrication of novel high performance nanowire devices a precise control of doping profile is indispensable. We use a multitip STM as nanoprober to reveal the electrical transport properties of freestanding GaAs nanowires. *p*-doped GaAs nanowires are grown by Au-assisted metal-organic vapor-phase epitaxy (MOVPE) on GaAs(111)B and GaP(111)B substrates. Conductance profiles along the nanowires were obtained with four point probe measurements. Nanowires grown on different substrates, using a two temperature step growth mode or constant substrate temperature, all exhibit highly nonlinear axial resistance profiles.

TT 26.6 Mon 17:15 POT 006

Investigation of the electrical properties of freestanding Zn-doped GaAs nanowires by a multitip STM — •Matthias Steidl[1], Hubertus Junker[2], Weihong Zhao[1], Stefan Korte[2], Werner Prost[3], Vasily Cherepanov[2], Bert Voigtländer[2], Peter Kleinschmidt[1], and Thomas Hannappel[1] — [1]Photovoltaics Group, Institute for Physics, Technische Universität Ilmenau, D-98684 Ilmenau — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, D-52425 Jülich and JARA-Fundamentals of Future Information Technology — [3]CeNIDE and Center for Semiconductor Technology and Optoelectronics, University of Duisburg-Essen, D-47057 Duisburg

The specific geometry of III-V semiconductor makes III-V semiconductor nanowires (NWs) to promising building blocks for novel semiconductor devices in future electronic and opto-electronic applications. In this context a homogeneous distribution of the dopant over the whole NW is of great importance. We have grown p-type Zn-doped GaAs-NWs on GaP(111)B using the Au-assisted vapor-liquid-solid growth mode in a metal-organic vapor phase apparatus with different growth procedures. For the electrical characterization we apply a multitip STM as a nanoprober and conduct four-point probe measurements on

single free-standing NWs. With this technique we are able to measure resistance profiles with a high spatial resolution over almost the whole length of a nanowire. These measurements reveal that the resistivity is both dependent on the growth condition and the part of the NW. Generally, the resistivity at the NW base is orders of magnitude larger compared to the upper part of the NW.

TT 26.7 Mon 17:30 POT 006

Investigation of top-gated InAs nanowires with HfO_2 dielectric — •Marion Rosien[1,2], Torsten Rieger[1,2], Sebastian Heedt[1,2], Torsten Jörres[1,2], Thomas Schäpers[1,2], Detlev Grützmacher[1,2], and Mihail Ion Lepsa[1,2] — [1]Peter Grünberg Institute - 9, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology

Electrical characteristics of top-gated InAs nanowire field effect transistors (FETs) with HfO_2 high-k gate dielectric are presented. The nanowires with diameters of about 60 to 80 nm are grown by molecular beam epitaxy (MBE) and coated with HfO_2. The HfO_2 is deposited ex-situ by atomic layer deposition (ALD), which benefits from a high conformity and a good thickness control. To investigate the impact of the gate, the oxide thickness is varied between 2 and 8 nm. Transfer times between the MBE and ALD are kept as short as possible to avoid any contamination. The nanowires are individually contacted by Ti/Au electrodes. The HfO_2 acts as an omega shaped gate dielectric with Ti/Au gate metal. The quality of the oxide and the interface between the nanowire and the dielectric is analyzed by DC electrical measurements of the FETs. In order to derive transport parameters from the measurements, the capacitance of the top gate is simulated for each individual nanowire. The carrier mobility and concentration, peak transconductance and the on/off ratio are presented and discussed.

TT 27: Topological Insulators: Mostly Interaction with Magnetic Fields (organized by HL)

Time: Monday 15:45–17:45 Location: POT 081

TT 27.1 Mon 15:45 POT 081

SQUID devices built form S-TI-S junctions based on mercury telluride (HgTe) — •Luis Maier, Manuel Grimm, Christopher Armes, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, 97074 Würzburg

In the search for Majorana fermions, one way to show their existence requires an interface of a s wave superconductor and a strong topological insulator (TI) [1]. It has already been shown, that a three-dimensional, strained layer of HgTe shows dominant surface conductance in magnetotransport measurements and thus is considered as a 3D-TI [2]. Here we investigate the interaction of superconducting contacts with Dirac Fermions.

S-TI-S junctions based on HgTe and Nb have already been fabricated and characterized successfully [3]. As a next step in this research we created SQUID structures to further study the current phase relation in these special devices. In this talk we are going to present our recent results searching for deviations from normal behaviour that could point to TI or Majorana interactions.

[1] L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008)
[2] C. Brüne et al., Phys. Rev. Lett. 106, 126803 (2011)
[3] J. Oostinga et al., Phys. Rev. X 3, 021007 (2013)

TT 27.2 Mon 16:00 POT 081

Quantum Interferences of Dirac fermions in Bi2Se3 nanostructures — •Louis Veyrat, Joseph Dufouleur, Romain Giraud, Hannes Funke, Silke Hampel, Christian Nowka, Joachim Schumann, and Bernd Büchner — IFW-Dresden, Dresden, Germany

Recently discovered Z2 topological insulators (TIs) are ideally conducting at their interface only, where a gapless band structure forms. In a strong 3D TI, such as Bi2Se3, surface states are spin-chiral Dirac fermions with an odd number of Dirac cones. However, in real materials, the finite bulk conductivity often prevents the study of surface-state transport. We show that mesoscopic transport measurements can unambiguously reveal the specific properties of spin-chiral Dirac fermions in a Bi2Se3 nanostructure [1]. The quantum conductance of a nanowire exhibits Aharonov-Bohm oscillations which result only from surface-state transport. At very low temperatures, the temperature dependence of their amplitude unveils the quasi-ballistic nature of charge transport, which is the signature of the weak coupling of quasi-particles to their environment. Our results further reveal the weak scattering by structural disorder, giving another evidence of the specific nature of spin-chiral Dirac fermions in a strong 3D TI. Furthermore, new physics evidenced in the study of UCF in a nanowire, could be the signature of a perfectly transmitted mode in a nanowire geometry [2].

[1] J. Dufouleur et al., Phys. Rev. Lett. 110, 186806 (2013)
[2] J. Bardarson et al., Phys. Rev. Lett. 105, 156803 (2010)

TT 27.3 Mon 16:15 POT 081

Thermal and Electrical Transport of Single-Crystalline Bismuth Telluride Nanowires — •Bacel Hamdou[1], Johannes Kimling[1], Johannes Gooth[1], August Dorn[1], Eckhard Pippel[2], Raimar Rostek[3], Peter Woias[3], and Kornelius Nielsch[1] — [1]Institute of Applied Physics, University of Hamburg, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]Department of Microsystems Engineering, University of Freiburg, Germany

Bi_2Te_3 is a topological insulator (TI), a phase of matter that has a bulk bandgap and gapless electronic surface states protected by time-reversal symmetry. Studying topological surface states via electrical transport measurements is still very difficult due to large bulk contribution to conductivity originating from unintentional doping and the small bulk band gaps, which are typical for TI materials. We report on thermal and electrical transport measurements on individual single-crystalline bismuth telluride nanowires (NWs), synthesized via catalytic growth and post-annealing in a Te-rich atmosphere. The resulting Bi_2Te_3 NWs show reproducible electronic transport properties that are close to those of intrinsic bulk Bi_2Te_3. Further, magnetoresistance measurements were performed at temperatures down to 2 K. The parallel magnetoresistance curves exhibit Aharonov-Bohm oscillations, which indicate the presence of topological surface states. Analyses of Subnikov-de Haas oscillations in perpendicular magnetoresistance yield extremely low two-dimensional carrier concentrations and effective electron masses, and very high carrier mobilities.

TT 27.4 Mon 16:30 POT 081

Ambipolar quantum Hall effect in strained bulk HgTe — •Cornelius Thienel, Jonas Wiedenmann, Steffen Wiedmann, Christoph Brüne, Christopher Ames, Hartmut Buhmann, and Laurens W. Molenkamp — Universität Würzburg, Experimentelle Physik III

Strained bulk HgTe has been identified as three-dimensional topological insulator [Phys. Rev. Lett. **106**, 126803 (2011)]. A Dirac-specific quantum Hall sequence can unambiguously be demonstrated in transport measurements. Furthermore we identify two subsets of Landau levels that originate from the topological surface states.
Improving the quality of the interfaces hosting the surface states by introducing additional buffer and cap layers to the structure increases the carrier mobilities in the topological states and makes it possible to observe the quantum Hall effect of electrons and holes in a wide gate voltage range. The detection of p-type QHE points towards a suppressed interaction between bulk and surface states.

TT 27.5 Mon 16:45 POT 081

Weak antilocalization effects in systems with Dirac-like energy dispersion — •Andreas Budewitz, Mathias Mühlbauer, Bastian Büttner, Grigory Tkachov, Ewelina M. Hankiewicz, Christoph Brüne, Hartmut Buhmann, and Laurens W. Molenkamp — Universität Würzburg, Lehrstuhl für experimentelle Physik III

HgTe quantum wells (QW) have been identified as topological insulator (TI) by appearence of the QSHE [1]. It has been shown that the band structure of HgTe QWs has to be described by a four band model revealing a Dirac like dispersion [2, 3]. Here now we investigate the weak antilocalization (WAL) effect in various n-conducting HgTe QWs. We analyse the magnetoresistance of a set of quasi one-

dimensional wires and clearly observe different WAL amplitudes for normal and inverted band ordering which does not depended on the structural inversion asymmetry (SIA). The data demonstrate that a non-universal Berry phase which exceeds π, the characteristic value for gapless Dirac fermions, is needed to explain the different observations in our measurements.

[1] M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi and S.-C. Zhang, Science 318, 766 (2007)

[2] B. A. Bernevig, T. L. Hughes and S. C. Zhang, Science 318, 1757 (2006)

[3] B. Büttner, C.-X. Liu, G. Tkachov, E. G. Novik, C. Brüne, H. Buhmann, E. M. Hankiewicz, P. Recher, B. Trauzettel, S.-C. Zhang, and L. W. Molenkamp, Nature Phys. 7, 418 (2011)

TT 27.6 Mon 17:00 POT 081

Giant Photocurrents in a Dirac Fermion System at Cyclotron Resonance — •C. Zoth[1], P. Olbrich[1], P. Vierling[1], K.-M. Dantscher[1], G.V. Budkin[2], S.A. Tarasenko[2], V.V. Bel'kov[2], D.A. Kozlov[3], Z.D. Kvon[3], N.N. Mikhailov[3], S.A. Dvoretsky[3], and S.D. Ganichev[1] — [1]Terahertz Center, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Institute of Semiconductor Physics, Novosibirsk, Russia

We report on the observation of giant photocurrents in HgTe/HgCdTe quantum wells (QW) of critical thickness at which a Dirac spectrum emerges [1]. Exciting QW of 6.6 nm width by terahertz radiation and varying an external magnetic field we detected a resonant photocurrent. Remarkably, the position of the resonance can be tuned from negative (-0.4 T) to positive (up to 1.2 T) magnetic fields by means of optical doping. The photocurrent data, accompanied by measurements of radiation transmission, as well as, magnetotransport, prove that the photocurrent is caused by cyclotron resonance in a Dirac fermion system. This allows us to obtain the effective electron velocity $v \approx 7.2 \times 10^5$ m/s. We develop a microscopic theory of the effect and show that the inherent spin-dependent asymmetry of light-matter coupling in the system of Dirac fermions causes the electric current to flow.

[1] P. Olbrich, C. Zoth, P. Vierling *et al.*, *PRB* **87**, 235439 (2013)

TT 27.7 Mon 17:15 POT 081

Quantum Oscillations of Photogalvanic Effect and Spin Orbit Interaction Effect in HgTe Quantum Wells — •K.-M. Dantscher[1], C. Zoth[1], P. Olbrich[1], V.V. Belkov[2], M.A. Semina[2], M.M. Glazov[2], L.E. Golub[3], D.A. Kozlov[3], Z.D. Kvon[3], N.N. Mikhailov[3], S.A. Dvoretsky[3], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Institute of Semiconductor Physics, Novosibirsk, Russia

We report on the observation of quantum oscillations in HgTe/HgCdTe quantum well (QW) structures of different widths, which are characterized by an inverted, normal and even Dirac like bandstructure [1,2]. Exciting the QWs by terahertz radiation and sweeping an external magnetic field we observed a resonant photocurrent [3] which shows pronounced oscillations. The photocurrent data are accompanied by measurement of photoconductivity, radiation transmission, as well as, magneto-transport. A comparison of the results shows that the photosignal is enhanced at cyclotron resonance position and is modulated by Shubnikov-De Haas oscillations. Furthermore we present a microscopic model of a magnetic field dependent oscillating current taking into account the oscillations of spin polarization and of conductivity.

[1] Z.D. Kvon *et al.*, *JETP Letters* **94**, 816-819 (2011)
[2] A. Bernevig *et al.*, *Science* **314**, 1757 (2006)
[3] P. Olbrich *et al. Phys. Lett B* **87**, 235439 (2013)

TT 27.8 Mon 17:30 POT 081

Strong Out-of-Plane Magnetic Anisotropy of Fe Adatoms on Bi_2Te_3 — •Thomas Eelbo[1], Marta Waśniowska[1], Marcin Sikora[2], Michal Dobrzański[2], Andrzej Kozlowski[2], Artem Pulkin[3], Gabriel Autès[3], Ireneusz Miotkowski[4], Oleg Yazyev[3], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Germany — [2]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland — [3]Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland — [4]Department of Physics, Purdue University, West Lafayette, USA

Topological insulators (TIs) are currently in the focus of fundamental physics. The interaction of magnetic impurities with TIs is widely unexplored on the local scale and might potentially entail interesting properties of the TIs in view of applications in spintronics. To this end, we studied the structural, electronic, and magnetic properties of individual Fe atoms adsorbed on a Bi_2Te_3(111) surface by means of scanning tunneling microscopy/spectroscopy (STM/STS), X-ray absorption spectroscopy and X-ray magnetic circular dichroism (XMCD) at low temperatures. STM reveals the existence of two different Fe species. Density functional theory-based calculations let us assign these to atoms adsorbed on the fcc/hcp hollow sites. STS proves the existence of characteristic resonances for each type and XMCD evidences a strong magnetic out-of-plane anisotropy of the Fe moments in agreement with our calculations.

TT 28: Focussed Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale II (organized by O)

Time: Monday 16:00–18:45 Location: TRE Ma

Topical Talk TT 28.1 Mon 16:00 TRE Ma

Simulating heat transport: from large scale molecular dynamics to first-principles calculations — •Davide Donadio — Max Planck Institute for Polymer Research, Mainz, Germany

The necessity to design materials and devices able to harness thermal energy, and possibly convert it into more amenable energy forms, has stimulated a major effort in the scientific community to understand heat transport at the mesoscale and the nanoscale. In this talk I will discuss different atomistic approaches to simulate nanoscale heat transport, ranging from large scale molecular dynamics simulations with classical empirical potentials at equilibrium and non-equilibrium conditions, to lattice dynamics calculations with force-constants computed by first principles. Applications will include silicon and carbon nanostructures, phase-change materials and molecular junctions.

TT 28.2 Mon 16:30 TRE Ma

First principles study of thermal conductivity cross-over in nano-structured Zinc-Chalcogenides — •Ankita Katre[1], Atsushi Togo[2], Ralf Drautz[1], and Georg K. H. Madsen[1] — [1]ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]ESISM, Kyoto University, Sakyo, Kyoto 606-8501, Japan

Nano-structured Zinc-Chalcogenides are interesting for thermoelectric applications due to their low thermal conductivity.[1] A simple model study has reported how the thermal conductivity of ZnS, ZnSe and ZnTe can potentially show a cross-over as a function of the maximal mean free path of the phonons.[2] We have applied the Boltzmann transport equation in the relaxation time approximation to verify this. We find that thermal conductivity of ZnS crosses ZnSe and ZnTe and explain this in terms of the different contributions of phonon modes in these materials. Furthermore, the cross-over is found to be strongly influenced by isotope scattering. The calculated thermal conductivity is found to be strongly dependent on the volume and we explain the observed differences between LDA and GGA calculations. We compare further calculated thermal properties, such as the thermal expansion coefficient, to experiment to validate our approach.

[1] L.Zhen, S.Qiao, D.Y.Xiang, H.Z.Zhong, and Q.L.Gao, J. Mater. Chem. 22, 22821 (2012). [2] N.Mingo and D.Broido, Phys. Rev. Lett. 93, 246106 (2004).

TT 28.3 Mon 16:45 TRE Ma

Density-functional perturbation theory for lattice dynamics with numeric atom-centered orbitals — •Honghui Shang, Christian Carbogno, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

The response of the electronic structure to atomic displacements gives rise to a variety of interesting physical phenomena, which can be

probed by experimental techniques such as infrared or Raman spectroscopy or neutron diffraction. The response can be conveniently computed from first principles by means of density-functional perturbation theory (DFPT). Here we present our implementation in the all-electron atom-centered numeric orbital code FHI-aims [1]. Our approach combines the accuracy of an all-electron full-potential treatment with the computationally efficiency of localised atom-centered basis sets that is necessary to study large and complex systems. We verified the accuracy of our DFPT implementation by comparing the vibrational frequencies to finite-difference reference calculations and literature values. Due to the atom-centered nature of the integration grids in FHI-aims, the portion of the grid that belongs to a certain atom also moves when this atom is displaced. Here we demonstrate that, unlike for first derivatives (i.e. forces) [2], this moving-grid-effect plays an important role for second derivatives (i.e. vibrational frequencies). Further analysis reveals that predominantly diagonal force constant terms are affected, which can be bypassed efficiently by invoking translational symmetry.

[1] V. Blum et al. Comp. Phys. Comm. 180, 2175 (2009)
[2] B. Delley, J. Chem. Phys. 94, 7245 (1991).

TT 28.4 Mon 17:00 TRE Ma

Breakdown of Fourier law in layered materials — •Andrea Cepellotti[1], Giorgia Fugallo[2], Francesco Mauri[3], and Nicola Marzari[1] — [1]THEOS, École Polytechnique Fédérale, Lausanne — [2]IMPMC, Universite Pierre et Marie Curie, Paris — [3]LSI, École Polytechnique, Paris

We compute the thermal conductivity in crystalline layered materials by solving the Boltzmann Transport Equation (BTE) for phonons [1], with the phonon-phonon collision rates obtained from density-functional perturbation theory. We find that in 2D materials, such as graphene and related compounds, and even in 3D layered materials, like bulk graphite, the single-mode relaxation time approximation (SMRTA) cannot describe heat transport correctly, underestimating by one order of magnitude or more thermal conductivities and phonons' mean free paths. Instead, we show that the exact self-consistent solution of the BTE provides results in excellent agreement with experimental measurements [2]. The shortcomings of the SMRTA lie in the assumption that heat flow is transferred only by individual phonon excitations, whereas in layered materials the transport can only be explained in terms of collective phonon excitations. The characteristic length of these collective excitations is often comparable with that of the experimental sample - as a result, Fourier's law become questionable, since its statistical nature makes it applicable only to systems larger than a few mean free paths.

[1] G. Fugallo et al., Phys. Rev. B, **88**, 045430 (2013).
[2] A. A. Balandin, Nat. Mater. **10**, 569 (2011).

TT 28.5 Mon 17:15 TRE Ma

High Temperature Thermal Conductivity from First Principles — •Christian Carbogno[1], Rampi Ramprasad[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, USA

In spite of significant research efforts, a first principles determination of the thermal conductivity at high temperatures has remained elusive. Under such conditions, Boltzmann transport techniques [1] that include anharmonic effects only perturbatively become inaccurate or even inapplicable. In this work, we overcome this limitation by performing first-principles Green-Kubo simulations [2], in which all orders of anharmonicity are incorporated by the means of *ab initio* molecular dynamics. The thermal conductivity is then assessed from the autocorrelation function of the heat flux in thermodynamic equilibrium. We discuss the details of our implementation and the definition of our heat flux that is based on the virial theorem. We validate our approach by presenting calculations for ZrO_2 that also showcase the importance of higher order anharmonic effects in materials with low thermal conductivities. Eventually, we discuss how our technique can be coupled to multi-scale models to achieve a computationally efficient and accurate description of the thermal conductivity at the nanoscale.

[1] D. A. Broido *et al.*, *Appl. Phys. Lett.* **91**, 231922 (2007).
[2] R. Kubo, M. Yokota, S. Nakajima, *J. Phys. Soc. Jpn.* **12**, 1203 (1957).

TT 28.6 Mon 17:30 TRE Ma

Accurate Modelling of the Polymorphism and Elastic Response of Molecular Materials from First Principles — •Anthony Reilly and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Molecular materials are of great fundamental and applied importance in science and industry, with numerous applications in pharmaceuticals, electronics, sensing, and catalysis. A key challenge for theory has been the prediction of their stability, polymorphism and response to perturbations. While pairwise models of van der Waals (vdW) interactions have improved the ability of density functional theory (DFT) to model these systems, quantitative and even qualitative failures often remain. Here, we show how a many-body description of vdW interactions can dramatically improve the accuracy of DFT for molecular materials, yielding quantitative description of stabilities and polymorphism for these challenging systems. Moreover, the role of many-body vdW interactions goes beyond stabilities to response properties. In particular, we have studied the elastic properties of a series of molecular crystals, finding that many-body vdW interactions can account for up to 30% of the elastic response, leading to quantitative and qualitative changes in elastic behavior. We will illustrate these crucial effects with the challenging case of the polymorphs of aspirin, leading to a better understanding of the conflicting experimental and theoretical studies of this system.

TT 28.7 Mon 17:45 TRE Ma

Surface chemistry on nanostructured oxides: do we have to go beyond hybrid DFT? — •Daniel Berger, Harald Oberhofer, and Karsten Reuter — Technische Universität München, Germany

Nanostructured oxide surfaces are promising candidates for a wide range of energy and catalysis applications. For first-principles modeling of corresponding surface chemical reactions the current state-of-the-art is generally defined by hybrid-level density-functional theory (DFT). Systematic work assessing the achieved accuracy at this level is nevertheless scarce, also owing to the fact that higher-level reference methods are often not available for standard periodic boundary condition supercell calculations. To this end, we present a study benchmarking semi-local and hybrid DFT against (renormalized) second-order perturbation theory (MP2,rPT2) as recently implemented in the FHI-aims package [1]. We make the efficient usage of the latter theories for oxide surfaces possible through a solid-state embedding framework, in which a central cluster region is described quantum mechanically, the long-range electrostatic interactions in the oxide are accounted for through a polarizable monopole field, and a shell of norm-conserving pseudopotentials correctly connects the two regions. We illustrate the performance of the various levels of theories using the water-splitting reaction at ideal and defected TiO_2(110) surfaces as showcase.

[1] X. Ren *et al.*, Phys. Rev. B **88**, 035120 (2013)

TT 28.8 Mon 18:00 TRE Ma

Atoms-in-solids perspective on polarizabilities and van der Waals coefficients in semiconductors — •Guo-Xu Zhang, Anthony M. Reilly, Alexandre Tkatchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

The calculation of response properties of solids including their polarizabilities and van der Waals (vdW) coefficients usually requires the knowledge of the full electronic bandstructure. For non-covalently bound solids, such as noble-gas and ionic crystals, atoms-in-solids model can be successfully utilized to define their polarizabilities. Here we critically assess the atoms-in-solids model for covalently-bound solids, ranging from wide-gap (10 eV) to narrow-gap (below 1 eV) semiconductors. We model their response by assigning a single quantum harmonic oscillator to every atom, where the parameters of the oscillators are defined as functionals of the electron density, following the Tkatchenko-Scheffler method [1]. The response function is then calculated by solving self-consistent screening equations of classical electrodynamics, without any explicit information about the electronic bandstructure [2]. The calculated polarizabilities and vdW coefficients for 23 semiconductors are compared with TDDFT and experimental benchmark data, revealing an overall agreement within 10%. The efficiency of our method and the accuracy of the calculated vdW parameters allows us to demonstrate the crucial role of vdW interactions in the cohesive properties of the 23 semiconductors.

[1] Tkatchenko and Scheffler, PRL (2009); [2] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012).

TT 28.9 Mon 18:15 TRE Ma

Adsorption at semiconductor surfaces - an energy analysis method — •Ralf Tonner and Marc Raupach — Fachbereich Chemie & Materials Sciences Centre, Philipps-Universität Marburg,

Germany

The chemical bond is one of the most fundamental concepts in chemistry. Classifications such as covalent, ionic or metallic bonding are central in discussing trends in different compounds and predicting new reactivity. Several very helpful concepts and methods were developed to understand the chemical bond at surfaces.[1] The question about energetic contributions to surface chemical bonds on the other hand did not receive great attention although energy changes are the ultimate driving force in bond formation.

Starting from preliminary work by Philippsen and Baerends,[2] we implemented all terms of an Energy Decomposition Analysis (EDA) to obtain quantitative data about energetic contributions to chemical bonding in periodic systems. This periodic EDA method was applied to questions of chemisorption of organic molecules at semiconductor surfaces where it can shed light on the nature of the surface-adsorbate bonds.

[1] a) A. Nilsson, L. G. M. Pettersson, J. Nørskov, Chemical Bonding at Surfaces and Interfaces, Elsevier, Amsterdam, 2007; b) A. Groß, Theoretical Surface Science, Springer, Berlin, Heidelberg, 2009. [2] P. H. T. Philipsen, E. J. Baerends J. Phys. Chem. B 2006, 110, 12470.

TT 28.10 Mon 18:30 TRE Ma

Non-local density functionals meet many-body dispersion: A hybrid approach for van der Waals interactions — •Jan Hermann, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Different approaches to treating van der Waals (vdW) interactions in density-functional theory can be loosely divided into the atom-based and the ones based on non-local functionals. The first type comprises a range of methods from atom-pairwise additive schemes by Grimme to many-body dispersion (MBD) approach of Tkatchenko et al. Usually, these methods require precalculated atomic parameters and thus rely on information not explicitly contained in the electron density. The other category consists of nonlocal functionals either of the Langreth and Lundquist or the Vydrov and van Voorhis (VV) type. In these approaches, the vdW interaction is obtained as a functional of the electron density and at most a few tuning parameters are needed.

Here, we show that these two contrasting approaches can be synergistically combined. We use the polarizability from the nonlocal functional of VV within the MBD method of Tkatchenko et al. Such a combination is worthy for several reasons. First, it is an atom-centered approach with no atomic parameters. Second, it puts aside the problem of partitioning electron density between atoms, which can be problematic in some cases. Third, it enables more direct comparison of so far unrelated methods. Fourth, it highlights the idea of combining working elements from different approaches.

TT 29: Graphene: Structural Properties (organized by O)

Time: Monday 16:00–19:00 Location: WIL C107

TT 29.1 Mon 16:00 WIL C107

Vertical height of quasi-free standing monolayer graphene on SiC(0001): an XSW study — •J. Sforzini[1], T. Denig[2], T. L. Lee[3], C. Kumpf[1], S. Subach[1], U. Starke[2], F. C. Bocquet[1], and F.S. Tautz[1] — [1]Peter Grünberg institute (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — [3]Diamond light source ltd, Harwell oxford, Didcot, Oxfordshire, United Kingdom

We investigated a quasi-free standing monolayer graphene sample[1] on SiC(0001) obtained by decoupling the buffer-layer from Si-terminated surface by hydrogen intercalation. We used X-ray Standing Wave technique (XSW), combining dynamical diffraction and X-ray photoelectron spectroscopy, to detect the coherent distribution of the chemically different species (Si and C) at the interface. Our analysis shows two different carbon species (C in the graphene layer and C in the SiC bulk); we find that the adsorption height of the graphene layer is slightly higher than theoretically predicted. The discrepancy, attributed to the very weak graphene-substrate intercation, is still challenging for theory[2].

[1]Riedl, et. al., PRL, 103, 246804 (2009)
[2]Deretzis , et. al., Nanoscale, 5, 671-680 (2012)

TT 29.2 Mon 16:15 WIL C107

Epitaxial graphene nanostructures on SiC — •Alexander Stöhr[1], Stiven Forti[1], Ulrike Waizmann[1], Thomas Reindl[1], Jens Baringhaus[2], Alexei Zakharov[3], Christoph Tegenkamp[2], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Institut für Festkörperphysik, Leibniz-Universität Hannover, Hannover, Germany — [3]MAX IV Laboratory, Lund University, Lund, Sweden

In recent years a lot of effort was put into the realization of graphene devices, in view of their unique electronic properties and the potential application in logical circuits. However, for the use in logical electronics a band gap would be required. This can be achieved by confining the electrons into quasi-onedimensional graphene stripes, called graphene nanoribbons. When patterning graphene, the altering of the electronic properties by the mechanical attack on the ribbon edges as well as residual resist is always an issue. For that matter we chose to structure the SiC-samples before growing graphene, using electron beam lithography and reactive ion etching. Subsequently, the graphene was grown at elevated temperatures, which also removed the residual resist. As a result onedimensional stripes could be obtained and were decoupled from the substrate by intercalation of hydrogen. Characterization by low-energy electron microscopy and angle-resolved photoemission spectroscopy proves the development of quasi-free standing monolayer graphene ribbons.

TT 29.3 Mon 16:30 WIL C107

Moiré-induced Brillouin zone backfolding of graphene phonons on Ir(111) — •Michael Endlich[1], Alejandro Molina-Sánchez[2], Henrique Miranda[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 moiré superstructure of graphene on Ir(111) leaves its characteristic footsteps in the phonon dispersion. Replica of the phonon dispersion branches of singly oriented graphene on Ir(111) have been determined throughout the entire surface Brillouin zone with angle-resolved inelastic electron scattering. These replica are rationalized in terms of phonon backfolding induced by the graphene moiré superlattice.

TT 29.4 Mon 16:45 WIL C107

Back Focal Plane Imaging of Raman Scattering from Graphene — •Harald Budde, Xian Shi, Nicolai Hartmann, and Achim Hartschuh — Department Chemie und CeNS, LMU München, Germany

Raman Scattering Spectroscopy is a powerful technique for studying graphene and other sp2 carbon materials [1]. We combined Raman Spectroscopy with back focal plane (BFP) imaging , a method used to visualize the angular distribution of emitted or scattered light. As an example BFP imaging allows to determine the orientation of single dipolar emitters [2, 3]. For graphene on glass Raman BFP images mainly reflect the polarization characteristics of the different phonon modes. On thin gold films emission from graphene leads to the excitation of propagating surface plasmon polaritons.

[1] A. Ferrari, D. Basko, Nat. Nanotech 8, 235-246, 2013.
[2] M. Lieb, J. Zavislan, L. Novotny, J. Opt. Soc. Am. B 21, 1210-1215, 2004.
[3] N. Hartmann, G. Piredda, J. Berthelot, G. Colas des Francs, A. Bouhelier, A. Hartschuh, Nano Lett. 12, 177-181, 2012.

TT 29.5 Mon 17:00 WIL C107

Ion Irradiation of Metal-Supported Graphene: Exploring the Role of the Substrate — •Charlotte Herbig[1], Harriet Åhlgren[2], Sabina Simon[1], Carsten Busse[1], Jani Kotakoski[2,3], Arkady V. Krasheninnikov[2,4], and Thomas Michely[1] — [1]II. Phys. Inst., Universität zu Köln, Germany — [2]Dept. of Phys., University of Helsinki, Finland — [3]Faculty of Phys., University of Vienna, Austria — [4]Dept. of Appl. Phys., Aalto University, Finland

Ion irradiation effects on 2D materials are an emerging subject, triggered by graphene's (Gr) potentials in applications. For supported Gr the effect of the substrate on ion beam damage and annealing is important. We investigate the behavior of high quality Gr, weakly coupled to Ir(111), to low energy noble gas ion irradiation by scanning tunneling microscopy (STM), molecular dynamics simulations, and density functional theory (DFT). For a freestanding layer, sputtered atoms leave the layer either in forward or backward direction. For metal-supported Gr, only C atoms carrying backward momentum are sputtered while atoms carrying forward momentum are trapped. As evident from STM and DFT, trapped C atoms form nm-sized Gr platelets at the interface upon annealing at 1000K, assisted by substrate defects. The incorporation into the Gr layer is suppressed due to high migration barriers, while diffusion into the Ir is energetically unfavorable. By measuring the area fraction of the platelets, we obtain the trapping yield, i.e., the number of trapped C atoms per incident ion. Interestingly, compared to the sputtering yield, the trapping yield for Gr on Ir(111) displays a distinctly different dependence on the ion beam angle of incidence.

TT 29.6 Mon 17:15 WIL C107

***Ab initio* study of graphene on O-intercalated Ir(111) surface and its functionalization via molecular adsorption** — •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

To integrate graphene in molecular electronics and spintronics devices it is crucial to understand how the strength of the graphene–metal electrode interaction can be specifically tuned. One possibility to loose or strengthen this interaction is to intercalate adatoms with different chemical reactivity between graphene and the metal surface in question. We will analyse this approach from first principles by considering the case of the O-intercalated graphene on Ir(111) [1]. Another path is to analyse how the adsorption of $\pi-$conjugated organic molecules can affect the electronic structure of a quasi-freestanding graphene layer. We investigated this issue by performing spin-polarized density functional theory (DFT) for a trioxotriangulene-derivate molecule [2] on graphene. Importantly, as already demonstrated in [3], for such systems it is mandatory to include the dispersion interaction and in our *ab initio* study these long-range van der Waals interactions were considered at a semi-empirical [4] or first-principle [5] level.

[1] E. Grånäs *et al.*, ACS Nano. **6**, 9951 (2012).
[2] Y. Morita *et al.*, Nat. Mater. **10**, 946 (2011).
[3] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).
[4] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).
[5] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).

TT 29.7 Mon 17:30 WIL C107

From two to three dimensions: The effect on the Coulomb interaction by increasing the dimensionality in layered 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 and Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [3]I. Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany — [4]Radboud University Nijmegen, Institute for Molecules and Materials, AJ Nijmegen, The Netherlands

We study the Coulomb repulsion and the dielectric screening in mono-, bi- and tetralayer graphene as well as in graphite. We discuss the transition from 2D systems to the bulk structure in layered materials with regard to the (non) local Coulomb interactions. Therefore, we use *ab initio* constrained random phase (cRPA) calculations to get reliable data in a first step. By tailoring the resulting Coulomb interaction in classical electrostatic models afterwards, we find the following: In addition to the effective height of each layer especially the direction dependence and the non-locality of the dielectric function are the keys to understand the screening effects in these structures. Thereby, we discuss models to estimate the Coulomb interaction of the 2D systems by using exclusively the bulk data as input. We apply these rules to calculate the Coulomb interaction in graphene on iridium and find a very good agreement with *ab initio* data.

TT 29.8 Mon 17:45 WIL C107

Graphene nanolithography with 2.5 nm precision: combining bottom-up and top-down techniques — •Antonio J. Martínez-Galera[1,2], Iván Brihuega[1,3], Ángel Gutiérrez-Rubio[1], Tobias Stauber[1,3], and José M. Gómez-Rodríguez[1,3] — [1]Departamento Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Present address: II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany. — [3]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

The selective modification of pristine graphene represents an essential step to fully exploit its potential. The work presented here overcomes one of the remaining challenges key for the comprehensive integration of graphene in real devices: the realization of lithography below 10 nm sizes. Specifically, we have developed a perfectly reproducible nanolithographic technique for graphene that allows, by means of an STM tip, to modify with 2.5 nm accuracy the electronic properties of graphene monolayers epitaxially grown on Ir(111) surfaces. This method can be carried out also on micrometer sized regions and the structures so created are stable even at room temperature. As a result, we can strategically combine graphene regions presenting large differences in their electronic structure to design graphene nanostructures with tailored properties. Therefore, this novel nanolithography method could open the way to the design of nanometric graphene-based devices with specific functionalities. In particular, we explore here the possibility of developing a new platform for plasmonics.

TT 29.9 Mon 18:00 WIL C107

Relaxation of compressive stresses in graphene through mobile nanoripples — •Peter Klaver, Shouen Zhu, Marcel Sluiter, and Guido Janssen — Delft University of Technology, Delft, Netherlands

Graphene monolayers have a far smaller thermal expansion coefficient than the Cu substrates on which they are often grown through CVD at high temperature. Once the Cu substrate and graphene monolayer are cooled down to room temperature, the Cu contracts 1.5-2.0% more than the graphene. Yet various experiments do not show graphene layers on Cu to be under significant compressive stress. We present molecular dynamics simulations that show that under compressive stress, small ripples of just a few nm wide appear that absorb the excess graphene area. These ripples are quite mobile, even at room temperature. Their movement offers a mechanism to remove the compressive stress in graphene while keeping it flat, by absorbing the ripples into larger ripples (like those that have formed around bunches of step edges) or by eliminating the ripples at the edges of graphene islands. The relaxation of stresses through the movement of nanoripples is somewhat analogous to flattening out a red carpet by gradually moving a wrinkle away to the carpet edge instead of pulling the entire carpet all at once. The ease with which stresses in graphene relax, is not directly determined by the corrugation energy.

TT 29.10 Mon 18:15 WIL C107

Epitaxial graphene nanoflakes on Au(111) and Ag(111) — •Julia Tesch[1], Philipp Leicht[1], Lukas Zielke[1], Riko Moroni[1], Bernd Illing[1], Luca Gragnaniello[1], Felix Blumenschein[1], Elena Voloshina[2], Lukas Hammerschmidt[3], Lukas Marsoner Steinkasserer[3], Beate Paulus[3], Yuriy Dedkov[4], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Institut für Chemie, HU Berlin — [3]Institut für Chemie und Biochemie, FU Berlin — [4]Fritz-Haber-Institut der MPG, Berlin

In zig-zag edge terminated graphene nanoribbons or nanoflakes (GNFs), confinement of electrons is predicted to give rise to edge states with magnetic moments. However, the experimental observation of edge effects is impeded by the inevitable presence of substrates that interact with the flake edges, hence masking the GNFs' intrinsic properties. In the attempt of reducing the graphene substrate interaction, we use an entirely UHV based approach for the preparation of GNFs on Au(111) and Ag(111) surfaces allowing for flake sizes down to 10 nm. GNFs on Ir(111) are prepared by temperature programmed growth [1] and subsequently covered by deposition of several nm of Au or Ag. After post-annealing, the flakes diffuse through the Au or Ag film and form embedded or floating graphene flakes. In scanning tunnelling microscopy (STM), the edges of floating GNFs are found to be singly hydrogen terminated and entire flakes can be laterally displaced with the STM tip on both Au and Ag surfaces, suggesting a considerable reduction of graphene-substrate interactions compared to other metals. [1] Coraux et al., New J. Phys. 11, 023006 (2009)

TT 29.11 Mon 18:30 WIL C107

Scatttering and electronic structure in graphene nanoflakes on Au(111) — •Philipp Leicht[1], Lukas Zielke[1], Samuel

Bouvron[1], Julia Tesch[1], Felix Blumenschein[1], Luca Gragnaniello[1], Lukas Marsoner Steinkasserer[2], Beate Paulus[2], Elena Voloshina[3], Yuriy Dedkov[4], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Institut für Chemie und Biochemie, FU Berlin — [3]Institut für Chemie, HU Berlin — [4]Fritz-Haber-Institut der MPG, Berlin

Confinement of electrons in graphene quantum dots and nano ribbons with atomically well defined edges represents an exciting field of research, owing to predicted peculiar electronic and magnetic properties.

Here, we present scanning tunneling microscopy (STM) investigations of graphene nano flakes (GNFs) prepared by temperature programmed growth on Ir(111) [1] and subsequent intercalation of Au for electronic decoupling. The electronic properties of the graphene flakes are addressed by scanning tunneling spectroscopy. Within our atomically resolved constant-energy maps we can probe the electronic states of the graphene electrons exploiting the intervalley scattering. The hereby obtained dispersion relation shows a linear behavior and can be unambiguously discriminated from the parabolic dispersion relation of the Au(111) surface state electrons. The intervalley scattering of graphene electrons forms discs in the Fourier transforms of constant-energy maps, which include additional scattering features compared to monolayer graphene.

[1] Coraux, J. et al., New J. Phys. 11, 023006 (2009)

TT 29.12 Mon 18:45 WIL C107

Improved effective theories for edge magnetism — •Cornelie Koop and Manuel Schmidt — Institut für Theoretische Festkörperphysik, RWTH Aachen University, Deutschland

We consider the effective interaction between edge states in graphene nanoribbons. Low-energy edge states come along with a strongly enhanced density of states near the graphene edges, which makes electron-electron correlation important and gives rise to the so-called edge magnetism. In a pristine nanoribbon in first order, there is a direct ferromagnetic intra-edge coupling and an antiferromagnetic interaction between opposite edges. We study the coupling by means of an effective model yielding a separation between edge and bulk states. In particular we investigate the influence of the bulk states on the effective edge state theory via a second order Schrieffer-Wolff transformation. Using both numeric and analytic methods, we calculate various correlation functions. We discuss the results for the effective correlations between smooth edges as well as between the strongly localized states at rough edge structures.

TT 30: Superconductivity - Poster Session

Time: Monday 15:00–19:00 Location: P2

TT 30.1 Mon 15:00 P2

Sample size dependence of the Josephson behavior of the interfaces in pyrolytic graphite — Ana Ballestar and •Pablo Esquinazi — Division of Superconductivity and Magnetism, University of Leipzig, Leipzig, Germany

Transport properties of TEM lamella graphite samples with embedded interfaces show evidence for granular superconductivity at elevated temperatures [1]. We show that the observed transition temperature decreases linearly with the sample/interface width, and finally vanishes for width size below 200 nm. We discuss the possible origin for this size dependence in terms of weak localization in two dimensions as found in superconducting/normal multilayers [2]. Our results clarify the different temperature dependence of the resistance in bulk pyrolytic graphite samples as well as the difference in the temperature region where a Josephson critical behavior is measured in graphite TEM lamellae.

[1] A. Ballestar et al., New Journal of Phys., 15, 023024 (2013)
[2] J. Guimpel et al., J Low Temp Phys 63, 151 (1986)

TT 30.2 Mon 15:00 P2

Organic crystals: From semi- to superconductors — •Antonia Morherr, Sebastian Witt, Christian Klein, Jan-Peter Bäcker, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt am Main, Deutschland

Intercalated aromatics became attractive in the last years as new class of organic superconductors [1]. Potassium-intercalated picene and phenanthrene showed superconducting transition temperatures of 18 and 5 K. Intercalated Dibenzopentacene reached a T_C of 33.1 K [2], Coronene T_Cs are between 3.5 K and 15 K [3]. So far, all experimental results are obtained on polycrystals, therefore the growth and investigation of single crystals of these materials are of importance for further research in superconductivity. We apply horizontal vapor growth and solution growth intercalation techniques for deeper understanding of the physical properties. Doping with potassium is achieved by co-crystallization and two zone gas transport. In this contribution, we present the physical and structural properties of intercalated single crystals and powder samples. To this end magnetization, resistivity and heat capacity was measured down to 1.8 K.

[1] R. Mitsuhashi et al., Nature 464, 76 (2010)
[2] M. Xue et al., Scientific Reports 2, 389 (2012)
[3] Y. Kubozono et al., Phys. Chem. Chem. Phys. 13, 16476 (2012)

TT 30.3 Mon 15:00 P2

Direct measurement of the magnetic anisotropy of thin sputtered MgB_2 films on MgO substrates in high magnetic fields — •Savio Fabretti[1], Inga-Mareen Imort[1], Timo Kuschel[1], Thomas Dahm[1], Andy Thomas[1,2], Veerendra K. Guduru[3], and Uli Zeitler[3] — [1]Bielefeld University, Bielefeld, Germany — [2]Johannes Gutenberg, Mainz, Germany — [3]Radboud University, Nijmegen, Netherlands

We investigated the magnetic anisotropy ratio of thin sputtered polycrystalline MgB_2 films on MgO substrates. Using high magnetic field measurements, we estimated an anisotropy ratio of 1.35 for T=0 K with an upper critical field of 31.74 T in the parallel case and 23.5 T in the perpendicular case. Direct measurements of a magnetic-field sweep at 4.2 K show a linear behavior, confirmed by a linear fit for magnetic fields perpendicular to the film plane. At an applied magnetic field parallel to the film plane, a deviation from the upper critical field of 3 T was observed by using magnetic sweep measurements; this deviation may be attributable to the different crystal sizes in the polycrystalline films. Furthermore, we observed a change of up to 12% of the anisotropy ratio in dependence of the film thickness.

TT 30.4 Mon 15:00 P2

High trapped fields in MgB_2 bulk samples — •Wolfgang Hässler[1], Günter Fuchs[1], Konstantin Nenkov[1], Juliane Scheiter[1], Axel Handstein[1], Bernhard Holzapfel[1,2], and Ludwig Schultz[1] — [1]Leibniz Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, P.O. Box 270116, 01171 Dresden — [2]Karlsruhe Institute of Technology (KIT), Institute for Technical Physics, P.O. Box 3640, 76021 Karlsruhe

MgB_2 is a promising superconductor for bulk trapped field magnets operating between 15 and 20 K. The absence of weak-link behavior in MgB_2 offers the advantage of a simple and cost-effective technique for fabrication of large bulks with high trapped fields. Bulk superconducting MgB_2 samples, 20 mm in diameter, were prepared by hot-pressing of high energy milled Mg and B powders using nanosized boron powders. High maximum trapped fields of 5.4 T were obtained at 12 K by Hall probe measurements at the centre of the bulk surface in one of the trapped field magnets (height 8 mm). For short MgB_2 samples (height 1.6 mm), trapped fields up to 3.2 T were achieved at 15 K. These high trapped fields are related to extremely high critical current densities up to 10^6 A/cm^2 at 15 K indicating strong pinning due to nano-crystalline MgB_2 grains. The measured trapped field of 5.4 T at 12 K is the highest reported so far. By increasing height and/or diameter of these bulk MgB_2 samples, even higher trapped fields are expected which demonstrates the large potential of MgB_2 trapped field magnets in the field of engineering applications at temperatures between 15 and 20 K

TT 30.5 Mon 15:00 P2

Thick $BaHfO_3$ doped $YBa_2Cu_3O_{7-\delta}$ films on textured Ni-W tapes — •Max Sieger[1], Jens Hänisch[1], Kazumasa Iida[1], Uwe Gaitzsch[1], Christian Rodig[1], Rainer Nast[2], Ludwig Schultz[1], Bernhard Holzapfel[2], and Ruben Hühne[1] — [1]Institute for Metallic Materials, IFW Dresden, PO Box 27 01 16, D-01171 Dresden, Germany — [2]Institute for Technical Physics, Karlsruhe Institute of Technology

(KIT), PO Box 36 40, D-76021 Karlsruhe

High-temperature superconductors grown on metallic tapes (coated conductors) might be used in a wide range of applications such as electric cables, MRI and fusion magnets. To achieve highest transport currents in magnetic fields, flux lines have to be immobilized by introducing nanoscaled pinning centres. In this study, we have prepared $YBa_2Cu_3O_{7-\delta}$ (YBCO) thick films (~ 1 μm) with different amounts of $BaHfO_3$ (BHO) on highly alloyed biaxially textured Ni-W tapes by pulsed laser deposition and discuss the effect of deposition parameters and BHO contents on the superconducting properties. X-Ray diffraction showed a good texture transfer from the nickel alloy tape via the buffer system to the superconducting layer. In general, a superconducting transition temperature T_c of about 88 K with a small transition width was determined. The incorporation of artificial pinning centres led to improved in-field critical current densities $J_c(\mu_0 H)$ and to an increase of the irreversibility field H_{irr}.

TT 30.6 Mon 15:00 P2

Ba_2YNbO_6 and Ba_2YTaO_6 doped $YBa_2Cu_3O_{7-\delta}$ films — •Lars Opherden[1], Jens Hänisch[1], Max Sieger[1], Marco Bianchetti[2], Judith MacManus-Driscoll[2], Ludwig Schultz[1], and Ruben Hühne[1] — [1]Institute for Metallic Materials, IFW Dresden, Dresden, Germany — [2]Department of Material Science and Metallurgy, University of Cambridge, Cambridge , UK

High-temperature superconductors might be applied in advanced electromagnets for the purpose of high field experiments. To realize such new types of superconducting magnets, the critical current density of high-temperature superconductors like $YBa_2Cu_3O_{7-\delta}$ (YBCO) needs to be improved. To achieve this goal, flux lines have to be immobilized in particular at the application temperature. Therefore, we introduce nanoscaled pinning centers applying YBCO targets mixed with different amounts of the secondary phases. The incorporation of Ba_2YNbO_6 and Ba_2YTaO_6 nanoparticles in the YBCO matrix leads to the formation of very fine self-assembled nanorods with significantly improved critical current densities $J_c(B,\theta)$[1,2]. To study this behavior in more detail, thin undoped and doped films were prepared on single crystalline substrates by pulsed laser deposition. X-ray diffraction and texture measurements were carried out to determine the crystal structure, whereas inductive and transport current measurements were performed to evaluate the superconducting properties T_c and $J_c(B)$ in different temperature regions.

[1] G. rcolano *et al.*, Supercond. Sci. Technol. **24** (2011) 095012
[2] S. A. Harrington *et al.*, Supercond. Sci. Technol. **22** (2009) 022001

TT 30.7 Mon 15:00 P2

Superconductivity in epitaxial Ru-doped $BaFe_2As_2$ thin films — •Marco Langer[1,2], Jan Engelmann[1,2], Vadim Grinenko[1], Eike Ahrens[2], Fabian Nitsche[3], Bernhard Holzapfel[1,4], Ludwig Schultz[1,2], and Ruben Hühne[1] — [1]Institute for Metallic Materials, IFW Dresden, PO Box 270116, D-01171 Dresden, Germany — [2]Dresden University of Technology, D-01062 Dresden, Germany — [3]Ludwig-Maximilians-University Munich, Department of Chemistry, D-81377 Munich, Germany — [4]Karlsruhe Institute of Technology, Institute for Technical Physics, D-76344 Eggenstein-Leopoldshafen, Germany

The iron pnictide $BaFe_2As_2$ (Ba122) exhibits superconductivity either by carrier doping, chemical pressure, strain or external pressure. The key parameter for controlling the phase diagram of Ba122 is still under debate.

In order to investigate the driving factor of superconductivity in more detail we prepared thin Ba122 films with different ruthenium doping levels on single-crystal substrates using pulsed laser deposition. Structural investigations were carried out using θ-2θ x-ray diffraction and texture measurements revealing an epitaxial growth of the thin films. Electronic transport and SQUID-susceptibility measurements were performed to determine the electronic phase diagram. The results will be discussed in comparison to published phase diagrams for bulk materials.

TT 30.8 Mon 15:00 P2

Delta-doped $La_{2-x}(Sr,Ba)_xCuO_4$ thin films grown by oxide molecular beam epitaxy — •Christopher Dietl, Federico Baiutti, Meng Wu, Georg Cristiani, Gennady Logvenov, Eva Benckiser, and Bernhard Keimer — Max-Planck-Institute for Solid-State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

We investigate the possibility of delta-doping LCO thin films by replacing selectively LaO-layers by SrO or BaO. In this fashion, a modulated dopant distribution is created, which is predicted to enhance spin fluctuations and thus T_C [1]. The necessary atomic layer-by-layer growth capability is achieved with a state of the art Molecular Beam Epitaxy (MBE) setup allowing to grow films with typical surface roughnesses of $\approx$ 5Å. Oxidization of copper under high vacuum is performed via ozone. The growth is monitored in-situ by Reflection High Energy Diffraction (RHEED) for qualitative stochiometry control. Characterization is performed via XRD, XRR and AFM. The superlattices show superconductivity with the highest critical temperature being $T_c = 35$K.

[1] T. Jarlborg, Appl. Phys. Lett. 94, 212503 (2009)

TT 30.9 Mon 15:00 P2

Photo-induced quasipersistent modification of the normal and superconducting properties of niobium thin films — •Daniel Kohlberger[1], Daniel Bothner[1], Elisabeth Koroknay[2], Michael Jetter[2], Peter Michler[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Collective Quantum Phenomena in LISA$^+$, Universität Tübingen, Germany — [2]Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, Universität Stuttgart, Germany

We report on the experimental investigation of resistive and superconducting transport properties of niobium thin films, which have been irradiated with an infrared laser at cryogenic temperatures. After irradiation, we find an increased normal state resistivity and a reduced transition temperature T_c to the superconducting state with respect to the values before irradiation. This photo-induced modification is completely reversible by raising the sample temperature to $T > 60$ K, but remains unchanged over large timescales at lower temperatures. In addition, we demonstrate that by a spatially periodic variation of the laser intensity across the niobium film, the reported effect can be used to generate a periodic pinning potential for Abrikosov vortices at $T < T_c$. This periodic potential is revealed by the occurrence of matching features in the dependence of the critical current I_c on an applied magnetic field B after laser irradiation. Finally, we discuss possible mechanisms of the observed effect.

TT 30.10 Mon 15:00 P2

Magneto-acoustic quantum oscillations in YNi_2B_2C — J. Nössler[1], •S. Yasin[1], S. Erfanifam[1], R. Seerig[1], G. Behr[2], S. Zherlitsyn[1], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, D-01069 Dresden, Germany

Magneto-acoustic quantum oscillations in the type-II superconductor YNi_2B_2C (T_c=15.5 K) have been investigated providing information about the effective mass and Dingle temperature for selected electron orbits. Remarkably, the quantum oscillations in the sound velocity have been observed not only in the normal state but even below the upper critical field, $B_{c2} = 8.2$ T, down to 3.6 T. Torque measurements performed with the same sample have revealed a complete suppression of the dHvA oscillations below B_{c2}. The marginal additional damping of the acoustic oscillations observed in the mixed state suggests that the corresponding electron band does not contribute to the superconductivity. This additional damping can be ascribed to the field inhomogeneity in the Shubnikov phase. Angular dependent ultrasound experiments in static (up to 18 T) and pulsed (up to 61 T) magnetic fields applied in the (010) plane have revealed four frequencies observed as well in earlier torque measurements and predicted from band-structure calculations. A new unknown frequency of 6756 T has been resolved from the pulsed-field ultrasound experiments.

TT 30.11 Mon 15:00 P2

Strong coupling behavior of the neutron resonance mode in unconventional superconductors — •Patrik Hlobil, Boris Narozhny, and Jörg Schmalian — Karlsruhe Institute of Technology

We analyze whether and how the neutron resonance mode in unconventional superconductors is affected by higher order corrections in the coupling between spin excitations and fermionic quasiparticles and find that in general such corrections cannot be ignored. In particular, we find that in two spatial dimensions(d=2) the corrections are of same order as the leading, weak coupling contributions demonstrating that the neutron resonance mode in unconventional superconductors is a strong coupling phenomenon. The origin of this behavior lies in the quantum-critical nature of the low energy spin dynamics in the su-

perconducting state and the feedback of the resonance mode onto the fermionic excitations. While quantum critical fluctuations occur in any dimensionality d<3, they can be analyzed in a controlled fashion by means of the epsilon-expansion (epsilon=3-d), such that the leading corrections to the resonance mode position are small. Even if higher order corrections are taken into account, the resonance mode emerges only if the phase of the superconducting gap function varies on the Fermi surface, making it a powerful tool to investigate the microscopic structure of the pair condensate.

TT 30.12 Mon 15:00 P2

Effect of reduced dimensionality on superconductivity in $CeCoIn_5$ probed by thermal expansion and magnetostriction measurements — •Kai Grube[1], Sebastian Zaum[1,2], Felix Eilers[1], Roland Schäfer[1], Eric D. Bauer[3], Joe D. Thompson[3], and Hilbert v. Löhneysen[1,2] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology, Physikalisches Institut, 76131 Karlsruhe, Germany — [3]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

In $CeCoIn_5$, a route towards reduced dimensionality is provided by an elongation of the unit cell along the *c*-axis. To determine the related strain dependences of T_c and B_{c2}, we measured thermal expansion and magnetostriction of $CeCoIn_5$ single crystals. The dependence of the strong-coupling parameter was estimated by the ratio between specific heat discontinuity at T_c and Sommerfeld coefficient. Our results show that B_{c2} grows with increasing *c*-axis lattice parameter due to an increase of the strong coupling nature of the superconductivity. This is in agreement with a recent study on artificial superlattices of alternating superconducting $CeCoIn_5$ and metallic $YbCoIn_5$ layers in which reducing dimensionality increases the ratio B_{c2}/T_c [1].
[1] Y. Mizukami et al., Nature Phys. 7, 849 (2011).

TT 30.13 Mon 15:00 P2

Strong electron-phonon coupling and the superconducting energy gap in $SrPt_3P$ — •Diego A. Zocco[1], Sven Krannich[1], Rolf Heid[1], Klaus-Peter Bohnen[1], Thomas Forrest[2], Alexei Bossak[2], and Frank Weber[1] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany. — [2]European Synchrotron Radiation Facility, F-38043 Grenoble Cedex, France.

We present a study of the lattice dynamical properties of the recently discovered superconductor $SrPt_3P$ ($T_c = 8.4$ K) via high-resolution inelastic x-ray scattering performed on a polycrystalline sample. Previous specific-heat measurements reveal evidence for very strong coupling *s*-wave superconductivity ($2\Delta/k_BT_c \sim 5$) [1], consistent with our *ab initio* calculations which yield a large electron-phonon coupling constant $\lambda \sim 2$. Our data suggests that a softening of a low-energy phonon mode occurs as temperature is lowered from 300 K to 10 K. Possible effects upon entering the superconducting state will also be discussed. Our insight into the pairing mechanism in this new superconducting compound will be important for the understanding of Pt-based superconductors in general, in particular the closely related heavy-fermion non-centrosymmetric superconductor $CePt_3P$.
[1] T. Takayama, Phys. Rev. Lett. **108**, 237001 (2012)

TT 30.14 Mon 15:00 P2

Multigap superconductivity in locally non-centrosymmetric SrPtAs as revealed by nuclear quadrupole resonance — •Felix Brückner[1], Rajib Sarkar[1], Marco Günther[1], Hans-Henning Klauss[1], Hannes Kühne[2], Hubertus Luetkens[3], Pabitra Biswas[3], and Titus Neupert[4] — [1]Technische Universität Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Paul Scherrer Institut, Villigen, Switzerland — [4]Princeton University, Princeton, USA

The recently discovered compound SrPtAs has awakened grown scientific interest, because it comprises an exceptional structural feature: it consists of non-centrosymmetric PtAs layers that are weakly coupled to each other. Theoretical calculations predict an unconventional chiral d-wave superconducting state which is unique in material science.

This is in line with evident breaking of time reversal symmetry in μSR experiments.

Our nuclear quadrupole resonance experiments reveal multigap superconductivity and a fully gapped state. In particular, we present spin-lattice relaxation rate ($1/T_1$) measurements and discuss possible pairing symmetries. These results are relevant to understand the pairing mechanism in this and similar compounds.

TT 30.15 Mon 15:00 P2

Fermi surface investigations on the filled skutterudite $LaRu_4As_{12}$ superconductor — •J. Klotz[1,2], K. Götze[1,2], V. Petzold[3], H. Rosner[3], T. Cichorek[4], Z. Henkie[4], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor (HLD), Helmholtz-Zentrum Dresden-Rossendorf — [2]Institut für Festkörperphysik, TU Dresden — [3]Max-Planck-Institut CPfS, Dresden — [4]INTiBS PAN, Wroclaw

Filled skutterudite compounds RT_4Pn_{12} (*R*: rare-earth element, T = Fe, Ru, Os, Pn = P, As, Sb) exhibit a large variety of phenomena such as exceptionally high thermoelectric power, heavy-fermion superconductivity or metal-insulator transition [1]. Within this class, $LaRu_4As_{12}$ features outstanding superconducting properties (T_c = 10.45 K and $\mu_0 H_{c2} \approx 10.2$ T). The magnetic-field dependence of the electronic specific-heat coefficient γ and the positive curvature of $H_{c2}(T)$ close to T_c indicate the existence of multiple superconducting gaps, making $LaRu_4As_{12}$ a rare example of a cubic superconductor displaying multiband effects [2]. Employing a capacitive torque magnetometer at temperatures down to 20 mK and in fields up to 35 T, we probed the angular dependence of the de Haas-van Alphen effect. We determined effective masses of different bands expecting enhanced masses due to the rather large γ = 59 mJ/mol K^2. In combination with density-functional band-structure calculations, our results provide detailed information about the Fermi surface of $LaRu_4As_{12}$.
[1] M. B. Maple, E. D. Bauer, *et al.*, Physica B, **328**, 29-33 (2003).
[2] L. Bochenek, R. Wawryk, *et al.*, Phys. Rev B. **86**, 060511(R) (2012).

TT 30.16 Mon 15:00 P2

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

We have demonstrated the coexistence of superconductivity and ferromagnetism in Bi_3Ni nanostructures which have been prepared by making use of novel chemical-reaction paths [1]. Here, we present recent experiments on novel nanostructures, such as supercrystals consisting of packed Bi_3Ni nanofibers. We have investigated their magnetic and electrical-transport properties by means of XMCD, SQUID magnetometry, pulsed-field susceptometry, and ac-resistance measurements in a wide field and temperature range. Resistivity measurements demonstrate that superconductivity persists well above the Pauli limiting field - with strong anisotropy. These results will be presented in the context of a coexistence of superconductivity and ferromagnetism.

Part of this work was performed at the NHMFL and ESRF beamline ID08.
[1] T. Herrmannsdörfer, R. Skrotzki, J. Wosnitza, D. Köhler, R. Boldt, M. Ruck, Phys. Rev. B 83, 140501 (R) (2011).

TT 30.17 Mon 15:00 P2

^{119}Sn NMR investigations on superconducting $Ca_3Ir_4Sn_{13}$ — •Rajib Sarkar[1], Felix Brueckner[1], Marco Günter[1], Cedomir Petrovic[2], Kefeng Wang[2], Hubertus Luetkens[3], Pabitra Biswas[3], Elvezio Morenzoni[3], Alex Amato[3], and Hans-Henning Klauss[1] — [1]IFP, TU Dresden, D-01069 Dresden, Germany — [2]CMPMS, BNL, Upton, NY-11973, USA — [3]PSI, CH-5232 Villigen PSI, Switzerland

$Ca_3Ir_4Sn_{13}$ was found to exhibit superconducting transition with $T_c \approx 7$ K. It received considerable attention due to the possible coexistence of superconductivity and ferromagnetic spin fluctuation as well as the three-dimensional charge density wave (CDW) from the superlattice transition. [1,2] While thermal, transport, and thermodynamic characterization of $Ca_3Ir_4Sn_{13}$ single crystals suggest that it is a weakly correlated nodeless superconductor, recent μSR investigation reveals that the electron-phonon pairing interaction is in the strong-coupling limit. Here we present ^{119}Sn NMR investigations on $Ca_3Ir_4Sn_{13}$ polycrystalline samples and discuss the symmetry of the superconducting order parameter together with the normal state properties. Our preliminary results of spin-lattice relaxation rate ($1/T_1$) indicate that this is a BCS superconductor with weak-coupling limit.
[1] J. Phys. Soc. Jpn. 19, 113705 (2010).

[2] Phys. Rev. Lett. 109, 237008 (2012).

TT 30.18 Mon 15:00 P2

Doping-induced superconductivity in germanium — •M. Naumann, R. Skrotzki, T. Herrmannsdörfer, R. Schönemann, V. Heera, J. Fiedler, M. Voelskow, A. Mücklich, B. Schmidt, W. Skorupa, M. Helm, and J. Wosnitza — Hochfeld-Magnetlabor Dresden (HLD) und Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O. Box 51 01 19, D-01314 Dresden, Germany

We report observations of superconductivity in highly doped germanium. High dopant concentrations of Al, B, Ga, In, Nb, P, or Sn have been introduced into nanolayers of Ge wafers via ion implantation. The electrical-transport properties of these thin-film samples strongly depend on the element type of dopant atoms, implantation dose, and on subsequent short-term annealing procedures. For Ge:Ga and Ge:In, we observe the emergence of superconductivity for certain sample-preparation conditions. In particular, the occurence of superconductivity requires well balanced flash-lamp or rapid thermal annealing conditions. On the one hand, the local temperature increase during annealing needs to be sufficiently intense to effectively activate dopant atoms as charge carriers. On the other hand, overheating and entire separation of dopant atoms in the germanium matrix needs to be avoided. Most likely, the superconducting state in highly doped germanium is triggered in dopant rich nano clusters and streched over their entire thin-film zone through percolation, tunneling, or proximity-effect networks.

TT 30.19 Mon 15:00 P2

Magnetic-field-dependent reentrant superconductivity in Ga-implanted Si — •R. Skrotzki, T. Herrmannsdörfer, R. Schönemann, V. Heera, J. Fiedler, E. Kampert, F. Wolff-Fabris, T. Förster, M. Voelskow, A. Mücklich, B. Schmidt, W. Skorupa, M. Helm, and J. Wosnitza — Hochfeld-Magnetlabor Dresden (HLD) und Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany

We have implanted Ga ions into Si wafers and thereby formed 10 nm thin films of densely-packed amorphous Ga clusters. Via short-term annealing we are able to trigger a structural superconductor-insulator transition. On its superconducting side ($T_c \approx 7$ K), we observe a reentrant transition where zero resistance is intermitted by finite resistance at 0.1 K $< T <$ 1 K. This phenomenon is accompanied by non-linear current-voltage characteristics and suppressed at in- and out-of-plane oriented magnetic fields $H > H_{\mathrm{reentrant}}$. Moreover, we find that $H_{\mathrm{reentrant}}$ accounts for up to 10 T and reveals the same anisotropy as H_{c2} indicating a strong dependence on the vortex density in this non-magnetic material. A detailed phase diagram is drawn from magneto-transport measurements in high magnetic fields of more than 40 T. We assume that fluctuations are responsible for paraconductivity of 2D Aslamazov-Larkin type at $T > T_c$ as well as for the reentrant phenomenon at $T < T_c$. The latter we discuss in terms of thermally activated phase-slip processes in conjunction with transport dynamics of resistively and capacitively shunted superconducting tunnel networks.

TT 30.20 Mon 15:00 P2

Electronic properties of undoped and doped aromatic hydrocarbon systems — •Friedrich Roth[1], Benjamin Mahns[2], Eric Müller[2], Bernd Büchner[2], and Martin Knupfer[2] — [1]Center for Free-Electron Laser Science / DESY, Notkestraße 85, D-22607 Hamburg, Germany — [2]Institute for Solid State and Materials Research Dresden, Helmholtzstraße 20, D-01069 Dresden, Germany

Tuning the electronic structure and carrier density by intercalation is crucial to modern day semiconductor technology. In general, the carrier density plays a pivotal role for the materials properties, because intercalation can induce, e. g., a charge transfer, a shift of the Fermi energy and in general wide-ranging changes in the electronic properties of the system. Furthermore, the prerequisite for the understanding of physical properties of new materials is the knowledge of the electronic structure, both in the undoped as well as in the intercalated phase. After the discovery of superconductivity in potassium doped picene with a rather high transition temperature (of 18 K) polyaromatic hydrocarbons came back into the focus of researcher. In this context, this work presents a summary of the investigations on the electronic structure of several aromatic hydrocarbon systems using electron energy-loss spectroscopy (EELS).

TT 30.21 Mon 15:00 P2

Investigation of the electronic properties of the dual-layered charge transfer salt κ-α'-(BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE) — •Michaela Altmeyer, Roser Valenti, and Harald O. Jeschke — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

In recent experimental work the synthesis of κ-α'-(BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE) was achieved, which was reported to be a superconductor below a critical temperature of 11.1K. The crystal is the first superconducting dual-layered charge transfer salt containing BEDT-TTF and consists of alternating layers of κ- and α'-type packed BEDT-TTF molecules. While there are superconductors in the family of (BEDT-TTF)$_2$X salts with a κ-type packing motif, the α'-type packed charge transfer salts tend to be Mott-Hubbard-insulators. Therefore we investigate the electronic properties of the dual-layered system within density functional theory. We compare the electronic structure to that of single-layered compounds with α'-type and with κ-type arrangement of BEDT-TTF molecules. This allows us to disentangle the more complex electronic structure of the title compound.

TT 30.22 Mon 15:00 P2

Stability of supercurrents and condensates in type I superconductors — Pavel Lipavsky[4], •Klaus Morawetz[1,2,3], Bretislav Sopik[5], 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 — [5]Central European Institute of Technology, Masaryk University, Kamenice 735, 62500 Brno, 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 Thouless approach based on the Galitskii T-matrix and the Kadanoff-Martin theory which is in many aspects equivalent to the BCS theory, both lead to zero critical velocity, what is in conflict with the mere existence of supercurrents. In contrast, the T-matrix with multiple scattering corrections provides the critical velocity of pair excitation which is p3-times larger than the critical velocity of pair breaking. This agrees with the experimentally well established fact that supercurrents in type I superconductors are limited by pair breaking, not by pair excitation

TT 30.23 Mon 15:00 P2

DFT Study on 122 pnictide superconductors and related compounds — •Tobias Förster[1], Helge Rosner[2], Andrey Polyakov[1], Marek Bartkowiak[1], Andrea D. Bianchi[3], and Jochen Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Deutschland — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Deutschland — [3]Départment de Physique and RQMP, Université de Montréal, Montréal H3C 3J7, Canada

The Fermi-surface topology of iron-pnictide superconductors stimulated many theories on the pairing mechanism in these materials. Especially the degree of nesting between quasi-two-dimensional hole and electron bands is regarded as a key ingredient. However, also more localized pictures and the duality of both itinerant and localized degrees of freedom of the Fe d electrons are considered. Here, we present a detailed electronic structure study of several AT_2P_2 (A =Ba, La, Ce; T =Fe, Rh, Ir) pnictides with $ThCr_2Si_2$ tetragonal structure type. Applying full potential density functional calculations in different approximations, we attempt to separate the influence of different parameters of the crystal structure on topology and character of the respective Fermi surfaces. For several compounds ($LaFe_2P_2$, $BaIr_2P_2$ und $CeFe_2P_2$), we will compare our calculated results with de Haas-van Alphen measurements and provide implications regarding their superconducting or magnetic properties.

TT 30.24 Mon 15:00 P2

Effect of weak disorder on the phase competition in iron pnictides — •Mareike Hoyer[1], Sergey Syzranov[1,2], and Jörg Schmalian[1,3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany —

[2]Department of Physics, University of Colorado, Boulder, Colorado, USA — [3]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany

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 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] Rafael M. Fernandes and Jörg Schmalian, Phys. Rev. B **82**, 014521

TT 30.25 Mon 15:00 P2

Manifestation of nematic degrees of freedom in the Raman response of pnictides — •Una Karahasanovic and Joerg Schmalian — Karlsruher Institut für Technologie, Wolfgang-Gaede-Str. 1 D-76131 Karlsruhe

The electronic nematic phase in pnictides, characterized by the broken C_4 symmetry, is believed to be generated by the presence of magnetic fluctuations associated with the striped phase [1], and occurs above the magnetic transition temperature. Detecting the presence of nematic fluctuations in iron-based superconductors is a difficult task, since it involves measuring four spin correlation functions. So far, these fluctuations were detected through the changes that they induce in the shear modulus (since the nematic order parameter couples to the orthorombic distortion). The presence of nematic fluctuations is felt even above the nematic transition, i.e. in the tetragonal phase.

Nematic degrees of freedom also manifest themeselves in the experimentally measurable Raman response function, which is a density-density correlation weighted by an appropriate form factor [2, 3]. We calculate the lineshape of the Raman response function in the tetragonal phase by considering Aslamazov-Larkin type of diagrams. We show that the reponse vanishes for the B_{2g} symmetry of the form factor, but not for the B_{1g} symmetry, as observed in the experiment.

[1] R. Fernandes and J. Schmalian, Supercond. Sci. Technol. 25, 084005 (2012).
[2] Y. Gallais et al, arXiv:1302.6255 (2013).
[3] S. Caprara et al, Phys. Rev. Lett. 95, 117004 (2005).

TT 30.26 Mon 15:00 P2

High-pressure synthesis of 1111-pnictides and related systems — •Agnes Adamski[1], Amir Haghighirad[1,2], Steffi Hartmann[1], Natalija van Well[1], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe University, Frankfurt am Main, — [2]University of Oxford, Department of Physics, Oxford

In 2008 Kamihara et al. found a new class of high-T_c superconductors: iron-based oxypnictides. A transition temperature of 26 K in F-doped LaFeAsO (1111-compound) was reported [1]. Replacing the nonmagnetic La ion by magnetic rare-earth elements in 1111-compounds leads to an increase of the superconducting transition temperatur up to ˜50 K. The crystal growth at high pressure/high temperature (HP/HT) conditions has been proven to be an effective method for the 1111-compounds [2][3].

We report on our progress to synthesize single crystals of these compounds under HP/HT conditions with a multi anvil apparatus, so called Walker-Type module. With this apparatus we can achieve rather hydrostatic pressures up to 8 GPa and temperatures up to 1750 K. We found that using NaCl/KCl as flux material is essential to avoid the formation of FeAs and to support the single crystal growth. The same Walker-Type module was used for the synthesis of related pnictides to search for new superconductors. It seems that high pressure is necessary to stabilized these compounds.

[1] Y. Kamihara et al., J. Am. Chem. Soc. 130, 3297 (2008)
[2] J. Karpinski et al., Physica C 469, 370 (2009)
[3] Z. Ren et al., Adv. Mater 21, 4584 (2009)

TT 30.27 Mon 15:00 P2

Microscopic investigations of the electronic phase diagram of $LaOFe_{1-x}Co_xAs$ — •Philipp Materne[1], Giacomo Prando[2], Hemke Maeter[1], Sabine Wurmehl[2,1], Bernd Buechner[2,1], Hubertus Luetkens[3], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]IFW Dresden, Postfach 270016, 01171 Dresden, Germany — [3]Paul-Scherrer-Institut, 5232 Villigen, Switzerland

The antiferromagnetic parent compound, LaOFeAs, can be tuned into a superconducting ground state by doping in the LaO- and in the FeAs-plane. We microscopically investigated the substitution of Fe by Co using muon-spin relaxation spectroscopy in the pure magnetic doping regime as well as in the coexistence regime. The results were compared with published data of $LaO_{1-x}F_xFeAs$ [1], $CeOFe_{1-x}Co_xAs$ and $CeO_{1-x}F_xFeAs$[2].

[1] H. Luetkens *et al.*, Nat. Mater. **8**, 305 (2009)
[2] G. Prando *et al.*, PRB **87**, 174519 (2013)

TT 30.28 Mon 15:00 P2

Antimony Substitution in Rare Earth 1111-Compounds — •Daniel Schmidt, Sebastian Wolf, and Hans F. Braun — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth

The rare earth iron arsenide 1111-compounds are well known oxypnictide high T_c superconductors. The phase diagram of the undoped compounds shows generally two parts, a magnetic and a superconducting phase. With sufficient electron doping in the charge carrier layer, that is substitution of oxygen with fluorine, the magnetic phase transition disappears and superconductivity arises. In our work we try to regain the magnetic phase from the superconducting one. Therefore we perform isostructural substitution at the iron arsenide layer by substituting As with Sb atoms in superconducting electron doped polycrystalline samples. We probe the doping level of Sb by observing the lattice parameters thus we can also test for impurity phases. The physical properties are observed by low temperature measurements of the resistivity and susceptibility.

TT 30.29 Mon 15:00 P2

Temperature dependent density of states study in stoichiometric LiFeAs — •Pranab Kumar Nag[1], Danny Baumann[1], Ronny Schlegel[1], Robert Beck[1], Sabine Wurmehl[1,2], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01171 Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — [3]Center for Transport and Devices of Emergent Materials, TU Dresden, 01069 Dresden

We present scanning tunneling microscopy / spectroscopy data for the stoichiometric iron arsenide superconductor LiFeAs. Temperature dependent tunneling spectra, obtained at a defined position on the surface, reveal a systematic closing of the superconducting gap with temperature, consistent with a bulk critical temperature of 16 K. We have observed a dip-hump structure in the quasiparticle density of states which is the indication of a strong electron-boson coupling in this material.

TT 30.30 Mon 15:00 P2

Induced magnetism in off-stoichiometric LiFeAs — •Robert Beck[1], Uwe Gräfe[1], Igor Morozov[1,2], Philipp Materne[3], Giacomo Prando[1], Hans-Joachim Grafe[1], Sabine Wurmehl[1,3], and Bernd Büchner[1,3] — [1]Leibniz Institute for Solid State and Material Research, D-01171 Dresden, Germany — [2]Moscow State University, Moscow, 119991 Russia — [3]Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany

We prepared a series of polycrystalline $Li_{1-y}Fe_{1+x}As$ samples in a wide range of nominal compositions ($0 < y < 0.1$ and $0 < x < 0.1$). The structure, composition and main characterization physical properties were studied in detail. Seemingly, the composition strongly affects the electronic ground state of the materials, ranging from superconductivity to bulk ferromagnetism. Concomitantly with the evolution of different ordering parameters as function of composition, we observe systematic trends in both line width and frequency of nuclear quadrupole resonance lines.

TT 30.31 Mon 15:00 P2

High-field NMR spectroscopy of the iron-based superconductor LiFeAs — •Hannes Kühne[1,2], Arneil P. Reyes[2], Philip L. Kuhns[2], Hans-Joachim Grafe[3], Saicharan Aswartham[3], Sabine Wurmehl[3], and Bernd Büchner[3] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA — [3]IFW Dresden,

Institute for Solid State Research, D-01171 Dresden, Germany

The iron-based compound LiFeAs exhibits superconductivity below $T_c \simeq 18$ K without introduction of chemical doping. From a number of macroscopic experiments, upper critical fields of 26 T or higher for a magnetic field orientation parallel to the FeAs planes were reported. So far, no local probe techniques were applied for the characterization of the microscopic electronic properties in this high-field parameter regime. We present the results of recently performed high-field NMR experiments on three high quality LiFeAs single crystals, implying upper critical fields much lower than 26 T. We discuss the signatures of the field-induced suppression of the superconducting order parameter, probed by the temperature dependent Knight shift, nuclear spin-lattice and spin-spin relaxation rates for fields and temperatures in the normal and superconducting state.

TT 30.32 Mon 15:00 P2

Local probe studies at copper containing 111 compounds — •Sirko Kamusella[1], Gohil S Thakur[2], Zeba Haque[2], Ashok K Ganguli[2], L C Gupta[2], Hubertus Luetkens[3], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Chemistry, Indian Institute of Technology,110016 New Delhi, India — [3]Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

The recently synthesized LiFeAs-related compounds CuFeAs and CuFeSb [1] are discussed in terms of bulk measurements, ^{57}Fe mössbauer spectroscopy and μSR, comparing it to antiferromagnetic LiFeAs samples. In the compounds presented here the alkali metal sites are replaced by the transition metal copper leading to a stretched Fe-As-bond and therefore deformed As-tetrahedra.

According to these structural differences, CuFeAs and LiFeAs show opposite temperature dependencies of the quadrupolar interaction at the iron site. Furthermore we can confirm the ferromagnetic behavior of CuFeSb [2] up to $T_N = 375$ K, but observe long range antiferromagnetic order below 10 K for CuFeAs, similar to Li-111 samples. Both LiFeAs and CuFeAs show an unusual magnetoelastic coupling, which might play an important role for superconductivity in the 111. We discuss doping options to achieve superconductivity and suggest pressure studies to clarify the effect of pnictide spacing on (anti)ferromagnetism.

[1] G. Thakur *et al.*, unpublished
[2] B. Qian *et al.*, Phys. Rev. B. **85** (2012) 144427

TT 30.33 Mon 15:00 P2

Dilatometric measurements of the detwinning process in $EuFe_2As_2$ — •Ina-Marie Pietsch, Christian Stingl, Hirale S. Jeevan, Jannis Maiwald, Nora Bach, and Philipp Gegenwart — I.Physikalisches Institut, Georg-August Universität, Göttingen, Germany

For the investigation of the anisotropic in-plane behavior of high temperature superconductors we need easy and practicable methods for detwinning single crystals. In our experiments the thermal expansion and magnetostriction has been used to analyze the detwinning process of $EuFe_2As_2$ in a magnetic field. This technique has the advantage that anisotropic behavior can be studied without applying external stress to the system. Using high-resolution capacitive dilatometry we can detect length changes related to the movement of domains due to an applied magnetic field. We examined the detwinning process for a large temperature range above and below the magnetic ordering transition of Eu spins at 19 K. Strikingly, the field-induced detwinning is permanent upon warming up to the structural transition at 187 K, which allows to investigate the anisotropic properties of the system over a wide temperature range.

TT 30.34 Mon 15:00 P2

Optical investigation of the in-plane anisotropy on the underdoped $EuFe_2(As_{1-x}P_x)_2$ single crystals — •shuai jiang[1], hirale s. jeevan[2], philipp gegenwart[2], and martin dressel[1] — [1]1.Physikalisches Institut, Universität Stuttgart, Deutschland — [2]I.Physikalisches Institut, Universität Göttingen, Deutschland

Applying uniaxial pressure enables us to detwin the iron-pnictide single crystal and detect the in-plane anisotropy. The effect of this external factor on the nematicity, however, is under debate. We have studied the in-plane anisotropy of as-grown $EuFe_2(As_{1-x}P_x)_2$ single crystals by optics measurements. The single crystal exhibits stripes in the micrometer range because of the birefringence of the twinned domains. Surprisingly, even without using the mechanical detwinning, the mid-infrared optical properties reveal an anisotropy that becomes pronounced below the structural transition temperature. The amplitude is comparable to the anisotropy of the fully detwinned single crystal. This observation is consistent with the SI-STM measurements on the atomic scale. Our in-situ study explores a new way to investigate the intrinsic dynamics of nematicity in iron pnictides.

TT 30.35 Mon 15:00 P2

A light scattering study of detwinned $BaFe_2As_2$ — •Andreas Baum[1], Andreas Walter[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 with a focus on lattice dynamics. Using uniaxial pressure to detwin the sample allows us to resolve anisotropic features as well as a separation of the structural and magnetic phase transitions.

The As A_{1g} phonon shows a resonance at high energies. With the polarizations aligned along either the antiferromagnetically or the ferromagnetically ordered direction the resonance profile is distinctly different.

The splitting of the E_g phonon at $135\,\mathrm{cm}^{-1}$ into two modes having B_{2g} and B_{3g} symmetry can be attributed to the transition into the magnetically ordered state rather than the structural transition.

TT 30.36 Mon 15:00 P2

Resistivity anisotropy measurements on $Ca(Fe_{1-x}Co_x)_2As_2$ — •Stephan Knöner[1], Bernd Wolf[1], Harald Schubert[1], Sheng Ran[2], Paul 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

Electronic nematicity has been discussed intensively in the research on iron-pnictide superconductors. Evidence for electronic nematicity has been reported from various experiments including magnetic torque measurements [1], scanning tunneling microscopy [2] as well as electronic transport [3]. The nematicity manifests itself in a strong anisotropy in electrical resistance of single crystals detwinned by the application of mild uniaxial strain [3]. Different experimental and theoretical studies support the idea that the transport anisotropy basically results from anisotropic scattering by dopant-induced impurity states [2]. In this contribution, we present measurements of the electrical resistance on detwinned high-quality single crystals of $Ca(Fe_{1-x}Co_x)_2As_2$ with different doping levels x. We discuss the size of the anisotropy, its dependence on the doping level and the effect of hydrostatic pressure tuning [4].

[1] S. Kasahara *et al.*, Nature **486**, 382 (2012)
[2] M. P. Allan *et al.*, Nature Physics **9**, 220 (2013)
[3] J. Chu *et al.*, Science **329**, 824 (2010)
[4] E. Gati *et al.*, PRB **86**, 220511(R) (2012)

TT 30.37 Mon 15:00 P2

Spin Reorientation and Resonance Mode in $Ba_{1-x}Na_xFe_2As_2$ — •Florian Wasser[1], Sabine Wurmehl[2], Saicharan Aswartham[2], Yvan Sidis[3], Astrid Schneidewind[4,5], Ji-Tae Park[5], Bernd Büchner[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany — [2]Institute for Solid State Research, IFW Dresden, D-01171 Dresden, Germany — [3]Laboratoire Léon Brillouin, CEA-CNRS, CEA Saclay, 91191 Gif-sur-Yvette Cedex, France — [4]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation At MLZ, D-85747, Garching, Germany — [5]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM-II), TU München, D-85747 Garching, Germany

Iron-pnictides are a novel class of superconductors displaying a close relation between structure, superconductivity and magnetism. Most parent compounds exhibit a coupled structural and magnetic transition that becomes suppressed upon doping. Here we present our neutron scattering studies on $Ba_{1-x}Na_xFe_2As_2$ which differs from the other systems: At intermediate Na concentrations we find clear evidence for a spin reorientation from in-plane to out-of-plane alignment of the ordered moments. The low-temperature phase with c-aligned moments is unique in this system but it qualitatively agrees with the single-ion anisotropy in pure $BaFe_2As_2$ where it costs less energy to rotate spins from the plane to the c direction than rotating them within the plane. In addition we find a sharp resonance feature in $Ba_{1-x}Na_xFe_2As_2$ at low energy and a broader upturn in intensity at energies comparable

to those of the resonance values in Co or Ni doped compounds.

TT 30.38 Mon 15:00 P2

Low-temperature specific heat of $K_{0.71}Na_{0.29}Fe_2As_2$ down to 20 mK — •Andreas Reifenberger, Marius Hempel, Andreas Fleischmann, Ruediger Klingeler, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, D-69120 Heidelberg

Specific heat measurements on $K_{1-x}Na_xFe_2As_2$ at very low temperatures are helpful for the understanding of the underlying symmetry and magnitude of the superconducting order parameter. To perform the measurements, we used a commercially available calorimeter which we calibrated in the temperature range $0.02\,\mathrm{K} \leq T \leq 0.8\,\mathrm{K}$. The data on $K_{0.71}Na_{0.29}Fe_2As_2$ imply the presence of a large T^2 contribution to the specific heat which gives evidence of d-wave symmetry of the superconducting order parameter on almost all Fermi-surface sheets. To extend these measurements to even lower temperatures, we have designed a novel calorimeter based on magnetic thermometry. We expect a temperature resolution $\Delta T \approx 0.1\,\mu\mathrm{K}$ and an addenda heat capacity of less than $200\,\mathrm{pJ/K}$ for $T < 100\,\mathrm{mK}$.

TT 30.39 Mon 15:00 P2

The electronic phase diagram of $Ba_{1-x}Rb_xFe_2As_2$ investigated by thermodynamic measurements — •D. Gruner[1], F. Steckel[1], V. Grinenko[1], S. Aswartham[1], C. Hess[1], A. U. B. Wolter[1], S. Wurmehl[1,2], and B. Büchner[1,2] — [1]Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01062 Dresden, Germany

After the discovery of a spin-density-wave (SDW) anomaly at 140 K in $BaFe_2As_2$ by Rotter et al., superconductivity (SC) was achieved in this material by hole-doping with potassium [1]. Since $RbFe_2As_2$ shows bulk SC at 2.6 K [2], via a partial substitution of Ba with Rb in Ba122 the crossover from SC to magnetism can be studied in detail. We have synthesized single crystals of $Ba_{1-x}Rb_xFe_2As_2$ by using the self-flux high temperature solution growth technique. Via AC-susceptibility, specific heat and electrical resistivity measurements the SDW and superconducting behavior was investigated. The corresponding electronic phase diagram of $Ba_{1-x}Rb_xFe_2As_2$ has been constructed. While the substitution of Ba^{2+} with Rb^{+} ions suppresses the SDW anomaly, SC is induced. A superconducting transition as high as ≈ 37.3 K is reached for an Rb content of $x \approx 0.3$. This T_c is comparable to K-doped Ba-122 with $x = 0.4$ and $T_c = 38$ K reported previously [3].

[1] M. Rotter, M. Tegel, and D. Johrendt, Phys. Rev. Lett. **101**, 107006 (2008)
[2] Z. Bukowski *et al.*, Physica C. **470**, Supplement 1, S328 - S329 Superconductivity, (2010)
[3] S. Avci *et al.*, Phys. Rev. B. **85**, 184507 (2012)

TT 30.40 Mon 15:00 P2

Strain experiments on Fe based superconductors using flexible substrates — •Stefan Richter, Sascha Trommler, Fritz Kurth, Kazumasa Iida, Jens Hänisch, Ludwig Schultz, and Ruben Hühne — IFW Leibnitz Institute for Solid State and Materials Research Dresden

Strain is known to have a significant influence on the superconducting properties. Especially uniaxial strain experiments are promising to provide insight in correlations between structure and superconducting properties of anisotropic materials like high temperature superconductors.
However, a systematic investigation of these effects is often difficult since the strain in the sample cannot be easily controlled.
Therefore, we constructed a special bending system that allows changing dynamically the strain in samples based on metallic substrates while simultaneously measuring the electronic properties. Highly textured $Ba(Fe_{(1-x)}Co_x)_2As_2$ thin films grown on flexible IBAD-MgO/Hastelloy substrates by pulsed laser deposition are used for these studies. Depending on the doping level, these films show a superconducting transition temperature of up to 20 K as well as high critical current densities. Based on the bending experiments we will discuss the influence of strain on the superconducting properties.

TT 30.41 Mon 15:00 P2

Preparation and characterization of thin films of the unconventional superconductor FeSe — Eike Venzmer, Alexander Kronenberg, and •Martin Jourdan — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, 55128 Mainz

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 by co-sputtering from separate Fe and Se targets. This method yield superconducting epitaxial thin films on MgO(100) as well as on $YAlO_3$(010) substrates whereas best results have been achieved on MgO(100). The influence of deposition rates and substrate temperature on phase formation, sample homogeneity, morphology and electronic transport properties are discussed. The main advantage of thin films made by sputterdeposition is an improved morphology which is promising for the future integration in planar tunneling junctions for spectroscopic investigations.

TT 30.42 Mon 15:00 P2

Applied dynamic strain on $FeSe_{0.5}Te_{0.5}$ through piezo-electric substrates. — •Sebastian Molatta, Sascha Trommler, Jens Hänisch, Kazumasa Iida, Michael Schulze, Sabine Wurmehl, Bernd Büchner, Ludwig Schultz, and Ruben Hühne — IFW Dresden, PF 27 01 16, 01171 Dresden

$FeSe_{1-x}Te_x$ is the structural most simple iron-based superconductor and shows a high sensitivity to applied strain. Typically, different substrates are used for the variation of static strain states in thin films to investigate the influence of the lattice parameters on the superconducting properties. However, this approach is restricted to thin layers ensuring a coherent growth. An alternative is to use epitaxial films on piezo-electric substrates, which allows the dynamic change of the lattice parameters to examine the influence of strain on the superconducting properties.

Therefore, we grew $FeSe_{0.5}Te_{0.5}$ films by pulsed laser deposition on different substrates. The epitaxial growth was first optimized on MgO single crystals and transferred afterwards to piezoelectric 0.72 $Pb(Mg_{1/3}Nb_{2/3})O_3$-0.28 $PbTiO_3$ (PMN-PT) substrates. In both cases an epitaxial growth and a superconducting transition T_c of more than 15 K were observed under optimized conditions. Finally, a shift in T_c of about 0.25 K for a change of 0.04% in the in-plane lattice-parameters was found in strain experiments for these $FeSe_0.5Te_0.5$-films grown on PMN-PT.

TT 30.43 Mon 15:00 P2

Preparation of planar SN and SNS‘ junctions on Ba-122 iron pnictide single crystals — •Noor Hasan[1], Stefan Schmidt[1], Sebastian Döring[1], Volker Tympel[1], Frank Schmidl[1], Paul Seidel[1], and Thomas Wolf[2] — [1]Friedrich-Schiller- Universität Jena , Institut für Festkörperphysik — [2]Karlsruhe Institute of Technology, Institut für Festkörperphysik

In order to understand the nature of the superconductivity in iron pnictides it is necessary to examine their electrical properties. Therefore we firstly have fabricated planar hybrid superconductor (S) - normal metal (N) - superconductor (SNS*) junctions with a Pb thin film as basis electrode. We used an artificial (barrier) layer which consists of thin normal conducting gold and titanium films. By oxygenation of the titanium we can add an insulating layer to the barrier system. A double layer film of Pb and In was used as the counter electrode. Then we fabricated the same junction type with a basis electrode using undoped $BaFe_2As_2$ single crystals which were produced with a self-flux method. After that we transferred the technology to superconducting Co-doped $BaFe_2As_2$ single crystals. For comparison between them we will present electrical measurements on these junctions. These include R*T measurements on each electrode and the different junction*s types itself as well as temperature dependent I-V characteristic and differential conductance respectively.

TT 30.44 Mon 15:00 P2

Long-range spin transport and spin-charge separation in nanoscale superconductors — Michael J. Wolf[1], Florian Hübler[1,2], Stefan Kolenda[1], Hilbert von Löhneysen[2,3], and •Detlef Beckmann[1] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie — [3]Physikalisches Institut, Karlsruher Institut für Technologie

We report on nonlocal transport in superconductor hybrid structures, with ferromagnetic as well as normal-metal tunnel junctions attached to the superconductor. In the presence of a strong Zeeman splitting of the density of states, we find signatures of spin transport over dis-

tances of several μm [1], exceeding other length scales such as the coherence length, the normal-state spin-diffusion length, and the charge-imbalance length [2]. The relaxation length of the spin signal shows a strong increase with magnetic field, hinting at a freeze-out of relaxation by the Zeeman splitting. Using a combination of ferromagnetic and normal-metal contacts, we demonstrate spin injection from a normal metal, and show a complete separation of charge and spin imbalance [3].

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[2] Hübler et al., Phys. Rev. B **81**, 184524 (2010)
[3] Wolf et al., Phys. Rev. B **87**, 024517 (2013)

TT 30.45 Mon 15:00 P2

Nonlocal transport and heating in superconductors under dual-bias conditions — •Stefan Kolenda[1], Michael J. Wolf[1], Dimitrij S. Golubev[1,2], Andrei Zaikin[1,3,4], and Detlef Beckmann[1] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie — [2]Low Temperature Laboratory (OVLL), Aalto University School of Science — [3]I. E. Tamm Department of Theoretical Physics, P. N. Lebedev Physics Institute, Moscow — [4]Laboratory of Cryogenic Nanoelectronics, Nizhny Novgorod State Technical University

We report on an experimental study of nonlocal transport in superconductor hybrid structures, where two normal-metal leads are attached to a central superconducting wire. Structures of this kind are of interest, since possibly they could serve as Cooper pair splitters, creating spin entangled electrons. With bias voltages below the gap we find s-shaped nonlocal conductance curves as a function of bias applied on both contacts, as predicted theoretically in the presence of dynamical Coulomb blockade (DCB) [1]. With bias voltages above the gap applied on both normal-metal electrodes we find surprisingly large nonlocal conductance signals, almost of the same magnitude as the local conductance. We show that under these conditions heating has a qualitativly similar effect as DCB on nonlocal conductance, mimicking the effect of Cooper pair splitting [2].

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[2] S. Kolenda et al., Phys. Rev. B **88**, 174509 (2013)

TT 30.46 Mon 15:00 P2

Superconductor-Insulator Transition in thin TiN-films — •Klaus Kronfeldner[1], Tatyana Baturina[2], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]A. V. Rzhanov Institute of Semiconductor Physics SB RAS, Novosibirsk 630090 Russia

We measured IV-characteristics and magnetoresistance of thin TiN-films in the vicinity of the disorder-tuned superconductor-insulator transition (SIT) for different square sizes (5μm to 240μm).

While the films are superconducting at $B = 0$T, at finite magnetic fields a SIT occurs with a magnetoresistance peak between $1\text{T} < B(R_{max}) < 2.6\text{T}$ for the different sizes. For temperatures higher than $T \approx 300$mK the magnetoresistance curves cross at a single point between $0.7\text{T} < B(R_{cross}) < 1.7\text{T}$ depending on the size and the $R(B)$ behaves linear for small B. For lower temperatures down to $T = 20$mK the $R(B)$ rises faster than exponential for $B < B(R_{max})$. The magnetoresistance of the smaller samples (5μm to 30μm) is significantly weaker than that of the bigger samples (60μm to 240μm).

The voltage-biased IV-characteristics reveal a highly non-monotonic behavior both at zero magnetic field and at $B(R_{max})$.

TT 30.47 Mon 15:00 P2

Large oscillations of the magnetoresistance in nanopatterned thin aluminum films — Christopher Espy[1], •Julian Braun[1], Omri Sharon[2], Elke Scheer[1], and Yosef Yeshurun[2] — [1]Universität Konstanz, Konstanz, Germany — [2]Bar-Ilan University, Ramat Gan, Israel

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

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

[1] W. A. Little and R. D. Parks, PRL **9**, 9 (1962)
[2] V. Vakaryuk, PRL **101**, 167002 (2008)
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[4] Sochnikov et al., Nat. Nanotech. **5**, 516 (2010)

TT 30.48 Mon 15:00 P2

Analytical solutions for the energy and eigenstates of the flux qubit — •Iris Conradi, Melanie Hauck, Andreas Heimes, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe

We analyze a gap tunable flux qubit and try to find an analytical solution for the eigenstates and their energy values. Using a semiclassical method we analyze the dependence of the potential energie spectrum on the parameters. Then we use a variation principle to determine analytical expressions for the eigenstates. As a first step we study the quartic potential. Here it is possible to find the e.g. the second excited state in good approximation. This allows us to estimate the anharmonicity of the flux qubit, which determines the speed of single qubit operations. Similarly we also find the second excited state of the double well potential.

TT 30.49 Mon 15:00 P2

The multidimensional eigenstates of the flux qubit — •Melanie Hauck, Iris Conradi, Andreas Heimes, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe

In order to show the influence of the second dimension of the gap-tunable flux qubit compared to the common one-dimensional description we construct the two-dimensional eigenstates using the eigenstates of the harmonic oscillator and the double-well potential. At first we analytically describe the eigenstates of the one-dimensional problem with different parameter configurations. Variations of the external flux through the main loop cause an asymmetry in the double-well potential. We find the eigenstate of the double well potential for various parameter regimes. We then numerically estimate how the eigenstates in two dimensions can be decomposed into eigenstates of the double well and an harmonic oscillator.

TT 30.50 Mon 15:00 P2

Tunneling and Relaxation of Single Quasiparticles in a Normal-Superconductor-Normal Single Electron Transistor — •Andreas Heimes[1], Ville Maisi[2,3], Dmitry Golubev[2,4], Michael Marthaler[1], Gerd Schön[1,4], and Jukka Pekola[2] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology, 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 — [4]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany

We investigate the properties of a hybrid single electron transistor, involving a small superconducting island sandwiched between normal metal leads, which is driven by dc plus ac voltages and works as a single electron turnstile. During the turnstile operation quasiparticles are injected onto the superconducting island, 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. Our low-temperature results compare well with recent experimental findings obtained for ac-driven hybrid single-electron turnstiles.

TT 30.51 Mon 15:00 P2

RF-SQUID mediated coupling between microwave resonators — •Fabian Koessel[1,2], Friedrich Wulschner[1], Jan Goetz[1], Borja Peropadre[3], Alexander Baust[1], Elisabeth Hoffmann[1,2], David Zueco[4], Frank Deppe[1,2], Edwin P. Menzel[1], Achim Marx[1], Juan Jose Garcia-Ripoll[3], and Rudolf Gross[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, TU München, Garching, Germany — [3]IFF-CSIC, Madrid, Spain — [4]CSIC-Universidad de Zaragoza and Fundacion ARAID, Spain

Networks of superconducting resonators are promising candidates for

the implementation of analog quantum simulators. In this context it is necessary realize a controllable coupling between nearest neighbor resonators. Furthermore, the coupling strength between the resonators has to be larger than the decay rates of the involved resonators. Here, we present experimental data from two microwave resonators which are coupled via an RF-SQUID. The coupling can be turned on and off by applying an external magnetic field, which changes the operation point of the RF-SQUID. Making use of chains of DC-SQUID intersected nonlinear resonators, these devices may pave the way to simulate bosonic many body Hamiltonians in the driven-dissipative regime.

We acknowledge support from the DFG via SFB 631, the German excellence initiative via NIM, and the EU via PROMISCE.

TT 30.52 Mon 15:00 P2

Squeezing physics and path entanglement of continuous-variable propagating microwaves — •E. P. Menzel[1], L. Zhong[1], R. Di Candia[3], P. Eder[1,2], M. Ihmig[4], A. Baust[1], M. Haeberlein[1,2], C. Schneider[1,2], K. Inomata[5], T. Yamamoto[5,6], Y. Nakamura[5,7], E. Solano[3], F. Deppe[1,2], A. Marx[1], and R. Gross[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, TU München, Garching, Germany — [3]University of the Basque Country UPV/EHU and IKERBASQUE Foundation, Bilbao, Spain — [4]TU München, Germany — [5]RIKEN Center for Emergent Matter Science, Japan — [6]NEC Smart Energy Research Laboratories, Japan — [7]The University of Tokyo, Japan

Josephson parametric amplifiers (JPA) have recently become promising devices in circuit quantum electrodynamics. We report on the detailed characterization of a flux-driven JPA at millikelvin temperatures and investigate its squeezing properties by two different detection techniques. By superimposing a squeezed vacuum and a vacuum state on a microwave beam splitter, we demonstrate a frequency-degenerate, continuous-variable path entanglement, which constitutes an essential resource in quantum information and communication protocols.

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TT 30.53 Mon 15:00 P2

Interference effects in superconducting coplanar waveguide structures — •J. Goetz[1], P. Summer[1,2], H.P. Gürtner[1,2], M.J. Schwarz[1], P. Eder[1], F. Wulschner[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

The freedom in designing superconducting coplanar waveguide (CPW) structures allows for the on-chip creation of electromagnetic fields with well defined spatial intensity distributions. Here we show the precise control of interfering fields which can be used for the control of gradiometer type tunable flux qubits. In addition we study the loss channels which our antenna structures add to CPW resonators. Our setup can be used to explore the manifold physics of gap tunable flux qubits coupled to CPW resonators.

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.

TT 30.54 Mon 15:00 P2

Time and Frequency Domain Characterization of the Superconducting Quantum Switch — •A. Baust[1], E. Hoffmann[1,2], P. Eder[1,2], J. Goetz[1], M. Häberlein[1,2], M. Fischer[1,2], M.J. Schwarz[1], F. Wulschner[1], E. Xie[1], L. Zhong[1], H. Huebl[1], K. Fedorov[1], E.P. Menzel[1], F. Deppe[1,2], A. Marx[1], R. Gross[1,2], E. Solano[3], D. Zueco[4], and J.J. Garcia-Ripoll[5] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, TUM, Garching, Germany — [3]Universidad del Pais Vasco and IKERBASQUE, Bilbao, Spain — [4]CSIC, Zaragoza, Spain — [5]Universidad Complutense, Madrid, Spain

Superconducting quantum circuits with transition frequencies of a few gigahertz form a powerful toolbox for the investigation of fundamental light-matter interaction, quantum simulation, and quantum information processing. For scalable architectures, it is important to establish controllable coupling between such circuits. To this end, we investigate how a three-Josephson-junction flux qubit mediates tunable and switchable coupling between two superconducting transmission line resonators. We demonstrate the switching behaviour in both time and frequency domain. In addition, we show that ultrastrong coupling between the qubit and a resonant mode is present in our system.

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TT 30.55 Mon 15:00 P2

Controlling the coupling between phosphorus donor spins and a superconducting resonator by light — •Kai Mueller[1,2], Christoph W. Zollitsch[1,2], 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

In the field of quantum information processing, phosphorus spin ensembles are discussed for information storage due to their exceptionally long spin coherence- and lifetimes of the order of seconds [1, 2]. On the other hand, their long lifetime limits the rate at which this quantum memory can be set. One strategy to overcome this problem is to shine light on the system to excite the phosphorus donor electrons. We investigate a spin ensemble consisting of phosphorus donors in silicon coupled to a superconducting coplanar waveguide resonator operating at GHz frequencies and below 1 K using microwave spectroscopy. When illuminating the silicon with 1050 nm light, we find that the coupling between the spin ensemble and resonator is reduced, which is compatible with the excitation of donor electrons to the conduction band. Additionally, we will discuss the time constants involved in this process. Financial support via SFB 631 and NIM is gratefully acknowledged.

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[2] G. Feher, Phys. Rev. **114**, 1245 (1959)

TT 30.56 Mon 15:00 P2

Collective Quantum Phase-Slip Dynamics in Superconding Nanowire Arrays — •Sebastian T. Skacel[1], Jan N. Voss[1], Tobias Bier[1], Lucas Radke[1], Martin Weides[1], Hannes Rotzinger[1], Hans E. Mooij[2,3], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, D-76131 Karlsruhe, Germany — [2]Center for Functional Nanostructures, Karlsruher Institut für Technologie, D-76128 Karlsruhe, Germany — [3]Kavli Institute of Nanoscience, Delft University of Technology, 2628 CJ Delft, The Netherlands

Superconducting nanowire arrays exhibit quantum phase-slip (QPS) phenomenon if the superconductor has a very high normal-state sheet resistance. We experimentally study QPS effects in arrays of nanowires embedded in a resonant circuit at GHz frequencies. We probe this circuit at ultra-low microwave power, applied flux and mK temperatures. The nanowires are fabricated utilizing aluminium grown in a precisely-controlled oxygen atmosphere. In this way, we aim to control the QPS rate for a given wire width. The wires are defined with conventional electron beam lithography down to a width of 20 nm. We will present the fabrication of the nanowire arrays and first microwave measurements at mK temperatures.

TT 30.57 Mon 15:00 P2

Towards tunable transmon chains with individual on-chip bias — •Peter Fehlner, Jochen Braumüller, Lucas Radtke, Saskia Meissner, Hannes Rotzinger, Martin Weides, and Alexey Ustinov — KIT, Karlsruhe, Germany

Superconducting qubits constitute the main building blocks for quantum circuits. In this work we study a multi-qubit architecture [1] consisting of transmon qubits [2].

Such multi-partite quantum systems composed of harmonic and anharmonic resonant circuits manipulate the propagation of electromagnetic waves on a single photon level. These qubits operate at a Josephson to charging energy ratio of a few hundred to preserve sufficient anharmonicity. We employ a coplanar waveguide geometry based on interdigitated finger capacitors containing two Josephson junctions in parallel for each qubit. The sputter-deposited overlap Al-AlO_x-Al tunnel junctions are e-beam lithographically patterned for junction ares of about $0.1\mu m^2$. The transmons are capacitively coupled to a half wavelength transmission line resonator. The on-chip bias lines provide individual σ_z control of each qubit in the chain. Resonator readout

and global σ_x, σ_y qubit manipulation is mediated by the resonator coupled to the feedline.

We will present sample design, microwave simulations and first results measured at cryogenic temperatures.

TT 30.58 Mon 15:00 P2

Investigation of a tunable transmon qubit in microstrip geometry — •Jochen Braumüller, Lucas Radtke, Oleksandr Lukashenko, Hannes Rotzinger, Martin Weides, and Alexey V. Ustinov — Karlsruhe Institute of Technology (KIT), Physikalisches Institut, 76131 Karlsruhe, Germany

Qubits constitute the main building blocks of a prospective quantum computer. The main challenge is given by their coherence times, determining the feasibility for quantum error correction and scalability. In this work we investigate a transmon qubit having lower sensitivity to charge noise and a reduced dephasing rate compared to a conventional Cooper pair box. The employed microstrip design reduces surface losses due to a decrease in field strength and by focussing of field lines into the substrate. The transmon's large shunt capacitance pads are connected by a split Josephson junction, corresponding to a dc-SQUID. The tunability of the transmon allows frequency selective coupling to other quantum systems. Our design features four frequency detuned microstrip resonators each capacitively coupled to a qubit, enabling frequency multi-plexed simultaneous qubit readout and better statistics of qubit parameters. Chip fabrication is done by sputter deposition of aluminum films and optical lithography. We will present Josephson junction transport characterizations, microwave simulations and qubit measurements.

TT 30.59 Mon 15:00 P2

Ultrasonic saturation of tunneling systems in superconducting circuits — •Saskia Meissner, Lucas Radtke, Jochen Braumüller, Hannes Rotzinger, Martin Weides, Alexey V. Ustinov, and Georg Weiss — Physikalisches Institut, KIT Karlsruhe

Atomic two-level tunneling systems (TLS) are well known to dominate the thermodynamic low temperature properties of amorphous solids. They are formed by an atom or a group of atoms tunneling between two configurations within the disordered solid. These TLS are also present in the disordered thin oxide layer of capacitors in superconducting resonators or tunnel barriers in Josephson junctions in superconducting circuits where they are known as a source of dielectric loss and qubit decoherence.

The resonant part of the dielectric loss, caused by TLS with energies fitting the measurement frequency, can be saturated at sufficiently high microwave power due to the reduction of the TLS's occupation number difference. Here we will exploit the coupling of the TLS to mechanical strain field to saturate them with high frequency ultrasonic waves.

The required ultrasonic waves in the GHz range are generated either by surface acoustic wave transducers directly integrated in the superconducting resonator circuit or by bulk acoustic wave transducers on the chip's backside. RF-sputtered zinc oxide is used as piezoelectric film. Chip design, simulation of the resonators and data will be presented.

TT 30.60 Mon 15:00 P2

Probing the Interaction of Individual Two-Level-Systems with Quasiparticles using a Superconducting Qubit — •Alexander Bilmes, Jürgen Lisenfeld, Georg Weiss, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institute of Technology and DFG-Center for Functional Nanostructures (CFN), D-76128 Karlsruhe, Germany

Two-Level-Systems (TLS) are solid state defects which constitute one of the main sources of decoherence in a variety of nanoscale devices while their physical nature remains yet unclear. TLS couple to the environment via their electrical dipole moment and the mechanical strain field. It is possible to use a superconducting phase qubit for coherent manipulation and measurement of TLS which reside inside the tunnel barrier of the qubit's Josephson junction. In order to verify theoretical TLS models, we investigate whether TLS interact with quasiparticles (QP) existing in the qubits circuit. We use an on-chip DC-SQUID to generate QP in-situ. The QP density can be calibrated according to their effect on the phase qubit, where they give rise to a change in energy relaxation time and plasma frequency as has been shown by the group of J.M. Martinis [1]. Here we present first results on the coherence of individual TLS in dependence of TLS asymmetry and QP density. We observe a strong enhancement of the TLS energy relaxation rate by injected QP.

[1] J. Wenner et al., Phys. Rev. Lett. 110, 150502 (2013)

TT 30.61 Mon 15:00 P2

Low-Vibration Design of a 4 K Pulse Tube Cooler operated on Helium Compressors of Small Input Power — Jens Falter[1,2], Bernd Schmidt[1], Andreas Euler[1], Marc Dietrich[1], André Schirmeisen[1,2], and •Günter Thummes[1,2] — [1]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany — [2]Institute of Applied Physics (IAP), Justus-Liebig-University Giessen, Germany

In comparison to conventional Gifford-McMahon coolers, Pulse Tube Coolers (PTC) offer the advantage of having no moving parts at low temperatures. This feature results in high reliability and reduced vibrations of the cold head, which makes the PTC very attractive for highly-sensitive applications. However, due to the periodic compression and expanding cycles in the cold head, also PTCs exhibit two intrinsic effects: (1) a periodic variation in temperature; (2) a periodic elastic deformation ("breathing") of the thin walled pulse- and regenerator-tubes, which leads to residual vibrations. Here we present a two-stage 4 K PTC cold head which was especially designed to work with compressors of low input power in order to minimize these intrinsic effects. Nevertheless, small variations in temperature and residual vibrations remain due to their intrinsic nature. Further reduction of the temperature oscillations can be achieved with metal plates of low thermal diffusivity and the residual vibrations can be further reduced by successfully decoupling the cooler from the experiment.

TT 30.62 Mon 15:00 P2

Ultra-thin TaN films on different substrates for superconducting detectors — •Ilya Charaev, Konstantin Ilin, and Michael Siegel — Institute of Micro- and Nanoelectronic Systems, Karlsruhe Institute of Technology, Hertzstrasse 16, Karlsruhe, Germany

Superconductors widely used for development of detectors with ultimate sensitivity. For example, Tantalum Nitride (TaN) is a promising material for superconducting nanowire single-photon detector (SNSPD) in a wide spectral range. We report on a study of superconducting, normal state and thermal properties of ultra-thin TaN films for SNSPD. The films with a thickness of 5.5 nm were deposited by reactive magnetron sputtering in an Ar+N_2 atmosphere on different substrates like Sapphire, Si, MgO and Si with AlN buffer layer. While the critical temperatures Tc and the critical current density j_c (4.2 K) of TaN films on sapphire and MgO substrates have been found almost identically (about 9.3 K and 4 MA/cm^2 correspondingly) the Tc values of the films on Si substrate were much lower (4.76 K). Using a buffer layer of AlN the T_c of TaN on Si (important for THz applications) has been increased up to 7 K. Thermal coupling (estimated from the hysteresis current density) between TaN films and MgO and Sapphire substrates has been found alike while on Si substrates with AlN buffer layer the coupling was much weaker. A detailed analysis of the influence of substrate material on properties of TaN films will be presented and the potential of TaN films for different applications will be discussed.

TT 30.63 Mon 15:00 P2

Thin NbN film nanowires on GaAs for single-photon detectors — •Ekkehart Schmidt[1], Ulrich Rengstl[2], Elisabeth Koroknay[2], Konstantin Ilin[1], Michael Jetter[2], Peter Michler[2], and Michael Siegel[1] — [1]Institut für Mikro- und Nanoelektronische Systeme (IMS), Karlsruher Institut für Technologie, Hertzstrasse 16, 76187 Karlsruhe, Germany — [2]Institut für Halbleiteroptik und funktionelle Grenzflächen (IHFG), Universität Stuttgart , Allmandring 3, 70569 Stuttgart, Germany

For photonic integrated circuits, on chip emitters as well as detectors are needed to provide efficient data processing. Therefore fast and efficient detectors compatible with large scale integration along with sources, microcavities, waveguides and interferometers based on GaAs technology are required. Due to their single-photon resolution, fast detection, high detection efficiency and low dark count rate, the Superconducting Nanowire Single-Photon Detectors (SNSPDs) seem very promising. We studied transport and superconducting properties of 6 nm thick NbN films on GaAs suitable for SNSPD development. The NbN films were deposited using reactive magnetron sputtering on heated GaAs substrates. A Tc $>$ 10 K of films has been achieved. SNSPDs were patterned using electron-beam lithography (EBL) and reactive-ion etching (RIE). The critical-current density of a 120 nm

wide nanowire at 4.2 K exceeds 1.4 MA/cm^2. Results on study of optical response of NbN nanowire on GaAs will be presented and potentials of SNSPD integration into GaAs based photonic circuits will be discussed.

TT 30.64 Mon 15:00 P2

High-T_c YBCO nanowires for detector applications — •Steffen Koch[1,2], Juliane Raasch[2], Konstantin Ilin[2], Bernhard Holzapfel[3], Kazumasa Iida[4], Marc Weber[1], and Michael Siegel[2] — [1]Institute for Data Processing and Electronics, Karlsruhe Institute of Technology (KIT) — [2]Institute of Micro- and Nanoelectronic Systems, KIT — [3]Institute for Technical Physics, KIT — [4]Leibniz Institute for Solid State and Materials Research Dresden, IFW Dresden

$YBa_2Cu_3O_{7-d}$ (YBCO) is a promising high-T_c material for the fabrication of superconducting detectors with ultimate sensitivity and ultrafast response in a broad spectral range. Due to its intrinsic interaction times of less than 2 ps [1] the timing jitter of the response of superconducting YBCO nanowire single-photon detectors (SNSPD) should be smaller than in NbN SNSPDs.

The design of a SNSPD made from YBCO requires the patterning of meander lines with widths of the nanowire below 300 nm. The required thickness of the YBCO films ranges from a few nanometers for the absorption of optical photons up to several hundred nanometers in the X-ray range.

We will present results on the development of a technology for YBCO nanowires with thicknesses below 40 nm, widths of a few hundred nanometers and lengths up to tens of micrometres. The superconducting transport properties of different nanowire geometries measured with and without applying a magnetic field will be presented.

[1] M. Lindgren et al., Appl. Phys. Lett. 74 , 853 (1999)

TT 30.65 Mon 15:00 P2

Advances in the development of microstructured Magnetic Penetration Thermometers (MPT) — •J. Geist, S. Kempf, L. Gastaldo, A. Fleischmann, and C. Enss — KIP Heidelberg University

We recently started the development of microfabricated calorimetric detectors with magnetic penetration thermometers (MPT). MPTs make use of the steep temperature dependence of the magnetic penetration depth and the critical magnetic field of a superconducting sensor to monitor its temperature. When the sensor is placed in a weak magnetic bias field, the temperature rise following the absorption of a particle in the detector leads to a change of magnetic flux density **B(r)** inside the sensor and in its vicinity, which is detected as a magnetic flux change in the pickup coil of a sensitive magnetometer and serves as a measure of the absorbed energy.

We present numerical design studies as well as first experimental tests of microfabricated MPT sensor layers, patterned to form arrays of micron wide lines and dots which can be read out e.g. using meander-shaped pickup coils. We show that hysteresis effects as previously observed in MPT devices with large-area superconducting films can be completely suppressed. We also show that elemental superconductors needs to be deposited with high film quality to allow for a high detector sensitivity and therefore energy resolution. Finally, we show that the requirements on the film quality is somehow relaxed when the MPT sensor is made of thick S/N bilayers such as Al/Au or Al/Ag.

TT 30.66 Mon 15:00 P2

Development of dc-SQUIDs for the readout of metallic magnetic calorimeters — •A. Ferring, S. Kempf, M. Wegner, A. Fleischmann, L. Gastaldo, and C. Enss — Kirchhoff-Institute for Physics, Heidelberg University.

The very large bandwidth, the quantum limited noise performance, as well as the compatibility with very low operation temperatures make superconducting quantum interference devices (SQUIDs) the devices of choice for the readout of low temperature microcalorimeters such as metallic magnetic calorimeters (MMCs). For many MMC, low inductance current sensing SQUIDs are used to either directly measure the detector output signal or to act as an ultra low noise amplifier in a multistage SQUID configuration. Due to the desire for devices that are optimized for the readout of state-of-the-art MMCs, we have recently started the development of low-T_c current sensing dc-SQUIDs employing an in-situ sputtered Nb/Al-AlO_x/Nb trilayer.

We discuss our various dc-SQUID designs as well as the properties of produced prototype SQUIDs. In particular, we compare SQUIDs made by three different fabrication processes that are based on selective Niobium etching which is optionally combined with chemical anodization. We investigate the noise performance of our devices with respect to the absolute value and the temperature dependence of the white noise level. Furthermore, we study the presence of an $1/f$-like noise contribution and its temperature dependent behaviour. Finally, we experimentally show that state-of-the-art MMCs can successfully be read out by our SQUIDs.

TT 30.67 Mon 15:00 P2

Microfabrication of Metallic Magnetic Calorimeters — C. Enss, A. Ferring, A. Fleischmann, L. Gamer, L. Gastaldo, J. Geist, •D. Hengstler, S. Kempf, M. Krantz, A. Pabinger, C. Pies, C. Schötz, V. Schultheiss, and T. Wolf — KIP Heidelberg University.

Metallic Magnetic Calorimeters (MMCs) are low temperature particle detectors that nowadays can reliably be produced with multilayer microfabrication techniques. Moreover, the consequent use of these techniques allows for the fabrication of thousands of virtually identical detectors as it is required for large detector arrays. Using various examples of current MMC detectors which are actively used for spectroscopic measurements, we present our state-of-the-art microfabrication processes. This includes the fabrication of micron wide Nb lines with critical current densities close to the bulk value, persistent current switches allowing for a preparation of a persistent current in these Nb lines, temperature sensors made of co-sputtered Au:Er with concentrations between 200 ppm and 900 ppm, as well as overhanging particle absorbers made of electroplated gold with thicknesses between 3 μm and 200 μm. We also discuss a process for thermal anchoring the detectors through a Si wafer by connecting both sides of the wafer with the help of a DRIE-ICP etch and a Au electroplating process. Finally, we discuss the fabrication of thin, large-area ($A > 1\,\mathrm{cm}^2$) free-standing absorbers which are connected to the solid substrate only via some stems with a very small diameter.

TT 30.68 Mon 15:00 P2

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

To study reactions like the dissociative recombination in laboratory environment, the MPI-K in Heidelberg is building a cryogenic storage ring to prepare molecular ions in their rotational groundstate. The kinematics of these processes can be resolved by a position and energy sensitive detection of the produced molecule fragments. Previously, we described a large-area MMC for position and energy sensitive detection of massive particles. The detector encompasses 16 large-area absorbers, the temperature of each is monitored by a paramagnetic sensor located at a short edge of the absorber. Due to the finite thermal diffusivity in the absorber material, the rise-time of the detector depends on the impact location of the particle. We compare the expected energy resolution and position sensitivity of this detector to experimental results where energy was deposited at different positions. We investigate the impact of backscattering, sputtering and lattice damage effects on the instrumental linewidth by means of Monte Carlo simulations and measurements performed with a similar detector that was irradiated with ions and small molecules. We find that the degradation of energy resolution is less than predicted and show that molecular fragments which differ by only 1 mass unit can clearly be resolved.

TT 30.69 Mon 15:00 P2

Design of a Large Solid Angle Array of Calorimetric Low Temperature Detectors for Applications in Heavy Ion Research — •Patrick Grabitz[1,2], Artur Echler[1,2,3], Peter Egelhof[1,2], and Saskia Kraft-Bermuth[3] — [1]GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany — [2]Johannes Gutenberg Universität, Mainz, Germany — [3]Justus-Liebig-Universität, Gießen, Germany

Calorimetric low temperature detectors (CLTDs) for heavy ion detection have been demonstrated to achieve an excellent relative energy resolution of $\Delta E/E = 1 - 2\mathrm{x}10^{-3}$ in a wide range of energies. Combined with time of flight detectors they were successfully applied in accelerator mass spectroscopy and stopping power measurements. They also have the potential to be applied for determination of fission fragment distributions as well as for mass identification of super heavy elements with $Z \geq 113$. At present a CLTD array consisting of eight individu-

ally temperature controlled pixels with an active area of 12x6mm^2 is used in different applications. To exploit the full potential of CLTDs in further experiments the active area has to be increased. The design of the new array with 25 individually temperature controlled pixels and an active area of 15x15mm^2 will be discussed. Results from the first performance tests will be presented.

TT 30.70 Mon 15:00 P2

Schutzdioden für supraleitende Magnete am KATRIN-Experiment — •Alexander Jansen — KIT - Institut für Kernphysik — Postfach 3640, 76021 Karlsruhe

Die absolute Neutrinomasse ist sowohl für die Astroteilchenphysik, als auch für die Kosmologie von großer Bedeutung. Ziel des KATRIN-Experiments ist die modellunabhängige Messung der Neutrinomasse mit einer Sensitivität von $0.2eV/c^2(90\%C.L.)$ über die Kinematik des Tritium-β-Zerfalls. Hierzu werden die Zerfallselektronen aus der fensterlosen, gasförmigen Tritiumquelle (WGTS) über eine differentielle Pumpstrecke (DPS) und eine kryogene Pumpstrecke (CPS) zum Spektrometerbereich (MAC-E-Filter) geführt, wo ihre Energie mit hoher Präzision gemessen wird.

Die Aufgabe der Transportstrecke (DPS und CPS) ist es, das gesamte Tritiumgas abzupumpen, bevor es das Spektrometer erreichen kann. Gleichzeitig werden die Zerfallselektronen adiabatisch zum Spektrometer geleitet. Der Elektronentransport erfolgt dabei mit Hilfe magnetischer Felder, die durch supraleitende Magnete erzeugt werden. Der sichere Betrieb der Anlage erfordert besondere Maßnahmen zum Schutz der Magnete im Quenchfall. Dabei muss die im Magnetfeld gespeicherte Energie sicher abgeführt werden. Hierzu wurde ein neues Design für die Schutzdioden mit verbesserter Wärmeankopplung konzipiert. Der Vortrag gibt einen Überblick über den Quell- und Transportbereich und stellt das Konzept der Schutzdioden inklusive Testmessungen vor.

Dieses Projekt wird vom BMBF unter dem Kennzeichen 05A11VK3 und von der Helmholtz-Gemeinschaft gefördert.

TT 31: Spin Properties of Graphene (organized by HL; with DS, MA, O, TT)

Time: Tuesday 9:30–12:15 Location: HSZ 02

Invited Talk TT 31.1 Tue 9:30 HSZ 02

Intrinsic magnetism in graphene — •Irina Grigorieva — School of Physics and Astronomy, University of Manchester, UK

I will review our recent experiments on inducing and controlling magnetic response in graphene via introduction of point defects such as vacancies and adatoms. Graphene is hailed as potentially an ideal material for spintronics due to its weak spin-orbit interaction and the ability to control its electronic properties by the electric field effect. We have demonstrated that point defects in graphene - both vacancies and adatoms - carry magnetic moments, leading to pronounced paramagnetic behaviour that dominates graphene's low-temperature magnetism. Even better, we show that the defect magnetism is itinerant (i.e. due to localisation of conduction electrons) and can be controlled by doping, so that the induced magnetic moments can be switched on and off. This not only adds important functionality to potential graphene devices but also has important implications for spin transport.

Invited Talk TT 31.2 Tue 10:00 HSZ 02

Defect Induced Magnetic Moments in Graphene — •Roland Kawakami — The Ohio State University, Columbus, OH, USA — University of California, Riverside, CA, USA

We utilize non-local spin transport measurements to detect the presence of defect induced magnetic moments in graphene. As shown in this talk, point defects such as hydrogen adatoms and lattice vacancies generate magnetic moments in graphene that have substantial exchange coupling with the conduction electrons. Therefore, this exchange coupling produces spin relaxation in the conduction electrons. Specifically, a characteristic field dependence of the non-local spin transport signal identifies the presence of the magnetic moments. Furthermore, Hanle spin precession measurements indicate the presence of an exchange field generated by the magnetic moments. The entire experiment including spin transport is performed in an ultra-high vacuum chamber, and the characteristic signatures of magnetic moment formation appear only after hydrogen adatoms or lattice vacancies are introduced.

Invited Talk TT 31.3 Tue 10:30 HSZ 02

Role of MgO barriers for spin and charge transport in Co/MgO/graphene spin-valve devices — •Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

We investigate the influence of MgO barriers on spin and charge transport in single (SLG) and bilayer (BLG) graphene spin-valve devices. Similar to previous studies on BLG [1], we observe a $1/\mu$ of the spin lifetime in SLG devices. This general trend is only observed in devices with large contact resistance area products $R_cA > 1\text{k}\Omega\mu\text{m}^2$. In devices with long spin lifetimes, we furthermore observe a second Dirac peak, which results from charge transport underneath the contacts. In contrast, all devices with $R_cA < 1\text{k}\Omega\mu\text{m}^2$ only exhibit a single Dirac peak. Additionally, the spin lifetime is significantly reduced indicating that an additional spin dephasing occurs underneath the electrodes. In the latter devices we achieve a gradual increase of R_cA values by successive oxygen treatments. With this manipulation of the contacts both spin lifetime and amplitude of the spin signal can significantly be increased by a factor of seven in the same device. Finally, we present a new method to fabricate graphene-based lateral spin valves on hexagonal boron nitride yielding spin lifetimes above 3 ns, spin diffusion length above 10 μm and large charge carrier mobilities above 30.000 cm^2/Vs.

This work was supported by DFG through FOR 912.

[1] T.-Y. Yang *et al.*, Phys. Rev. Lett. 107, 047206 (2011).
[2] F. Volmer *et al.* Phys. Rev. B 88, 161405(R)(2013).

Coffee break (15 min.)

Invited Talk TT 31.4 Tue 11:15 HSZ 02

Defect-Mediated Spin Relaxation and Dephasing in Graphene — Mark Lundeberg[1,2], Silvia Folk[1], and •Joshua Folk[1] — [1]University of British Columbia, Vancouver, Canada — [2]Institute of Photonic Sciences, Barcelona, Spain

This talk will describe a series of transport measurements that disentangle mechanisms of spin and orbital phase relaxation in graphene. The measurements are based on well-known quantum interference phenomena–weak localization and universal conductance fluctuations. We show that a careful analysis of the in-plane magnetic field and temperature dependences of these effects can separately quantify spin-orbit and magnetic scattering rates; this technique works especially well in graphene due to its single-atom thickness. Spin relaxation in exfoliated graphene on SiO_2 is found to be dominated by magnetic scattering (scattering off of magnetic defects), with a smaller contribution from spin-orbit interaction. A similar measurement performed in graphene on SiC suggests that both magnetic scattering and spin-orbit interaction are a factor of 10 stronger than in exfoliated graphene.

Invited Talk TT 31.5 Tue 11:45 HSZ 02

Electron spin relaxation in graphene: resonant scattering off local magnetic moments — •Jaroslav Fabian, Denis Kochan, and Martin Gmitra — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Dirac electrons in graphene should have large spin relaxation time, some microseconds, due to the weak spin-orbit coupling of its itinerant electrons. Yet experiments show spin lifetimes as short as 100 ps. Traditional spin relaxation mechanisms, Elliott-Yafet and Dyakonov-Perel, seem incapable to explain such short lifetimes, even though some external influences such as hydrogen adatoms seem to induce giant local spin-orbit coupling [1] and so enhance spin-orbit induced spin flips. We believe that the culprit may instead be local paramagnetic moments due to vacancies and some adatoms. As the local moments sit on resonance sites, the spin flip is resonantly enhanced. These resonant local moments are acting as spatial spin hot spots: they may contribute little to momentum relaxation of graphene, but dominate the spin relaxation. This new mechanism explains the observed 100 ps spin lifetimes with as little as 1 ppm of local moments [2]. We acknowledge support from DFG SFB 689, SPP 1285, GRK 1579, and EC under

Graphene Flagship (Contract No. CNECT-ICT-604391). [1] M. Gmitra, D. Kochan, and J. Fabian, Spin-orbit coupling in hydrogenated graphene, Phys. Rev. Lett. 110, 246602 (2013);[2] D. Kochan, M. Gmitra, and J. Fabian, Spin relaxation mechanism in graphene: resonant scattering by magnetic impurities, arXiv:1306.0230.

TT 32: Cryotechnique

Time: Tuesday 9:30–9:45 Location: HSZ 201

TT 32.1 Tue 9:30 HSZ 201

Efficient countermeasures against the intrinsic temperature oscillations of low vibration 4 K pulse tube cryo-coolers — •Jens Falter[1], Bernd Schmidt[1], Andreas Euler[1], Marc Dietrich[1], André Schirmeisen[1,2], and Günter Thummes[1,2] — [1]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany — [2]Institute of Applied Physics (IAP), Justus-Liebig-University Giessen, Germany

Within the family of regenerative cooling systems, Pulse Tube Coolers (PTC) provide long life operation and low vibrations due to the absence of moving parts inside the cold head. But as a consequence of the periodic compression and expansion cycles of the process gas (He), they exhibit an intrinsic temperature oscillation. Depending on the application, these variations can interfere with the distortion free cooling of detectors and superconducting voltage standards by use of PTCs. If only a low cooling power is needed, those oscillations can be passively damped by a metal plate of low thermal diffusivity. However, this damping fails when high cooling powers are required. Here we present an efficient method for damping the temperature variations which is suitable for applications demanding high cooling power near 4 K. The key component is a small pot located at the cold flange of the cold head. Small amounts of helium gas are precooled and liquefied into the pot. The high specific heat of liquid helium, together with the heat transfer by two-phase flow, allows an effective damping of the temperature oscillation without notable loss of cooling power. This new damping unit is a closed cycle system and maintenance free.

TT 33: Superconductivity: Vortex Physics

Time: Tuesday 9:45–11:00 Location: HSZ 201

TT 33.1 Tue 9:45 HSZ 201

Dynamics of superconductor vortices in finite-thickness Nb open microtubes — •Vladimir M. Fomin[1], Renat R. Dusaev[2], Roman O. Rezaev[2,3], and Oliver G. Schmidt[1,4] — [1]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany — [2]Tomsk Polytechnic University, Tomsk, 634050, Russia — [3]Moscow Engineering Physics Institute, Moscow, 115409, Russia — [4]Material Systems for Nanoelectronics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Combination of reduced dimensionality with curved geometry in rolled-up superconductor micro- and nanotubes is a rich source of novel vortex dynamics [1,2]. Numerical modeling of a realistic finite-thickness Nb open microtube in a magnetic field orthogonal to the tube axis has been performed within the Ginzburg-Landau approach. An increase of thickness enhances the vortex-vortex interaction which results in a steady configuration with a reduced number of vortices and extends the upper magnetic field, at which the vortex dynamics occur, by a factor of two at least. This leads to new vortex dynamics as compared to the zero-thickness model. In particular, a regime is revealed where a configuration of vortices is fixed in the region far from the tube ends, while in the vicinity of the ends vortices nucleate at the top and bottom sides and then move toward each other until they annihilate as a vortex-antivortex pair.

The work was supported by the BMBF-Russia research grant 01DS13009.

[1] V. M. Fomin, R. O. Rezaev, O. G. Schmidt, Nano Lett. 12, 1282 (2012)
[2] R. O. Rezaev, V. M. Fomin, O. G. Schmidt, Physica C 497, 1 (2014)

TT 33.2 Tue 10:00 HSZ 201

Neutron scattering studies of domain structures in type-II superconductor Niobium — •Tommy Reimann[1,2], Michael Schulz[1,2], Sebastian Mühlbauer[1], Christian Grünzweig[3], and Peter Böni[2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching (D) — [2]Physikdepartment E21, TU München, Garching (D) — [3]Paul-Scherrer-Institut, Villigen (CH)

In the intermediate mixed state (IMS) of a type II superconductor (SC), the sample splits up into Meissner domains and Shubnikov domains which carry the vortex lattice (VL). A detailed investigation of these domain patterns offers the possibility to study general characteristics of domain nucleation and morphology as well as the physical properties of vortex-vortex and vortex-pinning interactions. In this talk we show that ultra small angle neutron scattering (USANS) can be used for the identification of VL properties. We have studied the VL domain morphology in a Nb single crystal disc that exhibit strong vortex pinning. USANS is sensitive to structures with sizes up to 20 microns and is therefore capable to probe IMS domains which is not possible with the commonly used small angle neutron scattering (SANS). Futhermore, USANS averages over the whole sample and hence probes the bulk of the material in contrast to magneto optical methods. Our investigation on the IMS of Nb reveals a preferred domain size with a strong dependence on magnetic field and sample thickness. Surprisingly , the average domain size is nearly independent of the temperature in a field cooled measurement giving some hint on the nature of field expulsion in the IMS of samples with significant pinning.

TT 33.3 Tue 10:15 HSZ 201

Spatial-dependent critical magnetic field for the suppression of superconductivity in a single Pb island with non-uniform thickness — •Augusto Leon Vanegas[1], Agnieszka Stepniak[1], Michael Caminale[1], Hirofumi Oka[1], Dirk Sander[1], and Jürgen Kirschner[1,2] — [1]Max-Planck-Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg

We have studied the superconducting properties of Pb islands of $7-10$ layers thickness and sizes of $1600-10000$ nm^2 on Pb/Ag/Si(111) with a ^{3}He cooled scanning tunnelling microscope (^{3}He-STM) with a vector magnetic field. Spatially resolved scanning tunnelling spectroscopy(STS) at 1.8 K shows a uniform superconducting gap across the islands at 0 T. We have measured the differential conductance at zero bias (ZBC) across several islands with varying the magnetic field perpendicular to the island surface. We identify the vortex formation field (H_{C1}) for islands larger than 5000 nm^2 and the critical field for suppressing superconductivity (H_{C2}) in the islands. Below H_{C1} the islands remain superconducting with small spatial variations of the ZBC from the centre to the edge of the island, which we ascribe to Meissner screening currents along the island perimeter. Between H_{C1} and H_{C2} spectroscopy indicates the formation of a single vortex, with normal conductance at its centre. We observe that for islands with a non-uniform height, H_{C2} varies across the island. The thickest part of the island remains superconducting at higher magnetic field.

TT 33.4 Tue 10:30 HSZ 201

ac susceptibility investigation of vortex dynamics in nearly-optimally doped $Ba(Fe_{1-x}Co_x)_2As_2$ — •Giacomo Prando[1], Romain Giraud[1], Saicharan Aswartham[1], Oleksii Vakaliuk[1], Christian Hess[1], Sabine Wurmehl[1,2], Anja Wolter-Giraud[1], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, Germany — [2]Institut für Festkörperphysik, Technische Universität Dresden, Germany

In this contribution we will report about the dynamical features of the flux lines in single crystals of optimally-doped superconducting $Ba(Fe_{1-x}Co_x)_2As_2$ [1]. Investigations were performed by means of magneto-resistivity and first-harmonic ac susceptometry. The extremely high-quality of the sample allows 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 anomalous features of the magnetic relaxation and into the nature of the glassy phase. As a surprising output, non-negligible values of chemical doping ($x = 10$ %) act as a remarkable low level of quenched disorder for the vortices.
[1] G. Prando et al., Journ. Phys.: Cond. Matt. 25, 505701 (2013)

TT 33.5 Tue 10:45 HSZ 201

Interference of edge and bulk pinning mechanisms in ultra-thin superconducting NbN and TaN mesoscopic bridges — •Konstantin Ilin and Michael Siegel — Iinstitute of Micro- and Nanoelectronic Systems, Karlsruhe Institute of Technology (KIT), Hertzstraße 16, 76187 Karlsruhe, Germany

Ultra-thin superconducting films are widely used for development of different types of radiation detectors. Usually, the operation conditions of the detectors are very close to the critical ones. Therefore the critical current density jc and its dependence on temperature and magnetic fields B are interesting not only from the fundamental point of view but very important for different applications. We present results on experimental investigations of jc(B) dependencies in thin film bridges made from NbN and TaN ultra-thin films deposited on sapphire substrates. We have found that in bridges with a width much smaller than the Pearl length and with a thickness about the coherence length (5 nm) the jc(B) dependence is non-monotonic. The critical current density oscillates at B = Bs corresponding to transition from the Meissner (B < Bs) to a vortex state. Moreover in the vortex state at B > Bs the jc(B) dependence is weaker than that one expected from the edge pinning mechanism solely. The observed phenomena could be explained by a significant contribution of a bulk pinning mechanism to the critical state of the current carrying superconducting mesoscopic structures.

TT 34: Superconductivity: Heterostructures

Time: Tuesday 11:15–13:00 Location: HSZ 201

Invited Talk TT 34.1 Tue 11:15 HSZ 201

Giant Thermopower in the Emerging Field of Super-Spintronics — •Matthias Eschrig — Department of Physics, Royal Holloway, University of London, Egham, Surrey TW20 0EX, United Kingdom

Thermoelectric effects in metals and superconductors are usually negligibly small as they require a strongly asymmetric density of states. Thus, relatively little attention has been paid to these effects so far in the new emerging field of super-spintronics. This field combines the advantages of control of spin as basic principle in spintronics with that of macroscopic quantum interference, a hallmark of superconductivity. At the same time, non-local transport has been studied during the past decade in connection with so-called crossed Andreev reflection in a number of pivotal experiments. I will discuss how the idea of non-local transport has been generalised to include thermal currents in superconducting spintronics devices [1]. Surprisingly, it turns out that a dramatic enhancement of thermoelectric effects can be achieved when combining spin-dependent scattering phases with spin-filtering effects in superconductor-ferromagnet heterostructures. Thermopowers of the order of 100 μV/K can be achieved. We study a non-local setup with three terminals (two ferromagnetic, one superconducing), and show that a nonlocal version of the Onsager symmetry relations holds. We calculate all thermodynamic coefficients in diffusive as well as ballistic structures, and include non-equilibrium distribution functions as well as singlet-triplet mixing in the superconducting region.
[1] P. Machon, M. Eschrig, W. Belzig, PRL **110**, 047002 (2013).

TT 34.2 Tue 11:45 HSZ 201

Giant thermoelectric effects in proximity-coupled superconductor-ferromagnet devices — •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

The usually negligibly small thermoelectric effects in superconducting heterostructures can be boosted dramatically due to the simultaneous effect of spin-dependent scattering and spin-filtering [Phys. Rev. Lett. **110**, 047002 (2013)]. Using that principle, we propose realistic setups to measure the local thermoelectric effects combining superconducting and ferromagnetic elements. We find that a thermopower $\sim 100\mu V/K$ can be achieved if the setup allows to drain the thermal current. For applications in nano-cooling we show that the figure of merit can exceed one for realistic parameters at low temperatures.

Due to crossed Andreev reflections and coherent electron transfer, three terminal structures also provide nonlocal thermoelectricity, here discussed in clean and in disordered structures. Our results show that a nonlocal version of the Onsager's reciprocity relation holds in a three terminal quantum coherent device.

TT 34.3 Tue 12:00 HSZ 201

Features and functionalities of superconducting hybrids with mixed singlet and triplet states — •Pablo Burset[1], Felix Keidel[1], Yukio Tanaka[2], Naoto Nagaosa[3], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany — [2]Department of Applied Physics, Nagoya University, Nagoya, 464-8603, Japan — [3]Department of Applied Physics, University of Tokyo, Tokyo 113-8656, Japan

We propose a model for a superconductor where both spin-singlet and triplet pairing amplitudes can coexist. By solving the Bogoliubov-de Gennes equations with a general pair potential that accounts for both spin states we study experimental signatures of normal metal and superconductor hybrids. The interplay between the spin-singlet and triplet correlations manifests in the appearance of two effective gaps. This double gap structure can be detected in the conductance of an isolated normal-superconductor junction. Interestingly, depending on which spin state is dominant, the conductance presents a conventional gap structure or an unconventional zero-bias peak. The form of the Andreev bound states formed at a short ballistic Josephson junction strongly depends on the spin state of the pairing amplitude at each superconductor. The periodicity of the current flowing through the junction changes for a dominant singlet or triplet pairing. Remarkably, for an arbitrary mix of the spin states, the Josephson current can be spin polarized for a certain range of the phase difference between the superconductors.

TT 34.4 Tue 12:15 HSZ 201

Proximity effect in superconductor/conical magnet/ferromagnet heterostructures — •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 superconductor and a ferromagnetic metal spin-singlet Cooper pairs can penetrate into the ferromagnetic part of the heterostructure with an oscillating and decaying spin-singlet Cooper pair density. However, if the interface allows for a spin-mixing effect, equal-spin spin-triplet Cooper pairs can be generated that can penetrate much further into the ferromagnetic part of the heterostructure, known as the long-range proximity effect [1]. Here, we present results of spin-mixing based on self-consistent solutions of the microscopic Bogoliubov-de Gennes equations incorporating a tight-binding model. In particular, we include a conical magnet into our model heterostructure to generate the spin-triplet Cooper pairs and analyse the influence of conical and ferromagnetic layer thickness on the unequal-spin and equal-spin spin-triplet pairing correlations. It will be shown that, in agreement with experimental observations, a minimum thickness of the conical magnet is necessary to generate a sufficient amount of equal-spin spin-triplet Cooper pairs allowing for the long-range proximity effect [2].
[1] J. W. A. Robinson, J. D. S. Witt, and M. G. Blamire, Science **329**, 59 (2010).
[2] D. Fritsch and J. F. Annett, arXiv:1311.3278 (2013).

TT 34.5 Tue 12:30 HSZ 201

Multiply gapped density of states in a chaotic normal metal in contact with superconductors — •Johannes Reutlinger[1], Wolfgang Belzig[1], Yuli Nazarov[2], and Leonid Glazman[3] — [1]University of Konstanz, Department of Physics, 78457 Konstanz, Germany — [2]Kavli Institute of Nanoscience Delft, Delft University of Technology, 2628 CJ Delft, Netherlands — [3]Department of Physics, Yale University, New Haven CT 06511-8499, USA

The spectral properties of a normal metal adjacent to a superconductor are strongly dependent on the characteristic mesoscopic energy scale - the Thouless energy E_{Th} - and the strength of the connection. We predict that the local density of states (LDOS), besides the well known minigap $\sim E_{\mathrm{Th}}$, can exhibit a multiple gap structure. For ballistic contacts we calculate these secondary gaps analytically in the framework of the quantum circuit theory of mesoscopic transport. For a cavity coupled to two superconductors with phase difference φ the secondary gap $\sim \Delta^3/E_{\mathrm{Th}}^2$ for $E_{\mathrm{Th}} \gg \Delta$ with maximum width at $\varphi = 0$ disappears at a critical phase $\pm\Delta/E_{\mathrm{Th}}$. The existence of a critical ratio E_{Th}/Δ calls for a reconsideration of the level statistics in chaotic Andreev dynamics, which has previously only been addressed thoroughly for $E_{\mathrm{Th}} \ll \Delta$. For generic contacts, like diffusive connectors or dirty interfaces no gap exists, but the density of states is still suppressed around Δ. Analytical calculations relate the secondary gap to the transmission eigenvalue distribution at small transmissions.

[1] J. Reutlinger, L. Glazman, Yu. V. Nazarov, W. Belzig, arXiv:1308.2529 (2013)

TT 34.6 Tue 12:45 HSZ 201

Measuring local magnetic fields in superconductors via XMCD — •Claudia Stahl[1], Stephen Ruoss[1,2], Patrick Audehm[1], Markus Weigand[1], Gisela Schütz[1], and Joachim Albrecht[2] — [1]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Aalen University, Beethovenstraße 1, 73430 Aalen

We use soft ferromagnetic thin films in order to map the magnetic flux line distribution in superconductors. For that purpose amorphous CoFeB is directly deposited on top of high-T_c superconducting YBCO structures. The magnetic stray fields of supercurrents lead to a local reorientation of the magnetic moments in the ferromagnet.

Using polarized x-rays it is possible to measure the local magnetization via the XMCD effect. With XMCD spectroscopy we find a temperature-dependent signal in the CoFeB layer which can be attributed to the currents flowing in the superconductor. This signal can be additionally measured with high spatial resolution paving the way to x-ray microscopy of magnetic structures in superconductors. The measurements are carried out at our scanning x-ray microscope MAXYMUS and our own dedicated reflectometry endstation at Bessy II of the HZB in Berlin.

TT 35: Correlated Electrons: Quantum-Critical Phenomena - Experiment I

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

TT 35.1 Tue 9:30 HSZ 204

Optical non-Fermi-liquid behavior in $CeCoIn_5$ — •Marc Scheffler[1], Uwe S. Pracht[1], Martin Dressel[1], Masaaki Shimozawa[2], Ryota Endo[2], Takahito Terashima[3], Takasada Shibauchi[2], and Yuji Matsuda[2] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Department of Physics, Kyoto University, Kyoto, Japan — [3]Research Center for Low Temperature and Materials Science, Kyoto University, Kyoto, Japan

The non-Fermi-liquid metallic state of the heavy-fermion superconductor $CeCoIn_5$ is interpreted as a consequence of a nearby quantum-critical point. Spectroscopic studies of quantum-critical heavy fermions have yielded valuable information, but are experimentally challenging. This also holds for optical techniques: the required low energies, both in temperature and frequency, are hard to reach. We overcome these difficulties by combining high-quality thin films of $CeCoIn_5$ with THz transmission spectroscopy. We cover frequencies 0.2-1.1 THz at temperatures down to 3 K, i.e. matching energy scales.

The THz spectra of $CeCoIn_5$ indicate metallic behavior with unconventional features. Upon cooling, the transport relaxation rate decreases through our frequency window, but we never find a simple Drude response. Instead, at low temperatures we observe a strongly frequency-dependent relaxation rate which is clearly inconsistent with Fermi-liquid predictions and which we attribute to electronic correlations in this non-Fermi-liquid phase. We further address the frequency- and temperature-dependent effective mass, and we discuss possible scaling behavior in the quantum-critical regime.

TT 35.2 Tue 9:45 HSZ 204

Exploring new LuT_2In compounds: Evidence for a structural quantum critical point — •Thomas Gruner, Dongjin Jang, Raul Cardoso, Manuel Brando, Gerhard Fecher, and Christoph Geibel — MPI CPfS, 01187 Dresden, Germany

Finding novel compounds with unconventional properties is one of the most appealing tasks in modern solid state physics. We recently studied the compounds $LuPt_2In$ and $LuPd_2In$ and discover that they present an exceptional opportunity for studying a structural quantum critical point (QCP). Up to now QCPs have been intensively studied in magnetic systems, while structural QCPs are rather scarce.
We synthesized both compounds to study their structural and electronic properties. We found that at high temperatures both compounds crystalize in the simple cubic Heusler structure. While $LuPd_2In$ retains this structure down to lowest T, in $LuPt_2In$ susceptibility $\chi(T)$, resistivity $\rho(T)$ and T-dependent powder XR diffraction evidence a charge density wave type transition at about 450 K to a yet undetermined low T structure. The T dependence of the anomalies in $\chi(T)$ and $\rho(T)$ indicate a 2^{nd} order type transition. Substituting Pd for Pt in $Lu(Pt_{1-x}Pd_x)_2In$ results in a continuous decrease of T_{trans}, indicating a structural QCP at $x_{\mathrm{QCP}} \approx 0.55$. Most interestingly we observed bulk superconductivity in the whole alloy series, with a clear maximum in the SC transition temperature at x_{QCP}. Furthermore we found that the phonon contribution to the specific heat at low T also presents a clear maximum at x_{QCP}, suggesting critical phonon softening. These results provide new insight into structural QCPs.

TT 35.3 Tue 10:00 HSZ 204

The Spin-1/2 XXZ Chain System Cs_2CoCl_4 in a Transverse Magnetic Field — •Oliver Breunig[1], Markus Garst[2], Eran Sela[2,3], Benjamin Buldmann[2], Petra Becker[4], Ralf Müller[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln — [3]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University — [4]Institut für Kristallographie, Universität zu Köln

Cs_2CoCl_4 consists of $CoCl_4$ tetrahedra that form chains along the crystallographic b axis. Due to a strong single-ion anisotropy the Co^{2+} orbital S=3/2 ground state is split into two Kramers doublets. Thus, at low temperatures a description of the lower doublet in terms of an effective spin-1/2 with an additional easy-plane anisotropy arises. By comparing measurements of specific heat and thermal expansion to exact finite-size diagonalization, we show that Cs_2CoCl_4 at temperatures below 2 K realizes the spin-1/2 XXZ chain in a transverse field [1]. Our data indicate a quantum phase transition at a critical field of ~ 2 T before around 3.5 T the description in terms of an effective spin-1/2 chain becomes inapplicable. Considering both thermal as well as virtual excitations of higher crystal field states, we find that the spin chain is in the XY-limit with an anisotropy $J_z/J_\perp \approx 0.12$ substantially smaller than previously believed. This work has been supported by the Deutsche Forschungsgemeinschaft via SFB 608 and FOR 960.
[1] O. Breunig *et al.*, PRL **111**, 187202 (2013)

TT 35.4 Tue 10:15 HSZ 204

Anomalous quantum critical behavior in a 3d itinerant magnet $Sr_{1-x}Ca_xRuO_3$ — •Chien-Lung Huang[1,2], Dirk Fuchs[2], Markus Wissinger[2], Jörg Schmalian[3], Rudolf Schneider[2], Meng-Chieh Ling[3], and Hilbert von Löhneysen[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [3]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

The magnetization M and the specific heat C of polycrystalline

$Sr_{1-x}Ca_xRuO_3$ were investigated as a function of the Ca substitution x. The Curie temperature $T_C = 162$ K of $SrRuO_3$ decreases linearly with increasing x. Long-range ferromagnetic (FM) order is completely suppressed above the critical concentration $x_c \sim 0.7$ at which quantum critical behavior was observed. That behavior cannot be described by the conventional Hertz-Millis-Moriya thoery for an FM quantum critical point, nor by the existence of a Griffiths phase. Nevertheless, the electronic and magnetic specific heat $\delta C_{em}/T = (C_{em}(B) - C_{em}(0))/T$ after subtraction of the phonon contribution and the scaled magnetization M/T^{β} collapse onto single scaling functions $\mathcal{F}(B/T^{1.25})$ and $\mathcal{F}(B/T^{1.7})$, respectively. The anomalous critical behavior will be discussed in terms of magnetic inhomogeneity.

TT 35.5 Tue 10:30 HSZ 204

Frustration and Quantum Criticality in Ni-doped CePdAl — •Veronika Fritsch[1], Zita Huesges[2], Oliver Stockert[2], Christian Taubenheim[1], Wolfram Kittler[1], Chien-Lung Huang[1], Kai Grube[1], and Hilbert v. Löhneysen[1] — [1]Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

In heavy-fermion systems, magnetic quantum phase transitions (QPT) usually arise from the competition between RKKY and Kondo interaction. For large Kondo interactions the $4f$ states hybridize strongly with the conduction electrons, thus suppressing the magnetic ordering temperature to zero. Magnetic frustration is an alternative way to suppress the magnetic order, while keeping the local moments intact. Recently theoretical models were developed discussing additional frustration-induced fluctuations for heavy-fermion metals. We will examine the role of magnetic frustration at the QPT in the heavy fermion system CePdAl, which crystallizes in a hexagonal ZrNiAl-type structure, where the magnetic Ce-ions form a distorted kagomè lattice. The magnetic order, as revealed through previous neutron scattering experiments, is partially frustrated with one third of the Ce-ions not participating the long-range magnetic order. An external magnetic field turns the system toward a Fermi-liquid state. The substitution of Pd by Ni yields a QPT accompanied by non-Fermi-liquid behavior. We will present our recent experiments on single-crystalline $CePd_{1-x}Ni_xAl$, namely measurements of specific heat, thermal expansion, electrical resistivity and magnetization, as well as neutron scattering experiments.

TT 35.6 Tue 10:45 HSZ 204

Frustrated magnetic order in $CePd_{1-x}Ni_xAl$ studied by neutron diffraction — •Z. Huesges[1], S. Woitschach[1], O. Stockert[1], V. Fritsch[2], M.-H. Lemée-Cailleau[3], S. Capelli[3], S. Matas[4], K. Prokes[4], B. Pedersen[5], and H. von Löhneysen[2] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]Karlsruhe Insitute of Technology, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Helmholtz Zentrum Berlin, Germany — [5]FRM2, Technical University München, Germany

The heavy-fermion compound CePdAl might be a model system to study the influence of frustration on quantum criticality, which has recently become a much-discussed topic in theoretical condensed matter physics. The quantum critical point can be accessed by Ni doping on the Pd site, which reduces the Néel temperature from 2.7 K in the pure compound to zero for 14 % Ni substitution. The magnetic order of undoped CePdAl has previously been investigated by powder neutron diffraction, which revealed that only two thirds of the Ce spins order, while the ordered moment of the remaining third is zero even at very low temperatures. This frustration can be related to the quasi-Kagomé lattice of the Ce ions in the hexagonal basal plane. We have performed single crystal neutron diffraction for different alloys of the doping series $CePd_{1-x}Ni_xAl$. We found that the ordering vector remains unchanged upon doping and that the ordered moment is gradually suppressed. Furthermore, we observed short-range magnetic order which co-exists with the long-range order signal. The length scale of these fluctuations becomes much shorter on approaching the quantum critical point.

TT 35.7 Tue 11:00 HSZ 204

Single crystal growth of the ferromagnetic heavy fermion compound $YbNi_4P_2$ — •Kristin Kliemt and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt, 60438 Frankfurt am Main, Germany

In the heavy fermion metal $YbNi_4P_2$ a ferromagnetic (FM) transition at $T_C = 0.17$ K was observed recently [1]. This transition can be further suppressed by substituting As on the P site. Investigation of $YbNi_4(P_{1-x}As_x)_2$ showed the appearance of the first clear-cut example of a ferromagnetic quantum critical point in metals at $x \leq 0.08$ [2]. High quality single crystals are required to investigate this new compound in more detail.

Here, we report on the single crystal growth of $YbNi_4P_2$ in a Bridgman-type furnace. Because of the incongruent melting of $YbNi_4P_2$, the growth was done from a Ni-P self flux at about 1400°C. Subsequently, the flux was removed by centrifugation at 1000°C. The quality of the crystals was verified by resistivity and magnetic measurements from 300 to 2 K. In particular, we address the challenge, how to avoid the formation of impurity phases and flux inclusions by variation of crucible shapes and growth conditions like temperature, duration, velocity of cooling and flux composition. With this optimization we obtained single crystals suitable for several measurement techniques as e.g. ARPES, STM, NMR, ESR, and magnetization to unravel the nature of the ferromagnetism in $YbNi_4P_2$.

[1] C. Krellner et al., New J. Phys. 13, 103014 (2011)
[2] A. Steppke et al., Science 339, 933 (2013)

15 min. break.

TT 35.8 Tue 11:30 HSZ 204

Single crystal study of $SrCo_2P_2$: an unusual spin fluctuating system — •Christoph Bergmann, Christoph Geibel, Helge Rosner, and Deepa Kasinathan — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden Deutschland

Since the discovery of high temperature superconductivity in doped RFeAsO, transition metal pnictides have attracted considerable attention, especially those being close to a transition from a magnetic ordered to a non-magnetic ground state. $SrCo_2P_2$, a structural homologue of the AFe_2As_2 series of compounds, is such a system. Earlier investigation on polycrystals indicated a paramagnetic ground state, but a close proximity to magnetic ordering. Using a flux technique, we grew high quality single crystals with a residual resistivity ratio up to 140, and performed an in-depth study of the physical properties. Despite LDA calculation indicate a pronounced peak in the density of states at the Fermi level prone for electronic instability, we did not find any evidence for a phase transition. However we observed a quite unusual T dependence of the susceptibility with two distinct maxima, and Non-Fermi-liquid behavior in the resistivity at low T. Both features confirm $SrCo_2P_2$ to be a rather unusual spin fluctuating system close to a (quantum) critical point.

TT 35.9 Tue 11:45 HSZ 204

Competing order parameters in $NbFe_2$ — •Sven Friedemann[1], Max Hirschberger[1,2], William J Duncan[1], Andreas Neubauer[2], Thomas Bauer[3], Manuel Brando[3], Christian Pfleiderer[2], and F Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]Physik Department E21, TU München, Garching, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Quantum criticality in transition metal compounds imposes long-standing challenges: Near the border of magnetism at low temperature, T, prominent examples like the ferromagnets MnSi and $ZrZn_2$ obey unconventional power law-dependencies of the resistivity which cannot be understood within the standard magnetic fluctuation theory. Here, we present new results on $NbFe_2$ in which a $T^{3/2}$ dependence of the resistivity has also been observed [1]. $NbFe_2$ can be tuned by varying the composition, thus enabling detailed investigations not possible in pressure tuned systems. While slightly iron-rich samples are ferromagnetic at low $T < T_c$, T_c is suppressed to 0 on approaching stoichiometry and a new phase is observed above T_c. Using high-purity single crystals we conduct comprehensive studies of bulk magnetic, thermodynamic, and transport properties. These prove the presence of both ordered states. We show that our results are consistent with the competing order parameter theory of uniform and modulated magnetic states as proposed by Moriya and Usami [2]. We infer that the quantum critical behaviour in $NbFe_2$ is associated with the modulated magnetic order.

[1] Phys. Rev. Lett. **101**, 026401 (2008)
[2] Sol. State Comm. **23**, 935 (1977)

TT 35.10 Tue 12:00 HSZ 204

Microscopic study about the magnetic ground state of C14 systems: $Nb_{1-y}Fe_{2+y}$ and $Ta(Fe_{1-x}V_x)_2$ — •Daniela Rauch[1], Mathias Kraken[1], Jochen Litterst[1], Hubertus Luetkens[2], Manuel Brando[3], Michael Baenitz[3], William J Duncan[4], An-

dreas Neubauer[5], Christian Pfleiderer[5], Stefan Süllow[1], and F Malte Grosche[4] — [1]Institute of Condensed Matter Physics, TU Braunschweig, Braunschweig, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Villigen, Switzerland — [3]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [5]Physik Department E21, TU München, Garching, Germany

A large number of C14 Laves systems exhibits a complex magnetic phase diagram with ferromagnetic critical fluctuations. In this context, $Nb_{1-y}Fe_{2+y}$ and $Ta(Fe_{1-x}V_x)_2$ need to be discussed. $NbFe_2$ has been proposed to represent a very rare case of spin density wave order (SDW), which can be suppressed by slight changes to the stoichiometry to be ferromagnetic. Here, we present for the first time μSR of $Nb_{1-y}Fe_{2+y}$ and identify SDW and ferromagnetic phases on a microscopic scale and establish them as bulk magnetic phases. Moreover, we present a combined μSR study with the analysis of Mößbauer spectroscopy experiments on Fe-rich $Nb_{1-y}Fe_{2+y}$ and discuss the nature of the ground state magnetic phases. In addition, $Ta(Fe_{1-x}V_x)_2$ is of special interest because of ferromagnetic critical fluctuations, which evolved in the proximFor this reason, we report first Mößbauer experiments.

TT 35.11 Tue 12:15 HSZ 204

transport and torque magnetometry measurements on CeAuSb2 — •Lishan Zhao — University of St Andrews, St Andrews, Fife, UK

The tetragonal crystal CeAuSb2 has a layered structure and orders antiferromagnetically at T 6K. Under a c-axis magnetic field, the Neel temperature is gradually suppressed to zero at a possible field-tuned quantum critical point at about 6 T. Within this antiferromagnetic phase, between the QCP and about 2.8 T, there is an additional, novel phase[1]. We report transport measurements on purest-to-date single crystals of CeAuSb2, in fields of up to 15 T and from room temperature down to 100 mK. We also report torque magnetometry measurements. Unlike a recent report[2], we find single, sharp transitions into the novel phase. We discuss the nature of the novel phase.

[1] L. Balicas et al., Phys Rev B 72, 064422 (2005)
[2] K.-A. Lorenzer et al., Phys. Status Solidi B 250, 464 (2013)

TT 35.12 Tue 12:30 HSZ 204

Transport measurements in $Yb(Rh_{1-x}Co_x)_2Si_2$ with $x \leq 0.27$ — •Sandra Hamann[1], Stefan Lausberg[1], Christoph Klingner[1], Cornelius Krellner[2], Frank Steglich[1], Christoph Geibel[1], and Manuel Brando[1] — [1]Max Planck Institut for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Institute of Physics, Goethe University Frankfurt, Max-von-Laue Str. 1, 60438 Frankfurt (Main), Germany

$YbRh_2Si_2$ is considered one of the standard materials for studying quantum criticality. It shows antiferromagnetic (AFM) order below $T_N = 0.07\,K$ and unconventional behavior at the magnetic-field-induced quantum critical point (QCP). Due to the low T_N and the tiny size of the ordered moments ($\approx 10^{-3}\mu_B$) the exact magnetic structure could not be determined, yet. However, because of the strong magnetic anisotropy the moments are expected to lie in the *ab*-plane of the tetragonal crystalline structure, the magnetic easy plane. Cobalt substitution was used as chemical pressure to increase T_N and the size of the ordered moments in $Yb(Rh_{1-x}Co_x)_2Si_2$. Previous studies with magnetic field $B \perp c$ pointed to a possible AFM groundstate for the whole series. Surprisingly, ferromagnetic order was found for $x = 0.27$ with moments along the *c*-axis. This motivated a re-investigation of the groundstate for $x \leq 0.27$. We present a comprehensive study of the resistivity in single crystals with $x \leq 0.27$ and $B \parallel c$. We discuss our results considering the competition between in-plane antiferromagnetism and out-of-plane ferromagnetism and the consequences this might have for the quantum critical behavior of $YbRh_2Si_2$.

TT 35.13 Tue 12:45 HSZ 204

Fermi liquid breakdown and superconductivity in YFe_2Ge_2 — Yang Zou[1], Zhuo Feng[1,2], •Peter Logg[1], Jiasheng Chen[1], Giulio Lampronti[3], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE — [2]Dept. of Earth Sciences, University of Cambridge, Cambridge CB2 3EQ — [3]London Centre of Nanotechnology, University College London WC1H 0AH

The investigation of quantum critical phenomena associated with incipient antiferromagnetic or spin density wave order in transition metal compounds has been held back by the scarcity of candidate systems in this class of materials. The paramagnetic d-electron system YFe_2Ge_2 displays an unusually high Sommerfeld ratio of the specific heat capacity $C/T \simeq 100\,mJ/molK^2$ at low temperature and can be tuned to the border of spin density wave order by partial substitution of Y with isoelectronic Lu [1], suggesting that YFe_2Ge_2 is located close to a spin density wave quantum critical point. Our ambient pressure, low temperature measurements reveal signatures of Fermi liquid breakdown such as an increasing C/T on cooling and a 3/2 power law temperature dependence of the electrical resistivity. Moreover, samples of YFe_2Ge_2 with high residual resistance ratios display full superconducting transitions below $T_c \simeq 1.8\,K$ in the electrical resistivity and up to 80% Meissner volume fraction in bulk zero-field-cooled magnetisation measurements, or 20% in powdered samples [2].

[1] S. Ran et al., Phil. Mag. **91,** 4388 (2011).
[2] Y. Zou et al., arXiv:1311.0247 (2013).

TT 36: Focus Session: Advanced Algorithms for Strongly Correlated Quantum Matter

One of the aims of simulations of correlated electron systems is to understand the emergent collective phenomena inherent to this system class. The Focus Session will review recent highlights in this domain and address the following questions. What role can we expect quantum computing to play? Which models posses topologically ordered phases and how do we detect this exotic state of matter? How do we understand quantum phase transitions beyond the Landau paradigm, and can we find numerically solvable model systems which confirm exotic scenarios? Answers to the above questions are based on innovative algorithmic work in the domains of tensor networks, DMRG, and quantum Monte Carlo.

Organizer: Fakher Assaad (Uni Würzburg)

Time: Tuesday 9:30–12:15 Location: HSZ 03

Invited Talk TT 36.1 Tue 9:30 HSZ 03

Quantum Computing and Strongly Correlated Materials — •Matthias Troyer — ETH Zurich

Feynman's proposal of using quantum mechanics to solve hard quantum problem was the origin of the field of quantum computing. The same idea is at the heart of optical lattice quantum simulators, which can be viewed as special-purpose analog quantum computers. As successful as optical lattice quantum simulators are in emulating the Hubbard model and variants thereof, they suffer from several limitations: they can only simulate particular models that arise naturally from the underlying quantum system used to build the simulator, and reaching low effective temperatures is a challenge. Both of these problems can be overcome on (future) universal quantum computers. With small quantum computers becoming feasible in the next years it is time to think about how a quantum computer can help us solve strongly correlated electron problems. In this talk I will thus review quantum algorithms for the simulation of quantum systems and will estimate what size quantum computer could outperform a classical computer for these problems. I will also show that the exact ab-initio simulation of materials will be infeasible even on quantum hardware and that thus the model-based approach of first mapping materials to effective models will remain crucial.

Invited Talk TT 36.2 Tue 10:00 HSZ 03

Quantum Monte Carlo Simulations of Deconfined Quantum-

Criticality — •Anders Sandvik — Boston University, USA

I will discuss recent results, based on quantum Monte Carlo (QMC) simulations, for the quantum phase transition from the standard Neel state of a 2D antiferromagnet into a non-magnetic valence-bond solid state. The transition has been achieved in two different classes of models which are amenable to large-scale QMC simulations. These models can be defined with SU(N) spins for several different values of N, and results for these models can be compared with 1/N expansions of the quantum field-theory proposed to describe the "deconfined" transition. I will also discuss results for thermodynamics, which indicate that deconfined spinons can describe the excitation spectrum at criticality.

Invited Talk TT 36.3 Tue 10:30 HSZ 03

Characterizing Entanglement Entropy with Quantum Monte Carlo — •Roger Melko — University of Waterloo 200 University Ave. W. Waterloo, ON N2L 3G1

An understanding of entanglement across a bipartition can give novel perspectives on correlations in condensed matter systems. Entanglement probes geometric and topological properties of the bipartition, and resultant paradigms such as the "area" law have led to important resources for characterizing quantum phases and phase transitions. The full power of these resources has only recently been exploited in two dimensions and higher, since the advent of algorithms to calculation the Renyi entanglement entropies in quantum Monte Carlo (QMC). Estimators for the Renyi entropies, mostly based on replica-trick methods borrowed from quantum field theory, are now routinely exploited in almost all flavours of QMC, including Stochastic Series Expansion, T=0 Projector, Auxiliary Field, and Path Integral Monte Carlo for particles in the continuum. In this talk, I will discuss the common underpinning of all replica-trick methods, as well as some advanced algorithmic tactics required to obtain statistical control of the Renyi entropy estimators. Finally, I will illustrate the use of Renyi entropies as a resource in condensed matter systems, e.g. measurement of topological entanglement entropy in spin liquid phases, identification of broken continuous symmetries, and calculation of universal quantities at quantum critical points.

15 min. break.

Invited Talk TT 36.4 Tue 11:15 HSZ 03

Field-Induced Superfluids and Bose Liquids in Projected Entangled Pair States — •Didier Poilblanc — CNRS & University of Toulouse, Toulouse, France

In two-dimensional incompressible quantum spin liquids, a large enough magnetic field generically induces "doping" of polarized S=1 triplons or S=1/2 spinons. We review a number of cases such as spin-3/2 AKLT or spin-1/2 Resonating Valence Bond (RVB) liquids where the Projected Entangled Pair States (PEPS) framework provides very simple and comprehensive pictures. On the bipartite honeycomb lattice, simple PEPS can describe Bose condensed triplons (AKLT) or spinons (RVB) superfluids with transverse staggered (Neel) magnetic order. On the Kagome lattice, doping the RVB state with deconfined spinons or triplons (i.e. spinon bound pairs) yields uncondensed Bose liquids preserving U(1) spin-rotation symmetry. We find that spinon (triplon) doping destroys (preserves) the topological Z_2 symmetry of the underlying RVB state. We also find that spinon doping induces longer range interactions in the entanglement Hamiltonian, suggesting the emergence of (additive) log-corrections to the entanglement entropy.

[1] D. Poilblanc, N. Schuch, and J.I. Cirac, Phys. Rev. B 88, 144414 (2013) and references therein.

Invited Talk TT 36.5 Tue 11:45 HSZ 03

Nature of the Spin Liquid Ground State of the Kagome Model — •Uli Schollwoeck — Department of Physics, University of Munich

In this talk, I will discuss the identification of the spin liquid ground state of the Heisenberg antiferromagnet on a kagome lattice by ground state analysis, gap calculations and topological entanglement. All the numerical evidence obtained by the density-matrix renormalization group points to a Z_2 quantum spin liquid.

TT 37: Cold Atomic Gases

Time: Tuesday 9:30–12:45 Location: HSZ 304

Invited Talk TT 37.1 Tue 9:30 HSZ 304

Superfluidity and Collective Pairing in Polariton Microcavities — •Francesca Maria Marchetti — Departamento de Fisica Teorica de la Materia Condensada & IFIMAC, Universidad Autonoma de Madrid, Madrid 28049, Spain

Matter-light systems such as semiconductor microcavities have been witnessing remarkable advances, promoting them as ideal environments where to engineer and study novel collective quantum states. Since the first realisation of a polariton Bose-Einstein condensate, the field has grown at a high rate. Superfluid behaviour, the observation of full and half quantum vortices and solitons, the optical spin Hall effect, are just few examples of the most seminal results for polaritonic fluids obtained only in the last few years, a brief account of which will be given in the introduction of this presentation. Most recently, it has been possible to tune the interaction strength between polaritons with opposite polarisations via a bipolariton Feshbach resonance mechanism. This allows to access regimes of tunable pairing and strong correlations, opening a wealth of interesting possibilities. I will in particular show that microcavity polaritons present an ideal opportunity to study bosonic collective pairing phases: Exploring the theoretical phase diagram, I will show that, by using the photon-exciton detuning as the interaction tuning parameter, a novel phase transition between the regular polariton superfluid phase and a "molecular" (i.e. bipolariton) superfluid phase can be realised. Temperatures and detunings required for typical materials such as GaAs and ZnO are attainable, and I will discuss experimental signatures for detecting such novel phases.

TT 37.2 Tue 10:00 HSZ 304

Transport with ultra-cold atoms at constant density — •Christian Nietner, Gernot Schaller, and Tobias Brandes — Institut für theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate the transport through a few-level quantum system described by a Markovian master equation with temperature- and particle-density dependent chemical potentials. From the corresponding Onsager relations we extract linear response transport coefficients in analogy to the electronic conductance, thermal conductance and thermopower. Considering ideal Fermi and Bose gas reservoirs we observe steady-state currents against the thermal bias as a result of the non-linearities introduced by the constraint of a constant particle density in the reservoirs. Most importantly, we find signatures of the on-set of Bose-Einstein condensation in the transport coefficients.

TT 37.3 Tue 10:15 HSZ 304

Relaxation towards negative temperatures in bosonic systems: generalized Gibbs ensembles and beyond integrability — Stephan Mandt[1], Adrian E. Feiguin[2], and •Salvatore R. Manmana[3] — [1]Princeton Center for Complex Materials and Department of Physics, Princeton University, NJ 08544, USA. — [2]Department of Physics, Northeastern University, Boston, MA 02115, USA. — [3]Institute for Theoretical Physics, University of Göttingen, D-37077 Göttingen, Germany.

Motivated by the recent experimental observation of negative absolute temperature states in systems of ultracold atomic gases on optical lattices [Braun et al., Science 339, 52-55 (2013)], we investigate theoretically the formation of these states. More specifically, we consider the relaxation after a sudden inversion of the external parabolic confining potential in the one-dimensional inhomogeneous Bose-Hubbard model. First, we focus on the integrable hard-core boson limit which allows us to treat large systems and arbitrarily long times, providing convincing numerical evidence for relaxation to a generalized Gibbs ensemble at negative temperatures $T < 0$, being defined by us in this context. Second, going beyond one dimension, we demonstrate that the emergence of negative temperature states can be understood in a dual way in terms of positive temperatures, which relies on a dynamic symmetry of the Hubbard model. We complement the study by exact

diagonalization simulations at finite values of the on-site interaction.

TT 37.4 Tue 10:30 HSZ 304

Spin-Imbalanced Fillings for Fermions in a Trap — •Denis Morath, Stefan Söffing, and Sebastian Eggert — TU Kaiserslautern, 67663 Kaiserslautern, Germany

Recently it has become experimentally feasible to realize tunable few-fermion systems in an ultra cold gas setup. Besides the huge variability in interaction using the Feshbach Resonance people are now able to control the filling of different pseudo-spin species independently. This leads to interesting local magnetizations i.e. spin resolved local densities. We calculate these quantities on a discretized, one dimensional system using a Quantum Monte Carlo algorithm called Stochastic Series Expansion. This offers the opportunity to perform complete quantum many-body simulations in order to study the influence of finite interactions, filling and temperature on the density-distribution. We observe the formation of an anti-ferromagnetic arrangement, but this is only stable for small and intermediate interactions and small spin imbalances. For higher interactions a Wigner crystal forms, which has regular peaks in the density, that are independent of spin. Hence the density of one spin species typically has more peaks in the particle density than the actual number of particles in this case.

TT 37.5 Tue 10:45 HSZ 304

Zitterbewegung in the honeycomb lattice — •Michael Hauber[1], Benjamin Deissler[2], Johannes Hecker Denschlag[2], and Alejandro Muramatsu[1] — [1]Institut für Theoretische Physik III, Universität Stuttgart — [2]Institut für Quantenmaterie, Universität Ulm

We present simulations of the dynamics of relativistic fermions on a honeycomb lattice to investigate the Zitterbewegung in 2+1 dimensions under real conditions, such as finite lattice size and external potentials. Our results serve as a guide for an experimental realization of such systems with ultracold fermionic atoms (^6Li) on an optical lattice. From our simulations, Zitterbewegung should be observable in such a system with site-resolved imaging capabilities.

15 min. break.

TT 37.6 Tue 11:15 HSZ 304

2D Phase Space Crystals: artificial gauge fields in phase space — •Lingzhen Guo[1,2], Michael Marthaler[1,2], and Gerd Schön[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology(KIT), Karlsruhe, Germany — [2]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, Karlsruhe, Germany

We propose a new paradigm to study the properties of driven systems. We find the driving field in fact induces a lattice structure in phase space, which we call phase space crystals [1]. The discrete sysmmetry of phase space lattice allows us to apply the Bloch theorem in solid state physics to the study of driven systems. From this point of view, we investigate the gap openning mechanism of quasienergy spectrum different from that in solid state physics. Interestingly, because the two dimensions of phase space are intrinsically noncommutative, there exists an effective magnetic field in phase space. We explore the related physics due to the existence of this artificial magnetic field.
[1] Phys. Rev. Lett. 111, 205303 (2013)

TT 37.7 Tue 11:30 HSZ 304

Haldane phases of SU(N) spin chains and their realization in ultra-cold atom gases — •Thomas Quella — University of Cologne, Cologne, Germany

The general classification of SU(N) spin chains of Duivenvoorden and Quella predicts the existence of up to N-1 distinct non-trivial topologically protected phases. Each phase is characterized by a specific type of non-local string order and the emergence of fractionalized SU(N) spins at the boundary of the system.

In this talk, we analyze model Hamiltonians of AKLT type in which these phases are realized and discuss their relation to the Heisenberg Hamiltonians that arise as certain limits of suitably chosen Hubbard models. Our results indicate that it should be possible to realize at least one of the non-trivial topological phases in ultra-cold alkaline-earth atom gases if N is even. We also comment on the modifications of the previous Hamiltonians which are required to realize the remaining non-trivial topological phases.

TT 37.8 Tue 11:45 HSZ 304

Quantum phases of one-dimensional soft-core systems — •Marion Moliner, Davide Vodola, and Guido Pupillo — IPCMS (UMR 7504) and ISIS (UMR 7006), Université de Strasbourg and CNRS, 67000 Strasbourg, France

Rydberg-excited atoms trapped in optical lattices have provided an experimental realization of strong repulsive non-local van der Waals interactions [1]. These soft-core interactions engender exotic phases such as supersolid states in two and three dimensions. In one dimension, a very recent theoretical study showed the existence of critical quantum liquids beyond the Tomonaga-Luttinger liquid picture [2]. The particular feature of these liquids is the formation of clusters due to frustrating interactions.

In the present work, we investigate the effects of adding a 'spin' degree of freedom in order to mimic a magnetic behaviour. Such systems are described by a longer-range extended Hubbard model with frustrating couplings. By means of analytical and numerical methods we show the existence of other 'cluster Luttinger liquids' exhibiting different types of magnetic orders.
[1] N. Henkel, R. Nath, and T. Pohl, Phys. Rev. Lett. 104 195302 (2010)
[2] M. Mattioli, M. Dalmonte, W. Lechner and G. Pupillo, Phys. Rev. Lett. 111, 165302 (2013)

TT 37.9 Tue 12:00 HSZ 304

Repulsive to attractive interaction quenches for bosons in a one-dimensional trap — •Wladimir Tschischik, Roderich Moessner, and Masud Haque — Max-Planck-Institut für Physik komplexer Systeme, Dresden

We present a study of the non-equilibrium dynamics of attractively interacting bosons in a one-dimensional harmonic trap. We describe the physics in terms of many-body spectra. We focus on the highly excited 'super-Tonks-Girardeau' state that is accessed through a sudden quench from a positive to a negative interaction. We describe both lattice (Bose-Hubbard) and continuum (Lieb-Liniger) cases.

Topical Talk TT 37.10 Tue 12:15 HSZ 304

Mesoscopic Transport of Heat in Trapped-Ion Crystals — •Martin Bruderer[1], Alejandro Bermudez[1,2], and Martin B. Plenio[1] — [1]Institut für Theoretische Physik, Albert-Einstein-Allee 11, Universität Ulm, 89069 Ulm, Germany — [2]Instituto de Fisica Fundamental, IFF-CSIC, Calle Serrano 113b, Madrid E-28006, Spain

Measuring and controlling heat flow on the nanoscale poses formidable practical difficulties as elementary devices such as switches and 'ampere meters' for thermal currents are not available. We propose to overcome this problem by realizing heat transport through a chain of trapped ions, where steady-state currents of local vibrations (vibrons) are induced by a constant temperature difference between the edges of the chain. We show how to efficiently control and measure these currents by coupling vibrons to internal ion states, which can be easily manipulated in experiments. Trapped-ion crystals therefore provide a promising platform for studying heat transport, e.g., through thermal analogues of quantum wires and quantum dots. Specifically, elusive phenomena such as the onset of Fourier's law may be observable in trapped-ion systems.
[1] A. Bermudez, M. Bruderer and M. B. Plenio, Phys. Rev. Lett. **111**, 040601 (2013)

TT 38: Transport: Spintronics and Magnetotransport (organized by TT)

Time: Tuesday 9:30–10:30 Location: BEY 81

TT 38.1 Tue 9:30 BEY 81

Spin-population inversion in Co/Pd heterojunctions — •Torsten Pietsch, Stefan Egle, and Elke Scheer — Department of Physics, Universitätstraße 10, University of Konstanz, 78457 Konstanz, Germany

Herein, we investigate experimentally the magneto-transport properties of nanosized Co/Pd hetero contacts and show that a spin-population inversion can be created by resonantly exciting magnetic heterojunctions with high-frequency waves in the GHz and THz regime. Recently, spin-flip photoemission in such metallic, magnetic heterojunctions was predicted theoretically but has not been observed experimentally. When an external magnetic field is applied the Zeeman splitting in the normal metal lifts the spin-degeneracy. Under a large current bias, hot electrons from the ferromagnet can be injected into the upper Zeeman level, thus creating a spin-population inversion in the normal metal. This non-equilibrium spin-population inversion decays via spin-flip transitions, which results in the creation of magnons, scattering at magnetic impurities and, under certain circumstances, photoemission. In the later, case, the energy of the emitted photon corresponds to the Zeeman energy, which can be tuned by the external magnetic field; typical frequencies are in the range of 0.1GHz to 60GHz. By resonantly exciting the Co/Pd point contacts using an external RF source while monitoring the transport properties, we evaluate the parameter space, where a spin-population inversion can be created at the ferromagnet-normal metal interface.

TT 38.2 Tue 9:45 BEY 81

Tuning the ballistic anisotropic magnetoresistance in single-atom contacts via the apex atom — •Fabian Otte[1], Yuriy Mokrousov[2], and Stefan Heinze[1] — [1]Instiut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Peter Grünberg Institut and Institue for Advanced Simulation, Forschungszentrum Jülich und JARA, D-52425 Jülich, Germany

Recently, the tunneling anisotropic magnetoresistance has been demonstrated at the single-atom limit using scanning tunneling spectroscopy and was explained based on density functional theory calculations of the anisotropy of the vacuum local density of states (LDOS) [1]. In the contact regime the explanation via the LDOS breaks down due to overlap of the wave functions and therefore actual calculations of the conductance are necessary. Here, we report first-principles calculations of ballistic transport in model systems of such single-atom contacts using our recently developed Wannierfunction based approach [2]. We present the ballistic anisotropic magnetoresistance (BAMR) in contact and tunneling regime between two ferromagnetic Ni monowires terminated by single 4*d*- and 5*d*- transition metal apex atoms. We show that the BAMR in the tunneling regime can be enhanced by up to an order of magnitude from 20% for Ni- to 150% for 5*d*-apex atoms. We also observe a change of sign in the BAMR between tunneling and contact regime.

[1] N. Néel *et al.*, PRL **110**, 037202 (2013)
[2] B. Hardrat *et al.*, PRB **85**, 245412 (2012)

TT 38.3 Tue 10:00 BEY 81

Electrical tuning of spin-orbit interaction in InAs nanowires — •Zoltán Scherübl[1], Gergö Fülöp[1], Morten Hannibal Madsen[2], Samuel d'Hollosy[3], Christian Schönenberger[3], Jesper Nygård[2], and Szabolcs Csonka[1] — [1]Departement of Physics, Budapest University of Technology and Economic, Budapest, Hungary — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark — [3]Departement of Physics, University of Basel, Basel, Switzerland

InAs nanowires are a promising platform to fabricate various quantum electronic devices, for instance they have strong spin-orbit interaction (SOI). The controlled tuning of the SOI is needed in spin based qunatum devices, for example spintronic applications, spin qubits. In this study we investigated the possibility of tuning the SOI by electrostatic field. The sources of the electric field were two sidegates paralel to the wire axis. The strength of the SOI was analyzed by weak-antilocalization. We demonstrated that the SOI can be strongly tuned, by a factor of 3 with the electric field across the nanowire, while the average electron density in the nanowire was kept constant.

TT 38.4 Tue 10:15 BEY 81

Dissipationless spin current between two coupled ferromagnets — •Wei Chen, Peter Horsch, and Dirk Manske — Max Planck Institute for Solid State Research, Stuttgart, Germany

We demonstrate the general principle which states that a dissipationless spin current flows between two coupled ferromagnets if their magnetic orders are misaligned. This principle applies regardless the two ferromagnets are metallic or insulating, and also generally applies to bulk magnetic insulators. On a phenomenological level, this principle is analogous to Josephson effect, and yields a dissipationless spin current that is independent from scattering. The microscopic mechanisms for the dissipationless spin current depend on the systems, which are elaborated in details. A uniform, static magnetic field is further proposed to be an efficient handle to create the misaligned configuration and stabilize the dissipationless spin current.

TT 39: Transport: Quantum Coherence and Quantum Information Systems - Theory II

Time: Tuesday 10:45–13:00 Location: BEY 81

TT 39.1 Tue 10:45 BEY 81

Self-trapping of photons in circuit QED — •Sebastian Schmidt[1], James Raftery[2], Darius Sadri[2], Hakan Tureci[2], and Andrew Houck[2] — [1]Institute of Theoretical Physics, ETH Zurich, Switzerland — [2]Department of Electrical Engineering, Princeton University, USA

We discuss the theoretical proposal and recent experimental observation of a novel dissipation driven dynamical localization transition of strongly correlated photons in an extended superconducting circuit consisting of two coupled resonators, each containing a superconducting qubit. Interaction with an environment has been argued to provide a mechanism for the emergence of classical behavior from a quantum system. Surprisingly, homodyne measurements reveal the observed localization transition to be from a regime of classical oscillations into a macroscopically self-trapped state manifesting revivals, a fundamentally quantum phenomenon. This experiment also demonstrates a new class of scalable quantum simulators with well controlled coherent and dissipative dynamics suited to the study of quantum many-body phenomena out of equilibrium.

TT 39.2 Tue 11:00 BEY 81

Measurement and dephasing of a flux qubit due to heat currents — •Samuele Spilla[1,2,3], Fabian Hassler[2,4], and Janine Splettstoesser[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, D-52056 Aachen, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Dipartimento di Fisica e Chimica, Università di Palermo, I-90123 Palermo, Italy — [4]Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

The existence of a phase-dependent thermal current through a temperature-biased Josephson junction has been recently demonstrated experimentally. It is this phase-dependence of the thermal current, which makes it interesting to study its sensitivity and impact on the states of superconducting circuits for quantum computing, e.g., superconducting qubits. I will present an analysis of the thermal current through a superconducting persistent current qubit, made of a superconducting loop interrupted by three Josephson junctions, which is subject to a temperature gradient. It can be shown that the thermal current induced by the temperature gradient depends significantly on the state of the qubit. I will furthermore investigate the impact of the heat current on the coherence properties of the qubit state. We find that even small temperature gradients can lead to dephasing times of

the order of microseconds for the Delft-qubit design.

TT 39.3 Tue 11:15 BEY 81

Quantum annealing with qubits with poor decoherence properties — •Michael Marthaler, Philipp Rudo, Johannes Janssen, Matthias Hecker, and Gerd Schön — Institut für Theoretische Festkörperphysik, KIT, Karlsruhe

We analyse adiabatic quantum computing, and assume that each qubit is strongly coupled to an environment. This allows us to model the time evolution of the system simply as a rate equation. The coupling to the environment creates qubit flips, weighted by the energy differences of the eigenstates of the system. The resulting equation can be efficiently simulated by using kinetic monte carlo methods, even for rather large systems. We use our method to explicitly study recent experiments on 108 rf-SQUIDs.

TT 39.4 Tue 11:30 BEY 81

Applying stochastic Bloch-Redfield theory to transport in Josephson junction arrays — •Nicolas Vogt[1,2], Alexander Shnirman[1,2], and Jared H. Cole[3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Chemical and Quantum Physics, School of Applied Sciences, RMIT University, Melbourne, Australia

Electrical transport in Josephson junction arrays in the Coulomb-blockade regime has been studied using several different theoretical models. Frequently used models include the sine-Gordon equation for the charge on the capacitances in the array and kinetic Monte-Carlo simulations of the incoherent tunneling of the charge-carrier through the array. These models either include coherent Cooper pair tunneling or microscopic dissipation but not both. Simulations of the full quantum-mechanical system including decoherence are problematic due to the unfavourable scaling of standard master-equations with system size. We use a stochastic unraveling of the Bloch-Redfield equation analogous to the established quantum jump unravelling of the Lindblad equation to obtain the time-evolution of a Josephson junction array coupled to a solid-state environment.

TT 39.5 Tue 11:45 BEY 81

Multi-Stability, Criticality and Steady-State Entanglement in the Nuclear Spin Dynamics of a Double Quantum Dot — •Martin J. A. Schuetz[1], Eric M. Kessler[2,3], Lieven M. K. Vandersypen[4], Juan Ignacio Cirac[1], and Geza Giedke[1] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany — [2]Physics Department, Harvard University, Cambridge, MA 02318, USA — [3]ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA — [4]Kavli Institute of NanoScience, TU Delft, PO Box 5046, 2600 GA, Delft, The Netherlands

We propose a scheme for the deterministic generation of steady-state entanglement between the two nuclear spin ensembles in an electrically defined double quantum dot. Because of quantum interference in the collective coupling to the electronic degrees of freedom, the nuclear system is actively driven into a two-mode squeezed-like target state. The entanglement build-up is accompanied by a self-polarization of the nuclear spins towards large Overhauser field gradients. Moreover, the feedback between the electronic and nuclear dynamics leads to multi-stability and criticality in the steady-state solutions. Prospects for the experimental realization of this scheme and potential extensions towards steady-state entanglement between spatially separated quantum dots are also discussed.

TT 39.6 Tue 12:00 BEY 81

Maximal Rabi frequency of an electrically driven spin in a disordered magnetic field — •Gábor Széchenyi and András Pályi — Eötvös University, Budapest, Hungary

We present a theoretical study of the spin dynamics of a single electron confined in a quantum dot. Spin dynamics is induced by the interplay of electrical driving and the presence of a spatially disordered magnetic field, the latter being transverse to a homogeneous magnetic field. We focus on the case of strong driving, i.e., when the oscillation amplitude of the electron's wave packet is comparable to the quantum dot length. We show that electrically driven spin resonance can be induced in this system by subharmonic driving, i.e., if the excitation frequency is an integer fraction (1/2, 1/3, etc) of the Larmor frequency. At strong driving we find that (i) the Rabi frequencies at the subharmonic resonances are comparable to that at the fundamental resonance, and (ii) at each subharmonic resonance, the Rabi frequency can be maximized by setting the drive strength to an optimal, finite value. Our simple model is applied to describe electrical control of a spin-valley qubit in a weakly disordered carbon nanotube.
[1] arXiv:1310.7350

TT 39.7 Tue 12:15 BEY 81

Non-linear quantum optics and entanglement in arrays of optomechanical oscillators — •Steven Habraken, Zhijiao Deng, and Florian Marquardt — Institut für Theoretische Physik II, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstraße 7 91058 Erlangen

We consider arrays of coupled optomechanical cells, each of which consists of a laser-driven localized optical resonance interacting with a mechanical (vibrational) mode. The cells are coupled through photon tunneling. We characterize the phonon-mediated photon-photon interaction in such arrays. As an example, we focus on the case of three coupled optomechanical cells and show that such a setup can be used as a source of entangled photon pairs. We characterize such continuous variable entanglement and study its temperature dependence.

TT 39.8 Tue 12:30 BEY 81

Master equation approach for the description of the dynamics of an holmium atom on Pt(111) — •Christian Karlewski, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, KIT, 76128 Karlsruhe

We model a holmium atom located on a Pt(111) surface. This system was recently studied experimentally (Nature 503, 242 (2013)). Transitions between the two degenerated ground states are forbidden in first order due to several symmetries (time-reversal, internal symmetries of the total angular momentum, point symmetry of the local environment) yielding long life times. We simulate the dynamics of the whole set of 17 eigenstates (J=8) of the Ho-atom coupled to an environment with a master equation approach. To check the validity of our model it is compared to an experiment in which the system is driven out of equilibrium by a current and relaxes afterwards to one of the two degenerate ground states.

TT 39.9 Tue 12:45 BEY 81

Algebraic versus exponential decoherence in dissipative many-particle systems — Zi Cai[1] and •Thomas Barthel[1,2] — [1]LMU München — [2]Université Paris-Sud and CNRS

Until our recent study, it was assumed that, as long as the environment of a system is memory-less (i.e. Markovian), the temporal coherence decay in the system is always exponential – to a degree that this behavior was synonymously associated with decoherence. However, the situation can change if the system itself is a large many-body system with internal interactions.

I will discuss an open XXZ chain for which the decoherence time diverges in the thermodynamic limit. The coherence decay is then algebraic instead of exponential. In contrast, decoherence in the open transverse-field Ising model is found to be always exponential. In this case, the internal interactions can both facilitate and impede the environment-induced decoherence. The results are based on quasi-exact simulations using the time-dependent density matrix renormalization group (tDMRG) and explained on the basis of perturbative treatments.
[1] Z. Cai and T. Barthel, PRL 111, 150403 (2013)

TT 40: Multiferroics I (organized by MA)

Time: Tuesday 9:30–12:45 Location: BEY 118

TT 40.1 Tue 9:30 BEY 118

***Ab initio* study of electronic transport in the Co/PZT-based tunnel junctions** — •Vladislav Borisov[1], Sergey Ostanin[1], Igor Maznichenko[2], Arthur Ernst[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

Magnetoelectric coupling at the multiferroic interfaces FM/FE (FM=Co,Fe, FE=$PbTiO_3$,PZT) was studied from first principles. The magnetic interfacial effect, which is controlled by the FE polarization, originates from the charge transfer and *d*-orbital redistribution of Co/Fe and Ti mediated by the *p*-states of interfacial oxygens. In PZT, the presence of Zr dopants may locally enhance the effect. We analysed also the spin polarization of tunneling electrons in Co/PTO/Co and Fe/PTO/Co junctions, in which the calculated four-state conductance can account for the ferroelectrically switchable TMR signal observed recently in LSMO/PZT/Co [1].

[1] D. Pantel *et al.*, *NATURE MATERIALS* **11**, 289 (2012).

TT 40.2 Tue 9:45 BEY 118

Tunneling transport and memristive effects in PbTiO3- based multiferroic tunnel junctions — •Andy Quindeau, Marin Alexe, and Dietrich Hesse — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

A gradually tunable resistance effect based on the tunnel electroresistance (TER) of multiferroic tunnel junctions is investigated. The ferroelectric tunnel barrier comprises, a PbTiO3 layer of a few nm thickness, is embedded between two different ferromagnetic layers, viz. La0.7Sr0.3MnO3 and cobalt. In this capacitor geometry an electric bias, applied perpendicularly to the films, results in a direct tunneling current flowing between the two electrodes. The tunnel resistance is dependent on the polarization of the ferroelectric, which is switchable via relatively high voltage pulses. Due to the variation of the pulse parameters a variety of non-volatile resistance states can easily be achieved. These gradually tunable resistance states, characteristic for a memristor device, can be explained by a ferroelectric domain distribution inside the ferroelectric film: Domains with different polarities can coexist inside one capacitor after partial polarization switching and act as parallel connected tunnel barriers with different tunnel resistances. Temperature dependent measurements show the influence of different electron transport mechanisms, which will be discussed. The impact of the memristive states on the tunnel magnetoresistance (TMR) can be shown.

TT 40.3 Tue 10:00 BEY 118

Lattice and polarizability mediated spin activity in EuTiO3 — •Annette Bussmann-Holder[1], Kevin Caslin[1,2], Patrick Reuvenkamp[1], Zurab Guguchia[3], Hugo Keller[3], Reinhard Kremer[1], and Jürgen Köhler[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr.1, D-70569 Stuttgart, Germany — [2]Brock University, 500 Glenridge Ave., St. Catharines L2S-3A1, Ontario, Canada — [3]Physik-Institut der Universität Zürich, Winterthurerstr. 190, CH-8057 Zürich, Switzerland

EuTiO3 is shown to exhibit novel strong spin-charge-lattice coupling deep in the paramagnetic phase. Its existence is evidenced by an, until now, unknown response of the paramagnetic susceptibility at temperatures exceeding the structural phase transition temperature TS=282K. The extra features in the susceptibility follow the rotational soft zone boundary mode temperature dependence above and below TS. In addition, novel magnetostriction experiments and dielectric constant measurements have been performed which both reveal giant anomalies related to the antiferromagnetic phase transition at TN=5.7K and the structural phase transition at TS. The theoretical modeling consistently reproduces these anomalies and provides evidence that EuTiO3 has considerable analogies to SrTiO3 but also substantial differences stemming from the Eu 4f spins which are lattice activated at high temperatures far above TN.

TT 40.4 Tue 10:15 BEY 118

Magnetoelectric coupling in a composite multiferroic structure revealed by Ferromagnetic Resonance — •Alexander Sukhov[1], Paul P. Horley[2], Chenglong Jia[3], and Jamal Berakdar[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle/Saale, GERMANY — [2]Centro de Investigacion Materiales Avazados, S.C. (CIMAV), Chihuahua/Monterrey, MEXICO — [3]Lanzhou University, Lanzhou, CHINA

We theoretically study [1] a thin multiferroic junction related to a barium titanate (tetragonal or rhombohedral phase) layer in contact with an iron layer. Depending on the type of the magnetoelectric coupling at the interface - either due to screening charge or due to an epitaxial strain resulting in a strong magnetoelastic coupling - we present a detailed analysis of the response of the multiferroic structure to magnetic radio-frequency fields by means of ferromagnetic resonance as a function of the applied electric field.

[1] A. Sukhov, P.P. Horley, C.-L. Jia, J. Berakdar, J. Appl. Phys. **113**, 013908 (2013).

TT 40.5 Tue 10:30 BEY 118

Magnetoelectric monopoles in bulk periodic solids — •Michael Fechner[1], Eric Bousquet[1], Alexander Balatsky[2], Nicoal A. Spaldin[1], and Lars Nordström[3] — [1]ETH Zürich, Department for Materials Theory, Zürich, Switzerland — [2]NORDITA, KTH Royal Institute of Technology and Stockholm University, Stockholm, Sweden — [3]Department of Physics and Astronomy, Uppsala University, Sweden

The magnetoelectric (ME) response is described by a second rank tensor that can be decomposed into irreducible isotropic diagonal, antisymmetric and trace-free part. Here we show that the former component can be identified with a ferroic ordering of magnetoelectric monopoles[1]. We further develop a scheme to calculate the ME monopole in bulk periodic solids, by exploiting similarities to the ferroelectric polarization. Finally, as an example we present results for the series of lithium transition metal phosphate compounds ($LiMPO_4$, with M = Co, Fe and Ni), which include both ferromonopolar and antiferromonopolar ordered cases. We predict for the latter case a q-dependent diagonal ME effect.

[1] N . A. Spaldin et al., PRB 88, 094429 (2013)

TT 40.6 Tue 10:45 BEY 118

Different routes for enhanced control of ferroelectric polarization by magnetic field — •I. Fina[1,2], V. Skumryev[3,4], D. O'Flynn[5], G. Balakrishnan[5], N. Dix[2], J. M. Rebled[2,6], P. Gemeiner[7], X. Marti[8], F. Peiró[6], B. Dkhil[7], F. Sánchez[2], L. Fàbrega[2], and J. Fontcuberta[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Institut de Ciència de Materials de Barcelona, Catalonia, Spain — [3]Institució Catalana de Recerca i Estudis Avançats (ICREA), Catalonia, Spain — [4]Universitat Autònoma de Barcelona, Barcelona, Spain — [5]University of Warwick, Coventry, United Kingdom — [6]LENS - MIND/IN2UB, Barcelona, Spain — [7]Propriétés et Modélisation des Solides, Paris, France — [8]Faculty of Mathematics and Physics, Praha, The Czech Republic

I will focus on the direct magnetoelectric effect, control of polarization vector by magnetic field, in single-phase and composite multiferroic materials in thin film form.

In single-phase multiferroic materials, cycloidal magnet, we will see that strong coexistence of polar and non-polar regions allow large susceptibilities leading to a full control of the polarization vector by means of magnetic field [1]. In composite materials, ferromagnetic-ferroelectric heterostructures, the limiting factor is the substrate clamping effect. We will show that we can overcome this undesired effect, enhancing the presence of some small quantity of defects. These defects store the needed elastic energy, enhancing the magnetoelectric coupling, which result in huge effects near room temperature [2].

[1] I. Fina, et al., Phys. Rev. B 88, 100403(R) (2013). [2] I. Fina, et al., Nanoscale 5, 8037 (2013).

15 min. break

TT 40.7 Tue 11:15 BEY 118

Investigation of A-site Bismuth based double perovskites as potential room-temperature multiferroics — •Vikas Shabadi, Mehran VafaeeKhanjani, Mehrdad BaghaieYazdi, Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Ger-

many

A-site Bismuth based double perovskites ($Bi_2BB'O_6$), where ferroelectricity arises from the stereochemically active $6s^2$ lone pair of electrons on the Bi^{3+} cations, provide a vital test bed to engineer room temperature multiferroicity. Here, different combinations of 3d-3d or 3d-5d cations may be introduced at the B-site in order to obtain an effective ferri/ferromagnetic moment. The 3d-3d compound Bi_2FeCrO_6 (BFCO) has drawn a heightened interest due to its large experimentally reported ferroelectricity and divergent observations of its magnetic properties. We report epitaxial BFCO thin films grown by pulsed laser deposition on single crystal $SrTiO_3(100)$ substrates. Detailed structural characterization was performed by X-ray Diffraction and the magnetic properties were studied with a SQUID magnetometer. We show that BFCO adopts a superstructure with the same unit cell as the chemically ordered double perovskite. The magnetization is a function of chemical but not of structural order.

TT 40.8 Tue 11:30 BEY 118

Room temperature magnetism and ferroelectricity in eps-Fe2O3 thin films — •I. Fina[1], M. Gich[2], A. Morelli[1], F. Sánchez[2], M. Alexe[1], J. Fontcuberta[2], and A. Roig[2] — [1]Max Planck Institute of Microstructure Physics D-06120 Hallle/Salle, Germany — [2]Institut de Ciència de Materials de Barcelona ICMAB, Consejo Superior de Investigaciones Científicas CSIC, Campus UAB 08193 Bellaterra, Catalonia, Spain

The quest for magnetoelectric multiferroics is driven by the promise of a novel generation of devices combining the best characteristics of ferromagnetic and ferroelectric materials. These cherished applications require materials displaying a substantial magnetization and electric polarization which are coupled and coexist well above room temperature. These properties are not commonly fulfilled by single phase materials and firm candidates for the development of these technologies are still sought.

In this contribution, we will report on epitaxial eps-Fe2O3 thin films grown by Pulsed Laser Deposition on (111) SrTiO3 and present recent data on its structural, magnetic and dielectric characterization. The films are ferromagnetic and ferroelectric at room temperature and display magnetization and polarization values at remanence of about 50 emu/cm3 and 1 uC/cm2 with a long retention. A magnetocapacitive response has also been detected indicating that the films present coupling between both ferroic orders.

TT 40.9 Tue 11:45 BEY 118

Time-resolved analysis of switching in spiral multiferroics — •Jonas Stein[1], Tobias Cronert[1], Jeannis Leist[2], Karin Schmalzl[3], A Agung Nugroho[4], Alexander C Komarek[5], Götz Eckold[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Physikalische Chemie, Universität Göttingen — [3]JCNS at ILL, France — [4]Institut Teknologi Bandung, Indonesia — [5]MPI für chemische Physik fester Stoffe

Multiferroic crystals are promising materials for future memory devices with extremely low power consumption. The rise time between two states is a crucial parameter for a possible application and was investigated in the spiral spin multiferroic $TbMnO_3$. Polarized neutron diffraction is able to determine the ratio of chiral domains, which can be controlled by an external electric field. Using the stroboscopic technique we can follow the reversion of chiral domains in the timescale of a few 100 microseconds to hours. In $TbMnO_3$ we find a clear logarithmic relation between the rise time and temperature that is fulfilled over 5 decades.

TT 40.10 Tue 12:00 BEY 118

Thermodynamic properties of the new multiferroic material $(NH_4)_2[FeCl_5(H_2O)]$ — •Matthias Ackermann[1], Daniel Brüning[2], Thomas Lorenz[2], Petra Becker[1], and Ladislav Bohatý[1] — [1]Institut für Kristallographie, Universität zu Köln, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany

Multiferroic materials with coupled ferroelectric and (anti-)ferromagnetic order in the same phase have attracted considerable interest during the last decade. The search for new multiferroic materials is an important issue to further improve the understanding of the underlying coupling mechanisms. Here, we present a detailed investigation of the new multiferroic compound $(NH_4)_2[FeCl_5(H_2O)]$ [1]. Our measurements of pyroelectric currents reveal, that the electric polarization occuring in the antiferromagnetically ordered phase can drastically be influenced by applying magnetic fields. Based on the results of these dielectric investigations, together with measurements of thermal expansion, magnetostriction and specific heat, detailed magnetic field versus temperature phase diagrams are derived. Depending on the direction of the magnetic field up to three different multiferroic phases are identified, which are separated from the paramagnetic phase by a magnetically ordered, but non-ferroelectric phase.

This work was supported through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

[1] Ackermann M et al. 2013 *New J. Phys.* (in press, arXiv:1308.0285)

TT 40.11 Tue 12:15 BEY 118

Stoichiometric Effects on Crystal Quality in $LuFe_2O_4$ and $YbFe_2O_4$ — •Hailey Williamson[1,2], Geetha Balakrisnan[2], and Manuel Angst[1] — [1]Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, Forschungszentrum Jülich GmbH, Jülich, Germany. — [2]Department of Physics, The University of Warwick, CV4 7AL, Coventry, UK

The multiferroic rhombohedral $LnFe_2O_4$ (Ln=Lu, Y, Yb, Tm, Ho and Er) system, which can be described as stacked hexagonal Fe bilayers separated by Lu monolayers, has been in focus since the discovery of interesting magnetic and electrical characteristics in $LuFe_2O_4$. The specific CO configuration within the Fe bilayers was initially thought to produce a ferroelectricity through cross polarization of the two layers of the bilayer. However our recent investigations indicate that the CO configuration is actually non-polar. Extensive research highlighted a large sensitivity to oxygen stoichiometry, where crystals grown in an excess/deficient oxygen partial pressure environment exhibit smeared glassy magnetic transitions and diffuse CO. Through fine tuning of the atmospheric conditions, crystals exhibiting 3D CO and magnetism were produced. Interest then spread to isostructural $YbFe_2O_4$, which has currently few detailed investigations. Single crystals of $YbFe_2O_4$ were grown in four different partial pressure atmospheres to view the effects of oxygen stoichiometry on the magnetism and CO. A series of macroscopic and microscopic measurements provided a detailed look into the effects of oxygen stoichiometry on the intrinsic characteristics as well as a comparison to that of its predecessor $LuFe_2O_4$.

TT 40.12 Tue 12:30 BEY 118

Multiferroicity in Cu_2OSeO_3? — •Eugen Ruff[1], Stephan Krohns[1], Helmuth Berger[2], Peter Lunkenheimer[1], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg — [2]Institute of Physics of Complex Matter, École Polytechnique Fédérale de Lausanne

Skyrmions are topologically stable vortex-like objects, for the first time detected in the B20 alloy MnSi [1]. Their electrical controllability via small currents qualifies skyrmions for applications in high-density magnetic storage devices. The recent discovery of magnetoelectric skyrmions in the insulating chiral magnet Cu_2OSeO_3 leads to another promising route to electrical control [2]. This system is suggested to carry a local electrical dipole, which implies that the skyrmions should be controllable by an external electrical field without losses due to Joule heating. Here we provide a thorough analysis of the magnetic and polar phases of this material, using SQUID and pyrocurrent measurements. In order to investigate the possible ferroelectric properties of Cu_2OSeO_3, we have performed dielectric spectroscopy in various magnetic fields in a broad frequency range below 70 K. Combining all these different techniques, we address the question whether Cu_2OSeO_3 is magnetoelectric or multiferroic. [1] S.Mühlbauer *et al.*, Science **323**, 915 (2009). [2] S.Seki *et al.*, Science **336**, 198 (2012).

TT 41: Focus Session: Quantum Light Sources Based on Solid State Systems: Status and Visions I (organized by HL)

Non-classical quantum light sources with the ability to efficiently generate photon states with tailored properties (e.g. well defined photon-number Fock states, mutually highly indistinguishable photons, or high fidelity quantum entangled states, etc.) are among the fundamental building blocks of numerous proposed applications in the field of quantum information processing – particularly quantum computing and quantum cryptography. The aim of this focus session is to bring together the ideas, concepts and results of leading national and European research groups on semiconductor and solid state-based quantum light sources and to discuss the current status and future goals in this highly topical field of research.

Organizers: Sven Ulrich, Universität Stuttgart, and Christoph Becher, Universität des Saarlandes, Saarbrücken.

Time: Tuesday 9:30–11:15 Location: POT 251

Topical Talk TT 41.1 Tue 9:30 POT 251

Nonclassical light from semiconductor quantum dots — •Gregor Weihs[1,2], Tobias Huber[1], Harishankar Jayakumar[1], Thomas Kauten[1], and Ana Predojević[1] — [1]Institut für Experimentalphysik, Universität Innsbruck, Technikerstr. 25, 6020 Innsbruck, Austria — [2]Institute for Quantum Computing, University of Waterloo, 200 University Ave W, Waterloo, ON N2L 3G1, Canada

For fundamental tests of quantum physics as well as for quantum communications non-classical states of light are an important tool. In our research we focus on developing semiconductor-based and integrated sources of single photons and entangled photon pairs.

In this talk we will present our work on single InAs/GaAs quantum dots. For the highest degree of quantum control we use resonant two-photon excitation to deterministically trigger a biexciton-exciton cascade. We block the pump light from the detectors by using side excitation through the waveguide mode of a planar microcavity. We demonstrate Rabi oscillations, Ramsey interference and all-optical coherent control of the quantum dot resulting in single and paired photons with a high degree of indistinguishability [1]. Using novel quantum optical assessment tools we are then able to show the non-classical and non-Gaussian characteristics of the emitted photons.

This indistinguishability eventually results in time-bin entangled photon pairs through the biexciton-exciton cascade. Time-bin entanglement is a useful variant for long distance communication because it is robust against decoherence in optical fibers. Two successive coherent pulses excite the dot ei-ther in the early or in the late pulse. The emitted photons pass imbalanced interferometers for analy-sis in the energy basis. Through quantum state tomography we are able to demonstrate significant entanglement of the emitted pairs.

This work was supported by the ERC and CIFAR.

[1]H. Jayakumar, A. Predojevic, T. Huber, T. Kauten, G. S. Solomon & G. Weihs, Deterministic Photon Pairs and Coherent Optical Control of a Single Quantum Dot, Phys. Rev. Lett. 110, 135505 (2013).

TT 41.2 Tue 10:00 POT 251

On-demand generation of indistinguishable polarization-entangled photon pairs — •Markus Müller[1], Samir Bounouar[1], Klaus D. Jöns[1], Martin Gläßl[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institut für Theoretische Physik III, Universität Bayreuth, Universitätsstraße 30, 95440 Bayreuth, Germany

The development of quantum information science using linear optics has made substantial progress in the recent past. This advance is mainly based on the ability to generate high-quality photonic qubits from various kinds of different sources. Furthermore, for practical quantum information operations it is essential to create the qubits deterministically. In this work we show that semiconductor quantum dots (QDs) are suitable to fulfill both of this elementary requirements. To exploit their remarkable properties, a coherent resonant two-photon excitation scheme is applied. Thereby the biexciton state of an InGaAs QD is populated with a near unity preparation efficiency. Because of this individual and coherent addressing, the photons emitted by the biexciton-exciton cascade show enhanced optical and quantum-optical qualities. This is reflected in pure single-photon emission, long coherence times and high indistinguishability visibilities ($V_{\mathrm{HOM}} = 0.86 \pm 0.03$ and 0.71 ± 0.04) for the biexcitonic and excitonic emission, respectively. Taking advantage of a QD without fine structure splitting, we can demonstrate the on-demand generation (pair-efficiency $= 0.86 \pm 0.08$) of high fidelity (0.81 ± 0.02) polarization-entangled photon pairs.

TT 41.3 Tue 10:15 POT 251

Feedback-Enhanced Entanglement of Photons from a Biexciton Cascade — •Sven Moritz Hein[1], Franz Schulze[1], Alexander Carmele[2], and Andreas Knorr[1] — [1]Technische Universität Berlin, Institut für theoretische Physik, Nichtlineare Optik und Quantenelektronik, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Institut für Quantenoptik und Quanteninformation, Technikerstraße 21a, 6020 Innsbruck, Austria

Coherent quantum feedback [1] is a method to control and stabilize quantum-mechanical systems by the use of a feedback mechanism that does not rely on measurement, but is completely quantum-mechanical itself. We utilize such a feedback scheme to enhance the entanglement of photons from a biexciton cascade in a quantum dot. The achievable photon entanglement is usually diminished substantially by exciton fine-structure splitting. We demonstrate that it is possible to increase photon entanglement by feeding the emitted light back into the quantum dot after a certain feedback time, e.g. by using a mirror at a specific distance from the emitter [2]. The complex interplay between original and reflected field modifies the emission spectrum in a way that the achievable entanglement is strongly enhanced. We present a full quantum-mechanical theory of the system, including the feedback-induced modification of the photon mode continuum. We analyze the influence of feedback delay and phase and discuss the involved mechanisms in detail.

[1] S. Lloyd, Phys. Rev. A 62, 022108 (2000).
[2] A. Carmele et al., Phys. Rev. Lett. 110, 013601 (2012).

TT 41.4 Tue 10:30 POT 251

Emission of polarization-entangled photons from biexcitons: two-photon processes and phonon-assisted cavity feeding — •Dirk Heinze, Artur Zrenner, and Stefan Schumacher — Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, 33098 Paderborn

Semiconductor quantum dots are promising sources for generation of pairs of polarization-entangled photons. In [1] we have shown theoretically that using a direct two-photon emission process inside a high-quality optical microcavity, the degree of achievable polarization-entanglement can be rendered insensitive to exciton fine-structure splitting (in contrast to the usual cascaded emission). The results in [1] were obtained for realistic quantum-dot and cavity parameters but neglecting the influence of phonon-assisted cavity feeding. Here we extend our previous study and include the interaction with a bath of acoustic phonons in a Born-Markov approximation in the master-equation for the system density operator. Our analysis shows the detrimental influence of phonons on the polarization entanglement with increasing temperature. However, it also demonstrates that at low temperature the influence of phonons on the scheme proposed in [1] is strongly suppressed such that high degrees of entanglement can be achieved.

[1] S. Schumacher, J. Förstner, A. Zrenner, M. Florian, C. Gies, P. Gartner, and F. Jahnke. Cavity-assisted emission of polarization-

entangled photons from biexcitons in quantum dots with fine-structure splitting. Optics Express, **20**, 5335 (2012).

Topical Talk TT 41.5 Tue 10:45 POT 251
Taming single photons emitted by solid state systems — •Stephan Götzinger — Max Planck Institute for the Science of Light and Friedrich-Alexander-Universitaet Erlangen-Nuernberg (FAU), D-91058 Erlangen, Germany

In the first part of this talk we will discuss single-photon sources with near-unity efficiency. These sources are based on the concept of metallo-dielectric antennas. Then we will present experiments where photons and single solid state emitters strongly interact.

TT 42: Transport: Graphene (organized by TT)

Time: Tuesday 9:30–13:15 Location: WIL C107

Topical Talk TT 42.1 Tue 9:30 WIL C107
A First-Principles Perspective on Two-Dimensional Transition-Metal Dichalcogenides — •Udo Schwingenschlögl — KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

Layered transition-metal dichalcogenides recently are attracting great attention, because of the possibility to achieve two-dimensional (2D) materials, similar to the exfoliation of graphene from graphite. Using first-principles calculations, we study prototypical monolayer MoS_2 to obtain insight into the influence of defects and substitutional doping, for a wide range of transition-metal dopants. We also address polar transition-metal dichalcogenide monolayers with respect to their structural stability and the effects of the spin-orbit coupling. Heterojunctions of MoS_2 with unsaturated and saturated MXenes are studied; such hyrid systems are interesting for application in all-2D devices.
[1] Phys. Rev. B 87, 100401(R) (2013)
[2] EPL 102, 57001 (2013)
[3] Phys. Rev. B 87, 245307 (2013)

TT 42.2 Tue 10:00 WIL C107
Ab-initio simulations of local current flows in functionalized graphene flakes and ribbons — •Michael Walz, Alexei Bagrets, and Ferdinand Evers — Institute of Nanotechnology (INT) and Institut für Theorie der Kondensierten Materie (TKM), Karlsruhe Institut of Technologie (KIT), D-76131 Karlsruhe, Germany

Using our DFT-based transport framework AITRANSS [1,2], we calculate the transmission and the local current density in graphene flakes functionalized by adsorbed atoms, such as nitrogen or hydrogen.

We find that even a single nitrogen atom can almost completely suppress the conductance of a (gated) graphene armchair nano-ribbon. In this situation local ring currents emerge that result in local (orbital) magnetic moments.

As one expects, very wide ribbons (flakes, $W \gg L$) exhibit the bulk conductance $G = \frac{2e^2}{h}\frac{W}{\pi L}$ in the absence of adsorbants. With 20% hydrogen absorbants, we observe very complicated patterns of streamlines with many eddies and a broad distribution of local magnetic fields, $\mathbf{B}(\mathbf{r})$, that are induced by the dc-current flow. We plan to study the statistics of the conductance and $\mathbf{B}(\mathbf{r})$ of such large flakes and its dependency on the impurity concentration. Performing such calculations starting from first principles is challenging because of high computational costs. On this account, we parallelized our transport module AITRANSS using standard MPI and OpenMP techniques, also including Scalapack to treat systems up to 10.000 carbon atoms.
[1] A. Arnold *et al.*, J. Chem. Phys. **126**, 174101 (2007).
[2] J. Wilhelm, MW, *et al.*, Phys. Chem. Chem. Phys. **15**, 6684 (2013).

TT 42.3 Tue 10:15 WIL C107
Quantum transport simulations and Fabry-Perot interference patterns in multiple pn-junctions on graphene — •Fedor Tkatschenko[1], Ming-Hao Liu[1], Klaus Richter[1], Martin Drienovsky[2], Jonathan Eroms[2], and Dieter Weiss[2] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg

Advancements in experimental techniques have led to an amazing progress towards excellent graphene samples and to graphene devices with fascinating properties, ranging from narrow pnp junctions below 100 nm to large mean free paths up to micron scales. In such devices the charge carriers undergo multiple reflections at pn or np interface leading to interesting Fabry-Perot-type interference patterns in the conductance map[1,2]. We address the peculiar features of Fabry-Perot resonances in graphene. To this end we calculate the potential profiles for typical experimental setups[3] with the quantum capacitance model and perform transport calculations using the recursive Green's function technique. The numerical results are in good agreement with the experimental data. We further show that the leading contribution to the Fabry-Perot resonances in the conductance map originates from the first two pn junctions.
[1] A.F. Young and Ph. Kim, Nat. Phys. **5** (2009)
[2] P. Rickhaus, R. Maurand, M. H. Liu, M. Weiss, K. Richter and C. Schönenberger, Nat. Comm. **4** 2342 (2013)
[3] M. Drienovsky, F.-X. Schrettenbrunner, M. H. Liu, F. Tkatschenko, K.Richter, D. Weiss and J. Eroms, in preparation

TT 42.4 Tue 10:30 WIL C107
Ballistic interferences in suspended graphene — •Ming-Hao Liu[1], Peter Rickhaus[2], Romain Maurand[2], Markus Weiss[2], Klaus Richter[1], and Christian Schönenberger[2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Complex Fabry-Pérot interferences in ultraclean suspended graphene have been recently observed, with the ballistic origin confirmed by transport calculations well agreeing with experiment [1]. The observed conductance oscillations account for quantum interference of electron waves propagating ballistically over distances exceeding 1 μm. The complex interference patterns stem from Fabry-Pérot resonances within different cavities defined by electrically controlled pn junctions and the graphene-contact interfaces. In this talk, the theoretical part of this work [1], namely, the full modeling of the ballistic transport from contact to contact through the suspended graphene, will be illustrated at an appropriate depth.
[1] P. Rickhaus, R. Maurand, M.-H. Liu, M. Weiss, K. Richter, and C. Schönenberger, Nat. Commun. **4**, 2342 (2013)

TT 42.5 Tue 10:45 WIL C107
Ballistic transport in graphene nanoconstrictions — •Danny J. M. Jörger[1,2], Bernat Terrés[1,2], Stephan Engels[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], Slava V. Rotkin[1,4], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan — [4]Physics Department, Lehigh University, Bethlehem, Pennsylvania 18015, USA

Graphene nanodevices, such as for example nanoconstrictions are interesting systems for studying mesoscopic phenomena. Recent developments in the fabrication of graphene devices have revealed a significant increase in carrier mobility (e.g. 200.000 cm^2/Vs in bulk samples), making mean free path in the order of device dimensions accesible. This allows to investigate quantum interference effects and ballistic transport in nanostructured graphene. We discuss the differences in electrostatic coupling ($\alpha \approx 9.4 \times 10^{10}$ $cm^{-2}V^{-1}$) at high and low magnetic fields and the width-dependency of the overall conductance level at zero magentic field. Results confirm the Dirac fermion nature of confined charge carriers in graphene. We report on the observation of quasi one-dimensional subband transport characteristics in graphene nanoconstrictions encapsulated in hexagonal boron nitride. The ballistic nature of the transport in our devices ($l_m \geq 500$ nm) allows to study the interplay between confinement and Landau quantization and its crossover.

15 min. break.

TT 42.6 Tue 11:15 WIL C107
Optical conductivity of graphene — •Julia Link, Peter P.

Orth, and Jörg Schmalian — Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Graphene is a two-dimensional crystal of carbon atoms with a honeycomb structure, which has many fascinating optical and electronical properties. It has a high mobility of electrons at room temperature and a high transparency of light with 97.7%. In the optical domain, the value of the transparency does not depend on the frequency of white light being transmitted and is thus universal. This universality is linked to the fine structure constant $\alpha = 1/137$ and can be derived using non-interacting Dirac fermions.

We aim to understand the correction of the optical transparency due to Coulomb interaction. Since there is a long dispute about this correction in the literature [1-6], we try to resolve this controversy. Therefore we combine two different regularization schemes: dimensional regularization and a deformation of the Coulomb potential. We discuss the physical implication of the choice of the regularization.

[1] Herbut, Juricic, Vafek, Phys. Rev. Lett. **100**,046403 (2008)
[2] Mishchenko, Europhys. Lett. **83**, 17005 (2008)
[3] Sheey, Schmalian, Phys. Rev. B **80**, 193411 (2009)
[4] Juricic, Vafek, Herbut, Phys. Rev. B **82**, 235402 (2010)
[5] Rosenstein et al., Phys. Rev. Lett. **110**, 066602 (2013)
[6] Gazzola, Cherchiglia, Cabral, Nemes, Sampaio, Europhys. Lett. **104**, 27002 (2013)

TT 42.7 Tue 11:30 WIL C107

Polycrystalline graphene: mechanical, electrical and thermal properties — •Thomas Lehmann[1,2], Arezoo Dianat[1,2], Frank Ortmann[1,2], Dmitry Ryndyk[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, Germany

Large-area samples of graphene tend to be polycrystalline (PC) on some substrates. Grain boundaries with structural defects are expected to alter the structural and electronical properties of graphene. In this work, the mechanical properties of PC graphene are studied by means of density-functional theory and furthermore the electrical and thermal transport properties are addressed. To construct grain boundaries of zigzag and rotated armchair graphene sheets, molecular dynamics simulations are performed. The critical strain leading to structural failure of PC graphene nanoribbons is only half the value of pristine armchair nanoribbons. However we show that it can be significantly enhanced by the reaction of the chemically active grain boundaries with atmospheric gases. The transport properties of those systems are investigated, both parallel and perpendicular to the grain boundary, using an ab initio based atomistic model combined with Landauer transport theory and recursive Green function method. The electronic part is calculated within a tight-binding model and a force-constant approach has been applied for phonon transport.

TT 42.8 Tue 11:45 WIL C107

Electric field control of spin-polarized electron transport through zigzag graphene nanosheets — •Dirk Wiedmann[1], Marius Bürkle[2], and Fabian Pauly[1] — [1]Department of Physics, University of Konstanz, Germany — [2]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

We study the spin-polarized transport through a finite zigzag graphene nanoribbon, contacted by carbon-nanotube electrodes [1]. The electronic structure is determined from density functional theory, and Green's functions are used to compute the phase-coherent electric current within the Landauer scattering theory. We observe antiferromagnetically coupled edge states in the graphene nanosheet, which may lead to spin-polarized currents. We analyze how they depend on the position of the electrodes and on applied transverse electric fields. Our ab-initio results are rationalized with the help of a Hubbard model.

[1] D. Wiedmann, M. Bürkle, and F. Pauly, in preparation.

TT 42.9 Tue 12:00 WIL C107

Radiative damping and synchronization in a graphene-based terahertz emitter — •Andrey Moskalenko and Sergey Mikhailov — Institute of Physics, University of Augsburg, Germany

We investigate the collective electron dynamics in a recently proposed graphene-based terahertz emitter [1] under the influence of the radiative damping effect, which is included self-consistently in a molecular dynamics approach. We show that under appropriate conditions synchronization of the dynamics of single electrons takes place, leading to a rise of the oscillating component of the charge current. The synchronization time depends dramatically on the applied dc electric field and electron scattering rate, and is roughly inversely proportional to the radiative damping rate that is determined by the carrier concentration and the geometrical parameters of the device. The emission spectra in the synchronized state, determined by the oscillating current component, are analyzed. The effective generation of higher harmonics for large values of the radiative damping strength is demonstrated.

[1] S. A. Mikhailov, Phys. Rev. B 87, 115405 (2013)

TT 42.10 Tue 12:15 WIL C107

Non-vanishing Coulomb drag in clean double-layer graphene at the Dirac point — •Sven Aeschlimann[1], Michael Schütt[2], Igor Gornyi[1,2,3], Boris Narozhny[1], and Alexander Mirlin[1,2,4] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]A. F. Ioffe Physica-Technical Institute, St. Petersburg, Russia — [4]Petersburg Nuclear Physics Institute, St. Petersburg, Russia

Coulomb drag is the frictional effect of simple Coulomb interaction onto two currents driven through two spatially separated conducting layers. Initiating a current through one layer, causes a current or a voltage drop in the other.

Recent experiments revealed a suprising nonvanishing resistance at the Dirac point that was expected to be zero for symmetry considerations. We focus on the possibility of a non-vanishing resistance in clean samples due to third order interaction contributions to drag.

TT 42.11 Tue 12:30 WIL C107

Linear Magnetoresistance in bilayer graphene — •Ferdinand Kisslinger, Christian Heide, Christian Ott, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, ferdinand.kisslinger@physik.uni-erlangen.de

We investigate the magnetoresistance in bilayer graphene obtained by hydrogen intercalation of monolayer graphene grown on the SiC(0001) surface. Whereas in monolayer graphene electron-electron-interaction and weak localization can be observed at low temperatures, a strong linear contribution dominates the magnetoresistance for bilayer graphene. It is found to be nearly temperature independent.

A variation of charge carrier density using a bottom gate and the comparison of different samples is carried out. The entity of data agrees well with a theoretical model [1] that describes a resistance network of Van-der-Pauw resistors. Consistency with the experiment is achieved when a network of resistors with different resistances is assumed. There are several possibilities where such inhomogeneities may originate from. We can exclude some of them and propose dislocations recently found in bilayer graphene [2] as a good candidate causing this effect.

[1] M.M. Parish and P.B. Littlewood , Nature 426 (2003) 162
[2] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer and E. Spiecker, Nature (2013), accepted, DOI: 10.1038/nature12780

TT 42.12 Tue 12:45 WIL C107

Wigner Crystal phases in bilayer graphene — •Peter Silvestrov and Patrik Recher — Institut für Mathematische Physik, TU Braunschweig, Germany

It is generally believed that Wigner Crystal in single layer graphene can not exist because the magnitudes of the electron interaction and the kinetic energy scale similarly with the decreasing electron density. This scaling argument however does not work for the low energy states in bilayer graphene. We consider the Wigner Crystal in slightly doped bilayer graphene with a gap in spectrum opened by applying a perpendicular electric field. We argue that in this system the formation of the Wigner Crystal is not only possible, but a different phases of the crystal with very peculiar properties may exist here depending on the parameters.

TT 42.13 Tue 13:00 WIL C107

Half-metallic bilayer graphene — •Jie Yuan — Raum 26 A 407 RWTH Aachen Sommerfeldstrasse 26, D-52056, Aachen

Charge neutral bilayer graphene has very likely a gapped ground state, as transport experiments have demonstrated. The nature of the ground state is undertermined yet. One plausible ground state is the layered antiferromagnetic spin density wave (LAF) state, where the spins in the top and bottom layers have the same magnitude with opposite di-

rections. We propose that lightly doped bilayer graphene in an electric field perpendicular to the graphene plane may be a half-metal where only one spin direction lis conducting. By the special properties of the half-metal deriving from the LAF state, the primary source of the gap at charge neutrality may be distinguished from other competing ground states like the quantum spin-Hall state. We study this explicitly by using a mean-field theory on a two-layer Hubbard model.

TT 43: Topological Insulators (organized by O)

Time: Tuesday 10:30–13:15 Location: GER 38

TT 43.1 Tue 10:30 GER 38

Topological Insulator goes Elemental: α-Sn on InSb — •M. R. Scholz[1], A. Barfuss[1], L. Dudy[1], A. Fleszar[2], G. Bihlmayer[3], D. Wortmann[3], J. H. Dil[4], G. Landolt[4], M. Radovic[4], G. Li[2], R. Claessen[1], and J. Schäfer[1] — [1]Phys. Inst. and RCCM, Univ. Würzburg — [2]Inst. f. Theo. Physik u. Astronomie, Univ. Würzburg — [3]Peter Grünberg Inst. a. Inst. f. Advanced Simulation, FZ Jülich — [4]Swiss Light Source, Paul-Scherrer-Institut Villigen

We report on the topological insulator phase of epitaxially grown α-Sn on InSb substrates where compressive strain is induced by a slight lattice mismatch. The topological surface state (TSS) forms in the presence of an unusual band order not based on direct spin-orbit coupling, as shown in DFT and GW slab-layer calculations. Angle-resolved photoemission probes how the TSS emerges from the second highest bulk valence band. By means of spin-resolved photoemission we show that the surface state is highly spin-polarized with a counter-clockwise helicity below the Dirac point. The band situation in α-Sn closely resembles that of strained HgTe. Quantum well films of HgTe sandwiched between CdTe are a system where the topological properties have been successfully probed in DC transport [1]. The similarities to HgTe make α-Sn a promising candidate to exhibit the quantum spin Hall effect as well, if the film thickness is reduced to the 2D limit. Particularly, as a nontoxic elemental system, α-Sn is easier to fabricate which opens various pathways to access and manipulate the topological surface state. As a first step, we demonstrate the precise control of the Fermi level by dopants. [1] M. König et al., Science 318, 766 (2007).

TT 43.2 Tue 10:45 GER 38

Temperature effects in soft and hard x-ray photoemission from topological insulators — •Jürgen Braun, Jan Minar, and Hubert Ebert — Dept. Chemie, LMU Universität München, Germany

A brief introduction to the theory of temperature-dependent soft and hard x-ray angle-resolved photo electron spectroscopy (SARPES, HARPES) of solid materials is given with an emphasis on the so-called one-step-model of photoemission. The main aspects of the theory [1,2] and its implementation within the Munich SPR-KKR program package [3] will be reviewed. Our method, which is based on the Coherent Potential Approximation (CPA) alloy theory (alloy analogy model), goes well beyond the simple, but standard Debye-Waller approach to photoemission by including in particular the temperature dependence of the effective photoemission matrix elements as well. This allows among others to reproduce the so called XPS- or density of states limit in angle-resolved photoemission which occurs for high photon energies and/or high temperatures due to a full Brillouin zone averaging caused by phonon scattering. First examples of soft- and hard x-ray ARPES calculations at finite temperature for W(110), Sb_2Te_3 and Bi_2Se_3 will be presented.

1. A. Gray, J. Minár, J. Braun, H. Ebert, C. S. Fadley et al., Nature Materials, **10**, 759 (2011) and Nature Materials **11**, 957 (2012) 2. J. Braun, J. Minár, H. Ebert et al. Phys. Rev. B **88** 005400 (2013) 3. H. Ebert et al., The Munich SPR-KKR package, version 6.3, http://olymp.cup.uni-muenchen.de/ak/ebert/

TT 43.3 Tue 11:00 GER 38

Reorganization of a Topologically Protected Surface State: Theory for Au-Covered Bi_2Te_3(111) — Francisco Muñoz[1,2], •Jürgen Henk[2], and Ingrid Mertig[2] — [1]Facultad de Ciencias, Universidad de Chile, Chile — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

The electronic structure of Au-covered Bi_2Te_3 is investigated by first-principles calculations. The Dirac surface state of the topological insulator Bi_2Te_3 hybridizes with the Au sp states, which gives rise to strong reorganization of the surface electronic structure. Striking features of the modified Dirac surface state are (i) the introduction of new Dirac points within the fundamental band gap of Bi_2Te_3, (ii) an extremely weak dispersion, and (iii) an anisotropic number of conducting channels in the fundamental band gap of Bi_2Te_3 which leads to a complicated Fermi surface. Our findings have impact for spin-dependent surface transport.

TT 43.4 Tue 11:15 GER 38

Barrier-free sub-surface incorporation of magnetic impurities into the Bi(111) surface: Manipulation of the protected surface state - Experiment — •C. Klein[1], P. Zahl[2], N. Vollmers[3], U. Gerstmann[3], D. Lückermann[4], G. Jnawali[1], H. Pfnür[4], C. Tegenkamp[4], W.-G. Schmidt[3], P. Sutter[2], and M. Horn-von Hoegen[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, DE — [2]Center for Functional Nanomaterials, Brookhaven National Laboratory, New York, USA — [3]Department of Physics, University of Paderborn, DE — [4]Institut for Solid State Physics, University of Hannover, DE

Due to the large spin orbit coupling, electron backscattering within the Bi(111) surface states is strongly suppressed. In order to identify possible scattering mechanisms we performed low temperature scanning tunneling microscopy (LT-STM) measurements in which submonolayer amounts of 3d-metals (Fe, Co, Ni, Cu) were deposited at 5K. The metal atoms become immediately embedded in a sub-surface site, as they are not present in STM topography. They only become apparent in STS at tunneling conditions close to the Fermi-energy, as they are surrounded by a pronounced anisotropic threefold electronic scattering pattern with lateral dimensions of more than 10 nm. DFT calculations indeed confirm a barrier free incorporation of the 3d-metal impurities into the first Bi-Bilayer even at such low temperatures. This incorporation effect is limited to 3d-metals, as screening effects of the s- and p- orbitals are of great importance and leads to an effective reduction of the free surface energy of about 5 eV.

TT 43.5 Tue 11:30 GER 38

Efficient full-relativistic DFT calculations for large systems: Application to Bi-related surface states — •Uwe Gerstmann[1], Nora Jenny Vollmers[1], Wolf Gero Schmidt[1], Claudius Klein[2], Michael Horn-von Hoegen[2], Philipp Kröger[3], Daniel Lückermann[3], Herbert Pfnür[3], and Christoph Tegenkamp[3] — [1]Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn — [2]Center for Nanointegration CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [3]Institut for Solid State Physics, University of Hannover, Appelstr. 2, 30167 Hannover

Spin-orbit coupling is well-known to be the driving force behind ferromagnetism and can be used to control the functionality of electronic devices in spintronics. In asymmetric quantum wells and at surfaces spin-split electron gases may form and give rise to the Rashba-effect. In some cases, e.g. Bi(111) bilayers, the bandstructures are furthermore affected by k-point dependent shifts in the order of several eV. This effect may become crucial if adatoms are incorporated or adsorbed at the surface, strongly influencing the occupancy of the adatom-induced states and by this the magnetic moments and further magneto-transport properties of the resulting structures. In this work, we present an efficient pseudopotential-based method that allows a full-relativistic description of large systems containing several hundreds of atoms. The approach is used to describe the incorporation of a wide range of atomic species (3d-transition, coin-metal as well as rare-earth ions) into Bi(111) surfaces, where supercells with more than 200 atoms are needed to describe the resulting extended magnetic structures correctly.

TT 43.6 Tue 11:45 GER 38

Magnetic impurities on Bi thin films - Conductivity and surface diffusion — •Philipp Kröger[1], Daniel Lükermann[1], Sergii Sologub[2], Nora Vollmers[3], Uwe Gerstmann[3], Wolf Gero Schmidt[3], Herbert Pfnür[1], and Christoph Tegenkamp[1] —

[1]Leibniz Universität Hannover, Inst. für FKP, Appelstr. 2, 30167 Hannover — [2]Inst. of Ph., Nat. Acad. of Sc., Nauky Av. 46, 03028 Kyiv, Ukraine — [3]Universität Paderborn, Theoretische Physik, 33098 Paderborn

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as a low carrier concentration and a large mobility. The surface states reveal a pronounced Rashba splitting and the conductivity can be well discriminated from bulk contributions if thin films are grown epitaxially on Si(111) substrates, making surface related effects accessible even in macroscopic conductance measurements.
In this context the adsorption of the magnetic atom Cr (4,8 μ_B) on the Bi(111) surface will be discussed. In comparison to other adsorbates (Fe, Co, Tb) Cr exhibits the strongest scattering effect, accompanied by a transition from Weak Anti- to Weak Localization. This transition indicates strong impurity scattering, which lifts all spin-dependent selection rules. Furthermore, a significant increase of electron concentration due to hybridization effects has been found. For Tb and Cr surface diffusion of adsorbate-atoms even at T≈10 K needs to be considered.

TT 43.7 Tue 12:00 GER 38

Magnetic interaction and magnetic fluctuations in topological insulators with ordered and disordered magnetic adatoms — •MAIA G. VERGIORY[1,4], LEVAN CHOTORLISHVILI[2], ARTHUR ERNST[1], VITALI DUGAEV[1], ANDREAS KOMNIK[3], MIJAIL OTROKOV[4], EVGUENI CHULKOV[4], and JAMAL BERADKAR[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Institut fr Physik, Martin-Luther-Universitat Halle-Wittenberg, Germany — [3]Institut fr Theoretische Physik, Universitt Heidelberg, Germany, — [4]Donostia International Physics Center, Donostia - San Sebastian, Spain

Using a first-principles Green's function approach we study magnetic properties of the magnetic binary topological insulators Bi2Se3, Bi2Te23 and Sb2Te3 doped with 3d transition metals. We analyze the magnetic phase for each dopant, the exchange interaction, the Curie temperature and the Bloch spectral function. Furthermore, we observe that the interaction of magnons with surface electrons essentially renormalizes the electron energy spectrum. The renormalized spectrum is nonlinear and can be characterized by a negative effective mass of electrons and holes for any k point different from 0. The electron velocity near the Dirac point depends on the electron-magnon coupling.

TT 43.8 Tue 12:15 GER 38

The edge state at the dark side of the weak topological insulator $Bi_{14}Rh_3I_9$ probed by STM — •Christian Pauly[1], Bertold Rasche[2], Marcus Liebmann[1], Marco Pratzer[1], Klaus Koepernik[3], Manuel Richter[3], Michael Ruck[2], Jeroen van den Brink[3], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and Jara Fit, Germany — [2]Departement of Chemistry and Food Chemistry, TU Dresden, Germany — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Germany

Using scanning tunneling microscopy (STM) and spectroscopy (STS) at 6 K, we probe the local atomic and electronic structure of the weak topological insulator $Bi_{14}Rh_3I_9$ [1]. In [001]-direction, the material is built from stacks of intermetallic planes with non-trivial 2D topology and spacer layers in between. Thus, the surfaces of the intermetallic planes, which are the natural cleaving planes of the material, exhibit a trivial band gap however with topologically protected states at each step edge [1]. $Bi_{14}Rh_3I_9$ is cleaved at a base pressure of 10^{-10} mbar giving rise to several hundreds of nm large terraces of the intermetallic layer interrupted by step edges. Using STS, we identified the band gap on top of the intermetallic layer, which is in agreement with ARPES data, whereas at the step edges we directly mapped the edge state. The edge state appears continuously through the band gap and exhibits a spatial distribution of 0.4 nm FWHM. The observed spatial periodicity along the step edge is in line with the atomic structure confirming the Bloch type of this state. Partially, dispersive features appear which will be discussed. [1] B. Rasche et al., Nature Mater. 12, 422 (2013)

TT 43.9 Tue 12:30 GER 38

Evidence for topological band inversion of the phase change material $Ge_2Sb_2Te_5$ — •Marcus Liebmann[1], Christian Pauly[1], Alessandro Giussani[2], Jens Kellner[1], Sven Just[1], Jaime Sanchez-Barriga[3], Emile Rienks[3], Oliver Rader[3], Raffaella Calarco[2], Gustav Bihlmayer[4], and Markus Morgenstern[1] — [1]II. Inst. Phys. B, RWTH Aachen University — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin — [3]Helmholtz-Zentrum für Materialien und Energie, BESSY, Berlin — [4]Peter-Grünberg-Institut and Institute für Advanced Simulation, Forschungszentrum Jülich

We present an angle-resolved photoemission study of the ternary phase change material $Ge_2Sb_2Te_5$, epitaxially grown on Si(111) in the metastable cubic phase. This material serves, e.g., in DVDs as a fast switchable material (1 ns) between the metallic cubic and an insulating amorphous phase. The observed upper bulk valence band shows a minimum at $\bar{\Gamma}$ being 0.3 eV below the Fermi level E_F and a circular Fermi contour around $\bar{\Gamma}$ with a dispersing diameter of $0.27-0.36$ Å^{-1}. This is in agreement with density functional theory calculations of the Petrov stacking sequence of the cubic phase which is topologically nontrivial. Moreover, the results are in line with all previous calculations of $Ge_2Sb_2Te_5$ exhibiting the valence band maximum at Γ for a trivial $\mathbb{Z}_2$ topology and away from Γ for a non-trivial one. Scanning tunneling spectroscopy exhibits a band gap of 0.4 eV around E_F. Our finding opens the perspective of ns-switching between a topological crystalline and an insulating amorphous phase.

TT 43.10 Tue 12:45 GER 38

Step wise variation of the electrochemical potential at step edges of the Bi_2Se_3 surface — •Christian A. Bobisch, Sebastian Bauer, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Bi_2Se_3 is a 3D topological insulator (TI) whose surface states are protected from direct backscattering by time reversal symmetry [1]. However, step edges on a Bi_2Se_3 surface are predicted to work as an electron scatterer for other scattering angles than 180° backscattering [2]. We studied the electron transport on the surface of a 14.5 QL (quintuple layer) thick Bi_2Se_3 film grown on Si(111). By a distance dependent resistance measurement [3] in the μm range, we found a metallic character of the film with a sheet conductance of $2\times10^{-3}\Omega^{-1}$ which agrees well with recent literature [4]. By scanning tunneling potentiometry (STP) [5], we simultaneously analyzed the topography and the electrochemical potential μ_{ec} under real transport conditions. We observe on the microscopic scale a potential gradient which corresponds well the macroscopic conductance. In the vicinity of step edges we find a step-like variation of μ_{ec} which is a fingerprint of electron scattering at the step edge. For the given sample the electrical conductivity of a 1 QL step could be deduced to $3800\pm500\Omega^{-1}$cm^{-1}.

[1] M. Z. Hasan et al., Rev. Mod. Phys. 82, 3045 (2010). [2] W. Jing et al., Chin Phys. B 22, 067301 (2013). [3] P. Jaschinsky et al., J. Appl. Phys. 104, 094307 (2008). [4] A. A. Taskin et al., Phys. Rev. Lett. 109, 066803 (2012). [5] P. Muralt et al., Appl. Phys. Lett. 48, 514 (1986).

TT 43.11 Tue 13:00 GER 38

Quantum phase transitions of a disordered antiferromagnetic topological insulator — •Paul Baireuther[1], Jonathan M. Edge[1], Ion C. Fulga[1], Carlo W.J. Beenakker[1], and Jakub Tworzydlo[2] — [1]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [2]University of Warsaw, Hoza 69, 00-681 Warsaw, Poland

We have studied the effect of electrostatic disorder on the conductivity of a three-dimensional antiferromagnetic insulator (a stack of quantum anomalous Hall layers with staggered magnetization). The phase diagram contains regions where the increase of disorder first causes the appearance of surface conduction (via a topological phase transition), followed by the appearance of bulk conduction (via a metal-insulator transition). The conducting surface states are stabilized by an effective time-reversal symmetry that is broken locally by the disorder but restored on long length scales. A simple self-consistent Born approximation reliably locates the boundaries of this socalled "statistical" topological phase.

TT 44: Focus Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale III (organized by O)

Time: Tuesday 10:30–13:15 Location: TRE Ma

Topical Talk TT 44.1 Tue 10:30 TRE Ma

Ultrafast relaxation dynamics of Hubbard nanoclusters — •Michael Bonitz[1], Sebastian Hermanns[1], Christopher Hinz[1], and Denis Lacroix[2] — [1]Institut für Theoretische Physik und Astrophysk, CAU Kiel, Leibnizstr. 15, 24098 Kiel — [2]IPN Orsay, 15 Rue Georges Clemenceau, 91406 Orsay

With the growing availability of intense short-pulse radiation sources it becomes possible to drive interacting many-particle or few-particle systems out of equilibrium in a controlled way. The subsequent relaxation and equilibration dynamics is still poorly understood. From a theory point of view these processes are complicated due to the simultaneous dynamics of the occupation functions and of binary correlations. The problem becomes even more complicated when the system has finite size and is spatially inhomogeneous [1]. The Hubbard model is a prototype for treating correlation effects in condensed matter or molecular systems fully including finite size and inhomogeneity effects. We, therefore, concentrate on the relaxation dynamics of small 1D, 2D and 3D Hubbard clusters that contain from a few to several hundred electrons. We observe a complex multi-stage relaxation behavior that depends on the external excitation, on the coupling strength and on the geometry of the system. In this talk we present results from two complementary theoretical approaches: first, from nonequilibrium Green functions where we apply the Generalized Kadanoff Baym ansatz [1] and, second, from a stochastic mean field approach.

[1] K. Balzer, and M. Bonitz, "Nonequilibrium Green's Functions Approach to Inhomogeneous Systems", Lect. Notes Phys. **867** (2013)

TT 44.2 Tue 11:00 TRE Ma

Exact adiabatic approximation in TDDFT — •Jeiran Jokar and Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The use of functionals from static density functional theory in an adiabatic way in a time-dependent framework is known to cause various problems due to the resulting exchange-correlation kernel being frequency independent. In order to isolate the effects which are due to the adiabatic approximation we calculate the exact static potential for two electron systems. Before using this potential in an adiabatic way in a time propagation we need to ensure that the potential is well defined also at those parts of space where the density is small as they might become more populated at a later time. We use the exact adiabatic approximation to describe Rabi oscillations, i.e. the oscillation between the ground state and an excited state when a monochromatic laser with a frequency close to the resonance is applied.

TT 44.3 Tue 11:15 TRE Ma

Real-time propagation of coupled Maxwell-Schrödinger and time-dependent Kohn-Sham-Maxwell systems — •René Jestädt[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Based on the Riemann-Silberstein vector of the electromagnetic field, we formulate Maxwell's equations in a symplectic spinor representation similar to the Dirac equation. This spinor representation allows us to use standard unitary propagation techniques developed for the Schrödinger equation [1] also for Maxwell's equations and simplifies a coupled solution of Maxwell's and Schrödinger's equations. To illustrate our approach, we present the real-time evolution of atomic systems embedded in optical waveguides and dielectric nanostructures. The coupling of Maxwell's equations to the time-dependent Kohn-Sham equations is a basic ingredient for the development of a time-dependent density functional theory formulation of quantum electrodynamics [2]. As an extension of our work on coupled Maxwell-Schrödinger systems, we show first steps of an implementation of Maxwell's equations coupled to the time-dependent Kohn-Sham equations in the first principles real-space real-time code octopus [3].

[1] A. Castro et al., J. Chem. Phys. **121** (2004).
[2] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011); I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).
[3] X. Andrade et al., J. Phys. Cond. Mat. **24** (2012).

TT 44.4 Tue 11:30 TRE Ma

Nonlinear optics by means of the dynamical Berry phase: Application to second- and third-harmonic generation — •Claudio Attaccalite[1] and Myrta Gruning[2] — [1]Univ. Grenoble Alpes/CNRS, Institut Neel, F-38042 Grenoble, France — [2]School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK

We present an real-time approach to study nonlinear optical properties in Condensed Matter systems that is especially suitable for crystalline solids. The equation of motions and the coupling of the electrons with the external electric field are derived from the Berry phase formulation of the dynamical polarization. Many-body effects are introduced by adding single-particle operators to the independent-particle Hamiltonian. Specifically we include crystal local field effects, renormalization of the energy levels and excitonic effects. The approach is validated by calculating the second and third harmonic generation of bulk semiconductors. Finally we present second-harmonic generation spectrum of h-BN or MoS2 monolayers and show that correlation effects double the signal intensity at the excitonic resonances with respect to the contribution from independent electronic transitions.

References: [1] Nonlinear optics from ab-initio by means of the dynamical Berry-phase http://arxiv.org/abs/1309.4012 [2] Second Harmonic Generation in h-BN and MoS2 monolayers: the role of electron-hole interaction http://arxiv.org/abs/1310.7459

15 min. break

TT 44.5 Tue 12:00 TRE Ma

Accurate Correlation Energies from Adiabatic Time-Dependent Density Functional Theory with Renormalized Kernels — •Thomas Olsen[1] and Kristian S. Thygesen[2] — [1]Universidad del Pais Vasco — [2]Center for Atomic-scale Materials Design (CAMD), Technical University of Denmark

We demonstrate the accuracy of electronic correlation energies obtained from the adiabatic connection and Time-Dependent Density Functional Theory (TDDFT) using a non-empirical renormalized gradient-corrected exchange-correlation kernel. The method can be viewed as a natural step beyond the Random Phase Approximation (RPA) and captures the short-range correlation effects which are poorly described in RPA. In particular, we show that for molecules and solids the renormalized kernel gives a four and five fold improvement in binding energies respectively when compared to RPA. We also consider examples of barrier heights in chemical reactions, molecular adsorption and graphene interacting with metal surfaces, which are three examples where RPA has provided highly accurate results. In these cases, our novel kernel provides results that are of equal quality or even slightly better than RPA, with a similar computational cost. We finally note that the renormalization procedure can be applied to any known semi-local exchange-correlation functional and thus defines an entire new class of adiabatic non-local functionals for ground state calculations within TDDFT.

TT 44.6 Tue 12:15 TRE Ma

Low scaling algorithm for the random phase approximation — •Merzuk Kaltak, Jiri Klimeš, and Georg Kresse — University of Vienna, Computational Material Physics

The computationally most expensive step in conventional RPA implementations is the calculation of the independent particle polarizability χ. We present an RPA algorithm that calculates χ using the Green function G in real space and imaginary time. The systematic construction of optimized time and frequency grids for G is obtained by means of solving a fitting problem. Furthermore a non-uniform discrete Fourier transform between the two grids is introduced, which converges exponentially. We show that the usage of the Green function approach in combination with the optimized grids can be used for the calculation of the RPA correlation energy for large systems.

TT 44.7 Tue 12:30 TRE Ma

Long range correlation energy from coupled atomic response functions — •Alberto Ambrosetti and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Faradayweg 4-6 14195 Berlin, Ger-

many

Electron correlation is an elusive and ubiquitous energy contribution that arises from transient collective electron fluctuations. Its reliable (accurate and efficient) modeling is central to the correct description of cohesive, structural, and response properties of molecules and solids. In this regard, the main challenge is to model the long-range correlation energy beyond (semi-)local density-functional approximations. Here we propose a very efficient method to compute the long-range correlation energy for non-metallic molecules and solids within a density functional theory framework, by using coupled atomic response functions (ARF). Extending the recent MBD method [1], we separate the coupling between ARFs into short and long range, allowing for a seamless many-body treatment of weakly and strongly polarizable systems. Thorough benchmarking on large data sets including small molecules (S22, S66x8), large supramolecular complexes (S12L), molecular crystals (X23) and bulk graphite shows consistently good agreement with high level theoretical and experimental reference binding energies (within the order of 6%). The uniform accuracy for molecules and solids represents a strong validation of our method, and further confirms the importance of modeling the truly collective nature of the long-range correlation energy. [1] A. Tkatchenko et al. PRL **108** 236402 (2012).

TT 44.8 Tue 12:45 TRE Ma

The exact Hohenberg-Kohn functional for a lattice model — •Tanja Dimitrov[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Standard local exchange-correlation and semi-local functionals in ground-state density functional theory are known for their shortcomings in describing correct charge transfer, dissociation energies of molecular ions, and barriers of chemical reactions [1,2]. To understand the failures of approximate functionals and to gain insight into the behavior of the exact functional, we investigate the exact solution of the many-body Schrödinger equation for a lattice model. Using exact diagonalization, we explicitely construct the exact Hohenberg-Kohn functional and the mapping from densities to wavefunctions. Besides the normal inter-system derivative discontinuity widely discussed in the density-functional theory community, we observe a new feature of the exact functional in the low-density limit. This "intra-system derivative discontinuity" resembles the inter-system derivative discontinuity, but is within the system (work in progress [3]). The description of many physical phenomena linked to charge-transfer processes (both in the static and dynamical regimes) require a proper account of this "intra-system derivative discontinuity".

[1] A. J. Cohen et al. Science **321**, 792 (2008).
[2] P. Mori-Sanchez et al., Phys. Rev. Lett. **100**, 146401 (2008).
[3] T. Dimitrov, H. Appel, A. Rubio to be published

TT 44.9 Tue 13:00 TRE Ma

Incorporating static correlation effects into density functional theory — Nektarios N. Lathiotakis[1], •Nicole Helbig[2], Nikitas I. Gidopoulos[3], and Angel Rubio[4,5] — [1]Theoretical and Physical Chemistry Institute, NHRF Athens, Greece — [2]Peter-Grünberg Institut, Forschungszentrum Jülich, Germany — [3]Department of Physics, Durham University, United Kingdom — [4]Nano-Bio Spectroscopy group, Universidad del Pais Vasco and DIPC, San Sebastian, Spain — [5]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present a novel idea that builds on the knowledge acquired in Reduced density matrix functional theory (RDMFT) to construct a density-functional scheme which accurately incorporates static and left-right correlation effects. At the same time, the new scheme preserves the high quality of a density functional description at the equilibrium and keeps the computational costs at an acceptable level comparable to the costs when using hybrid functionals. Within this scheme the natural orbitals, i.e. the eigenfunctions of the one-body density matrix, are constrained to be solutions of a single-particle Schrödinger equation with a local effective potential. This provides a natural way to connect an energy eigenvalue spectrum to the natural orbitals. This energy spectrum is found to reproduce the ionization potentials of different atoms and molecules very well. In addition, the dissociation limit of diatomic molecules is well described without the need to break any spin symmetry, i.e. this attractive feature of RDMFT is preserved. The present scheme can be easily implemented in all first principles codes for electronic structure calculations.

TT 45: Superconductivity: Fe-based Superconductors - 1111,111, FeSe

Time: Tuesday 14:00–16:00 Location: HSZ 201

TT 45.1 Tue 14:00 HSZ 201

In-plane vs. out-of-plane doping and disorder in CeFeAsO — •Oleksii Vakaliuk[1], Giacomo Prando[1], Sabine Wurmehl[1], Christian Hess[1,2], and Bernd Buechner[1,2] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstr. 20, 01069 Dresden Germany — [2]Center for Transport and Devices of Emergent Materials, TU Dresden, 01069 Dresden, Germany

In this contribution we will discuss the effect of the in-plane Fe/Co and the out-of-plane O/F chemical dilutions on the electronic phase diagram of CeFeAsO. Both substitutions lead to a quantitatively identical suppression of the spin density wave (SDW) phase upon doping, regardless of the actual degree of in-plane disorder. We detected two distinct regimes at low-doping levels: a long-range (LRO) followed by a short-range (SRO) ordered magnetic phase, the latter coexisting with superconductivity within a certain range of doping. In contrast, such in-plane disorder dramatically affects superconductivity and, in particular, the optimal-doping value of T_c [1]. Moreover, the magnetic ordering of the *Ce* ions is preserved throughout the entire phase diagram in $CeFe_{1-x}Co_xAsO$, at variance with what is observed in $CeFeAsO_{1-x}F_x$. Intriguingly, the ordering temperature T_N^{Ce} as a function of doping exhibits a dome-like shape in correspondence with the actual superconduting dome.
[1] G. Prando, *et.al.*, Phys. Rev. **B 87**, 174519 (2013)

TT 45.2 Tue 14:15 HSZ 201

Effects of hydrostatic pressure on the superconducting properties of $LaFeAsO_{1-x}F_x$ — •Giacomo Prando[1], Wolf Schottenhamel[1], Samuele Sanna[2], Rustem Khasanov[3], Zurab Guguchia[4], Anja Wolter-Giraud[1], Sabine Wurmehl[1,5], and Bernd Büchner[1,5] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, Germany — [2]Dipartimento di Fisica and Unità CNISM di Pavia, Università di Pavia, Italy — [3]Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [4]Physik-Institut der Universität Zürich, Winterthurerstrasse 190, Switzerland — [5]Institut für Festkörperphysik, Technische Universität Dresden, Germany

The most typical way of sweeping the electronic phase diagram of 1111 oxy-pnictides is to induce a gradual charge doping via chemical substitutions such as, e. g., out-of-plane $O_{1-x}F_x$ or in-plane $Fe_{1-x}Co_x$. However, it is well known that external pressure qualitatively mimics the charge doping across the whole phase diagram. In this contribution we will review the effect of pressure in $LaFeAsO_{1-x}F_x$ under different conditions of chemical doping x as examined by means of μ^+ spin spectroscopy. The suppression of the magnetic phase in the undoped compound will be addressed [1] as well as the phase segregation achieved at the crossover between magnetism and superconductivity [2]. Recent studies will be reported dealing with the superconducting side of the phase diagram. The evolution of both the critical temperature and the superfluid density will be discussed in detail.
[1] R. De Renzi et al., Supercond. Sci. Technol. 25 084009 (2012)
[2] R. Khasanov et al., Phys. Rev. B 84 100501 (2011)

TT 45.3 Tue 14:30 HSZ 201

Microscopic insight into the poisoning effect of Mn in $LaFe_{1-x}Mn_xAsO_{0.89}F_{0.11}$ — •Franziska Hammerath[1,2], Pietro Bonfá[3], Samuele Sanna[1], Giacomo Prando[1,2], Roberto De Renzi[3], Pietro Carretta[1], Yoshiaki Kobayashi[4], and Masatoshi Sato[4] — [1]Dipartimento di Fisica and Unitá CNISM di Pavia, I-27100 Pavia, Italy — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Germany — [3]Dipartimento di Fisica and Unitá CNISM di Parma, I-43124 Parma, Italy — [4]Department of Physics, Division of Material Sciences, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan

We investigate the extraordinary poisoning effect of Mn on superconductivity (SC) in $LaFe_{1-x}Mn_xAsO_{0.89}F_{0.11}$ [1] by means of muon spin rotation (μSR) and nuclear quadrupole resonance (NQR) on compounds with $x = 0.025\,\%$ up to $x = 0.75\,\%$. We find that the iron plane electronic environment is extremely sensitive to the addition of Mn, even though charge doping effects can be neglected. Already $0.2\,\%$ Mn suppress SC completely, while static magnetism is observed for $x = 0.1\,\%$ and becomes enhanced upon further Mn substitution. This re-entrant magnetism is found to be intrinsic to the FeAs plane. A progressive increase of low energy spin fluctuations, expressed in an enhanced NQR spin-lattice relaxation T_1^{-1}, is observed upon Mn substitution. The analysis of T_1^{-1} for the sample closest to the the crossover between SC and magnetism points towards an antiferromagnetic quantum critical point at this crossover.
[1] M. Sato *et al.*, JPSJ **79**, 014710 (2010).

TT 45.4 Tue 14:45 HSZ 201

Magnetic Vortices in LiFeAs as seen by Scanning Tunneling Spectroscopy — Ronny Schlegel[1], Pranab Kumar Nag[1], Danny Baumann[1], Robert Beck[1], Sabine Wurmehl[1,2], Bernd Büchner[1,3], and •Christian Hess[1,3] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01171 Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, 01069 Dresden — [3]Center for Transport and Devices of Emergent Materials, TU Dresden, 01069 Dresden, Germany

We performed investigations of the Shubnikov phase of LiFeAs in high magnetic fields up to 12 Tesla using scanning tunneling microscopy and spectroscopy. In our measurements the location of individual magnetic vortices can clearly be identified from the spatial variation of the zero bias differential conductance. We determine the Ginzburg-Landau coherence length from our data, as well as the nearest neighbor lattice constant, which we compare with results from complementary methods.

TT 45.5 Tue 15:00 HSZ 201

Incommensurate antiferromagnetic fluctuations in superconducting LiFeAs — •Navid Qureshi[1], Paul Steffens[2], Daniel Lamago[3,4], Yvan Sidis[3], Oleg Sobolev[5], Russell Ewings[6], Luminita Harnagea[7], Sabine Wurmehl[7], Bernd Büchner[7], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut Laue Langevin, Grenoble — [3]Laboratoire Léon Brillouin, C.E.A. Saclay — [4]Institut für Festkörperphysik, Karlsruhe — [5]Technische Universität München, FRM-II — [6]ISIS Facility, Rutherford Appleton Laboratory, Didcot — [7]Institut für Festkörper- und Werkstoffforschung, Dresden

We present an inelastic neutron scattering study on single-crystalline LiFeAs devoted to the characterization of the previously reported incommensurate antiferromagnetic fluctuations [1]. Time-of-flight measurements show their presence up to an energy transfer of 60 meV, while polarized neutrons in combination with longitudinal polarization analysis on a triple-axis spectrometer prove the pure magnetic origin of this signal. The normalization of the scattered intensity to an absolute scale yields that the magnetic fluctuations in LiFeAs are by a factor 8 weaker than in nearly optimally Co-doped $BaFe_2As_2$, although a factor 2 is recovered due to the incommensurability. The longitudinal polarization analysis gives hints for a weak spin-space anisotropy with slightly stronger out-of-plane component between 6 and 14 meV. Furthermore, our data suggest a fine structure of the magnetic signal most likely arising from two nesting vectors.
[1] N. Qureshi et al., Phys. Rev. Lett 108 117001 (2012)

TT 45.6 Tue 15:15 HSZ 201

Phase diagram characterization of $NaFe_{1-x}Rh_xAs$ by electrical transport — •Frank Steckel[1], Robert Beck[1], Dirk Bombor[1], Maria Roslova[1,4], Igor Morozov[1,4], Sabine Wurmehl[1,3], Bernd Büchner[1,2], and Christian Hess[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden — [2]Center for Transport and Devices, TU Dresden, 01069 Dresden — [3]Institut für Festkörperphysik, TU Dresden, 01069 Dresden — [4]Moscow State University, 119991 Moscow

The electronic properties of single crystals from the pure and Rh-doped unconventional high temperature pnictide superconductor NaFeAs are probed by resistivity and Hall effect measurements. Typical transition temperatures for the undoped parent compound are found and their evolution upon $4d$-electron doping up to $x = 6\%$ in $NaFe_{1-x}Rh_xAs$ are investigated. The structural and magnetic transition signatures are strongly suppressed upon Rh-doping. Already at $x = 1.8\%$ no sign of the aforementioned phase transitions are found. Optimal doping is found at $x = 2\%$ doping level with $T_C \sim 19.6$ K. A temperature-composition phase diagram is constructed from the resistivity, Hall coefficient and magnetization data. The comparison to the $3d$-electron doped $NaFe_{1-x}Co_xAs$ phase diagram yields astonishing similarities as found before in Rh- and Co- doped $BaFe_2As_2$. Thus, we suggest a generic behavior upon Rh- and Co-doping in Fe-based superconductors. Accordingly the structural and antiferromagnetic transition temperatures as well as the superconducting transition may depend only on the doping level and the doped charge.

TT 45.7 Tue 15:30 HSZ 201

Magnetoresistance and Hall effect of $Fe_{1.01}Se$ — •Sahana Roessler, Cevriye Koz, Ulrich Schwarz, and Steffen Wirth — Max Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden

The simplest member of Fe-based superconductor $Fe_{1.01}Se$ displays a superconducting transition at $T_c \approx 8$ K [1] and a structural transition at $T_s \approx 90$ K [2]. Here we present magnetoresistance, Hall effect, and magnetic susceptibility of $Fe_{1.01}Se$ single crystals. The onset of negative magnetoresistance below T_s indicates a strong change to the Fermi surface topology at the structural phase transition. The Hall resistivity ρ_{xy} is negative below 55 K indicating electron dominated transport, and non-linear in magnetic field down to 12 K. The magnetic susceptibility also displays a minimum close to 30 K suggesting a strong enhancement of antiferromagnetic fluctuations. This behavior is in agreement with the temperature dependence of spin-fluctuation susceptibility in NMR measurements [3]. These results suggest that the pairing correlations in $Fe_{1.01}Se$ are enhanced by antiferromagnetic fluctuations.
[1] F. C. Hsu et al. Proc. Natl. Acad. Sci (USA) 105, 14262 (2008)
[2] T. M. McQueen et. al. Phys. Rev. Lett. 103, 057002 (2009)
[3] T. Imai et. al. Phys. Rev. Lett. 102, 177005 (2009)

TT 45.8 Tue 15:45 HSZ 201

Orbital-selective metal-insulator transition and gap formation above T_c in superconducting Rb_{1-x} $Fe_{2-y}Se_2$ — •Zhe Wang[1], Michael Schmidt[1], Jonas Fischer[1], Vladimir Tsurkan[1], Markus Greger[2], Dieter Vollhardt[2], Alois Loidl[1], and Joachim Deisenhofer[1] — [1]Experimentalphysics 5, Univ. Augsburg, Germany — [2]Theoreticalphysics 3, Univ. Augsburg, Germany

We report on a hierarchy of temperatures $T_c < T_{gap} < T_{met}$ in superconducting Rb_{1-x} $Fe_{2-y}Se_2$ observed by THz spectroscopy. Above $T_{met} = 90$ K the material reveals semiconducting characteristics. Below T_{met} a coherent metallic THz response emerges. This metal-to-insulator-type, orbital selective transition is indicated by an isosbestic point in the temperature dependence of the optical conductivity and dielectric constant at THz-frequencies. At $T_{gap} = 61$ K a gap opens in the THz regime and then the superconducting transition occurs at $T_c = 32$ K. This sequence of temperatures seems to reflect a corresponding hierarchy of the electronic correlations in the different bands.

TT 46: Low-Dimensional Systems: Molecular Conductors

Time: Tuesday 14:00–16:00 Location: HSZ 204

TT 46.1 Tue 14:00 HSZ 204

Tuning the hole injection barrier in the intermolecular charge-transfer compound DTBDT-F_4TCNQ at metal interfaces — Dennis Bayer[1], Sandra Diehl[1,2,4], Martin Baumgarten[3,4], Klaus Müllen[3,4], •Torsten Methfessel[1,4], and Hans-Joachim Elmers[1,4] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, 55128 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [4]SFB/TR49

The codeposition of the organic molecules dithienobenzodithiophene (DTBDT)[1] and tetrafluorotetracyanoquinodimethane (F_4TCNQ) on metal surfaces in ultrahigh vacuum leads to the formation of a novel organic charge-transfer (CT) salt. By scanning tunneling spectroscopy at room-temperature we determined the energetic positions of the highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals of acceptor (F_4TCNQ) and donor (DTBDT) in the pure and in the mixed phase. The mixed phase exhibits a new HOMO close to the Fermi energy depicting a charge-transfer of less than one elementary charge in agreement with earlier results of the CT-salt TMP-TCNQ[2]. The binding energy of this new orbital varies in dependency on the underlying metal substrate, i.e. 0.4 eV on C(R15 × 3)/W(110) , 0.25 eV on a monolayer Co/W(110) and 0.16 eV on hcp Co(0001), thus revealing the possibility of tuning the hole injection barrier.

[1] P. Gao et al., Advanced Materials 21, 213 (2009)
[2] K. Medjanik et al., Physical Review B 82, 245419 (2010)

TT 46.2 Tue 14:15 HSZ 204

The Search for Massless Dirac Fermions — •Rebecca Beyer[1], Armin Dengl[1], Tomislav Ivek[1,2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Institut za fiziku, P.O. Box 304, HR-10001 Zagreb, Croatia

The quasi-two dimensional organic conductor α-(BEDT-TTF)$_2$I$_3$ is a semimetal at high temperature and low pressure. At $T_{MI} = 136$ K (ambient pressure) it undergoes a metal-insulator transition and becomes charge ordered. Pressure is known to reduce the transition temperature and theory predicts a Zero-Gap-Semiconducting (ZGS) state once the transition is fully suppressed. This ZGS state was thoroughly investigated in terms of Landau Levels: many different experiments prove the existence of a zero-energy Landau-Level at high pressures ($p > 15$ kbar) and low temperatures ($T < 10$ K). Only few studies comment on the evolution of the ZGS and the linear dispersion relation in the band structure with pressure or temperature. For example first principle band structure calculations predict a Dirac cone even at room temperature and ambient pressure but with a finite chemical potential.

We present infrared reflectivity measurements under intermediate hydrostatic pressures ($0 < p < 10$ kbar) on α-(BEDT-TTF)$_2$I$_3$ between room temperature and 10 K. We show the evolution of the insulating gap and investigate the possible coexistence of massless and normal charge carriers in one of the few bulk materials with a ZGS state.

TT 46.3 Tue 14:30 HSZ 204

Charge-carrier dynamics at the Mott transition in κ-(BEDT-TTF)$_2$X-Salts — •Benedikt Hartmann[1], David Zielke[1], Jana Polzin[1], Robert Rommel[1], John A. Schlueter[2], Takahiko Sasaki[3], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL, USA — [3]Institute for Materials Research, Tohoku University, Sendai, Japan

The nature of criticality at the Mott transition recently has been in the focus of intense experimental and theoretical research. The quasi-2D organic charge-transfer salts κ-(ET)$_2$X are considered as model systems for studying the Mott metal-insulator transition (MIT) in reduced dimensions. We investigated partially deuterated κ-[(H$_8$-ET)$_{0.2}$(D$_8$-ET)$_{0.8}$]$_2$Cu[N(CN)$_2$]Br, which is located very close to the critical pressure p_0 and further utilized the possibility to reversibly tune the 'chemical pressure' by employing different cooling rates shifting the system to the critical region of the generalized phase diagram. By means of fluctuation (noise) spectroscopy as a powerful new tool for studying charge-carrier dynamics without injecting additional electrons, we observe a pronounced and sudden slowing down of the dynamics near the finite-temperature critical endpoint (p_0, T_0) of the Mott transition. A striking divergence of the low-frequency resistance fluctuations at T_0 for certain cooling rates is accompanied by a signature in higher-order statistical moments (second spectrum) being a hint to spatial correlations. We dicuss this in terms of glassiness of the electronic system which may be an universal feature of MITs.

TT 46.4 Tue 14:45 HSZ 204

STM investigations of κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br — •Sandra Diehl[1,2,3], Torsten Methfessel[1,3], Jens Müller[3,4], Michael Lang[3,4], and Hans-Joachim Elmers[1,2,3] — [1]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, 55128 Mainz — [3]SFB/TR 49 — [4]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main

We investigate the organic charge-transfer salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br as an example for an organic superconductor. The superconducting properties strongly deviate from BCS theory but resemble the properties of high-T_c cuprates which has been attributed to their two dimensional structure leading to electronic correlation effects [1]. In order to understand their electronic properties we measured temperature dependent differential conductivity spectra using scanning tunneling spectroscopy. With this method the shape of the superconducting gap can be determined. In addition to the superconducting gap of the expected size we observe a second, much wider gap indicating a surprisingly large correlation effect. Furthermore, we present STM images showing the alternating structure of conducting and insulating layers. All investigations were done under UHV-conditions ($5 \cdot 10^{-11}$ mbar) using a low temperature scanning tunneling microscope. The surface of the crystals was prepared by in-situ cleaving.

[1] R. H. McKenzie, Science **278**, 820 (1997)

TT 46.5 Tue 15:00 HSZ 204

Low temperature phase diagram of κ-(BETS)$_2$FeCl$_4$ — •Michael Kunz[1], Werner Biberacher[1], Karl Neumaier[1], Natasha D. Kushch[2], and Mark V. Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Institute of Problems of Chemical Physics, Chernogolovka, Russia

The organic charge transfer salts of the (BETS)$_2$FeX$_4$ (X = Cl or Br) family are a subject of intensive research due to interesting correlation effects and magnetic ordering coexisting with superconductivity. κ-(BETS)$_2$FeCl$_4$ is an antiferromagnetic (AFM) metal with a Néel temperature $T_N \approx 0.45$ K. Interlayer resistance measurements were used to track the behavior of the phase boundaries with a magnetic field applied in different directions. Thus the low temperature phase diagram of κ-(BETS)$_2$FeCl$_4$ under applied magnetic field, which shows some remarkable features, was obtained. Shubnikov-de Haas oscillations below the Néel temperature reveal a significant impact of antiferromagnetism on the Fermi surface.

TT 46.6 Tue 15:15 HSZ 204

Studying the Mott criticality via thermal expansion under ^{4}He-gas pressure — •Rudra Sekhar Manna[1], Elena Gati[1], Ulrich Tutsch[1], Takahiko Sasaki[2], and Michael Lang[1] — [1]Physics Institute, Goethe University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany — [2]Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

Quasi-2D organic charge-transfer salts κ-(ET)$_2$X show a variety of ground state properties accessible upon either changing the anion X or by applying hydrostatic pressure. The T-P phase diagram includes a first-order Mott transition line which terminates at a second-order critical end point. Interestingly, deuterated κ-(d8-ET)$_2$Cu[N(CN)$_2$]Br (κ-d8 in short) lies on the verge of the Mott transition line at ambient pressure. Thus, for this material temperature sweeps are sufficient to experimentally access the critical end point and thereby to study the controversy surrounding the Mott criticality. Recent scaling theory [1] applied to previous thermal expansion data on κ-d8 crystals [2] speaks in favor of a 2D Ising universality class. Here we present thermal expansion measurements performed under ^{4}He-gas pressure [3] on κ-d8 crystals along the in-plane a-axis. The aim of this work is to pressure-

tune the system in the vicinity of the Mott critical end point and to compare the results with theoretical predictions [1, 4].
[1] L. Bartosch *et al.*, Phys. Rev. Lett. **104**, 245701 (2010).
[2] M. de Souza *et al.* Phys. Rev. Lett. **99**, 037003 (2007).
[3] R. S. Manna *et al.*, Rev. Sci. Instrum. **83**, 085111 (2012).
[4] M. Zacharias *et al.*, Phys. Rev. Lett. **109**, 176401 (2012).

TT 46.7 Tue 15:30 HSZ 204

Photo-induced phase transition in TTF-CA — •Patricia Haremski, Tobias Peterseim, Tomislav Ivek, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Germany

30 years ago, the first experiments on photo-induced phase transitions on the quasi 1D organic mixed-stacked TTF-CA salt paved the way for numerous experimental and theoretical studies on nonequilibrium states. TTF-CA shows a neutral (N) to ionic (I) phase transition at $T_{NI} = 81.5\,\mathrm{K}$ with a change of ionicity from 0.2 (N) to 0.6 (I) and a dimerization of TTF and CA molecules along the stacking direction. Step-Scan FTIR spectroscopy was used to investigate the photo-induced transitions in TTF-CA by pulsed laser excitation. For different temperatures below T_{NI} and different laser intensities, temporal changes of the infrared reflection spectrum with polarization parallel and perpendicular to the stacking direction were recorded. The reduction of the a_g-modes intensity indicates that the dimerization is dissolved and metastable domains are created. The temporal evolution of the changes in reflectivity can be described by a non-exponential decay function and exhibits similarities to the decay process observed in 1D random-walk annihilation process in photo-excited polyacetylen. Due to the multi-instability in the vicinity of T_{NI}, large domains are formed with an extended lifetime in the microsecond range.

TT 46.8 Tue 15:45 HSZ 204

Electronic transport through defective carbon nanotubes — •Fabian Teichert[1], Andreas Zienert[1], and Jörg Schuster[2] — [1]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Continuing the miniaturization, microelectronics will ultimately approach the atomic scale. One prominent example are carbon nanotubes (CNT), which could be used for transistors and interconnects. So far CNTs cannot be grown or deposited in an ideal and reproducible way inside a device. As one consequence they contain defects.

The present work aims to describe the transport properties of defective armchair CNTs. The focus is set on monovacancies and divacancies. The calculation of the transmission spectrum and the conductivity is done by a fast recursive equilibrium Green's function formalism, which scales linearly with the length of the tube, allowing to treat large systems. The electronic structure is described by the density functional based tight binding model. Single defects, double defects and the behavior of single configurations with many defects are studied. Furthermore, the mean influence of certain defect densities and the diameter of the CNT is investigated within a statistical analysis. It is shown that in the limit of small transmission the system is in the regime of strong localization, where the conductivity scales exponentially with the number of defects. Consequently, a localization length can be extracted, which depends on the defect density and on the CNT diameter.

TT 47: Correlated Electrons: Spin Systems and Itinerant Magnets - Frustrated Magnets III

Time: Tuesday 14:00–16:00 Location: HSZ 03

TT 47.1 Tue 14:00 HSZ 03

Spin Heat-Conductivity of Two-Dimensional Antiferromagnets coupled to Phonons — •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 present results of a study of thermal transport due to magnons in two dimensional spin-1/2 Heisenberg antiferromagnets on the square lattice, subject to dissipation by lattice degrees of freedom. The spin phonon scattering is described in terms of magnetoelastic coupling to either acoustic of optical lattice modes. The thermal conductivity and transport relaxation rates will be evaluated using both, a memory function approach and Boltzmann equations. The temperature dependence of the transport will be analyzed in terms of various asymptotic scattering processes. Implications for recent observations of magnetic thermal transport in layered cuprate materials will be discussed.

TT 47.2 Tue 14:15 HSZ 03

Spin-current autocorrelations from single pure-state propagation — •Robin Steinigeweg[1], Jochen Gemmer[2], and Wolfram Brenig[1] — [1]Institute for Theoretical Physics, Technical University Braunschweig, Germany — [2]Department of Physics, University of Osnabrück, Germany

We study spin dynamics in the anisotropic and antiferromagnetic spin-1/2 Heisenberg chain in the long-wavelength limit. To this end, we numerically calculate the spin-current autocorrelation function by propagating only a single pure state in time, which is a "typical" representative of the quantum statistical ensemble. By comparing to short-time data from time-dependent density matrix renormalization group, we show that quantum typicality is fulfilled extremely well. This quantum typicality allows us to determine almost exactly the long-time Drude weight for chains as long as $L = 33$ sites, i.e., with a $8192\times$ larger Hilbert space than the typically considered $L \sim 20$ sites within the range of exact diagonalization. Therefore we can shed light on the Drude weight in the thermodynamic limit at both, high and low temperatures. Even though we apply our approach to an integrable quantum system in one dimension, it is applicable to non-integrable models in a much more general framework.

TT 47.3 Tue 14:30 HSZ 03

Microscopic magnetic modeling for the spin-$\frac{1}{2}$ kagome compound $[\mathbf{NH_4}]_2[\mathbf{C_7H_{14}N}][\mathbf{V_7O_6F_{18}}]$ — •Oleg Janson[1,2], Alexander Tsirlin[1,2], Ioannis Rousochatzakis[3], Helge Rosner[1], and Raivo Stern[2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia — [3]Leibniz Institute for Solid State and Materials Research, Dresden, Germany

In the recently synthesised compound $[NH_4]_2[C_7H_{14}N][V_7O_6F_{18}]$, magnetic $S{=}\frac{1}{2}$ V^{4+} atoms form an ideal kagome lattice [1]. Very recent μSR studies indicate the emergence of a gapless spin liquid state as a result of magnetic frustration [2]. Using density functional theory calculations, we address the microscopic magnetic model of this low-dimensional compound. We show that its peculiar symmetry gives rise to two inequivalent nearest-neighbor couplings. The behavior of the resulting quantum spin model is studied using exact diagonalization and compared to the experiments. OJ and AT were supported by the Mobilitas program of the ESF, grant numbers MJD447 and MTT77, respectively.
[1] F. H. Aidoudi *et al.*, Nature Chem. **3**, 810 (2011)
[2] L. Clark *et al.*, Phys. Rev. Lett. **110**, 207208 (2013)

TT 47.4 Tue 14:45 HSZ 03

The Spin-1 Kagome Antiferromagnet $\mathbf{Ca_{10}(Cr^{V}O_4)_6(Cr^{VI}O_4)}$ — •Christian Balz[1,2], Bella Lake[1,2], Nazmul Islam[1], Manfred Reehuis[1], and Yogesh Singh[3] — [1]Helmholtz Zentrum Berlin, 14109 Berlin, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [3]Indian Institute of Science Education & Research Mohali, 140306 Mohali, India

The mixed valence compound $Ca_{10}(Cr^{V}O_4)_6(Cr^{VI}O_4)$ consists of ferromagnetically coupled pairs of spin-1/2 Cr^{5+} ions which form dimers along the c-axis. These dimers form an effective spin-1 Kagome arrangement in the a-b-plane. Besides Cr^{5+} there are also Cr^{6+} ions in the structure which are non-magnetic. We have grown single crystals of $Ca_{10}(Cr^{V}O_4)_6(Cr^{VI}O_4)$ and have performed DC susceptibility, magnetization and heat capacity measurements as well as powder and single crystal neutron diffraction and powder X-ray diffraction experiments. Our magnetization and diffraction confirm the ordered arrangement of Cr^{5+} and Cr^{6+} ions in the ratio 6:1, while the heat capacity and susceptibility show the absence of long-range magnetic order down to 50 mK. We have also performed inelastic neutron scattering which reveals diffuse excitations which are gapless everywhere

and are highly two-dimensional. Two bands of scattering are observed, the low energy band (0-0.7 meV) corresponds to excitations of the spin-1 Kagome and the higher energy band (0.7-1.4 meV) corresponds to excitations of the dimer bond. Thus, the Kagome antiferromagnet $Ca_{10}(Cr^{V}O_4)_6(Cr^{VI}O_4)$ is a promising candidate for a Spin-Liquid ground state.

TT 47.5 Tue 15:00 HSZ 03

Impact of vacancies on the Kagome Antiferromagnet — •Siegfried Guertler — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

The Kagome lattice Heisenberg model, has been the subject of discussions over a long time. Recently strong indication for a spin-liquid ground state has been found numerically. The exact type of spin-liquid is still debated, as is the question whether it is gapped or not.
An interesting point is how perturbations in the form of vacancies change the picture. This is relevant for experimental detection techniques on compounds (photo-doping), the possible design of new compounds (chemical doping) and as well for experiments applying pressure and therefore changing the coupling constants.
In this talk I present numerical investigations by variational Monte-Carlo of the role of vacancies regarding this problem, particularly the t-J and Hubbard model on this lattice. For the t-J model a particular form of a valence bond crystal appears and can be understood by a few observed short range effects (as reported in PRB 84, 174409 (2011) and PRL 111, 097204 (2013)) the Hubbard model in the low-U limit seems to have a rich phase-diagram including various exotic phases and magnetically ordered phases (to appear soon on cond-mat).

TT 47.6 Tue 15:15 HSZ 03

Strongly Correlated Fermions on the Kagome Lattice — •Krishanu Roychowdhury and Frank Pollmann — MPIPKS, Dresden, germany

We consider an extended fermionic Hubbard model on the kagome lattice and show that this model exhibits exciting phenomena at certain fractional filling factors. The strong coupling regime of the model, described by an effective low-energy Hamiltonian, includes competing interactions, i.e., fermionic ring exchange as well as an antiferromagnetic Heisenberg term. We find that the interplay between spin and charge degrees of freedom enforces a quantum phase transition between phases with different spin and charge ordering at 1/3 filling. Following a similar spirit, we also discuss the spin polarized case at 1/6, 1/3 and 1/2 filling and focus on the influence of longer ranged interactions. The possibilities to stabilize topologically ordered phases are explored in detail.

TT 47.7 Tue 15:30 HSZ 03

Investigation of the strongly correlated one-dimensional magnetic behavior of $NiTa_2O_6$ — •Joseph M Law[1] and Reinhard K Kremer[2] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

$NiTa_2O_6$ has been previously shown to be a 2D system.[1] Herein, we re-investigated magnetic properties of $NiTa_2O_6$ by magnetic susceptibility, specific heat, electron paramagnetic resonance, neutron powder diffraction and pulse field magnetization measurements. In contrast to the previous findings we found $NiTa_2O_6$ to be a quasi-1D Heisenberg S = 1 spin chain with a nearest neighbor spin exchange interaction of 18.92(2) K with a g-factor of 2.14(1).
[1] E. G. Santos, J. B. M. da Cunha, O. Isnard, C. Lacroix, and M. A. Gusmao, J. Phys.: Condens. Matter 24, 496004 (2012)

TT 47.8 Tue 15:45 HSZ 03

Flat-band ferromagnetism and Pauli-correlated percolation — •Mykola Maksymenko[1], Andreas Honecker[2], Roderich Moessner[1], Johannes Richter[3], Oleg Derzhko[4], and Kirill Shtengel[5] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [3]Institut für theoretische Physik, Universität Magdeburg — [4]Institute for Condensed Matter Physics of NAS of Ukraine — [5]University of California at Riverside

Flat-band ferromagnetism is a special case of magnetism due to correlated itinerant electrons in a number of geometrically frustrated lattices. We develop an exact mapping between ground states of this many-body problem and a novel site-percolation problem. This allows us to study the ferromagnetic transition using tools from equilibrium statistical physics. In the case of the Hubbard model on the Tasaki lattice, we provide a complete analytical treatment of the 1D case and show that for D > 1, the paramagnetic phase persists beyond the usual threshhold for uncorrelated percolation point. When the transition to an unsaturated ferromagnetic phase finally occurs, it is in the form of a first-order jump to an unsaturated ferromagnetic phase.

TT 48: Transport: Topological Insulators I (organized by TT)

Time: Tuesday 14:00–16:00 Location: HSZ 304

TT 48.1 Tue 14:00 HSZ 304

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 specular phenomena occurring at the surface 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.

To protect the surface integrity an all in- ultra-high-vacuum study is crucial. High quality thin films of Bi_2Te_3 were grown on well lattice matched $BaF_2(111)$ substrates using Molecular Beam Epitaxy. The preparation, characterization by RHEED, LEED, XPS and ARPES and especially transport measurements, were performed all in-situ under ultra-high-vacuum conditions.

Results of this study and the effect of air exposure on the electronic structure and transport properties will be presented.

TT 48.2 Tue 14:15 HSZ 304

Finite width effect on weak antilocalization in MBE grown Bi_2Te_3 thin films — •Christian Weyrich[1,2], Tobias Merzenich[1,2], Igor E. Batov[3], Gregor Mussler[1,2], Jörn Kampmeier[1,2], Jürgen Schubert[1], Thomas Schäpers[1,2], and Detlev Grützmacher[1,2] — [1]Peter Grünberg Institute (PGI-9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Virtual Institute for Topological Insulators (VITI), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [3]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, 142432, Moscow Distr., Russia

The weak antilocalization effect is measured in Bi_2Te_3 layers under various tilt angles of the magnetic field with respect to the layer surface. The investigated Bi_2Te_3 layer was prepared by molecular beam epitaxy. For a magnetic field oriented perpendicularly to the layer the weak antilocalization effect at different temperatures can be well-fitted by the Hikami-Larkin-Nagaoka model. From the fit a phase coherence length of about 200 nm is obtained at a temperature of 2 K. A clear signature of weak antilocalization is also observed when the magnetic field is oriented parallel to the Bi_2Te_3 layer. This effect is compared to classical models as well as a recently developed theory, which takes into account the finite penetration depth of the surface or interface states into the bulk.

TT 48.3 Tue 14:30 HSZ 304

Band structure and magnetotransport in strained HgTe — •Jan Böttcher and Ewelina M. Hankiewicz — Universität Würzburg, Faculty for Physics and Astronomy, Am Hubland, D-97074 Würzburg

Strained mercury telluride is a 3D topological insulator with negligible bulk conductivity [1]. Here we report on band structure calculations using a six-band Kane model with a self-consistent Poisson solver. We find that while the surface states lie within the band gap, the Dirac point lies deep in the heavy hole subbands. We study this system as

a function of gate voltage and give possible explanations of exciting experimental observations of the Landau level structures in high magnetic fields as well as oscillations in the Shubnikov-de Hass data at low magnetic fields.

We acknowledge financial support via grant HA 5893/4-1 within SPP 1666.

[1] C. Brüne, C. X. Liu, E. G. Novik, E. M. Hankiewicz, H. Buhmann, Y. L. Chen, X. L. Qi, Z. X. Shen, S. C. Zhang, and L. W. Molenkamp, Phys. Rev. Lett. 106, 126803 (2011)

TT 48.4 Tue 14:45 HSZ 304

Photoemission investigation of the predicted topological Kondo insulator behavior of SmB_6 — •Peter Hlawenka[1], Emile Rienks[1], Konrad Siemensmeyer[1], Eugen Weschke[1], Andrei Varykhalov[1], Natalya Shitsevalova[2], Slavomir Gabani[3], Karol Flachbart[3], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Institute for Problems of Material Science, Kiev, Ukraine — [3]IEP, Slovak Academy of Science, Kosice

The system SmB_6 is known for its unusual resistivity which increases exponentially with decreasing temperature and saturates below 3 K [1]. This has recently been attributed to topological-Kondo-insulator behavior where a topological surface state is created by Sm4f-5d hybridization and is responsible for the transport [2]. The local-density-approximation + Gutzwiller calculations of the (100) surface predict the appearance of three Dirac cones in the surface Brillouin zone [2]. We perform angle-resolved photoemission (ARPES) below 1 K and do not observe the predicted Dirac cones at $\overline{\Gamma}$ or $\overline{X}$. Moreover, the Fermi surface is made up of steeply dispersing bulk Sm5d states. The Sm^{2+} 4f band and the hybridization gaps where the surface states are expected [2] are too far ($\sim$ 20 meV) below the Fermi energy in order to contribute to the transport. These results will be discussed in comparison to other ARPES studies.

[1] J. C. Cooley, M. C. Aronson, Z. Fisk, P. C. Canfield, Phys. Rev. Lett. 74, 1629 (1995)
[2] F. Lu, J. Zhao, H. Weng, Z. Fang, Xi Dai, Phys. Rev. Lett. 110, 096401 (2013)

TT 48.5 Tue 15:00 HSZ 304

Excitations of surface and bulk states in spin orbit dominated materials — •Peter Lemmens[1], Vladimir Gnezdilov[1,2], Dirk Wulferding[3], Patrik Recher[4], Helmuth Berger[5], Yoichi Ando[6], R Sankar[7], and Fang-Cheng Chou[7] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE, Kharkov, Ukraine — [3]POSTECH, Korea — [4]IMAPH, TU-BS, Braunschweig — [5]EPFL, Lausanne, Switzerland — [6]ISIR, Osaka, Japan — [7]CCMS, National Taiwan Univ., Taipei, Taiwan

Using Raman scattering experiments we probe inelastic processes in the giant Rashba material BiTeI, the topological semimetal Cd_3As_2 and several topological insulators. By comparing surface with bulk scattering processes we notice the dominance of quantum well states. With exception to Cd_3As_2 all materials show pronounced resonances in the Raman scattering cross section.

TT 48.6 Tue 15:15 HSZ 304

Josephson Effect in Topological Insulator Planar, Nanostep and Edge Junctions — •Jennifer Nussbaum, Rakesh Tiwari, Thomas Schmidt, and Christoph Bruder — University of Basel, Switzerland

Topological insulators are states of quantum matter which are characterized by a full insulating gap in the bulk and gapless surface states which are protected by time-reversal symmetry. By using the superconducting proximity effect on a Bi_2Se_3 topological insulator, a topological superconductor - topological insulator - topological superconductor (SIS) junction can be engineered. By solving the Dirac-Bogoliubov-De-Gennes equation in such a junction the maximal supercurrent that can flow through the surface of the Bi_2Se_3 topological insulator with heavily doped superconducting electrodes is calculated. In this manner, short and wide nanostep Josephson junctions involving different side surfaces of the 3D topological insulator are investigated. The results are compared to the Josephson response of a junction involving only one side surface. The comparison reveals, for example, that a step setup leads to a non-trivial scaling of the Josephson current.

TT 48.7 Tue 15:30 HSZ 304

Parity measurement in topological Josephson junctions — •François Crépin and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

We study the properties of a topological Josephson junction made of both edges of a 2D topological insulator. We show that, due to fermion parity pumping across the bulk, the global parity of the junction has a clear signature in the periodicity and critical value of the Josephson current. In particular, we find that the periodicity with the flux changes from 4π in a junction with an even number of quasi-particles to 2π in the odd sector. In the case of long junctions, we exhibit a rigorous mathematical connection between the spectrum of Andreev bound-states and the fermion parity anomaly, through bosonization. Additionally, we discuss the rather quantitative effects of Coulomb interactions on the Josephson current.

TT 48.8 Tue 15:45 HSZ 304

PN junctions of Topological Insulators — •Sourin Das[1] and Disha Wadhawan[2] — [1]MPIPKS, Dresden, Germany & University of Delhi, India — [2]University of Delhi, India

Spin textures of surface states of topological insulators (TI) open up possibilities for designing ultra fast electrically controllable spin transistor. In this context I will discuss spin-valve effect associated with a gating induced PN junction designed on the surface state of 2D and 3D TI. I will show that *conduction to conduction* and *conduction to valence* band transport in a PN junction is topologically distinct resulting in asymmetric electrical transport. The topological distinction is shown to be quantifiable in term of the Pancharatnam geometric phase.

TT 49: Spintronics (organized by MA)

Time: Tuesday 13:45–16:00 Location: HSZ 401

TT 49.1 Tue 13:45 HSZ 401

Sound Waves in a Magnon Bose Einstein Condensate — •Patryk Nowik-Boltyk[1], Oleksandr Dzyapko[1], Vladislav E. Demidov[1], Sergej O. Demokritov[1], Vasyl Tyberkevych[2], and Andrej N. Slavin[2] — [1]Institute of Applied Physics, University of Muenster, Muenster, Germany — [2]Department of Physics, Oakland University, Rochester, USA

Magnon Bose-Einstein condensation (mBEC) in Yttrium-Iron-Garnet films is a spectacular room-temperature macroscopic quantum phenomenon, which is under investigation since recently [1]. Although the basic properties of mBEC such as temporal [2] and spatial [3] coherence have extensively been studied during the last 5 years, the perturbed dynamics of the condensate have not been addressed so far. Here we report an experimental study of sound waves in a magnon gas, above and below the threshold for mBEC, performed using a space- and time-resolved Brillouin light scattering technique. The magnon gas was prepared using microwave pumping of magnons, while the sound waves were excited by, an additional, localized, oscillating, RF magnetic field. We show that at small wave vectors sound waves exhibit a linear dispersion law with a density independent group velocity, while at large wave vectors the dispersion changes from a linear dependence into a quadratic one at the threshold for mBEC. We demonstrate that this sudden change is due to an additional scattering mechanism that arises when an mBEC is formed. [1] S.O. Demokritov et al. Nature 443, 430 (2006) [2] V.E. Demidov et al. Phys. Rev. Lett. 100, 047205 (2008) [3] P. Nowik-Boltyk et al. Nature Sci. Rep. 2, 482 (2012)

TT 49.2 Tue 14:00 HSZ 401

Antiferromagnetic spintronics — •I. Fina[1,2], X. Marti[3,4,5], D. Yi[3], C. Rayan-Serrao[3], J. Liu[3], J.-H. Chu[3], S.J. Suresha[3], J. Zelezny[5], T. Jungwirth[5,6], J. Fontcuberta[3], and R. Ramesh[3] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, Halle Germany — [2]Institut de Ciencia de Materials de Barcelona, ICMAB-CSIC, 08193 Bellaterra, Spain — [3]Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA

— [4]Dept. Condensed Matter Physics Charles University in Prague — [5]Institute of Physics ASCR, v.v.i., Cukrovarnick 10, 162 53 Praha 6, Czech Republic — [6]School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom

Magnetic semiconductors entwine two of the most successful concepts in both fundamental physics and industrial applications. Recently antiferromagnets have been proposed as new and atractive material systems. Antiferromagnetic spintronics have been demonstrated by the fabrication of tunnel devices, atomic-size proof-of concepts, even devices without auxiliary ferromagnetic layers. Here we present the control of the electrical conductivity of an antiferromagnetic semiconductor by manipulating the magnetic state of a contiguous ferromagnetic.

We present an oxide-based fully epitaxial heterostructure, its structural characterization and the electrical measurements showing a direct link between state of the ferromagnetic gate and ohmic resistance of the semiconductor, even displaying distinct remnant resistance states. We will also show that distinct remnant states can also been obtained at room temperature, promising potential applicability.

TT 49.3 Tue 14:15 HSZ 401

Calculating spin transport and magnetization dynamics parameters in textured magnetic materials — •Zhe Yuan — Faculty of Science and Technology, University of Twente, Enschede, The Netherlands — Institute of Physics, Johannes Gutenberg-University Mainz, Mainz, Germany

First-principles calculations allow us to understand the electronic and magnetic properties of real materials in terms of their chemical composition, atomic structure and magnetic configuration by numerically solving the quantum mechanical equations that describe the motion of the electrons. We have developed a unique first-principles formalism of scattering theory that can be used to calculate quantities such as the resistivity, Gilbert damping, and spin-transfer torque for a wide variety of material systems. In this talk, I will focus on how magnetic domain walls (DWs) modify the above transport and magnetization dynamics properties in real materials. Taking the technologically important Ni80Fe20 magnetic alloy, as an example, we have studied the change in its resistance due to the presence of a DW. The Gilbert damping in a DW is found to be anisotropic and drastically enhanced by the magnetization gradient, which has significant effects on field- and/or current-driven DW motion.

TT 49.4 Tue 14:30 HSZ 401

Spin Solar Cell for Spin Injection into Semiconductors. — Bernhard Endres, Mariusz Ciorga, Maximilian Schmid, Martin Utz, Dominique Bougeard, Dieter Weiss, Christian Back, and •Günther Bayreuther — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

Optical spin pumping allows to create spin-polarized carriers in III-V semiconductors, but requires circularly polarized light of a well-defined wavelength. Here we describe a spin-generating solar cell without such limitations [1,2]. The device consists of a p-n junction with highly n-doped GaAs at the n-side and ferromagnetic (Ga,Mn)As at the p-side. Illuminating this junction creates a photo-voltage causing electrons to tunnel across the narrow barrier from the n-GaAs into the (Ga,Mn)As. Due to the spin-dependent tunneling probability a spin accumulation occurs in the n-GaAs. This spin solar cell effect is demonstrated with a laser beam generating electron-hole pairs and detecting the spin accumulation via the polar magneto-optic Kerr effect and by measuring non-local voltages. On applying a large negative bias the sign of the photo-induced spin polarization is reversed as expected due to the suppression of the tunneling current through a wider barrier. This mode of operation corresponds to a spin photodiode. The spin solar cell effect should equally work for metallic ferromagnets with a high Curie temperature and allow to convert unpolarized light into a spin current also in semiconductors without a direct band gap like Si and Ge.

[1] B. Endres et al., Nature Commun. 4, 2068 (2013).
[2] R. Jansen, Nature Mater. 12, 779 (2013)

TT 49.5 Tue 14:45 HSZ 401

Magnetic anisotropy in CoFe/MgO/CoFe magnetic tunnel junctions with ultrathin electrode layers and its composition dependence — •Jia Zhang, Christian Franz, Michael Czerner, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University, Giessen, Germany

MgO based magnetic tunnel junctions (MTJs) with ultrathin CoFeB magnetic electrodes can have perpendicular magnetic anisotropy and a low switching current. In addition, MgO-MTJs with perpendicular anisotropy may also be easier to switch by thermal spin transfer torque and may pave its potential application in Spincaloritronics. In this talk, the magnetic anisotropy in CoFe/MgO/CoFe-MTJs on different substrates for instance Cu, Au, MgO etc. and different CoFe alloy composition are discussed using full relativistic Korringa-Kohn-Rostoker and coherent potential approximation (CPA) first-principles calculations. The magnetic anisotropy energy (MAE) in CoFe/MgO/CoFe-MTJs was calculated by employing magnetic force theory. The calculated MAE in Co_xFe_{1-x}/MgO/Co_xFe_{1-x}-MTJs decreased with the increasing of Co composition. The $d_{zx}(d_{yz})$ and $d_{xy}(d_{x^2-y^2})$ orbital and its evolution in the spin down channel was found to be responsible for the rise of magnetic anisotropy and the composition dependence. The shape anisotropy energy was also calculated and thus the phase diagram with perpendicular anisotropy versus composition and thickness was determined. Finally, we will give a brief discussion on magneto resistance and spin-transfer torque in CoFe/MgO/CoFe-MTJs with perpendicular easy axis.

TT 49.6 Tue 15:00 HSZ 401

Magnetic and electronic properties of $Ni_2S_2O_2N_6C_{57}H_{78}P^+$ on Au(111) — •Kai Trepte, Claudia Martin, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, Germany

The electronic and magnetic properties of a Ni^{2+} dimer including a PPh_3- ligand in contact with a Au(111) surface have been measured [1]. We will present theoretical calculations using DFT (with and without van der Waals interactions) including only the PPh_3- ligand binding on the Au(111) surface in order to determine the magnetic exchange and anisotropy. We will discuss charge transfer and the bonding situation for the favored binding position in more detail. Finally we will compare these results with a calculation of the dimer on the surface including geometry changes and charge transfer.

[1] M. Golecki et al. Chemisorption of exchange-coupled $[Ni_2L(dppba)]^+$ complexes on gold by using ambidentate 4-(diphenylphosphino)benzoate co-ligands. *Chemistry - A European Journal*, 19(24):7787-7801, 2013.

TT 49.7 Tue 15:15 HSZ 401

Manipulating the coupling between metal and molecule in hybrid structures by changing of organic anchor groups — •Simon Liebing, Torsten Hahn, and Jens Kortus — Institut of Theoretical Physics, TU Bergakademie Freiberg, 09599 Freiberg

There are theoretical and experimental works which propose to the use of amino anchor groups [1] instead of the more often used thiol [2] ones. So far there is no systematic study comparing the properties of different anchor groups. The present study investigates the properties of amino, cyano, furan, hydroxyl, pyrol thiol and thiophen in a break junction like geometry. The anchor groups are attached to a novel molecular system based on an anthraquinone-core with conjugated spacers to form a model system. These anchor groups include also some that could form π-like bonds and allow fully and cross-conjugated electron systems.

The molecular structures are constructed with Avogadro [3] and optimized by all-electron DFT-code NRLMOL [4]. The device structures are than optimized with the GPAW program package [5] an plane wave augmented wave again. The same software is used for the calculation of the transport properties by means of the NEGF-formalism.

References

1 Angela. D. et. al. Nano Letters 10, no. 7 (2010), 2 Markussen, T. et al. JCP 132 , 224104 (2010), 3 Hanwell, M. D. et al. Journal of Cheminformatics 4, 17 (2012), 4 Pederson, M. et. al. Phys. Status Solidi b 217, 197. (2000), 5 Enkovaara, J. et al. Journal of Physics: Condensed Matter 22, 253202 (2010)

TT 49.8 Tue 15:30 HSZ 401

Barrier dependent tunneling magnetoresistance in carbon nanotubes — •Carola Meyer[1,2], Cate Morgan[1,2], Dominik Metten[3], Sebastian Heedt[1,2], Thomas Schäpers[1,2], and Claus M. Schneider[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA - Fundamentals of Future Information Technologies — [3]Institut de Physique et Chimie des Matériaux de Strasbourg and NIE, UMR 7504, Université de Strasbourg and CNRS, France

Carbon nanotubes (CNTs) are a material of interest in spintronics, because in addition to exhibiting ballistic transport, the low atomic number and low abundance of ^{13}C nuclei in CNTs is expected to lead

to low spin orbit coupling and hyperfine interaction indicating a long spin relaxation time. However, the size of the magnetoresistance (MR) observed depends strongly on the current regime and on the type of CNT device measured. In the single-electron-tunneling regime, typically only a few percent MR can be reached. MR in multiwalled CNTs with a large diameter has shown to be as large as 60% for contacts with high polarization [1].

We present a way to compare the MR of different devices from single-wall and multiwalled CNTs with respect to the current regime. Temperature dependent data confirm tunneling MR as the main effect. The size of the MR measured depends on the strength of the tunnel barrier and follows the Slonczewski model. Finally, the presence of the Hanle effect proves successful spin injection.

[1] L. E. Hueso et al., Nature 445, 410 (07)

TT 49.9 Tue 15:45 HSZ 401

Transport properties of multiferroic tunnel junctions in an embedded Green-function approach — •Andera 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

Multiferroics tunnel junctions are promising structures for spintronic devices due to their transport properties. From the theoretical point of view the study of transport in Metal/Ferroelectric/Metal needs to deal with several degrees of freedom. Structural distortions at the interface, polarization and magnetization directions, presence of oxides at the interface and strong correlations must be taken into account. We focus on the tunneling properties of a Fe/BTO/Fe barrier obtained in an embedded Green-function approach [1] implemented with the framework of the full-potential linearized augmented plane-wave (FLAPW) method `FLEUR` [2]. Electronic charge self-consistency is achieved in the same approach. 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 50: Correlated Electrons: Quantum-Critical Phenomena - Theory

Time: Tuesday 14:00–16:00 Location: BEY 81

TT 50.1 Tue 14:00 BEY 81

Detailed analysis of critical points in coupled spin dimer systems — •Sebastian Eggert[1], Dominik Strassel[1], and Peter Kopietz[2] — [1]Fachbereich Physik, Technische Universität Kaiserslautern — [2]Fachbereich Physik, Goethe Universität Frankfurt

Spin dimer systems are a promising playground for the detailed study of quantum phase transitions. In many cases it is sufficient to use the magnetic field as the tuning parameter in order to reach interesting non-trivial critical points. Depending on the temperature it is in principle possible to observe a crossover from the characteristic scaling near the critical point to the behavior of a finite temperature phase transition. In order to quantitatively demonstrate those effects and inspired by recent experiments we have started large scale quantum Monte Carlo simulations in order to analyze several different physical quantities in spin dimer systems, namely the susceptibility, the magneto-caloric effect, the structure factor and the spin stiffness. We discuss in detail how the phase transitions (quantum and finite temperature) are manifest in the characteristic scaling behavior near critical points by comparing them with interacting boson theories. The results give a unified picture of the full quantum and finite temperature phase diagram.

TT 50.2 Tue 14:15 BEY 81

Quantum Monte Carlo Simulations of Trimerized Antiferromagnetic Systems — •Dominik Strassel and Sebastian Eggert — Department of Physics and Research Center Optimas, Technical University Kaiserslautern, 67663 Kaiserslautern, Germany

We study linear clusters of three strongly coupled spins $\mathcal{S} = \frac{1}{2}$ (trimers), which are connected more weakly in a two dimensional lattice using *Stochastic Series Expansion Quantum Monte Carlo* simulations of the Heisenberg model in a magnetic field. In general these systems show a magnetization plateau at $\frac{1}{3}$ saturation, which is already known from strongly coupled three-leg ladders. Interestingly, the origin of the plateau is very similar to the $\frac{1}{3}$ plateau in frustrated lattices (e.g. the triangular lattice) so that the analogous phase transitions can be analyzed using non-frustrated systems, which do not suffer from the infamous minus sign problem. With increasing coupling between the trimers, the plateau vanishes and a critical point can be identified. We also analyze the behavior in the limit of weak inter-trimer coupling.

TT 50.3 Tue 14:30 BEY 81

Excitonic Instability at Spin-State Transition — •Jan Kuneš and Pavel Augustinský — Institute of Physics, ASCR, Prague, Czechia

We report a newly observed instability of the half-filled two-band Hubbard model in the vicinity of the spin-state transition. [1] Using dynamical mean-field theory we have performed a unbiased search for divergent particle-hole susceptibilities. Depending on the bandwidths ratio the system was found to establish a checker-board order of high- and low-spin sites, breaking the discrete translational symmetry, or to undergo a condensation of spinful excitons, breaking a continuous gauge symmetry. Besides numerical results we provide an analytic description in the strong-coupling limit where the problem maps of a variate of the bosonic t-J model.

[1] Kunes and Augustinsky, arXiv:1310.0669

TT 50.4 Tue 14:45 BEY 81

Critical phenomena of the two-channel spin-boson model — •Benedikt Bruognolo[1], Andreas Weichselbaum[1], Jan von Delft[1], and Matthias Vojta[2] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, 80333 München, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

In recent years bosonic quantum impurity models have attracted significant attention in the context of quantum phase transitions. Numerical approaches to study the critical properties in such models face additional challenges arising from the bosonic nature of the bath modes, that are not present in purely fermionic systems.

Guo et al. [1] presented a powerful numerical method based on a combination of NRG and DMRG, which overcomes the problem of a diverging bosonic state space by variationally constructing an optimized boson basis on each site of the Wilson chain. We discuss a symmetry improved application of this method to the sub-ohmic spin-boson model with two symmetrically coupled bosonic baths and focus on its critical properties, which so far had been an open question. We present the first numerical study of the critical points, which in combination with RG results allows a description of the critical phenomena of this model for a wide range of parameters.

[1] C. Guo, A. Weichselbaum, J. von Delft, M. Vojta, Phys. Rev. Lett. 108, 160401 (2012)

TT 50.5 Tue 15:00 BEY 81

Interplay of fermion and boson induced critical Kondo destruction — •Farzaneh Zamani[1,2], Pedro Ribeiro[1,2,3], and Stefan Kirchner[1,2] — [1]MPI-PKS, Dresden, Germany — [2]MPI-CPFS, Dresden, Germany — [3]CFIF-IST, Universidade de Lisboa, Lisboa, Portugal

An increasing number of experiments have indicated that the traditional approach to continuous zero-temperature phase transitions in strongly correlated electrons systems is inadequate. In the context of intermetallic rare-earth compounds this approach does e.g. not account for the linear-in-temperature relaxation rates observed in a number of systems in the charge- and spin-response near criticality. A widely discussed alternative to the standard approach picture is local Kondo destruction, where Kondo screening becomes critical concomittantly with the lattice. We study the phenomenon of critical Kondo destruction in the pseudogap Bose-Fermi Kondo model where a quan-

tum spin is coupled to a fermionic and a bosonic bath. Each of the baths by itself is capable of critically destroying Kondo screening, allowing us to study the dynamic interplay of the two. We employ a dynamic large-N limit and obtain asymptotically exact solutions at zero temperature. We also report full scaling equations at all critical points and discuss the ensuing relaxation rates. Finally, we revisit the issue of 'conformal scaling' of the imaginary-time correlation functions at criticality and relate our findings to their counterpart in the easy-axis pseudogap pseudogap Bose-Fermi Kondo model.

TT 50.6 Tue 15:15 BEY 81

Corrections to scaling in the critical theory of deconfined criticality — •Lorenz Bartosch — Institut für Theoretische Physik, Universität Frankfurt, 60438 Frankfurt am Main, Germany

Inspired by recent conflicting views on the order of the phase transition from an antiferromagnetic Néel state to a valence bond solid, we use the functional renormalization group to study the underlying quantum critical field theory which couples two complex matter fields to a non-compact gauge field. In our functional renormalization group approach we only expand in covariant derivatives of the fields and use a truncation in which the full field dependence of all wave-function renormalization functions is kept. While we do find critical exponents which agree well with some quantum Monte Carlo studies and support the scenario of deconfined criticality, we also obtain an irrelevant eigenvalue of small magnitude, leading to strong corrections to scaling and slow convergence in related numerical studies.

TT 50.7 Tue 15:30 BEY 81

Heavy fermion quantum critical point from AdS/CFT correspondence — •Mihailo Čubrović — Institute for Theoretical Physics, University of Cologne, Germany

We propose a holographic (AdS/CFT) approach to strongly correlated electrons and study a quantum phase transition from small to large Fermi surface phase in a model "heavy fermion" system. AdS/CFT is a duality which maps the correlation functions from field theory to solutions of the equations of motion for classical fields in a curved spacetime, i.e. in general relativity. The appealing side of this approach is its nonperturbative nature: the calculations on the gravity side are essentially an expansion in inverse coupling strength and indeed work best in the strong coupling regime. We construct a gravity dual of a Fermi liquid system which shows a mass enhancement of the order of several hundred times the bare mass. At zero temperature, the system exhibits a continuous quantum phase transition to another Fermi liquid with different effective mass and Fermi momentum. The difference in sizes of the Fermi surfaces (i.e. Fermi momenta), as well as the fact that the transition happens at finite wavevector agree with the intuition on heavy fermion transitions. While the picture resembles the fractionalization scenario, we.do not introduce any emergent gauge fields. The shrinking of the Fermi surface can best be interpreted as formation of bound states between electrons and exotic bosonic excitations near the quantum critical point.

TT 50.8 Tue 15:45 BEY 81

Anderson Metal-Insulator Transitions With Classical Magnetic Impurities — •Daniel Jung[1], Keith Slevin[2], and Stefan Kettemann[1,3] — [1]School of Engineering and Science, Jacobs University Bremen, 28759 Bremen, Germany. — [2]Department of Physics, Graduate School of Science, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan. — [3]Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), Pohang 790-784, South Korea.

We study the effects of classical magnetic impurities on the Anderson metal-insulator transition numerically [1, 2]. In particular we find that while a finite concentration of Ising impurities lowers the critical value of the site-diagonal disorder amplitude W_c, in the presence of Heisenberg impurities, W_c is first enhanced with increasing exchange coupling strength J due to time-reversal symmetry breaking. The resulting scaling with J is analyzed and compared to analytical predictions by Wegner [3]. We discuss the relevance of our findings for systems like phosphor-doped silicon, which are known to exhibit a quantum phase transition from metal to insulator driven by the interplay of both interaction and disorder, accompanied by the presence of a finite concentration of magnetic moments [4].

[1] D. Jung, and S. Kettemann, AIP conf. proceed., submitted.
[2] D. Jung, K. Slevin, and S. Kettemann, to be published.
[3] F. Wegner, Nucl. Phys. B **280**, 210 (1987).
[4] H. von Löhneysen, Adv. Solid State Phys. **40**, 143 (2000)

TT 51: Quantum Wires: Optical Properties (organized by HL)

Time: Tuesday 14:30–16:15 Location: POT 112

TT 51.1 Tue 14:30 POT 112

Continuous Wave Lasing in Sn:CdS Nanowires — •Marcel Wille[1,2], Robert Röder[2], Sebastian Geburt[2], Carsten Ronning[2], Mengyao Zhang[3], and Jia Grace Lu[3] — [1]Institut für Experimentelle Physik II/Halbleiterphysik, Universität Leipzig — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena — [3]Department of Physics and Electrical Engineering, University of Southern California

Semiconductor nanowires (NWs) are promising candidates for future optoelectronic applications due to their possibility of light generation, optical waveguiding and light amplification. The controlled modification of their electrical and optical properties by doping will continue the consequent progress in NW research. In a modified VLS growth process using tin (Sn) as catalyst the in-situ doping of cadmium sulphide (CdS) NWs was demonstrated. Optical investigations using temperature dependent photoluminescence and cathodoluminescence technique were correlated with electrical transport measurements in field-effect-transistor geometry [1]. Furthermore, these NWs exhibit ideal Fabry-Pérot resonator morphology necessary for the occurrence of laser oscillations under continuous wave excitation. The continuous wave lasing mode is proven by the evolution of the emitted power and spectrum with increasing pump intensity [2]. The high temperature stability up to 120 K at given pumping power is determined by the decreasing optical gain necessary for lasing in an electron hole plasma.
[1] Zhang, M., Wille, M. et al., Submitted to Nano Letters, 09.2013 [2] Röder, R., Wille, M. et al., Nano Letters 2013, 13, 3602-3606

TT 51.2 Tue 14:45 POT 112

Phonon-assisted lasing in ZnO microwires — •Stefan Lange, Tom Michalsky, Christof P. Dietrich, Helena Franke, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

In this work we present the investigation of the lasing properties of ZnO microwires. The spectral distribution of the lasing modes reveals a strong exciton-phonon interaction as the main lasing mechanism. These findings are supported by former results measuring a strong exciton-phonon interaction in ZnO [1,2] and showing indications for an increase of the coupling strength with reduced structure size [2]. Photoluminescence and coherence measurements under varying excitation density prove the transition from spontaneous to stimulated emission.

[1] D.C. Reynolds et al., J. Appl. Phys. 89, 6189 (2001)
[2] H.C. Hsu et al., J. Crystal Growth 261, 520 (2004)

TT 51.3 Tue 15:00 POT 112

Phonons in PbSe nanostructures — •Efterpi Kalesaki and Ludger Wirtz — Physics and Materials Science Research unit, University of Luxembourg, Luxembourg

The prospect of efficient utilization of lead chalcogenides in optoelectronic, photovoltaic and thermoelectric devices has brought PbSe into the spotlight of scientific research. Bulk PbSe exhibits a plethora of intriguing characteristics, in terms of structural, electronic and vibrational properties, which have been the subject of intense investigation. In particular, the phonon dispersion displays a near-Kohn anomaly of the LO mode at Γ [1]. However, attempts to understand the vibrational properties of corresponding nanostructures are limited.

We present results of ab-initio calculations on the phonon dispersions of <001> - oriented PbSe slabs of various thicknesses. The latter are correlated with the phonon modes of bulk PbSe via the quantum confinement model [2]. Quantum confinement and strain effects are identified as parameters critically affecting the lattice dy-

namics of PbSe nanostructures. In contrast to most nanocrystalline materials, where the Raman active phonon modes shift down in frequency, a blueshift of the longitudinal optical mode with decreasing layer thickness is recorded for PbSe nanostructures, validating recent experimental results of Raman spectra for lead selenide nanocrystals [2]. Softening of the TO mode in the slabs is an indication of near-ferroelectric behaviour in PbSe nanostructures.

[1] O. Kilian et al., Phys. Rev. B 80, 245208 (2009)
[2] J. Habinshuti et al., Phys. Rev. B 88, 115313 (2013)

TT 51.4 Tue 15:15 POT 112

Picosecond time-resolved photocurrents in single semiconductor nanowires — •Stefan Zenger[1,2], Nadine Erhard[1], and Alexander Holleitner[1] — [1]Walter Schottky Institute and Physik-Department, Technische Universität München, Germany — [2]stefan.zenger@wsi.tum.de

Conventional scanning photocurrent microscopy experiments on semiconductor nanowires are typically limited to timescales exceeding several tens of picoseconds. Yet, it is known from optical experiments that carrier relaxation and transport processes can occur on much faster timescales in semiconducting nanowires. We apply a recently developed pump-probe photocurrent spectroscopy to investigate the photocurrent dynamics in single nanowires made out semiconductors, such as InAs, GaAs, and InGaN, with an on-chip THz-time domain spectroscopy [1]. Hereby, the ultrafast photocurrent response of the nanowire is sampled at a field probe in a stripline circuit a picosecond time-resolution. We discuss ultrafast thermoelectric, displacement, and carrier lifetime limited currents as well as the time-resolved transport of photogenerated holes.

[1] N. Erhard, P. Seifert, L. Prechtel, S. Hertenberger, H. Karl, G. Abstreiter, G. Kobelmueller,and A. Holleitner, Ann. Phys. (Berlin) 525, 180 (2013).

We gratefully acknowledge financial support from the ERC-grant NanoREAL.

TT 51.5 Tue 15:30 POT 112

Combined optical and electrical characterization of single AlGaN/GaN nanowire heterostructures — •Jan Müssener, Pascal Becker, Svenja van Heesvijk, Markus Schäfer, Pascal Hille, Jörg Schörmann, Jörg Teubert, and Martin Eickhoff — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

We report on the photoluminescence characterization of single GaN nanowires (NWs) with embedded AlGaN/GaN heterostructures under the influence of an external electric field. Group III-nitrides exhibit strong internal polarization-induced electric fields which influence the optical properties via the quantum confined Stark effect (QCSE). While the presence of the QCSE in NWs has been proven, a controlled modification of the QCSE via external axial electric fields on a single NW basis has not been achieved up to now. NWs were grown along $[000\bar{1}]$ by plasma assisted molecular beam epitaxy on a Si(111) substrate. Their geometry consists of a single ND embedded in AlGaN barriers and surrounded by Ge-doped GaN contacts. We performed numerical simulations of the three dimensional quantum confinement to optimize the sample structure with respect to its opto-electrical properties. Single NWs were isolated for μ-PL measurements and contacts were formed using electron beam lithography to allow application of external axial electric fields. The effect of current induced heating on the low temperature μ-PL spectra was investigated. The application of axial electric fields leads to a suppression or an enhancement of the QCSE which corresponds to the polarity of the NWs.

TT 51.6 Tue 15:45 POT 112

Nanospectroscopic imaging of twinning superlattices in individual Beryllium-doped GaAs/AlGaAs core-shell nanowires — •Alexander Senichev[1], Igor Shtrom[2], Vadim Talalaev[1,3], George Cirlin[2,4], Christoph Lienau[5], Jörg Schilling[3], and Peter Werner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]St. Petersburg Academic University RAS, St. Petersburg, Russia — [3]Martin-Luther-Universität, ZIK "SiLi-nano", Halle, Germany — [4]Ioffe Physico-Technical Institute, St. Petersburg, Russia — [5]Institut für Physik, Carl von Ossietzky University, Oldenburg, Germany

We report on subwavelength-resolution near-field photoluminescence (PL) spectra and transmission electron microscopy (TEM) images taken from the very same single p-GaAs/AlGaAs core-shell nanowire grown on silicon.By correlation with the TEM images, we distinguish between the emission spectra of pure ZB-type regions and those of periodic twinning plane superlattices (TSL). Emission from the ZB region is governed by direct interband recombination whereas the TSL spectra are split into two peaks, separated in energy by the hole confinement at a single WZ-type quantum disk. Blue-shifts of the local emission spectra reveal electron quantum confinement in twinning superlattices and allow us to trace spatial variations of the TSL period by all-optical means. Our results provide direct and quantitative insight into the correlations between morphology and optics of TSL nanowire and hence present an important step towards band gap engineering of GaAs nanowires by controlled crystal phase formation.

TT 51.7 Tue 16:00 POT 112

Optical characterization and enhanced luminescence properties of InAs-InAsP core-shell nanowires — •Thomas Stettner[1], Julian Treu[1], Michael Bormann[1], Hannes Schmeiduch[1], Stefanie Morkötter[1], Markus Döblinger[2], Sonja Matich[1], Peter Wiecha[1], Kai Saller[1], Benedikt Mayer[1], Max Bichler[1], Markus Christian Amann[1], Jonathan Finley[1], Gerhard Abstreiter[1,3], and Gregor Koblmüller[1] — [1]Walter Schottky Institut and Physik Department, TU München, Garching, Germany — [2]Department of Chemistry, Ludwig-Maximilians-Universität München, Munich, Germany — [3]TUM Institute for Advanced Study, Garching, Germany

Using optical spectroscopy InAs nanowires (NW) grown by molecular beam epitaxy (MBE) and subsequently overgrown and passivated with an $InAs_{1-x}P_x$-shell by a hybrid metal-organic vapor phase epitaxy (MOVPE) process are studied in detail. With a microphotoluminescence (PL) setup designed for the mid infrared spectral range we demonstrate up to 100x enhancement of the InAs core signal [1]. By systematically varying both the shell thickness and the phosphorus content x(P) we show that it is possible to further tune the emission energy >100meV for comparatively low x(P) due to strain effects, which is confirmed by numerical simulation. For even higher P-content an asymmetric shell growth leads to a drastic reduction in PL efficiency/blueshift due to an onset of plastic relaxation which proves the importance to engineer a high quality InAs-InAsP core-shell interface for future use in photonic and optoelectronic devices like solar cells.

[1] J. Treu, et al., Nano Lett.2013, dx.doi.org/10.1021/nl403341x

TT 52: Focus Session: Quantum Light Sources Based on Solid State Systems: Status and Visions II (organized by HL)

Continuation of 'Quantum light sources based on solid state systems: Status and visions I'

Organizers: Sven Ulrich, Universität Stuttgart, and Christoph Becher, Universität des Saarlandes, Saarbrücken.

Time: Tuesday 14:00–15:45 Location: POT 251

Topical Talk TT 52.1 Tue 14:00 POT 251

Quantum network challenges for solid-state spins and photons — •Mete Atature — University of Cambridge, Cambridge, United Kingdom

Spins confined in solids, such as quantum dots and atomic impurities provide interesting and rich physical systems. Their inherently mesoscopic nature leads to a multitude of interesting interaction mechanisms of confined spins with the solid state environment of spins, charges, vibrations and light. Implementing a high level of control on these constituents and their interactions with each other creates exciting opportunities for realizing stationary and flying qubits within the context of spin-based quantum information science. I will provide a snapshot of the progress and challenges for optically interconnected spins, as well as first steps towards hybrid distributed quantum networks.

TT 52.2 Tue 14:30 POT 251

Indistinguishable single photons from quasi-resonantly pumped quantum dots in adiabatic micropillar cavities — •Sebastian Unsleber[1], Michael Dambach[1], Matthias Lermer[1], Sven Höfling[1,2], Christian Schneider[1], and Martin Kamp[1] — [1]Technische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Present address: SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Single, indistinguishable photons are very important for applications in quantum networks and communication as well as linear optical quantum computing. Due to their atom-like emission properties quantum dots are promising candidates for photon sources matching this characteristics. Furthermore quantum dots can be implemented in nanostructured waveguides and microcavities leading to higher emission rates of single, indistinguishable photons.

We report on the emission of single and indistinguishable photons generated from quantum dots under quasi-resonant excitaion. The quantum dots are implemented in a adiabatic cavity design where we applied Bloch-wave engeneering to realize submicron diameter high quality factor GaAs/AlAs micropillars. Single photons emission with $g^{(2)}(0)$-values as low as 0.036 are observed and quantum interference of the quantum dots leads to visibility as high as 76%. Furthermore we studied the influence of the quantum dot cavity detuning on the indistinguishability of the emitted photons.

TT 52.3 Tue 14:45 POT 251

Indistinguishable photons generated from deterministic quantum light sources fabricated by in-situ electron-beam lithography — •Tobias Heindel, Luzy Krüger, Elisabeth Schlottmann, Manuel Gschrey, Marc Seifried, Ronny Schmidt, Jan-Hindrik Schulze, Sven Rodt, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623, Germany

Quantum communication technology relies vitally on efficient non-classical light sources emitting single indistinguishable photons on demand. A promising approach to realize such light sources is based on single self-assembled semiconductor quantum dots (QDs) embedded into microcavity systems. The main challenge of this approach is the precise control of the coupling between the statistically grown QD and the optical mode of the microcavity. In this work we tackle this issue by using in-situ electron-beam lithography to embed target QDs deterministically into sub-μm mesa structures [1] as well as microlenses with enhanced photon extraction efficiency. The huge potential of this device technology is demonstrated by quantum optical studies which reveal distinct excitonic emission lines with resolution limited linewidths below 10 μeV and a strong suppression of multi-photon emission events associated with $g^{(2)}(0) < 0.04$. Furthermore, Hong-Ou-Mandel type two-photon interference experiments are used to analyze the indistinguishability of the emitted photons.

[1] M. Gschrey et al., APL 102, 251113 (2013).

TT 52.4 Tue 15:00 POT 251

Bright quantum dot single photon source based on a low Q defect cavity — •Sebastian Maier[1], Peter Gold[1], Alfred Forchel[1], Niels Gregersen[2], Sven Höfling[1,3], Christian Schneider[1], and Martin Kamp[1] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074, Würzburg, Germany — [2]DTU Fotonik, Department of Photonics Engineering, Technical University of Denmark, Building 343, DK-2800 Kongens Lyngby, Denmark — [3]present address: SUPA, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Efficient light outcoupling in quantum dot single photon sources is critical and usually complicated resonator geometries, lithographic steps and spatial alignment are necessary. In this paper we demonstrate a quantum dot based quasi-planar single photon source with a high extraction efficiency of 42% measured with a numerical aperture of 0.7. Our sample was fabricated via molecular beam epitaxy (MBE) and contains a λ-thick cavity which is sandwiched between two distributed Bragg reflector (DBRs), consisting of 18 (5) bottom (top) layers of AlAs/GaAs mirror pairs. The high efficiency is caused by the self-aligned formation of oval defects on top of the quantum dots which is interesting for a possible scalable sample layout. Besides the high extraction efficiency the sample shows a high purity with a g2(0) value of 0.023. Due to the absence of any etched and exposed lateral semiconductor-air interfaces, such cavities are nearly ideal for spin manipulation and readout experiments.

TT 52.5 Tue 15:15 POT 251

On-demand single-photon emission from electrically pumped, site-controlled quantum dots based on buried stressors — •Alexander Schlehahn, Waldemar Unrau, David Quandt, Jan-Hindrik Schulze, Tobias Heindel, Tim D. Germann, Ole Hitzemann, Udo W. Pohl, Dieter Bimberg, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, TU Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Single photons, emitted on demand, is one of the most basic needs in quantum information technology. We present pulsed operation of a lately introduced electrically driven source based on single quantum dots, deterministically aligned to a strain-inducing and current-path-restricting oxide aperture. The aperture is formed by oxidation of an AlAs/AlGaAs sandwich structure. The modification of its crystalline structure leads to geometry dependent strain in the topping GaAs-layer. Due to this strain modulation at the surface, an accumulation of quantum dots occurs above the aperture when depositing InGaAs. These QDs show excellent optical properties regarding the emission linewidth ($FWHM < 25\mu$eV) and the single photon purity ($g^{(2)}(0) < 0.05$), and outclass the reported characteristics of QDs grown by other prepositioning methods. The sample characterization is facilitated by an automatized micro-electroluminescence setup which includes a He-flow cryostat with an internal high-frequency probe in combination with a precise x-y-z-stage. This system allows for efficient sample testing without the need for wire bonding.

TT 52.6 Tue 15:30 POT 251

Integrated quantum optics in coupled quantum-dot micropillar cavities — •Pierce Munnelly — Institut für Festkörperphysik, Technische Universität Berlin

The development of novel concepts for integrated photonics has become an area of intensive research in the field of semiconductor nanotechnology. The overall goal is to integrate light sources, waveguides, non-linear optical elements and detectors into compact and externally controllable optical networks. Up till now, most approaches for integrated nanophotonics have relied on planar waveguide structures and photonic crystal membranes, where the integration of active and pas-

sive areas on the same chip or the definition of electrical contacts is challenging. In an alternative approach for 'free space' integrated optics we take advantage of the fact that electrically contacted micropillar cavities allow for efficient in-plane emission of light via whispering gallery modes. Using this very appealing feature, we demonstrate that electrically driven micropillar lasers can act as integrated light sources to perform cavity quantum electrodynamics experiments in laterally coupled micropillar cavities. Moreover, electrical contacts at the coupled micropillars allow for resonance tuning using the quantum confined Stark effect and for integrated light detection via on-chip photocurrent measurements.

TT 53: Superconductivity: Fe-based Superconductors - 122

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

TT 53.1 Wed 9:30 HSZ 201

The Pauli-limited multiband superconductor $RbFe_2As_2$ — •Felix Eilers, Diego A. Zocco, Thomas Wolf, Peter Schweiss, Kai Grube, and Hilbert v. Löhneysen — Karlsruher Institut für Technologie, Institut für Festkörperphysik, Karlsruhe, Germany

The compounds AFe_2As_2 - where A denotes an alkali metal element like K or Rb - offer the possibility to probe the unconventional superconductivity in iron pnictides. The upper critical magnetic fields H_{c2} are easily accessible and no additional chemical disorder is introduced by substitutional atoms. We measured the thermal expansion and magnetostriction of a $RbFe_2As_2$ single crystal at temperatures T between 50 mK and 4 K and magnetic fields $\mu_0 H$ up to 14 T. The quantum oscillations observed in our magnetostriction measurements indicate a strongly correlated electron system in accordance with the enhanced Sommerfeld coefficient and Pauli susceptibility of KFe_2As_2 [1]. In addition, they reveal, together with the thermal expansion, the multiband character of the electronic structure and superconductivity. The T-H phase diagram constructed from our field-dependent measurements shows the typical behavior of an orbitally limited superconductor for H parallel to the c-axis, while for H within the ab-plane the superconducting phase transition becomes discontinuous below $T = 1.2$ K. For this field direction the orbital limit strongly exceeds $H_{c2}(T = 0)$, thus pointing to a Pauli-limited upper critical field like in KFe_2As_2 [2].

[1] F. Hardy et al., PRL 111, 027002 (2013)
[2] D. A. Zocco et al., PRL 111, 057007 (2013)

TT 53.2 Wed 9:45 HSZ 201

Single 20-meV boson mode in KFe_2As_2 as seen by point-contact spectroscopy — Y. Naidyuk[1], O.E. Kvitnitskaya[1], N.V. Gamayunova[1], L. Boeri[2], S. Aswartham[3], G. Fuchs[3], S. Wurmehl[3], •D.V. Efremov[3], and S.-L. Drechsler[3] — [1]B. Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, 61103, Kharkiv, Ukraine — [2]Technische Universität Graz, 5150 Institut für Theoretische Physik-Computational Physics, 8010 Graz, Austria — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e.V.,P.O. Box 270116, D-01171 Dresden, Germany

We investigate the electron-boson interaction in KFe_2As_2 by point-contact spectroscopy. The point-contact spectrum or the derivative of the differential resistance dR/dV exhibits a pronounced maximum at about 20 meV and surprisingly a featureless behavior at lower and higher energies in our point-contact spectra. We discuss phonon and nonphonon (excitonic) mechanisms for the origin of this peak, which may be important for the understanding of serious puzzles of superconductivity in this type of compounds.

TT 53.3 Wed 10:00 HSZ 201

Superconducting specific heat jump $\Delta C \propto T_c^{\beta}$ ($\beta \sim 2$) and gapless Fermi surfaces in $K_{1-x}Na_xFe_2As_2$ — •V. Grinenko[1], D.V. Efremov[1], S.-L. Drechsler[1], S. Aswartham[1], D. Gruner[1], M. Roslova[1], I. Morozov[1], K. Nenkov[1], S. Wurmehl[1,2], A.U.B. Wolter[1], B. Holzapfel[1,3], and B. Büchner[1,2] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, D-01171 Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

We present a systematic study of the electronic specific heat jump ($\Delta C_{\rm el}$) at the superconducting transition temperature T_c of $K_{1-x}Na_xFe_2As_2$. Both T_c and $\Delta C_{\rm el}$ monotonously decrease with increasing x. The jump scales approximately with a novel power-law: $\Delta C_{\rm el} \propto T_c^{\beta}$ with $\beta \approx 2$ determined by the impurity scattering rate. This finding is in sharp contrast to most of all iron-pnictide superconductors with a cubic Bud'ko-Ni-Canfield (BNC) scaling. Our observations, also, suggests that disorder diminishes the small gaps leading to partial gapless superconductivity which results in a large residual Sommerfeld coefficient in the superconducting state for $x > 0$. Both T-dependence of $C_{\rm el}(T)$ in the superconducting state and the nearly quadratic scaling of $\Delta C_{\rm el}$ at T_c are well described by the Eliashberg-theory for a single-band d-wave superconductor with weak pair-breaking due to nonmagnetic impurities having reduced the density of superconducting quasi-particles.

TT 53.4 Wed 10:15 HSZ 201

Coupled order parameters in $Ca_{1-x}Na_xFe_2As_2$ — •Philipp Materne[1], Sirko Bubel[1], Hemke Maeter[1], Rajib Sarkar[1], Johannes Spehling[1], Luminita Harnagea[2], Sabine Wurmehl[2,1], Bernd Buechner[2,1], Hubertus Luetkens[3], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]IFW Dresden, Postfach 270016, 01171 Dresden, Germany — [3]Paul-Scherrer-Institut, 5232 Villigen, Switzerland

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 in terms of order parameter interaction in the coexistence region as well as electronic properties in the pure magnetic and superconducting parts of the phase diagram. The results were compared with recently published data of $Ba_{1-x}Na_xFe_2As_2$ [1].

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

TT 53.5 Wed 10:30 HSZ 201

Specific heat of $Ca_{0.32}Na_{0.68}Fe_2As_2$ single crystals: unconventional $s_{\pm}$ multi-band superconductivity with intermediate repulsive interband coupling and sizable attractive intraband couplings — •S.-L. Drechsler[1], S. Johnston[1], H. Rosner[2], M. Abdel-Hafiez[1], V. Grinenko[1], L. Harnagea[1], Y. Krupskaya[1], D. Bombor[1], S. Wurmehl[1], C. Hess[1], A. Wolter[1], and B. Buechner[1] — [1]IFW-Dresden, Germany — [2]MPI CPfS-Dresden, Germany

We report a low-temperature specific heat study of single crystals of the heavily hole doped superconductor $Ca_{0.32}Na_{0.68}Fe_2As_2$. This compound exhibits bulk superconductivity with a transition temperature $T_c \approx 34$ K, which is evident from the magnetization, transport, and specific heat measurements. The zero field data manifests a significant electronic specific heat in the normal state with a Sommerfeld coefficient γ ≈53 mJ/mol K^2. Using a multi-band Eliashberg analysis, we demonstrate that the dependence of the zero field specific heat in the superconducting state is well described by a three-band model with an unconventional $s_{\pm}$ pairing symmetry and gap magnitudes Δ_i of about 2.35, 7.48, and -7.50 meV. Our analysis indicates a non-negligible attractive intraband coupling,which contributes significantly to the relatively high value of T_c. The Fermi surface averaged repulsive and attractive coupling strengths are of comparable size and outside the strong coupling limit frequently adopted for describing high-T_c iron pnictide superconductors. We further infer a total mass renormalization of the order of five, including the effects of correlations and electron-boson interactions.

TT 53.6 Wed 10:45 HSZ 201

ARPES of iron-based superconductors: from low- to high-energy edge of 3d band — •Daniil Evtushinsky, Volodymyr Zabolotnyy, Janek Maletz, Bernd Büchner, and Sergei Borisenko — Institute for Solid State Research, IFW Dresden, P. O. Box 270116, D-01171 Dresden, Germany

An overview of the available angle-resolved photoemission spectroscopy (ARPES) measurements of iron-based superconductors will be given. Large variety of Fermi surface shapes and topologies as well as superconducting gap momentum distributions was observed. At the same time one can point out several common tendencies for iron high temperature superconductors - band renormalization, often a two-gap behavior, presence of an electronic coupling to the low-energy bosonic modes. A correlation between the superconducting gap magnitude and orbital origin of the electronic states was found; further analysis of the electronic structures of different iron arsenides consistently points to the significance of $3d_{xy,yz}$ bands for superconductivity in these materials. The recently revealed high-energy anomalies in the electronic spectra of iron superconductors are very reminiscent of the corresponding structures for cuprates. This implies that physical processes with energy scales of the whole 3d band might be important for the emergence of superconductivity with highest transition temperatures.

TT 53.7 Wed 11:00 HSZ 201

Electronic structure and quantum criticality in $Ba(Fe_{1-x-y}Co_xMn_y)_2As_2$, an ARPES study. — •J. Fink[1], E.D.L. Rienks[2], T. Wolf[3], K. Koepernik[1], I. Avigo[4], P. Hlawenka[2], C. Lupulescu[5], T. Arion[6], F. Roth[7], W. Eberhardt[7], and U. Bovensiepen[4] — [1]Leibniz-Institute for Solid State and Materials Research, Dresden, Germany — [2]Helmholtz-Zentrum, Berlin, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]Universität Duisburg-Essen, Duisburg, Germany — [5]Technische Universität Berlin, Berlin, Germany — [6]Universität Hamburg, Hamburg, Germany — [7]Center for Free-Electron Laser Science, Hamburg, Germany

We used angle-resolved photoemission spectroscopy (ARPES) and density functional theory calculations to study the electronic structure of $Ba(Fe_{1-x-y}Co_xMn_y)_2As_2$ for x=0.06 and $0 \leq y \leq 0.07$. From ARPES we derive that the substitution of Fe by Mn does not lead to hole doping, indicating a localization of the induced holes. An evaluation of the measured spectral function does not indicate a diverging effective mass or scattering rate near optimal doping. Thus the present ARPES results indicate a continuous evolution of the quasiparticle interaction and therefore question previous quantum critical scenarios.

15 min. break.

TT 53.8 Wed 11:30 HSZ 201

Spin Fluctuations in doped Ba122 probed by NMR Spin Lattice Relaxation Rate — •Uwe Gräfe[1], Hannes Kühne[2,3], Saicharan Aswartham[1], Philip Kuhns[2], Arneil Reyes[2], Sabine Wurmehl[1,4], Bernd Büchner[1,4], and Hans-Joachim Grafe[1] — [1]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany — [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden High Magnetic Field Laboratory, P.O. Box 510119, D-01314 Dresden, Germany — [4]TU-Dresden, Institute for Solid State Physics, D-01062 Dresden, Germany

In this talk we take a closer look on Co doped Ba122 by the local probe technique of NMR. Like many other iron pnictides Co doped Ba122 shows an increased spin lattice relaxation rate (SLR) above the superconducting transition temperature which hints at enhanced antiferromagnetic spin fluctuations (SF). These fluctuations are debated to play a crucial role for the pairing mechanism of superconductivity (SC). However, evidence for progressive slowing of SF in F doped La1111 (PRB 88, 104503) as well as evidence for cluster spin glass behavior in underdoped Ba122 (PRL 111, 207201) points at a competition of SC and antiferromagnetic order. We investigated the field dependence of the SLR in optimally Co doped Ba122 in detail to gain insights into the nature of spin fluctuations and their relevance for SC.

TT 53.9 Wed 11:45 HSZ 201

Effects of transition metal doping on the electronic structure of $BaFe_2As_2$ — •Jan Trinckauf[1], Klaus Koepernik[1], Sai Aswartham[1], Vladimir Strocov[2], Sabine Wurmehl[1], Bernd Büchner[1], and Jochen Geck[1] — [1]IFW Dresden, Germany — [2]Paul-Scherrer Institute, Villigen, Switzerland

We have performed resonant soft X-ray ARPES measurements on Co and Ni doped $BaFe_2As_2$ on the $L_{2,3}$ absorption edge of the dopant. We find that the 3*d* contribution of the TM dopant is shifted towards higher binding energies compared to the Fe bands and this shift increases with increasing atomic number. No considerable dispersion can be detected in the resonance features. We compared our data to DFT supercell calculations and see a similar trend in the 3*d* bandweights and the local DOS of the dopant. Most importantly, we observe in the calculations a shift of the Fermi level by the amount expected from the additional electrons on the TM sites, while simultaneously the total Fe 3*d* DOS stays constant. The additional electrons are counted solely towards the dopant. Referring to a model of local scatterers in a one-dimensional metallic chain and a two dimensional square lattice, we find that, while the electronic structure of the model as a function of the impurity potential behaves similar to what is observed in $BaFe_2As_2$, the effective doping behaves very different. This suggests that the almost rigid band like shift of the chimcal potential with doping, even in case of Cu, that is observed both theoretically and experimentally is a peculiarity of the compound, which has strong implications for the developement of superconductivity.

TT 53.10 Wed 12:00 HSZ 201

Analysis of the sub-dominant *d*-wave pairing channel in iron-based superconductors — •Thomas Böhm[1], Florian Kretzschmar[1], Rudi Hackl[1], Thomas P. Devereaux[2], and Alexander F. Kemper[3] — [1]Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, 85748 Garching, Germany — [2]SLAC National Accelerator Laboratory, Stanford Institute for Materials and Energy Sciences, 2575 Sand Hill Road, Menlo Park, California 94025, USA — [3]Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA

An analysis of the light scattering spectra of optimally doped $Ba_{0.6}K_{0.4}Fe_2As_2$ is presented. On the basis of a realistic band structure as derived from LDA calculations it is shown that the narrow feature found experimentally in the B_{1g} ($d_{x^2-y^2}$) Raman spectra can be reproduced quantitatively and be identified as a Bardasis-Schrieffer exciton. The theoretical description of the spectra shows that the coupling strength in the subdominant $d_{x^2-y^2}$ channel is as strong as 60% of that of the dominant s_{+-} channel.

TT 53.11 Wed 12:15 HSZ 201

Raman study of SDW order and band-folding in twin-free $BaFe_2As_2$ — •Florian Kretzschmar[1], Thomas Böhm[1], Bernhard Muschler[1], Andreas Baum[1], Rudi Hackl[1], Alexander F. Kemper[2,3], Thomas P. Devereaux[3,4], James G. Analytis[5], Jiun-Haw Chu[5,6], and Ian R. Fisher[3,4] — [1]Walther Meissner Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — [3]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [4]Geballe Laboratory for Advanced Materials, Stanford University, Stanford, California 94305, USA — [5]Department of Physics, University of California, Berkeley, California 94720, USA — [6]Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

We present results of electronic Raman scattering experiments on detwinned $BaFe_2As_2$ above and below the transition into the spin-density-wave (SDW) state. We observe signatures of the SDW gap in all symmetries. The spectra indicate a strong mixing of the bands due to backfolding along the SDW vector. For analysis we calculated the Raman susceptibility on the basis of a 5 band tight binding model using the effective mass approximation. Prominent features in the Raman response can be traced back to a few interband transitions.

TT 53.12 Wed 12:30 HSZ 201

Tracing the $s_{\pm}$ symmetry in iron pnictides — •Micha Schilling[1], Sina Zapf[1], Boris Gorshunov[1,2,3], Andreas Baumgartner[1], Kazumasa Iida[4], Valery A. Dravin[5], Kirill V. Mitsen[5], Dimitri Efremov[6], Oleg Dolgov[7], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Institute of General Physics, RAS, Russia — [3]Moscow Institute of Physics and Technology, Russia — [4]Institut für Metallische Werkstoffe, IFW Dresden, Germany — [5]Lebedev Physical Institute, Moscow, 119991 Russia — [6]Institute for theoretical physics, IFW, Dresden — [7]Max-Planck Institut für Festkörperforschung, Stuttgart, Germany

For multiband iron pnictides, the symmetry of the superconducting order parameter is still under debate. It was suggested [1] that in the case of $s_{\pm}$ symmetry, a disorder-induced crossover from $s_{\pm}$ to s_{++} symmetry could occur, meaning that the smaller superconducting gap Δ_1 first closes and then reopens. To that end, we have step-wise ir-

radiated a $Ba(Fe_{0.9}Co_{0.1})_2As_2$ thin film with protons and measured its complex conductivity in the terahertz frequency range. Our preliminary results show that the irradiation with protons is capable to linearly decrease the critical temperature of the film, while Δ_1 gets suppressed faster. Thus, further irradiation might reveal the reopening of Δ_1 and thus proof the $s_\pm$ symmetry of the superconducting order parameter.

[1] D.V. Efremov *et al.*, Phys. Rev. B **84**, 180512 (2011)
[2] B. Gorshunov *et al.*, Phys. Rev. B **81**, 060509 (2010)

TT 53.13 Wed 12:45 HSZ 201

Measuring detwinned $EuFe_2As_2$ without external pressure — •Jannis Maiwald[1], Christian Stingl[1], Sina Zapf[2], Shuai Jiang[2], Nora Bach[1], Kirk Post[3], Hirale S. Jeevan[1], David Neubauer[2], Anja Löhle[2], Conrad Clauss[2], Dimitri Basov[3], Martin Dressel[2], and Philipp Gegenwart[1] — [1]I.Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]1.Physikalisches Institut, Universität Stuttgart, Germany — [3]Department of Physics, UC San Diego, USA

The formation of twin domains in the low temperature state of high-temperature superconductors is impeding the investigation of the in-plane anisotropy of these materials. Due to the applied pressure, mechanical clamps—commonly used to detwin crystals—induce artificial anisotropy and thus complicate the interpretation of acquired data. In case of the iron pnicides, application of typical laboratory magnetic fields did not lead to a substantial detwinning. In this talk we present a novel way to detwin $EuFe_2As_2$ by brief application of a small magnetic field of ~ 1 Tesla. We will discuss magnetoresistance, magnetostriction/themal expansion and thermopower measurements, revealing that the Eu^{2+} moments support the detwinning not only below, but also above their magnetic ordering at 19K. After removing the field the system remains detwinned up to the structural and electronic phase transition at 190 K, providing a unique possibility to study the in-plane anisotropic properties of this material without the application of any external force.

TT 53.14 Wed 13:00 HSZ 201

Permanent Detwinning of $EuFe_2As_2$ by indirect magnetoelastic coupling — •Sina Zapf[1], Christian Stingl[2], Kirk Post[3], Jannis Maiwald[2], Shuai Jiang[1], Hirale S. Jeevan[2], Nora Bach[2], David Neubauer[1], Anja Löhle[1], Conrad Clauss[1], Dimitri N. Basov[3], Philipp Gegenwart[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Uni Stuttgart, Germany — [2]I. Physikalisches Institut, Uni Göttingen, Göttingen — [3]Department of Physics, UC San Diego, USA

In order to examine the in-plane anisotropy of high-temperature superconductors, sophisticated methods had to be developed for detwinning single crystals. Unfortunately, in the case of iron pnictides, typical laboratory magnetic fields do not yield an imbalance of twin domains by more than a few percent. Here we present a novel way of permanently detwinning $EuFe_2As_2$ single cystals in magnetic fields of less than 1 Tesla. We will discuss magneto-optical and magnetization measurements, revealing that the Eu^{2+} moments actually support the detwinning not only below, but also above their magnetic ordering at 19 K, probably by an indirect magnetoelastic coupling via the Fe^{2+} spins. Most strikingly, the detwinning remains even when the magnetic field is switched off and the resulting ratio of unbalanced twin domains of about 1:3 is robust against heating to the structural and electronic phase transition at 190 K. This provides a unique possibility to study the low temperature in-plane anisotropy of iron pnictides without the application of any external force, suitable for a wide variety of experimental techniques.

TT 54: Correlated Electrons: Heavy Fermions

Time: Wednesday 9:30–11:00 Location: HSZ 204

TT 54.1 Wed 9:30 HSZ 204

Charge fluctuations in SmB_6 — •Chul-hee Min[1,2], Peter Lutz[1,2], Sebastian Fiedler[1,2], Boyoun Kang[3], Beongki Cho[3], Hyung-do Kim[4], Hendrik Bentmann[1,2], and Friedrich Reinert[1,2] — [1]Universität Würzburg, Experimentelle Physik VII & Röntgen Research Center for Complex Material Systems, 97074 Würzburg, Germany. — [2]Karlsruhe Institut für Technologie, Gemeinschaftslabor für Nanoanalytik, 76021 Karlsruhe, Germany. — [3]School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Gwangju 500-712, Korea. — [4]Department of Physics and Astronomy, Center for Correlated Electron Systems, Institute for Basic Science, Seoul National University, Seoul 151-747, Republic of Korea.

Kondo insulators can have nontrivial Z_2 topology because their energy gap opens at the Fermi energy (E_F) by the hybridization between an odd parity- renormalized f band and an even parity- conduction d band. Samarium hexaboride (SmB_6) is a promising candidate for the realization of such a correlated topological insulator. Here, we present the electronic structure of SmB_6 by angle-resolved photoemission spectroscopy. Our spectra reveal that the bottom of the odd parity- d-f hybridized band at the X point gradually shifts from below to above E_F with decreasing temperature. Moreover, by comparison with theoretical calculations, the signatures of nontrivial surface states are observed. Our results indicate that charge fluctuations play a major role during the gap evolution, and can be important in determining its Z_2 topological indices.

TT 54.2 Wed 9:45 HSZ 204

Intense ferromagnetic fluctuations in the heavy-fermion antiferromagnet CeB_6 — •D. Inosov[1,2], H. Jang[2], G. Friemel[2], J. Ollivier[4], A. V. Dukhnenko[3], N. Yu. Shitsevalova[3], V. B. Filipov[3], and B. Keimer[2] — [1]Inst. für Festkörperphysik, TU Dresden, Germany. — [2]MPI für Festkörperforschung, Stuttgart, Germany. — [3]Inst. for Problems of Material Sciences, Kiev, Ukraine. — [4]Inst. Laue-Langevin, Grenoble, France.

Heavy-fermion metals exhibit a plethora of low-temperature ordering phenomena, among them the so-called hidden-order phases that in contrast to conventional magnetic order are invisible to standard neutron diffraction. One of the oldest and structurally simplest hidden-order compounds, CeB_6, is famous for an elusive phase attributed to the antiferroquadrupolar ordering of Ce 4f moments. In its ground state, CeB_6 also develops a more usual antiferromagnetic (AFM) order. Hence, its essential low-temperature physics was always considered to be governed by AFM interactions between the dipolar and multipolar Ce moments. Our recent inelastic neutron scattering experiments overturned this established perspective by uncovering an intense ferromagnetic (FM) low-energy collective mode that dominates the magnetic excitation spectrum of CeB_6, thus placing CeB_6 much closer to a FM instability than could be anticipated. This propensity of CeB_6 to ferromagnetism may account for much of its unexplained behavior, such as the existence of a pronounced electron spin resonance, and should lead to a substantial revision of existing theories that have so far largely neglected the role of FM interactions.

TT 54.3 Wed 10:00 HSZ 204

Surface Properties of Rare Earth Hexaborides Studied by X-Ray Spectroscopy — •Nadine Heming[1], Uwe Treske[1], Dmytro S. Inosov[2,3], Martin Knupfer[1], Bernd Büchner[1], Natalya Yu. Shitsevalova[4], Volodymyr B. Filipov[4], Emile Rienks[5], and Andreas Koitzsch[1] — [1]IFW Dresden — [2]TU Dresden — [3]MPI Stuttgart — [4]Frantsevich Inst. Kiev — [5]HZB, Berlin

Rare earth hexaborides (RB_6) are a group of materials that have unique crystal structures but a striking variety of physical properties. SmB_6, for example, is a mixed valence heavy fermion compound and well known for its anomalous low temperature resistivity behavior. Transport experiments have evidenced, that its unusual residual conductivity occurs only at the surface, making this compound the prime candidate for the proposed new material class of "Topological Kondo Insulators". However, it is known for decades that the surface undergoes valence changes and reconstructions, which may influence the properties of the material and could even form the basis of alternative scenarios. Here we use x-ray spectroscopy (XPS, XAS) to explicitly study surface properties of SmB_6 and CeB_6. The heavy fermion compound CeB_6 is known for many years for its unusual magnetic properties at low temperatures, in particular the elusive antiferroquadrupolar ordering at $T_Q = 3.2$ K. To study its electronic structure surface sensitive techniques such as ARPES and STM are in order, which benefit from deeper knowledge of the surface properties as well.

TT 54.4 Wed 10:15 HSZ 204

Magnetic phases in the heavy-fermion system $Yb(Rh_{1-x}Co_x)_2Si_2$ — •A. Hannaske[1], O. Stockert[1], C. Klingner[1], N. Mufti[1], C. Krellner[2], A. Hoser[3], J.-U. Hoffmann[3], S. Matas[3], S. Capelli[4], M.-H. Lemee-Cailleau[4], K. Kaneko[5], 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 — [5]Japan Atomic Energy Agency, Tokai, Japan

One route to get insight into the unusual magnetic properties of quantum critical $YbRh_2Si_2$ is to study magnetism in the alloying series $Yb(Rh_{1-x}Co_x)_2Si_2$. Isoelectronic doping of Co on the Rh site leads to a stabilization of the magnetic order. The magnetic phases in $Yb(Rh_{1-x}Co_x)_2Si_2$ have been investigated in detail by thermodynamic measurements and neutron scattering. In pure $YbCo_2Si_2$ the occurrence of antiferromagnetic domains plays an important role in understanding the magnetic $B-T$ phase diagram. While for $Yb(Rh_{1-x}Co_x)_2Si_2$ with high Co content our measurements clearly reveal an incommensurate magnetically ordered phase below T_N followed by a commensurate phase at low T, the magnetic order drastically changes below about $x \approx 0.58$ where surprisingly ferromagnetic behavior was observed. We will discuss this finding and its impact on the quantum criticality in $YbRh_2Si_2$.

TT 54.5 Wed 10:30 HSZ 204

Valence determination in CeMIn$_5$ (M=Co, Rh, and Ir) and CeT_2Al$_{10}$ (T=Fe, Rh, and Os) using HAXPES — •M. Sundermann[1], F. Strigari[1], M.W. Haverkort[2], Y. Muro[3], T. Takabatake[3], E.D. Bauer[4], J.D. Thompson[4], Y.F. Liao[5], K.-D. Tsuei[5], L.H. Tjeng[2], and A. Severing[1] — [1]University of Cologne, Institute of Physics II, 50937 Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Department of Quantum Matter, AdSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan — [4]Los Alamos National Laboratory, Los Alamos, New Mexico, USA — [5]National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan

The hybridization of $4f$ electrons and the conduction band (cf-hybridization) is an important ingredient for the versatile physics of Ce compounds. In the CeMIn$_5$ superconductivity appears in the vicinity of a quantum critical point where the $4f$ moments are magnetically ordered on one side and more itinerant due to the stronger cf-hybridization on the other. In the antiferromagnetic Ce Kondo semiconductors CeT_2Al$_{10}$ the ordered moments are *not* aligned along the easy axis and they have unusually high ordering temperatures. There are speculations that the cf-hybridization has an impact on the magnetic ordering. — We performed the bulk sensitive hard x-ray photoemission spectroscopy (HAXPES) for CeMIn$_5$ and CeT_2Al$_{10}$ and obtained the occupancy of the $4f$ states and important parameters like the cf hybridization by analyzing the data within an Anderson impurity Ansatz which contains the full multiplet theory.

TT 54.6 Wed 10:45 HSZ 204

XMCD-Signatures of Kondo and Heavy Fermion Behaviour in the Surface Intermetallic $CePt_5$/Pt(111) — Christian Praetorius, •Martin Zinner, and Kai Fauth — Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg

In this contribution, we explore the detection of magnetic signatures of Kondo and heavy fermion physics by x-ray spectroscopy and study the anisotropic paramagnetic Ce-$4f$ response in $CePt_5$, prepared on Pt(111). Qualitatively, the magnetic behaviour above $T \gtrsim 20$ K is readily understood in terms of a hexagonal crystal field (CF), acting on weakly interacting, considerably screened Ce-$4f$ moments. A quantitative description necessitates distinct CF parameters for 'inner' and 'surface' atomic layers. This approach is strongly supported by complementary structural information (LEED-IV). Treating both CF and Kondo physics within a simplified NCA approach [1] proved unsuccessful and we therefore resort to a more ad-hoc kind of Hamiltonian.

The paramagnetic response displays an anomaly ($T^* \approx 18$ K), which we shall discuss as signalling the transition towards the coherent heavy fermion state . Well below T^* we find Ce $4f$ saturation moments much smaller than the free ion values. Their occurrence, too, can be understood to be characteristic of the coherent state and associated with a Lifshitz transition as predicted theoretically [2]. X-ray spectroscopy thus proves valuable for investigating strongly correlated electron systems in case sufficiently well-defined surfaces can be obtained.

[1] G. Zwicknagl, V. Zevin und P. Fulde, *Z. Phys. B* **79**, 365 (1990)
[2] K. S. D. Beach and F. F. Assaad, *Phys. Rev. B* **77**, 205123 (2008)

TT 55: Correlated Electrons: Quantum-Critical Phenomena - Experiment II

Time: Wednesday 11:15–12:30 Location: HSZ 204

TT 55.1 Wed 11:15 HSZ 204

Electronic structure investigations in β-$LuAlB_4$ — •Pascal Reiss[1], Sven Friedemann[1], Michael Sutherland[1], Swee K. Goh[2], Kentaro Kuga[3], Eoin O'Farrell[3], Hisatomo Harima[4], Satoru Nakatsuji[3], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, CB3 0HE, United Kingdom — [2]Chinese University of Hong Kong, Shatin, N.T., Hong Kong — [3]Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan — [4]Kobe University, Kobe 657-8501, Japan

The β-phase of $YbAlB_4$ is the first Yb based heavy fermion compound which features both superconductivity and quantum critical behaviour without the need of tuning by magnetic field, pressure or doping [1]. Quantum oscillation (QO) measurements can help decide whether at low temperature the relevant 4f states in $YbAlB_4$ form a band and contribute to the Fermi surface, or whether they should be regarded as localised [2]. Here, we use β-$LuAlB_4$ as a reference compound: both compounds have the same crystal structure, and Lu features a full 4f shell, which prevents the f-states from contributing to the Fermi surface volume. We present QO measurements on β-$LuAlB_4$ and compare them to detailed calculations based on LDA-DFT. Whereas our calculations agree in detail with the observed frequencies and their angular dependence in β-$LuAlB_4$, they differ significantly from the QO spectra observed in β-$YbAlB_4$. These findings strongly suggest itinerant 4f electron character in $YbAlB_4$ further supporting the conclusions reported in [2].

[1] S. Nakatsuji et al, Nature Phys. **4**, 603 (2008)
[2] E.C.T. O'Farrell et al, PRL 102, 216402 (2009)

TT 55.2 Wed 11:30 HSZ 204

Spin dynamics in the Haldane compound $SrNi_2V_2O_8$ — Vladimir Gnezdilov[1,2], •Peter Lemmens[1], Anup Kumar Bera[3], ATM Nazmul Islam[3] und Bella Lake[3] — [1]TU-BS, Braunschweig — [2]ILTPE NAS, Ukraine — [3]HZBME, Helmholtz-Zentrum, Berlin

We present a Raman scattering study of the quasi-one-dimensional Haldane chain compound $SrNi_2V_2O_8$. In contrast to simple expectations, complex temperature-dependent magnetic excitations exist. Our observations provide strong evidence that $SrNi_2V_2O_8$ is indeed close to the phase boundary that separates a spin-liquid and an Ising-like ordered state on the Sakai-Takahashi phase diagram.

TT 55.3 Wed 11:45 HSZ 204

Anisotropy and quantum criticality in $CeTi_{1-x}V_xGe_3$ single crystals — •Wolfram Kittler[1], Veronika Fritsch[1], Paul C. Canfield[2], and Hilbert v. Löhneysen[1] — [1]Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Ames Laboratory, US DOE, and Dept. of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA

$CeTiGe_3$ is a heavy-fermion ferromagnet with the Curie-temperature $T_C \approx 14$ K [1]. It crystallizes in a hexagonal structure with space group P63/mmc. The magnetic moments are located at the Ce sites pointing along the c-axis [2]. Partial substitution of Ti by V leads to a suppression of T_C toward zero. Thus $CeTi_{1-x}V_xGe_3$ seems to be one of the few ferromagnetic systems that can be driven to a quantum critical point at a critical V concentration $x_c \approx 0.38$.
We will present detailed measurements of magnetization, electrical resistivity and specific heat on flux-grown single crystals showing the highly anisotropic Ising-like magnetism in this system. Furthermore we will demonstrate signatures of non-Fermi-liquid behavior when approaching the critical concentration.

[1] P. Manfrinetti et al., Sol. State Comm. **135** (2005) 444

[2] W. Kittler et al., Phys. Rev. B **88** (2013) 165123

TT 55.4 Wed 12:00 HSZ 204

Binary Cr-Ge systems close to a magnetic quantum critical point — •Katharina Weber, Marcus Peter Schmidt, Walter Schnelle, Michael Baenitz, Helge Rosner, and Christoph Geibel — Max Planck Institute for Chemical Physics of Solids, Dresden

Systems close to the transition between a magnetic-ordered (MO) and a paramagnetic (PM) ground state are of strong interest, because some very peculiar phenomena, like unconventional superconductivity, quantum critical points, and non-Fermi liquids haven been observed in connection with such transitions. While quite a lot of research has been devoted to compounds based on late transition metals, as Fe or Cu, only limited work has been published on Cr-based systems. Here we present a deeper investigation of CrGe and $Cr_{11}Ge_8$. Previous studies indicate both compounds to be close to a magnetic instability, but information on physical properties were limited. CrGe single crystals were grown by vapor phase transport, while polycrystalline $Cr_{11}Ge_8$ was prepared by arc melting and subsequent annealing. Physical properties were studied by means of susceptibility χ(T), resistivity, and specific heat measurements. Both compounds show a Curie-Weiss behavior at high temperatures, with sizeable effective moments of about $2\mu_B$/Cr. CrGe presents a broad, but clear maximum in χ(T) at about 60 K, while in $Cr_{11}Ge_8$ χ(T) increases continuously down to low T. This suggest both compounds to be in the PM regime, $Cr_{11}Ge_8$ being extremely close to the transition to a MO state, while CrGe is slightly further away. The Sommerfeld coefficients are quite large for 3d systems, of the order of 20 mJ/K^2 mol-Cr, supporting strong correlations.

TT 55.5 Wed 12:15 HSZ 204

Thermoelectric properties at a Quantum Phase Transition in $Mn_{1-x}Fe_xSi$ — Marlies Gangl[1], •Anna Kusmartseva[1,2], Marco Halder[1], Andreas Bauer[1], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik Department E21, Garching, Germany — [2]Loughborough University, Physics Department, Loughborough, UK

MnSi is a B20 transition metal compound that has been traditionally a model system to study helical modulation in magnetism and weak itinerant ferromagnetism. In particular, the behaviour to different transition metal doping with Fe, Co as well as studies under pressure had been of vast interest to the research community.

Here we present resistivity, thermopower and thermal conductivity on high-quality Fe-doped single crystals of MnSi over a wide range in temperatures from 2 to 300K under magnetic fields up to 14T. The growth and purity of the single crystals $Mn_{1-x}Fe_xSi$ was investigated previously in detail [1]. We report the appearance of Non-Fermi Liquid behaviour in the resistivity of doped Mn1-xFexSi samples and discuss how these results relate to the respective measurements of thermopower and thermal conductivity. Comparisons and parallels to studies reported under pressure are also made [2,3].

[1] A. Bauer, A. Neubauer, C. Franz, W. Muenzer, M. Garst, and C. Pfleiderer, Phys. Rev. B, 82, 57011 (2010)
[2] J.-G. Cheng, F. Zhou, J.-S. Zhou, and J.B. Goodenough, Phys. Rev. B, 82, 214402 (2010)
[3] S. Arsenjevic, C. Petrovic, L. Forro, and A. Akrap, Euro. Phys. Lett., 103, 57015 (2013)

TT 56: Focus Session: Electronic Properties of Spin-Orbit Driven Oxides

Relativistic correlated materials such as iridates present a substantial challenge to theory and experiments since several relevant energy scales converge to the level of 0.5–1 eV: one-electron hopping t, spin-orbit coupling λ, onsite Coulomb repulsion U, and Hund's rule magnetic coupling J. This is often accompanied by nontrivial geometries, such as honeycomb, pyrochlore or triangular lattice structures. Many phenomena, intuitively understood in the non-relativistic $3d$ transition metal oxides or weakly relativistic $4d$ systems, become highly nontrivial and challenging in $5d$ materials. This Focus Session will review recent progress made in this internationally active field of research.

Organizers: Roser Valenti (Uni Frankfurt), Jeroen van den Brink (IfW Dresden)

Time: Wednesday 9:30–12:15 Location: HSZ 03

Invited Talk TT 56.1 Wed 9:30 HSZ 03

Exotic Magnetism of J_{eff}=1/2 Iso-Spins in Complex Ir Oxides — •Hidenori Takagi — Department of Physics, University of Tokyo, Tokyo, Japan — Max Planck Institute for Solid State Research, Stuttgart, Germany

In 5d Iridium oxides, a large spin-orbit coupling of 0.5 eV, inherent to heavy 5d elements, is not small as compared with other relevant electronic parameters including Coulomb U, transfer t and crystal field splitting D, which gives rise to a variety of exotic magnetic ground states. In the layered perovskite Sr_2IrO_4, spin-orbital Mott state with J_{eff}=1/2 is realized due to the novel interplay of those energy scales [1, 2]. Despite the strong entanglement of spin and orbital degrees of freedom, surprisingly isotropic, two-dimensional Heisenberg character of J_{eff}=1/2 iso-spins was observed in Sr_2IrO_4 with 180 deg Ir-O-Ir bonds, by the recent resonant magnetic x-ray diffuse scattering and the magnetic susceptibility measurements [3]. Complex Na-Ir oxides with honeycomb and more recently identified hyper-honeycomb lattices, where 90 deg Ir-O-Ir bonds are realized, are candidates for Kitaev spin liquid. Such exotic magnetism was recently shown to be tailored using super-lattice structure [4]. In this talk, we review these phases of interest.

[1] B. J. Kim et al., Phys. Rev. Lett. 101, 076402 (2008)
[2] B. J. Kim et al., Science 323, 1329 (2009)
[3] S. Fujiyama et al. , Phys. Rev. Lett. 108, 247212 (2012)
[4] J. Matsuno et al., submitted.

Invited Talk TT 56.2 Wed 10:00 HSZ 03

Isospin Dynamics in Sr_2IrO_4 Revealed by Resonant Inelastic X-Ray Scattering — •Jungho Kim — Argonne National Lab, Argonne, IL, 60565 USA

Iridium oxides with strong relativistic spin-orbit coupling have received much attention due to intriguing sets of novel electronic and magnetic phases and phenomena, which were imagined for a long time but not realized in real world. Among many materials, Sr_2IrO_4 provides a model case for investigating essential aspects of the magnetic exchange interactions of the so-called J_{eff}=1/2 isospin states, which were established by various spectroscopic studies such as angle-resolved photoemission and magnetic x-ray scattering. In this talk, I will review on resonant inelastic x-ray scattering (RIXS) technique at the Ir absorption edges and novel aspects of iridium oxides with strong relativistic spin-orbit coupling. Low energy excitation spectra of Sr_2IrO_4 by RIXS will be discussed. The J_{eff}=1/2 isospin dynamics of Sr_2IrO_4 can be well described by the isotropic Heisenberg model, which renders the low-energy effective physics of Sr_2IrO_4 much akin to that in superconducting cuprates. Higher dd excitations between J_{eff}=1/2 and 3/2 are found to be dispersive in the same way as the single hole propagates in an antiferromagnetic background.

Topical Talk TT 56.3 Wed 10:30 HSZ 03

Honeycomb Lattice Iridates — •Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

Iridates, in particular those crystallizing in a honeycomb structure have recently created much interest due to the proposal of new topological states such as Kitaev-Heisenberg magnet with dynamic spin liquid phase or correlated topological (quantum spin Hall) states. Experimentally, both Na_2IrO_3 and Li_2IrO_3 are Mott insulators with antiferromagnetic ground states. We report single crystal structural, microscopic and magnetic experiments in combination with band-structure calculations for variously doped honeycomb iridates to explore the possibility of tuning these systems into topological states.

Work in collaboration with Soham Manni, Friedrich Freund, Yogesh Singh, Sungkyun Choi, R. Coldea, F. Luepke, M. Wenderoth, M. Altmeyer, H.O. Jeschke, I. Mazin and R. Valenti. Financial support through DFG SPP 1666 and the Helmholtz virtual institute 521 is acknowledged.

15 min. break.

Topical Talk TT 56.4 Wed 11:15 HSZ 03

Novel Magnetic States in Spin-Orbit Coupled Mott Insulators — •Giniyat Khaliullin — Max-Planck-Institut FKF, Stuttgart

In late transition metal compounds such as Ir, Rh, Os oxides, large spin-orbit coupling entangles the spin and orbital subspaces and may lead to unusual interactions and ground states. In this talk, after some basic introduction to spin-orbital physics, the following topics will be addressed: (i) Magnetic ordering and excitations in single layer Sr_2IrO_4 and bilayer $Sr_3Ir_2O_7$ iridium perovskites; (ii) Exchange interactions in a hexagonal lattice iridates, Kitaev-Heisenberg model, its phase diagram including spin-liquid states; (iii) Excitonic magnetism and spin-orbit driven magnetic QCP in Van Vleck-type d4 Mott insulators.

Topical Talk TT 56.5 Wed 11:45 HSZ 03

Electronic Structure of Honeycomb Iridates and Rhodates from a Density Functional Theory Perspective — •Harald O. Jeschke[1], I. I. Mazin[2], K. Foyevtsova[1], D. Khomskii[3], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Germany — [2]Naval Research Laboratory, Washington, USA — [3]II. Physikalisches Institut, Universität zu Köln, Germany

Taking a complementary point of view to previous studies that classify the hexagonal iridate Na_2IrO_3 as a realization of the Heisenberg-Kitaev model with dominant spin-orbit coupling, we show that this system represents a highly unusual case in which the electronic structure is dominated by the formation of quasi-molecular orbitals (QMOs), with substantial quenching of the orbital moments [1]. The QMOs consist of six atomic orbitals on an Ir hexagon, but each Ir atom belongs to three different QMOs. We discuss both limiting descriptions for Na_2IrO_3, the itinerant QMO limit valid at small SO coupling and the localized relativistic orbitals limit at large SO coupling and show that the description of Na_2IrO_3 lies in an intermediate regime [2]. We demonstrate that the electronic structure of Na_2IrO_3 is exceptionally sensitive to structural details and analyze role of the various structural distortions. We discuss the application of the QMO picture to Li_2RhO_3 [3].

[1] I. I. Mazin, H. O. Jeschke, K. Foyevtsova, R. Valenti, D. I. Khomskii, Phys. Rev. Lett. **109**, 197201 (2012)
[2] K. Foyevtsova, H. O. Jeschke, I. I. Mazin, D. I. Khomskii, R. Valenti, Phys. Rev. B **88**, 035107 (2013)
[3] I. I. Mazin *et al.*, Phys. Rev. B **88**, 035115 (2013)

TT 57: Transport: Molecular Electronics I

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

TT 57.1 Wed 9:30 HSZ 304

Electrical transport through ferrocene molecules using MCBJ — •Karthiga Kanthasamy, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik (ATMOS), Leibniz Universität Hannover

In order to understand the electrical behavior of molecules we fabricate a stable atomic gold contact by Mechanically Controllable Break Junction(MCBJ). We study the electrical transport through ferrocenedithiol (FDT) molecules because of its rotational flexibility with respect to two cyclopentadienyl(Cp) rings without activation threshold and high conductance.

The molecules are chemisorbed on the Au atomic contact, as confirmed by XPS characterization on Au thin film. After insertion of FDT molecules, measuring conductance versus contact distance at constant voltage 1 mV there are characteristic stepwise changes below 1 G_0 with a very pronounced plateau at 0.4 G_0. In the range 0.1 G_0 < conductance < 0.4 G_0, we measured IV-curves at room temperature and 80 K. Detailed analysis of IV-curves exhibit characteristic peak in the first derivative. The voltage at the maxima can be identified with the excitation of C-H bending, C-H stretching vibrational modes indicating resonantly enhanced conductance by vibrational excitation. The influence of different anchoring groups in the electronic transport will be shown.

TT 57.2 Wed 9:45 HSZ 304

Multi-orbital STM theory for π-conjugated molecules on thin insulating films — •Benjamin Siegert, Andrea Donarini, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg

We present a multi-orbital extension of our STM theory [1,2,3], based on the reduced density matrix formalism, which is capable of describing electronic transport through π-conjugated molecules on thin insulating films. In order to investigate spin-dependent transport effects using the example of a Cu-Phthalocyanine molecule, we set up an effective many-body Hamiltonian including exchange and spin-orbit interaction. The transport dynamics is calculated by evaluating a Generalized Master Equation including all diagonal and off-diagonal elements of the reduced density matrix of the molecule. Examples are shown of how many-body effects, like interference between degenerate many-body states, can affect the transport properties of π-conjugated molecules on thin insulating films in an STM setup.

[1] S. Sobczyk, A. Donarini, and M. Grifoni, PRB **85**, 205408 (2012).
[2] A. Donarini, B. Siegert, S. Sobczyk, and M. Grifoni, PRB **86**, 155451 (2012).
[3] B. Siegert, A. Donarini and M. Grifoni, pss (b) **250**, 2444 (2013)

TT 57.3 Wed 10:00 HSZ 304

Gate-controlled shift of CoPc orbitals on graphene in a STM junction — •Samuel Bouvron[1], Philipp Erler[1], Alexander Graf[1], Romain Maurand[2], Luca Gragnaniello[1], Dirk Wiedmann[1], Fabian Pauly[1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Department of Physics, University of Basel

One of the most promising aims of molecular electronics is the fabrication of a molecular transistor. Such a device necessarily requires a gate-electrode, which allows to set the molecule into a controllable electric field, therefore tuning the energy of the molecular orbitals relevant for charge transport. Moreover since the very first year of the development of the scanning tunneling microscope (STM), it has been proposed to use its extremely high lateral resolution to study molecules and record $I(V)$ or $I(z)$ characteristics of the tunnel contacts formed. However, the geometric constrains of the microscope make the implementation of a third gate-electrode challenging. Here we investigate the electronic properties of cobalt phthalocyanine (CoPc) molecules on graphene on SiO_2/Si, where graphene and Si serve as drain and gate electrode, respectively. We report on site-dependent and gate-dependent tunnel transport through the CoPc molecules. The influence of the gate voltage on the energy position of the molecular orbitals is discussed and the orbital structure is assigned. Finally this STM-tip/molecule/graphene/SiO_2/Si device geometry opens a possibility to combine the spatial resolution of the STM with the additional control of the electric field commonly used in transport measurements.

TT 57.4 Wed 10:15 HSZ 304

Laser pulse induced transient currents in a molecular junction — •Yaroslav Zelinskyy[1,2] and Volkhard May[1] — [1]Institut für Physik, Humboldt Universität zu Berlin — [2]Bogolubov Institute for Theoretical Physics, National Academy of Science of Ukraine

The investigation of transient phenomena in molecular junctions is of increasing interest. As an example, computations are presented on femtosecond laser pulse excitations and subsequent transient current formation. A single molecule sandwiched between two spherical leads is considered[1,2]. Optical excitation of the leads is accounted for by their collective plasmon excitations which may also couple to the molecular excitations. While this coupling may be strong the electron transfer coupling of the molecule to the leads is considered to be small to stay in the regime of sequential charge transmission. All the calculations of transient currents are performed in the framework of a

density matrix theory. As a quantity detectable in the experiment the averaged dc–current resulting from a huge sequence of laser pulses is also calculated . The obtained transient currents are confronted with those induced by voltage pulses[3].

[1] L. Wang and V. May, Phys.Chem.Chem.Phys. 13, 8755 (2011)
[2] Y. Zelinskyy and V. May, Nano Lett. 12, 446 (2012)
[3] Y. Zelinskyy and V. May, J. Chem. Phys. (submitted)

TT 57.5 Wed 10:30 HSZ 304

Theory of molecular junction electroluminescence: plasmon-enhancement and emission narrowing due to multiple molecules — •Yuan Zhang and Volkhard May — Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489, Germany

Photoemission of a molecular junction formed by up to five individual molecules and placed in the proximity of an Au nanosphere is studied theoretically. Charge transmission through the molecules at a finite applied voltage induces an electronic excitation while an energy transfer coupling to the nanosphere is responsible for plasmon excitation and enhancement effects. The consideration of several molecules and larger currents results in an increased electroluminescence intensity compared to earlier studies [1,2].The used density matrix description accounts for the entanglement of different molecular excitations due to their simultaneous coupling to the Au nanosphere. The obtained emission line narrowring with increasing number of molecules is related to the SPASER mechanism.

[1]Y. Zhang, Y. Zelinskyy, and V. May, J. Chem. C **116**, 25962 (2012)
[2]Y. Zhang, Y. Zelinskyy, and V. May, Phys. Rev. B **88**, 155426 (2013)

TT 57.6 Wed 10:45 HSZ 304

Polarization dependent, surface plasmon induced photoconductance in gold nanorod arrays — Sandra Diefenbach[1], •Lisa Kugler[1], Nadine Erhard[1], Johannes Schopka[1], Alfonso Martin[2], Christoph Karnetzky[1], Daniela Iacopino[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München — [2]Tyndall National Institute, University College Cork, Lee Maltings Complex, Dyke Parade, Cork, Ireland

We report on the photoconductance properties of two-dimensional arrays of gold nanorods which are formed by a combination of droplet deposition and stamping methods. The photoconductance of the nanorod arrays is strongly enhanced through the excitation of longitudinal surface plasmons. Hereby, the photoconductance is polarization dependent with a maximum signal for the electric field of the exciting photon being aligned with the longitudinal axis of the nanorods [1]. We interpret the observations by a plasmonically induced, bolometric enhancement of the conductance, but we also discuss a possible hot-electron emission induced by the plasmons.

We gratefully acknowledge support from the European (FP7) 263091 project HYSENS.

[1] S. Diefenbach et al., arXiv:1311.1002 (2013)

15 min. break.

Invited Talk TT 57.7 Wed 11:15 HSZ 304

Quantum Transport at Molecular Scales — •Ferdinand Evers — Karlsruhe Institute of Technology, Germany

The quantum transport on molecular scales is a wide and very complex research area. It connects to phenomena in experimental disciplines as diverse as the surface sciences, organic electronics, spintronics, catalysis, electrochemistry, strongly correlated systems and even the life sciences. An important motivation in the sub-discipline Molecular Electronics is to single out a single molecule and use it to investigate in detail aspects of the elementary charge transfer processes involved.

The first part of the presentation offers an overview about recent experimental and theoretical developments and new directions in Molecular Electronics. The second part will embark on effects of molecular magnetism. It will deal with the Kondo-effect in molecular adsorbates and explains, how a non-magnetic molecule (hydrogen-phtalocyanine) brings about a giant magnetoresistance.

TT 57.8 Wed 11:45 HSZ 304

Kondo-effect in binuclear metal-organic molecules — •Dimitra Xenioti[1,2], Alexej Bagrets[1], Richard Korytár[1], Lei Zhang[1,3], Frank Schramm[1], Mébarek Alouani[2], Mario Ruben[1,2], Wulf Wulfhekel[1,3], and Ferdinand Evers[1,4] — [1]Institute of Nanotechnology (INT), KIT, Karlsruhe, Germany — [2]Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), Strasbourg, France — [3]Physikalisches Institut (PI), KIT, Karlsruhe, Germany — [4]Institut für Theorie der Kondensierten Materie (TKM), Karlsruhe, Germany

Low-temperature STM measurements performed on a binuclear metal-organic molecule ($(Ni(hfacac)_2)_2(bpmd)$ ("Ni_2") deposited on a Cu surface reveal that the system undergoes a Kondo effect with $T_K \sim 10$K and a spin located nearby Ni atoms. The physics in play is intriguing, because the molecule does not have anchoring groups, which could be responsible for the formation of a chemical bond with the Cu surface. By comparing experimental data with simulated STM images, we have identified possible adsorption geometries. Our simulations show that some observed STM images and large T_K could be attributed to a distorted "Ni_2" complex, which is bound to Cu(001) via the bipyrimidine (bpmd) unit. Other images may be interpreted as arising from molecular fragmentation, suggesting a $Ni(hfacac)_2$ moiety to be seen in the experiment. In the latter case our analysis of the DFT+U (Kohn-Sham) spectral function show that the S=1 type Kondo effect arises mainly due to unpaired electrons populating d_{xy} and d_{z^2} orbitals of Ni^{2+} ion. In the case of "Ni_2", our calculations suggest that the Kondo effect originates from a pair of weakly coupled S=1 Ni^{2+} spins.

TT 57.9 Wed 12:00 HSZ 304

Heat dissipation and thermopower in atomic-scale junctions — •Fabian Pauly — Department of Physics, University of Konstanz, Germany

In this talk, I will present recent combined experimental and theoretical efforts to understand the heat dissipation in atomic-scale junctions [1,2]. Using custom-fabricated scanning probes with integrated nanoscale thermocouples, we find that if the junctions have transmission characteristics that are strongly energy dependent, this heat dissipation is asymmetric (that is, unequal between the electrodes) and also dependent on both the bias polarity and the identity of the majority charge carriers. In contrast, junctions consisting of only a few gold atoms, whose transmission characteristics show weak energy dependence, do not exhibit appreciable asymmetry. Our results unambiguously relate the electronic transmission characteristics of atomic-scale junctions to their heat dissipation properties, establishing a framework for understanding heat dissipation in a range of mesoscopic systems where transport is elastic.

[1] W. Lee, K. Kim, W. Jeong, L. A. Zotti, F. Pauly, J. C. Cuevas, and P. Reddy, Nature 498, 209 (2013).
[2] L. A. Zotti, M. Bürkle, F. Pauly, W. Lee, K. Kim, W. Jeong, Y. Asai, P. Reddy, and J. C. Cuevas, New J. Phys. (accepted); arXiv:1307.8336.

TT 57.10 Wed 12:15 HSZ 304

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], we consider substantially larger wires and explore different lattice orientations. In combination with experiments we recently provided evidence that one can build a fatigue-resistant two-terminal switch with the reversible rearrangement of single atoms[2].

[1] M. Dreher, F. Pauly, J. Heurich, J. C. Cuevas, E. Scheer, and P. Nielaba, Phys. Rev. B 72, 075435 (2005)
[2] C. Schirm, M. Matt, F. Pauly, J. C. Cuevas, P. Nielaba and E. Scheer, Nature Nanotechnology 8, 645 (2013)

TT 57.11 Wed 12:30 HSZ 304

Large Fluctuation of Conductance in Oligo(phenylene ethynylene)-Based Molecular Junctions — •Daijiro Nozaki[1], Cormac Toher[2], and Gianaurelio Cuniberti[1,3,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Department of Mechanical Engineering and Materials Science, Duke University — [3]Center for Advancing Electronics Dresden (cfAED), TU Dresden, 01062 Dresden, Germany — [4]Dresden Center for Computational Materials Science

(DCCMS), TU Dresden, 01062 Dresden, Germany

Oligo(phenylene ethynylene)s (OPEs) are widely used as conductive building blocks in molecular electronics. It is known that a phenylene unit in OPEs has low energy barrier (100 meV) for its rotation along the axis of the molecule. We have modeled an OPE-based molecular junction where an OPE oligomer is connected between conducting leads, and calculated the conductance of the junction using gDFTB code [1]. We show that the conductance at the Fermi energy significantly changes as a function of rotation angle of the phenylene unit yielding the on/off ratio over 10^4. We have also performed the ab initio MD at room temperature and obtained the similar result. This result implies that a special attention needs to be paid to the relationship between conductance and fluctuation of molecular framework.

[1] D. Nozaki, C. Toher, and G. Cuniberti, J. Phys. Chem. Lett. **4**, 4192 (2013)

TT 57.12 Wed 12:45 HSZ 304

A Simple Graphical Model to Predict and to Control of Quantum Interference in T-shaped Molecular Junctions — •Daijiro Nozaki[1], Haldun Sevincli[2], Stanislav M. Avdoshenko[3], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1,4,5] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany. — [2]Department of Micro- and Nanotechnology, TU Denmark, DK-2800 Kgs. Lyngby, Denmark — [3]School of Materials Engineering, Purdue University, Indiana 47907, USA — [4]Center for Advancing Electronics Dresden (cfAED), TU Dresden, 01062 Dresden, Germany. — [5]Dresden Center for Computational Materials Science (DCCMS), TU Dresden, 01062 Dresden, Germany

Quantum interference (QI) effect in molecular devices introduces an abrupt dip in the transmission spectra, thus it can be used to a series of applications such as molecular switches and molecular thermoelectric devices. For the development of the QI-based molecular devices, it is important to give the guideline to predict and to control the shape and positions of QI in transmission spectra. For this purpose, we present a simple graphical approach (called as "parabolic model") to predict the appearance, shape, and energy position of the QI in transmission spectra for T-shaped molecular devices. We show that this "parabolic model" enables one to visualize the relationship between key electronic parameters and the shape of transmission functions without calculating transmission functions.

[1] D. Nozaki, *et al.*, Phys. Chem. Chem. Phys. **15**, 13951 (2013).

TT 58: Multiferroics II (organized by MA)

Time: Wednesday 9:30–13:00 Location: HSZ 04

TT 58.1 Wed 9:30 HSZ 04

An Engineered Polar Oxide Heterostructure Built from Isosymmetric Magnetically Ordered Components — •Matthew S Dyer[1], Jonathan Alaria[1], Pavel Borisov[1,5], Troy D Manning[1], Serban Lepadatu[2], Markys G Cain[2], Elena D Mishina[3], Natalia E Sherstyuk[3], N A Ilyin[3], Joke Hadermann[4], David Lederman[5], John B Claridge[1], and Matthew J Rosseinsky[1] — [1]University of Liverpool, Liverpool, UK — [2]National Physical Laboratory, Teddington, UK — [3]Moscow State Technical University, Moscow, Russia — [4]University of Antwerp, Antwerp, Belgium — [5]West Virginia University, Morgantown, USA

Theory predicts that certain layered heterostructures consisting of perovskite blocks have non-centrosymmetric structures. The breaking of spatial inversion symmetry arises through a combination of octahedral tilting and A site ordering. Following this prediction, we grow a thin-film of the $[(YFeO_3)_5(LaFeO_3)_5]_{40}$ heterostructure using RHEED monitored pulsed layer deposition. Polar domains are present in the thin-film, as demonstrated by second harmonic generation and piezoelectric force microscopy measurements. We experimentally confirm that the heterostructure is also magnetically ordered at room temperature with a finite magnetization, retaining the magnetic structure of the individual $YFeO_3$ and $LaFeO_3$ components.

TT 58.2 Wed 9:45 HSZ 04

First-principles study of the $BaTiO_3/BaFeO_3$ perovskite interface — •Igor Maznichenko[1], Sergey Ostanin[2], Arthur Ernst[2], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Epitaxial growth can combine a robust ferroelectric, such as $BaTiO_3$, and strong ferromagnets into the so called composite multiferroic films. The switching properties of artificial multiferroics sandwiched between metallic contacts make them excellent candidates for the room temperature four-state memories.

Regarding the ferromagnetic side of composite multiferroics, we suggest to use the cubic perovskite $BaFeO_3$ whose epitaxial growth has been recently reported. Here, from the basis of *ab-initio* electronic structure calculations, within the Korringa-Kohn-Rostoker method, we study the magnetic properties of bulk $BaFeO_3$. The approach allows us to accurately monitor the evolution of the Curie temperature upon both the tetragonal distortions and presence of oxygen vacancies. Finally, we examine magnetoelectricity at the $BaTiO_3/BaFeO_3$ interface.

TT 58.3 Wed 10:00 HSZ 04

Behaviour of Raman modes in $BiFeO_3$ epitaxial thin films with respect to azimuthal orientation — •Andreas Talkenberger[1], Cameliu Himcinschi[1], Ionela Vrejoiu[2,3], Florian Johann[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09596 Freiberg, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [3]Max Planck Institute for Solide State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

$BiFeO_3$ (BFO) is an interesting candidate for multiferroic applications. In this work we focus on the Raman spectroscopic investigation of epitaxially grown thin films of BFO by pulsed laser deposition on different substrates, belonging to the group of scandates ($DyScO_3$, $SmScO_3$, $GdScO_3$). The Raman spectra were recorded using the 442 nm emission line of a He-Cd laser. Some phonon modes show changes in the position, full width at half maximum (FWHM) and intensity depending on the azimuthal angle. We found a 90 degree periodicity of the peak position and of the FWHM for particular modes. For both parallel and crossed polarisation the four maxima in positions correspond to the minima in FWHM. Such a behaviour can be explained considering a twin family of domains with a very well defined orientation to each other. Our results are supported by piezoresponse-force microscopy and X-ray diffraction measurements as well.

TT 58.4 Wed 10:15 HSZ 04

$BiFeO_3/LaFeO_3$: a magnetoelectric multiferroic — •Zeila Zanolli[1,3], Jacek Wojdel[2], Jorge Iniguez[2], and Philippe Ghosez[3] — [1]Forschungszentrum Jülich, PGI and IAS, Jülich, Germany — [2]ICMAB-CSIC, Bellaterra, Spain — [3]Université de Liège, Physics Department, Liegé, Belgium

Transition-metal oxides of perovskite structure present a wide variety of physical properties. In particular, there is a strong interest in multiferroic materials that are simultaneously ferroelectric and magnetic (*magnetoelectrics*). Due to the scarcity of natural magnetoelectric multiferroics and thanks to recent advances in epitaxial growth techniques, designing new magnetoelectric multiferroic heterostructures is a promising way to succeed in this quest.

First-principles techniques are used to investigate electric control of the magnetization in the $BiFeO_3/LaFeO_3$ perovskite oxide superlattice (SL) on a (001)-$SrTiO_3$ substrate. Our results [1] show that the $BiFeO_3/LaFeO_3$ SL exhibits a trilinear coupling of a polar mode with two different rotations of the oxygen cages (*hybrid improper ferroelectricity*). Non-collinear spin calculations reveal that the ferroelectric ground state also presents weak ferromagnetism with easy axis along the [1 -1 0] direction. The microscopic mechanism allowing one to manipulate the magnetization with an electric field in such systems is presented and its dependence on strain and chemical substitution is discussed. The $BiFeO_3/LaFeO_3$ SL is found to be a good candidate to attain electric switching of magnetization at room temperature.

[1] Phys. Rev. B **88**, 060102(R) (2013)

TT 58.5 Wed 10:30 HSZ 04

The influence of strain on the optical properties of pseudo-tetragonal $BiFeO_3$ thin films — •Cameliu Himcinschi[1], Akash Bhatnagar[2], Andreas Talkenberger[1], Dietrich R.T. Zahn[3], Jens Kortus[1], and Marin Alexe[2,4] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [3]Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [4]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

Tetragonally distorted $BiFeO_3$ recently attracted a lot of attention because of its interesting multiferroic properties and the larger spontaneous polarization as compared to its rhombohedral counterpart. Highly strained (when grown on $LaAlO_3$ substrates) and nearly pseudomorphic (when grown on $TbScO_3$ substrates) $BiFeO_3$ films were deposited by pulsed laser deposition. The symmetry of the tetragonally distorted $BiFeO_3$ films is discussed based on polarisation dependent Raman measurements and the comparison with Raman spectra measured for films deposited on $TbScO_3$. The evaluation of ellipsometric spectra reveals that the films deposited on $LaAlO_3$ are optically less dense and the dielectric function is blue-shifted by more than 0.3 eV as compared to the films deposited on $TbScO_3$. By analyzing the absorption edge using a bandgap model, bandgaps of 3.10 eV and 2.75 eV were determined for the films deposited on $LaAlO_3$ and $TbScO_3$, respectively. This work is supported by the German Research Foundation DFG HI 1534/1-1.

TT 58.6 Wed 10:45 HSZ 04

Electrically induced magnetic transiton at the LSMO/BTO interface — •Markus Schmitz, Alexander Weber, Paul Zakalek, Markus Waschk, and Thomas Brückel — Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich Germany

The magnetoelectric coupling is one of the most fascinating and active research areas today. The control of the magnetism due to an applied electric field may lead to new device concepts. First principles calculations of $La_{(1-x)}Sr_xMnO_3/BaTiO_3(001)$ interfaces show magnetic reconstructions due to the change of the polarization of BTO by applying an external electric field. The different electron densities influence the equilibrium between super- and double-exchange favoring a ferromagnetic or an antiferromagnetic order at the interface for the two different orientations of the polarization. Here we report on LSMO/BTO, grown with an Oxide Molecular Beam Epitaxy system. The epitaxial layer-by-layer growth was confirmed by in-situ RHEED analysis and the crystalline quality of the surface was investigated by LEED and Atomic Force Microscopy. The structural characterization was carried out by X-ray reflectometry and diffraction. We could prove the possibility to electrically polarize $BaTiO_3$ substrates due to an applied voltage of 400V by optical methods. The macroscopic magnetic properties were determined by MOKE and SQUID magnetometry. The magnetic formation at the interface with respect to the polarization of the $BaTiO_3$ was investigated by Polarized Neutron reflectometry measurements performed at MARIA (FRM II).

15 min. break

TT 58.7 Wed 11:15 HSZ 04

Growth and structure characterization of double perovskite Sr2FeMoO6 thin films — •Hakan Deniz[1], Dietrich Hesse[1], Marin Alexe[1], Robert Lowndes[2], and Lucian Pintilie[2] — [1]Max-Planck Institute of Microstructure Physics, Weinberg 2, D-06120, Halle (Saale), Germany — [2]National Institute of Materials Physics, Atomistilor 105bis, Magurele 077125, Romania

The double perovskite Sr2FeMoO6 (SFMO) has drawn considerable attention recently owing to some of its unique features such as high Curie temperature (˜410K) and half-metallic ferrimagnetic nature with a high saturation moment of 4μB. The low-field room temperature magnetoresistance observed in SFMO makes it an attractive candidate for oxide spintronics applications. However, the broad distribution of results reported so far on SFMO films suggests that an optimal structure is attainable only within a narrow window of growth conditions; and magnetic/transport properties are highly akin to Fe and Mo atomic site disorder. Pulsed laser deposition was employed to grow SFMO thin films on vicinal SrTiO3 substrates from a custom-made stoichiometric target using argon as ambient gas. X-ray diffraction data revealed that the SFMO films were grown epitaxially with respect to the substrate, including, however, a small percentage of secondary phases. The morphology of the films shows flat plains with embedded grain- or needle-like structures, which are most likely the result of spurious phases. The nature of these defects and their interfaces with the SFMO matrix are under investigation by transmission electron microscopy. This work is supported by the EU-FP7 project IFOX.

TT 58.8 Wed 11:30 HSZ 04

Magnetic Anisotropy in Multiferroic Lu_2MnCoO_6 — •Martin Lonsky[1], Merlin Pohlit[1], María Antonia Señarís Rodríguez[2], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — [2]Dpto. Química Fundamental U. Coruña, Coruña, Spain

Lu_2MnCoO_6 recently has been introduced as a new type-II multiferroic with ferroelectricity due to charge ordering and magnetostriction related to magnetic Mn^{4+} and Co^{2+} ions which are arranged alternately in the form of Ising chains along the c-axis of the crystal [1]. The magnetic properties, however, remain puzzling, which in particular is due to the lack of measurements on single crystals, that have not yet successfully been synthesized. Here, we present for the first time measurements of the magnetic anisotropy by employing micro-Hall magnetometry on a few micrograins of dimensions $\sim 1\,\mu$m only. Our results reveal a strong dependence of magnetic hysteresis on temperature and the applied field direction. This anisotropy is also reflected in the observation of a variety of unusual effects as for instance wasp-waisted hysteresis loops, sharp jumps in magnetization at about $T = 300\,$mK and an exchange bias, ocurring in each case in only one field direction. Additionally, the observation of a pronounced maximum in the coercive field at $T_{SF} \sim 12\,$K indicates a significant change in the spin dynamics of the system below T_{SF}, similar to the behavior of the related compound $Ca_3Co_{2-x}Mn_xO_6$ ($x \approx 0.95$) [2].

[1] S. Yáñez-Vilar et al., Phys. Rev. B. 84, 134427 (2011).
[2] T. Lancaster et al., Phys. Rev. B 80, 020409 (2009).

TT 58.9 Wed 11:45 HSZ 04

The multiferroic $CuCrO_2$ compound: interlayer exchange and domain population — •Matthias Frontzek — Laboratory for Neutron Scattering, Paul Scherrer Institut, 5232 Villigen-PSI, Switzerland

Multiferroic materials have become of interest for their unusual low-temperature properties in general, and the tunability of the magnetic structure through an electric field and the electric polarization through a magnetic field in particular. The most promising candidates for such controllable multiferroics have been found among the materials with inherent geometric magnetic frustration.

Among these, the delafossite $CuCrO_2$, which crystallizes in the rhombohedral $R\bar{3}m$ space group, is a multiferroic compound with an apparent strong coupling of spin and charge. In contrast to other multiferroic compounds $CuCrO_2$ shows a spontaneous electric polarization upon antiferromagnetic ordering without an accompanying structural phase transition, thus the magnetic ordering alone breaks the inversion symmetry. The peculiar magnetic structure of $CuCrO_2$ allows the direct quantitative analysis of the domain population.

In our contribution, we present a detailed study on $CuCrO_2$ single crystals using neutron diffraction in applied electric and magnetic fields. With the fields we were able to tune the multiferroic states in $CuCrO_2$ and could directly relate them to the underlying domain physics. Our results allow the re-interpretation of macroscopic measurements and show that the $p-d$ hybridization is the dominant spin-charge coupling mechanism.

TT 58.10 Wed 12:00 HSZ 04

Structure and Magnetic Coupling in $YBaFeCuO_5$ — •Andrea Scaramucci[1], Mickael Morin[2], Ekaterina Pomjakushina[2], Marek Bartkowiak[2], Denis Sheptyakov[2], Lukas Keller[2], Juan Rodriguez-Carvajal[3], Michel Kenzelmann[2], Kazimierz Conder[2], Marisa Medarde[2], and Nicola A. Spaldin[1] — [1]Materials Theory, ETH-Zurich, Zurich, Switzerland — [2]Paul Scherrer Institute, Villigen, Switzerland — [3]Institute Laue Langevin, Grenoble, France

We theoretically study the structure and exchange couplings in multiferroic $YBaFeCuO_5$ (YBFCO). Using density functional theory we calculate energies of configurations with various Fe^{3+}/Cu^{2+} orderings in the bilayered perovskite structure of YBFCO. We find that configurations with different distribution of Fe^{3+} and Cu^{2+} ions fall into two groups with distinctly different energies. The energies of those in the lowest energy group are close to that of the ground state (relative to the growth temperature) suggesting Fe^{3+} and Cu^{2+} to be disordered in YBFCO. Finally, we calculate exchange coupling constants for all

the low energy configurations and show that the magnetic ordering resulting from these couplings is compatible with the experimentally-observed high-temperature magnetic ordering. However, they do not explain the existence of the experimentally observed low-temperature incommensurate magnetic structure.

TT 58.11 Wed 12:15 HSZ 04

Hybrid-functional study of the structural, magnetic and electronic properties of rare-earth nickelates — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Rare-earth nickelates ($ReNiO_3$) are very promising functional perovskite crystalline materials, exhibiting metal-insulator (MI) transition, which can be continuously controlled by composition, bi-axial strain and(or) electric field. Unfortunately, conventional *ab initio* DFT+U results fail to reproduce their magnetic ground state as well as the effect of epitaxial strain on MI transition temperature. We present results of our comprehensive study of structural, magnetic and electronic properties of bulk $ReNiO_3$ (Re=Y, Gd, Eu, Sm, Nd and Pr) and strained $SmNiO_3$ films [1], performed with HSE06 functional. We show correlation between MI transition temperature and structural parameters of bulk and films, which nicely fits known experimental data. We also analyze the difference in the electronic structure obtained in DFT+U and with the hybrid functional and their influence on the resulting magnetic ordering in the ground state.

We acknowledge the support by Helmholtz Young Investigators Group Programme VH-NG-409, JSC and JARA-HPC.

[1] F.Y. Bruno, K.Z. Rushchanskii, S. Valencia, Y. Dumont, C. Carrétéro, E. Jacquet, R. Abrudan, S. Blügel, M. Ležaić, M. Bibes, and A. Barthélémy, Phys. Rev. B 88, 195108 (2013).

TT 58.12 Wed 12:30 HSZ 04

Magnetic properties of multiferroic $TbMnO_3$ — •Natalya Fedorova, Andrea Scaramucci, Claude Ederer, and Nicola Spaldin — ETH Zurich, Materials Theory, Wolfgang-Pauli-Strasse 27, CH-8093 Zurich, Switzerland

We use ab-initio calculations to investigate the magnetic properties of multiferroic $TbMnO_3$.

At low temperatures $TbMnO_3$ demonstrates an incommensurate spiral ordering of Mn spins which is accompanied by appearance of spontaneous electric polarization driven by applied magnetic field [1]. The establishment of such spin ordering is usually described within the framework of a Heisenberg model with competing nearest-neighbor and next-nearest-neighbor exchange interactions. However, our theoretical estimations of these interactions by ab-initio calculations demonstrate a clear deviation from Heisenberg model.

We consider first the coupling between magnetic and orbital orderings as a main source of non-Heisenberg behavior in $TbMnO_3$, but conclude that it does not explain the observed deviation. We find that higher order interactions (biquadratic and four-body spin couplings) should be taken into account for proper treatment of the magnetism in $TbMnO_3$.

[1] T. Kimura et al., Nature 426, 55-58 (2003)

TT 58.13 Wed 12:45 HSZ 04

Coupling of epitaxial strain and point-defect formation in perovskites — •Ulrich Aschauer, Philipp Baumli, and Nicola A. Spaldin — Materials Theory, ETH Zurich, Zürich, Switzerland

Using density functional theory calculations we recently established the existence of a strong coupling between epitaxial strain and the formation energy of oxygen vacancies in the model perovskite $CaMnO_3$ (Phys. Rev. B. 88, 054111, 2013). Here we investigate the generality of this concept for other oxides including metallic perovskites and also investigate the effect of strain on the formation of cation vacancies. We find that in general the response of the defect profile follows the behavior expected from chemical-expansion arguments, with tensile strain favoring oxygen vacancies and compressive strain favoring cation vacancies. We show, however, that material-specific details of the electronic structure can cause deviations from this trend under both tensile and compressive strain.

TT 59: Low-Dimensional Systems: 2D - Theory (organized by TT)

Time: Wednesday 9:30–13:00 Location: BEY 81

TT 59.1 Wed 9:30 BEY 81

Critical theory of the spin quantum Hall transition — •Roberto Bondesan — Institute of theoretical physics, Köln, Deutschland

The spin quantum Hall (SQH) transition is a 2+1 dimensional Anderson transition between topological phases distinguished by different integer values of the spin conductance. In contrast to the celebrated integer quantum Hall transition, in the SQH case, critical exponents governing low moments of observables are known exactly. In this talk I will address the problem of characterizing completely the exponents of the theory beyond low moments. For this puropouse I will explain recent insights on the classification of scaling fields at Anderson transitions, which allow to perform efficient numerical studies and conjecture the multifractal spectrum of the theory.

TT 59.2 Wed 9:45 BEY 81

Pure scaling operators at the integer quantum Hall plateau transition — Roberto Bondesan, •Daniel Wieczorek, and Martin Zirnbauer — Universität zu Köln, Institut für theoretische Physik, Zülpicher Straße 77, 50937 Köln

Despite considerable effort, the conformal field theory underlying the integer quantum Hall plateau transition is still not known. We circumvent the fact that conductances in the Chalker-Coddington model do not show pure scaling behaviour by introducing a new family of scattering observables corresponding to n-point functions of conformal primary fields at the plateau transition. Disorder averages of these observables correspond to lattice pure scaling operators in the supersymmetric vertex model. We also present numerical results for the multifractal spectra of 2 and 3 point functions.

TT 59.3 Wed 10:00 BEY 81

Plasmons due to the interplay of Dirac and Schrödinger fermions — •Stefan Jürgens, Paolo Michetti, and Björn Trauzettel — Institute of Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

We study the interplay between Dirac and Schrödinger fermions in the polarization properties of a two-dimensional electron gas (2DEG). Specifically, we analyze the low-energy sector of narrow-gap semiconductors described by a two-band Kane model. In the context of quantum spin Hall insulators, particularly, in Hg(Cd)Te quantum wells, this model is named Bernevig-Hughes-Zhang model. Interestingly, it describes electrons with intermediate properties between Dirac and Schrödinger fermions. We calculate the dynamical dielectric function of such a model at zero temperature within random phase approximation. Surprisingly, plasmon resonances are found in the intrinsic (undoped) limit, whereas they are absent – in that limit – in graphene as well as ordinary 2DEGs. Additionally, we demonstrate that the optical conductivity offers a quantitative way to identify the topological phase of Hg(Cd)Te quantum wells from a bulk measurement.

TT 59.4 Wed 10:15 BEY 81

Correlated spinless fermions on the honeycomb lattice — •Martin Hohenadler[1] and Maria Daghofer[2] — [1]University of Würzburg, Germany — [2]IFW Dresden, Germany

We study the phase diagram of spinless fermions on the honeycomb lattice with nearest– (V_1) and next-nearest neighbour repulsion (V_2) using numerical methods. At the mean-field level, this model has been shown to describe an interaction-generated quantum anomalous Hall (QAH) phase with nonzero Chern index [Raghu *et al.*, PRL **100**, 156401 (2008)]. Our exact results reveal that this phase is completely suppressed by quantum fluctuations. However, for small V_2, we find that V_2 enhances bond order correlations that resemble the mean-field bond order in the QAH phase. This weak-coupling tendency toward a QAH state suggests that the phase may be realized in other models.

TT 59.5 Wed 10:30 BEY 81

The π flux honeycomb lattice: a topological crystalline in-

sulator. — •Martin Bercx, Martin Hohenadler, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg

We consider the Kane-Mele-Hubbard model with intrinsic spin-orbit coupling λ supplemented by a π flux threading each honeycomb plaquette. At $U = 0$ and in each spin sector the band structure is characterized by a Chern number $C = \pm 2$. Furthermore fine tuning of λ leads to a point of quadratic band crossing associated with a topological phase transition. Bulk quantum Monte Carlo simulations reveal a magnetically ordered phase which extends to weak couplings at the value of λ where the quadratic band crossing occurs. Although the spinful model carries two helical edge states and is explicitly shown to be a Z_2 trivial insulator, its edge states are robust due to protection by lattice translation symmetry. We present quantum Monte Carlo calculations which reveal that well defined edge states remain even in the case of strong interactions.

TT 59.6 Wed 10:45 BEY 81

Density Functional Description of Two-Dimensional Fermi Gases — •Martin-Isbjörn Trappe[1], Hui Khoon Ng[1], Cord Axel Müller[2], and Berthold-Georg Englert[1] — [1]Centre for Quantum Technologies, National University of Singapore — [2]Department of Physics, University of Konstanz, Germany

Several methods suggest the gradient corrections beyond the Thomas-Fermi (TF) kinetic energy functional to vanish for two-dimensional systems at zero temperature. However, the TF functional does not coincide with the exact functional, implying the existence of corrections. We present a systematic derivation of such first order gradient corrections by means of the Wigner function and test the result employing the exactly known particle density of spin-1/2-fermions in a two-dimensional harmonic trap.

TT 59.7 Wed 11:00 BEY 81

Renormalization group approach to non-analytic corrections in Fermi liquid theory — •Casper Drukier[1,2], Philipp Lange[1,2], and Peter Kopietz[1,2] — [1]Institut für Theoretische Physik, J.W.Goethe-Universität Frankfurt, Frankfurt am Main, Germany — [2]Department of Physics, University of Florida, Gainesville, Florida, USA

We calculate the leading non-analytic magnetic field dependence of the free energy and spin-susceptibility of a two-dimensional Fermi liquid using functional renormalization group methods, with bosonized particle-hole fluctuations. At weak coupling we recover the perturbative results of Maslov and Chubukov [PRB 79, 075112 (2009)]. We go beyond perturbation theory by including self-energy and vertex corrections within a truncated vertex expansion and present explicit results for the leading non-analytic correction to the spin-susceptibility and other Fermi liquid parameters as a function of interaction strength.

15 min. break.

TT 59.8 Wed 11:30 BEY 81

From infinite to two dimensions through the functional renormalization group — Ciro Taranto[1], Sabine Andergassen[2], Johannes Bauer[3], Karsten Held[1], Andrey Katanin[4], Walter Metzner[5], Georg Rohringer[1], and •Alessandro Toschi[1] — [1]Institute for Solid State Physics, Vienna University of Technology 1040 Vienna, Austria — [2]Faculty of Physics, University of Vienna, 1090 Vienna, Austria — [3]Department of Physics, Harvard University, 17 Oxford St., MA 02138, USA — [4]Institute of Metal Physics, Russian Academy of Sciences and Ural Federal University, Ekaterinburg, Russia — [5]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

We present a novel scheme[1] for an unbiased and non-perturbative treatment of strongly correlated fermions. The proposed approach combines two of the most successful many-body methods, i.e., the dynamical mean field theory (DMFT) and the functional renormalization group (fRG). Physically, this allows for a systematic inclusion of non-local correlations via the flow equations of the fRG, after the local correlations are taken into account non-perturbatively by the DMFT. To demonstrate the feasibility of the approach, we present numerical results for the two-dimensional Hubbard model at half-filling.
[1] C. Taranto, S. Andergassen, J. Bauer, K. Held, A. Katanin, W. Metzner, G. Rohringer, and A. Toschi, arXiv: 1307.3475.

TT 59.9 Wed 11:45 BEY 81

Efficient 2D density matrix renormalization group in mixed real- and momentum-space representation — •Johannes Motruk[1], Michael P. Zaletel[2], Roger S. K. Mong[3], and Frank Pollmann[1] — [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

Density matrix renormalization group (DMRG) is a powerful numerical technique for both 1D and 2D systems. The traditional implementation for a 2D system requires an ordering of sites to form an effective 1D chain for simulation. We present a variation of the DMRG technique that utilizes a real-space representation in one direction and momentum-space representation in the perpendicular direction of the lattice. We demonstrate how the mixed representation reduces the computational costs by using momentum as a conserved quantity—and as a by product—produces the momentum-resolved entanglement spectrum. As an application, we map out the phase diagram of a tight-binding model of spinless fermions with nearest-neighbour interactions on the square lattice. For this model, we give performance benchmarks comparing the mixed basis to the traditional real-space basis.

TT 59.10 Wed 12:00 BEY 81

Dimensional-Crossover-Driven Mott Transition: A Variational Cluster Approach — •Benjamin Lenz and Thomas Pruschke — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

The dimensional-crossover-driven Mott transition has been studied recently for a frustrated Hubbard model with next-nearest neighbor hopping at finite temperatures [Raczkowski, Assaad, PRL 109 (2012)]. Here, we study this crossover from one to two dimensions at zero temperature by means of the variational cluster approximation (VCA) for fixed frustration as function of the interaction. The transition at zero temperature is found to be continuous, and results for various dynamic and static quantities are discussed as a function of cluster size.

TT 59.11 Wed 12:15 BEY 81

Superconductivity in the two-dimensional t-t'-Hubbard model — •Andreas Eberlein and Walter Metzner — Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Using a recently developed renormalization group method for fermionic superfluids, we determine conditions for d-wave superconductivity in the ground state of the two-dimensional Hubbard model at moderate interaction strength, and we compute the pairing gap in the superconducting regime. A pairing instability signaled by a divergent flow in the Cooper channel leads to a superconducting state in all studied cases. The next-to-nearest neighbor hopping t' plays a crucial role in the competition between antiferromagnetism and superconductivity. A sizable t' is necessary to obtain a sizable pairing gap.

TT 59.12 Wed 12:30 BEY 81

Unconventional superconductivity in the two dimensional Edwards model — •Dai-Ning Cho and Steffen Sykora — Institute for Theoretical Solid State Physics, IFW Dresden, D-01069 Dresden, Germany

The nature of charge transport within a correlated background medium can be described by spinless fermions coupled to bosons in the model introduced by Edwards. Employing the analytical projector-based renormalization method (PRM), we obtain a solvable effective Hamiltonian $\tilde{\mathcal{H}}$ which consists of a decoupled system of renormalized conduction electrons and a bosonic term with renormalized dispersion $\tilde{\omega}_{\mathbf{q}}$ which is generated naturally within the renormalization procedure. This method has been applied successfully to the 1D Edwards model where unbiased numerical results could be confirmed by the PRM. For the 2D model we show results for the effective one-particle dispersions of electrons and bosons in the whole Brillouin zone and for different values of the electron filling. In particular, we find strong dispersion of boson modes indicating a quantum phase transition to an unconventional superconducting state mediated by strong charge fluctuations. We show that the pairing changes its character from s- to d-wave symmetry.

TT 59.13 Wed 12:45 BEY 81

Phase diagram of the square lattice bilayer Hubbard model: A Variational Monte Carlo study — Robert Rüger[1,2], •Luca Fausto Tocchio[1,3], Roser Valentí[1], and Claudius Gros[1] —

[1]University of Frankfurt, Germany — [2]Scientific Computing & Modelling NV, Amsterdam, The Netherlands — [3]SISSA, Trieste, Italy

We investigate the phase diagram of the square lattice bilayer Hubbard model at half filling with the variational Monte Carlo method for both the magnetic and the paramagnetic case as a function of interlayer hopping $t_\perp$ and on-site Coulomb repulsion U. With this study we resolve some discrepancies in previous calculations based on the dynamical mean field theory, and we are able to determine the nature of the phase transitions between metal, Mott insulator and band insulator. In the magnetic case we find only two phases: An antiferromagnetic Mott insulator at small $t_\perp$ for any value of U and a band insulator at large $t_\perp$. At large U values we approach the Heisenberg limit. The paramagnetic phase diagram shows at small $t_\perp$ a metal to Mott insulator transition at moderate U values and a Mott to band insulator transition at larger U values. We also observe a reentrant Mott insulator to metal transition and metal to band insulator transition for increasing $t_\perp$ in the range of $5.5t < U < 7.5t$. Finally, we discuss the obtained phase diagrams in relation to previous studies based on different many-body approaches.

TT 60: Focus Session: Chiral Domain Walls in Ultrathin Films (organized by MA)

Organizer: Stefan Blügel (Forschungszentrum Jülich)

During the past years we witnessed a breakthrough in the observation and application of chiral domain walls to spintronics. In chiral domain walls the magnetization rotates from one domain to the next with a preferred handedness. They are a result of the Dzyaloshinskii-Moriya interaction originating from spin-orbit interaction in combination with the lack of inversion symmetry of the atomic structure e.g. due to the presence of interfaces. The presence of Néel-type chiral domain walls in thin perpendicularly magnetized ferromagnetic films has been pointed out by theory and they were observed first by spin-polarized scanning tunneling microscopy (SP-STM). Recent low-energy electron microscopy (LEEM) experiments show that the formation of this novel type of wall may be a rather general phenomenon in thin films with structure-asymmetry and that the chirality of the domain wall can be engineered using different materials combinations and stackings. It was demonstrated that the Dzyaloshinskii-Moriya interaction stabilizes the domain wall during motion and the current-induced wall motion is very efficient for this type of wall. The origin of the torque the current exerts on the magnetization when driving the domain wall motion, i.e. the degree of spin-transfer torque (STT) and spin-orbit torque (SOT) is currently a matter of debate. Chiral domain walls provide unprecedented opportunities for the development of spintronic devices and in the focus session we try to illuminate different aspects including their observation, the dynamics and applications.

Time: Wednesday 9:30–12:15 Location: BEY 118

Topical Talk TT 60.1 Wed 9:30 BEY 118

On the rediscovery of the Dzyaloshinskii-Moriya interaction—A review — •Matthias Bode — Physikalisches Institut, Experimentelle PhysikUniversität Würzburg II, , Am Hubland, D-97074 Würzburg, Germany

Even though it had already been theoretically predicted in 1960 [1,2] that the spin-orbit–driven Dzyaloshinskii–Moriya interaction (DMI) may lead to chiral spin structures in magnetic systems with broken inversion symmetry, this term was largely ignored for decades. This is particularly astonishing as experimental progress allowed the preparation of increasingly subtle magnetic structures which feature surfaces and interfaces or even—as in the case of magnetic nanostructures—exclusively consist of surfaces and interfaces. Obviously, in all these sample geometries inversion symmetry is broken and a sufficiently strong spin-orbit coupling should lead to chiral magnetism [3]. In this talk I will review why the importance of the DMI interaction in thin film and nano magnetism was overlooked for so long, and how scientific persistence [4] eventually led to irrefutable evidence that it not only exists [5] but in some (if not many) cases strongly influences [6,7] or even dominates magnetic order.

[1] I.E. Dzialoshinskii, Sov. Phys. JETP **5**, 1259 (1957).
[2] T. Moriya, Phys. Rev. **120**, 91 (1960).
[3] A. Bogdanov and A. Hubert, J. Magn. Magn. Mat. **138**, 255 (1994).
[4] A. Bogdanov and U. Rößler, Phys. Rev. Lett. **87**, 037203 (2001).
[5] M. Bode *et al.*, Nature **447**, 190 (2007).
[6] M. Heide *et al.*, Phys. Rev. B **78**, 140403 (2008).
[7] S. Meckler *et al.*, Phys. Rev. Lett. **103**, 157201 (2009).

Topical Talk TT 60.2 Wed 10:00 BEY 118

Chiral Magnetic Domain Wall Structure in Epitaxial Multilayers — •Yizheng Wu[1], Gong Chen[2,1], Jie Zhu[1], Alpha T. N'Diaye[2], Tianping Ma[1], HeeYoung Kwon[3], Changyeon Won[3], and Andreas. K. Schmid[2] — [1]Physics Department,Fudan University, Shanghai, China — [2]NCEM, LBNL, Berkeley, California, USA — [3]Department of Physics, Kyung Hee University, Seoul , Korea

In ultrathin film, the inversion symmetry broken at interface will induce Dzyaloshinskii-Moriya interaction (DMI). In this talk, we will show that the DMI at interface will induce the chiral Néel type domain wall in perpendicularly magnetized films. The spin structure in magnetic domain wall was identified in real-space at room temperature by spin-polarized low energy electron microscopy (SPLEEM). The chiral Néel-type domain wall was identified in the magnetic stripe domain phase in Fe/Ni/Cu(001), and the chirality can switch from the right-hand cycloid in Fe/Ni/Cu(001) to the left-hand cycloid in Ni/Fe/Cu(001), which indicates that the chirality is caused by the DMI mainly located at the Fe/Ni interface [1]. The chiral domain wall structure can also be observed in [Co/Ni]n multilayer grown on Pt(111) and Ir(111)[2]. by inserting an Ir layer between the Co/Ni stack and the Pt substrate and varying the thickness of the Ir layer, we prove that domain wall chirality together with the sign and strength of the DMI can be tuned through the interface engineering, which may enable more possibility for designing of new spintronics devices.

[1] G. Chen, et al., Phys. Rev. Lett. 110, 177204 (2013) [2] G. Chen, et al., Nature Communication, 4,2671(2013)

15 min. break

Topical Talk TT 60.3 Wed 10:45 BEY 118

'Dzyaloshinskii domain walls' in ultrathin magnetic films — •André Thiaville[1], Stanislas Rohart[1], Emilie Jué[2], Olivier Boulle[2], Vincent Cros[3], Albert Fert[3], Stefania Pizzini[4], and Jan Vogel[4] — [1]Lab. Phys. Solides, CNRS, Univ. Paris-Sud, 91405 Orsay, France — [2]SPINTEC, INAC, CEA-CNRS-UJF-INPG, 38054 Grenoble, France — [3]UMP CNRS-Thales & Univ. Paris-Sud, 91767 Palaiseau, France — [4]Institut Néel, CNRS-UJF, 38042 Grenoble, France

In ultrathin magnetic films with perpendicular anisotropy and vertical structural inversion asymmetry, we have recently proposed [1] that the domain walls are chiral Néel walls with a peculiar dynamics. This results from a Dzyaloshinskii-Moriya interaction (DMI) of the interfacial type, predicted by A. Fert long ago and observed on monolayers by SP-STM [2]. Several recent experimental observations of the dynamics of domain walls in such samples, under fields and current, are in agreement with this picture, with the effect of current incorporated

by the spin Hall effect in an adjacent layer [3].

After recalling the main characteristics of these Dzyaloshinskii domain walls, I will describe additional features that occur at large values of the DMI (but still in the region where an isolated domain is stable), namely the tilt of such walls in nanostrip-shaped samples. This affects the statics and dynamics of these walls [4].

[1] A. Thiaville et al., EPL 100, 57002 (2012) [2] P. Ferriani et al., PRL 101, 027201 (2008) [3] S. Emori, et al., Nature Mater. 12, 611 (2013) [4] O. Boulle et al., PRL 111, 217203 (2013)

Topical Talk TT 60.4 Wed 11:15 BEY 118

Current-driven dynamics of chiral ferromagentic domain walls — •Geoffrey Beach — MIT Dept. of Mater. Sci. and Eng., Cambridge, MA, USA

In most ferromagnets the magnetization rotates from one domain to the next with no preferred handedness. However, broken inversion symmetry can lift the chiral degeneracy, leading to topologically rich spin textures such as spin-spirals and skyrmions via the Dzyaloshinskii-Moriya interaction (DMI) [1-3]. Here we show that in ultrathin metallic ferromagnets sandwiched between a heavy metal and an oxide, the DMI stabilizes chiral domain walls (DWs) whose spin texture enables extremely efficient current-driven motion [4-6]. We show that spin torque from the spin Hall effect drives DWs in opposite directions in Pt/CoFe/MgO and Ta/CoFe/MgO, which can be explained only if the DWs assume a Néel configuration with left-handed chirality. We directly confirm the DW chirality and rigidity by examining current-driven DW dynamics with magnetic fields applied perpendicular and parallel to the spin spiral [4,6]. This work identifies the origin of efficient current-driven domain wall motion in heavy metal/ferromagnet bilayers, and highlights a new path towards interfacial design of spintronic devices. In collaboration with S. Emori, U. Bauer, and E. Martinez.

[1] M. Bode, et al., Nature 447, 190 (2007). [2] S. Heinze, et al., Nature Physics 7, 713 (2011). [3] A. Thiaville, et al., Europhys. Lett. 100, 57002 (2012). [4] S. Emori, et al., Nature Mater. 12, 611 (2013). [5] E. Martinez, et al., APL 103, 072406 (2013). [6] S. Emori, et al., arXiv:1308.1432 (2013).

Topical Talk TT 60.5 Wed 11:45 BEY 118

Phenomenology of current-induced spin-orbit torques — •Kjetil M. D. Hals — The Niels Bohr International Academy, Niels Bohr Institute, 2100 Copenhagen, Denmark

Recent developments have shown that currents can cause magnetization torques via relativistic, intrinsic spin-orbit coupling, often referred to as spin-orbit torques (SOTs). A detailed understanding of the SOTs requires improved theoretical models that exceed the present phenomenological framework used to model current-induced magnetization dynamics. In this talk, I present a novel phenomenology of current-induced torques that is valid for any strength of intrinsic spin-orbit coupling [1]. In Pt|Co|AlOx, I demonstrate that the domain walls move in response to a novel relativistic dissipative torque that is dependent on the domain wall structure and that can be controlled via the Dzyaloshinskii-Moriya interaction. Unlike the non-relativistic spin-transfer torque, the new torque can, together with the spin-Hall effect in the Pt-layer, move domain walls by means of electric currents parallel to the walls.

[1] K. M. D. Hals and A. Brataas, Phys. Rev. B 88, 085423 (2013).

TT 61: Graphene: Transport (organized by HL)

Time: Wednesday 9:30–12:15 Location: POT 051

TT 61.1 Wed 9:30 POT 051

Ratchet effects in graphene with a lateral potential — •Josef Kamann[1], Leonid Golub[2], Matthias König[1], Jonathan Eroms[1], Felix Fromm[3], Thomas Seyller[3], Dieter Weiss[1], and Sergey Ganichev[1] — [1]University of Regensburg, Germany — [2]Ioffe Physical-Technical Institute of the RAS, St. Petersburg, Russia — [3]Technical University of Chemnitz, Germany

We report on the observation of terahertz radiation induced ratchet effects in graphene with a lateral periodic potential. These effects generate a dc electric current from an ac electric field. To probe ratchet effects, a metal grating has been deposited on top of epitaxially grown graphene. This lattice contains periodically deposited stripes with different widths and spaces and, therefore, has no inversion symmetry.

We demonstrate that the ratchet effect is generated only in the modulated area and does not arise in unpatterned graphene. This proves the symmetry breaking induced by the asymmetric lateral potential. Additional effects like edge currents or the circular ac Hall effect are excluded by the geometry of the samples and by illumination under normal incidence. The ratchet signal is studied with respect to the polarization and the wavelength of the radiation. We show that the ratchet effect is sensitive to both linear and circular polarization and conducted calculations for different elastic-scattering processes to compare them to our experimental findings.

TT 61.2 Wed 9:45 POT 051

Magnetic quantum ratchet effect in graphene — •Christoph Drexler[1], Sergey Tarasenko[2], Peter Olbrich[1], Johannes Karch[1], Marion Hirmer[1], Florian Müller[1], Martin Gmitra[1], Jaroslav Fabian[1], Rositza Yakimova[3], Samuel Lara-Avila[4], Sergey Kubatkin[4], Minjie Wang[5], Junichiro Kono[5], and Sergey Ganichev[5] — [1]THz Center, University of Regensburg, Germany — [2]Ioffe Physical-Technical Institute, St. Petersburg, Russia — [3]Linköping University, Sweden — [4]Chalmers University, Göteborg, Sweden — [5]Rice University, Houston, USA

We report on the experimental observation of the magnetic quantum ratchet effect in epitaxial- and CVD- grown graphene layers excited by pulsed terahertz (THz) - laser radiation [1]. Our experimental findings can be well understood in terms of asymmetric carrier scattering in graphene in presence of an in-plane magnetic field yielding strong structure inversion asymmetry (SIA) in graphene. The SIA stems from the fact that graphene is deposited on a substrate and/or is sensitive to chemical bonding of adatoms on the surface. Considering hydrogen atoms on top of carbon we calculated the magnitude of the photocurrent being in good agreement with the data obtained from the experiments. The amplitudes of the current differ significantly for the used material systems whereas its sign can be influenced by the post-groth treatment of the samples. The ratchet current can be calibrated to measure the strength of the SIA, which plays an important role in graphene ferromagnetism and spintronics.

[1] C. Drexler et al, Nat. Nano. 8 104-107, 2013.

TT 61.3 Wed 10:00 POT 051

Spin transport in arrays of graphene nanoribbons — Matthias Berl, Bastian Birkner, Andreas Sandner, Silvia Minke, Dieter Weiss, and •Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany

We performed non-local spin valve and Hanle measurements in arrays of graphene nanoribbons in both single and bilayer graphene. Nanoribbons were patterned by electron beam lithography and oxygen-based reactive ion etching. By fabricating several sets of electrodes, we can compare spin transport data in bulk and nanoribbons on the same graphene flake. Due to band-gap opening in the nanoribbons at low temperatures, spin transport measurements were only possible at 200 Kelvin. For single layer graphene we observe that while nanopatterning decreases the electron mobility, the spin lifetime increases from 200 ps to 500 ps. This is consistent with a Dyakonov-Perel-like contribution to spin relaxation. In bilayer graphene, we observe a low electron mobility and high spin lifetimes of about 1 ns in both bulk and nanoribbons, again consistent with Dyakonov-Perel-like spin relaxation. Attempting to see an influence of possible magnetic moments at the sample edges, no clear signature was detected in the Hanle data at 200 Kelvin.

TT 61.4 Wed 10:15 POT 051

THz radiation interacting with epitaxial graphene — •Christian Sorger, Sascha Preu, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We investigate the interaction between terahertz (THz) radiation and periodically doped graphene ribbons. We find a remarkable polarization dependence. The Drude response of graphene can be probed with

THz electric fields parallel to the ribbons. This results in a high-pass filter-like behavior with a 3dB-frequency in the THz range. The exact value depends on carrier mobility and carrier concentration. For THz electric field perpendicular to the ribbons we detect rather high transmission as the response is dominated by plasmonic effects. Utilizing the material system epitaxial graphene on silicon carbide (SiC) we show that no lithographic patterning is required to couple light into the two-dimensional electron gas (2DEG). As the interaction strength depends on the geometry of the 2DEG and its electronic properties, respectively, this strategy allows for a characterization of the AC conductivity in epitaxial graphene.

TT 61.5 Wed 10:30 POT 051

Numerically exact approach to transport properties of disordered two-dimensional materials — •Stefan Barthel[1,2], Malte Rösner[1,2], Fernando Gargiulo[3], Oleg V. Yazyev[3], and Tim O. Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Germany — [3]Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

We present a numerical method for modeling electron transport in disordered two-dimensional materials such as graphene with resonant impurities. Covalently bonded adatoms, such as hydrogen, modify the electronic structure and transport properties of graphene in the diffusive as well as localized regime in which quantum corrections become important. The electronic structure is described using a tight-binding model involving pz-orbitals on a honeycomb lattice, whereas the transport properties are evaluated in the linear response approximation (Kubo-Greenwood) using the kernel polynomial method as a solver. By combining these methods we gain access to large systems containing up to 10ˆ6 atoms. These results are compared to the ones obtained using the Landauer-Büttiker approach in the above-mentioned transport regimes.

TT 61.6 Wed 10:45 POT 051

Quantum Hall Effect in Chemically Functionalized Graphene: Defect-Induced Critical States and Breakdown of Electron-Hole Symmetry — •Nicolas Leconte[1,2], Jean-Christophe Charlier[2], and Stephan Roche[1] — [1]ICN2 - Institut Catala de Nanociencia i Nanotecnologia, Campus UAB, 08193 Bellaterra (Barcelona), Spain — [2]Université catholique de Louvain (UCL), Institute of Condensed Matter and Nanoscience (IMCN), Chemin des étoiles 8, 1348 Louvain-la-Neuve, Belgium

Unconventional magneto-transport fingerprints in the quantum Hall regime (with applied magnetic field from one to several tens of Tesla) in chemically functionnalized graphene are reported. Upon chemical adsorption of monoatomic oxygen (from 0.5% to few percents), the electron-hole symmetry of Landau levels is broken, while a double-peaked conductivity develops at low-energy, resulting from the formation of critical states conveyed by the random network of defects-induced impurity states. Scaling analysis suggests an additional zero-energy quantized Hall conductance plateau, which is here not connected to degeneracy lifting of Landau levels by sublattice symmetry breakage. This singularly contrasts with usual interpretation, and unveils a new playground for tailoring the fundamental characteristics of the quantum Hall effect. The study on oxygen is complemented with a study on a simplified divacancy model, confirming the percolation of impurity states leading to delocalized states.

Coffee break (15 min.)

TT 61.7 Wed 11:15 POT 051

Ultra long spin decoherence times in graphene quantum dots with a small number of nuclear spins — •Moritz Fuchs[1], John Schliemann[2], and Björn Trauzettel[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg — [2]Institut für Theoretische Physik, Universität Regensburg, 93053 Regensburg

We study the dynamics of an electron spin in a graphene quantum dot, which is interacting with a bath of less than ten nuclear spins via the anisotropic hyperfine interaction. Due to substantial progress in the fabrication of graphene quantum dots, the consideration of such a small number of nuclear spins is experimentally relevant. This choice allows us to use exact diagonalization to calculate the longtime average of the electron spin as well as its decoherence time. We investigate the dependence of spin observables on the initial states of nuclear spins and on the position of nuclear spins in the quantum dot. Moreover, we analyze the effects of the anisotropy of the hyperfine interaction for different orientations of the spin quantization axis with respect to the graphene plane. Interestingly, we then predict remarkable long decoherence times of more than 10ms in the limit of few nuclear spins.

TT 61.8 Wed 11:30 POT 051

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

We investigate the ultrafast dynamics of low-energetic Dirac electrons in graphene under Landau quantization [1]. In a joint experiment-theory study, we provide calculations based on the density matrix formalism [2] as well as measurements of the relaxation dynamics via differential transmission spectroscopy.

As a consequence of the linear dispersion at the Dirac points, graphene exhibits a non-equidistant Landau level spectrum which allows to address specific transitions by optical pumping. Exploiting this to selectively excite the energetically lowest Landau levels, we employ pump-probe spectroscopy to explore the carrier dynamics in this regime. A surprising sign reversal in differential transmission spectra is observed both in experiment and theory and provides evidence for strong Auger scattering on a picosecond timescale. Our calculations even predict the occurrence of a substantial carrier multiplication in Landau quantized graphene [3].

[1] M. Mittendorff et al., (in preparation).

[2] E. Malic, A. Knorr, Graphene and Carbon Nanotubes: Ultrafast Optics and Relaxation Dynamics, (Wiley-VCH, Berlin, 2013).

[3] F. Wendler, A. Knorr, and E. Malic, (submitted).

TT 61.9 Wed 11:45 POT 051

Polarization dependence of optical carrier excitation in graphene — •Martin Mittendorff[1,2], Torben Winzer[3], Ermin Malic[3], Andreas Knorr[3], Harald Schneider[1], Manfred Helm[1,2], and Stephan Winnerl[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Technische Universität Berlin, Hardenbergstraße 36 10623 Berlin, Germany

We present near-infrared pump-probe measurements to investigate the polarization dependence of optical carrier excitation in graphene. Excitation with linearly polarized radiation leads to an anisotropic distribution of the nonequilibrium carriers in momentum space. This anisotropy can be revealed by the comparison of pump-probe signals for different polarization configurations. In parallel configuration the probe beam has the same polarization with respect to the pump beam, for the perpendicular configuration the polarization of the probe beam is rotated by 90°. The signal amplitude of the parallel configuration is about twice as large as compared to the perpendicular configuration. The initial relaxation process is faster for the parallel polarized probe beam, which leads to identical signals about 150 fs after excitation. At this time delay an isotropic carrier distribution is reached by electron-phonon scattering. These findings are confirmed by microscopic calculations.

TT 61.10 Wed 12:00 POT 051

Anisotropic photoinduced current injection in graphene — •Julien Rioux[1], John Sipe[2], and Guido Burkard[1] — [1]University of Konstanz — [2]University of Toronto

Quantum-mechanical interference effects are considered in carrier and charge current excitation in gapless semiconductors using coherent optical field components at frequencies ω and 2ω. Due to the absence of a bandgap, excitation scenarios outside of the typical operation regime are considered; we calculate the polarization and spectral dependence of these all-optical effects for single- and bilayer graphene. For linearly-polarized light and with one-photon absorption at ω interfering with 2ω absorption and ω emission, the resulting current injection is five times stronger for perpendicular polarization axes compared to parallel polarization axes. This additional process results in an anisotropic current as a function of the angle between polarization axes, in stark contrast with the isotropic current resulting from the typical interference term in graphene [Rioux et al., PRB 83, 195406 (2011)]. Varying the Fermi level allows to tune the disparity parameter $d = \eta_I^{xyyx}/\eta_I^{xxxx}$ closer to typical values in GaAs [$|d| \approx 0.2$, Rioux and Sipe, Physica E 45, 1 (2012)]: from -1, when the additional process is fully Pauli-blocked, to $-3/7$, when it is fully accessible, thus facilitating polarization sensitive applications.

TT 62: Spintronics I (organized by HL)

Time: Wednesday 10:15–12:00 Location: POT 006

TT 62.1 Wed 10:15 POT 006

Spin dynamics on the metallic side of the metal to insulator transition — •Jan G. Lonnemann, Kim Niewerth, Jens Hübner, and Michael Oestreich — Leibniz Universität Hannover - Abteilung Nanostrukturen, Hannover, Germany

Several theoretical works treat the spin dynamics in zinc-blende semiconductors, like GaAs, around the metal-to-insulator transition. Most of them fail to explain the extremely long lifetimes experimentally observed [1]. Recently, it was argued that the Dyakonov-Perel mechanism (DP), usually only applicable in the conduction band, can be extended towards hopping transport (HT) present in the impurity band [2]. The theoretical calculations predict a dependence on the carrier density differing strongly from the DP spin relaxation expected for the conduction band electrons. We present extremely low excitation Hanle depolarization measurements on precisely n-doped MBE grown samples in the range of carrier concentrations from 2 to $10 * 10^{16}$ cm^{-3}. The density dependence of the spin lifetimes extracted from our measurements indicates that the dephasing due to HT is not the dominant mechanism. Remarkably, there is no significant difference in the spin lifetimes obtained from measurements on MBE material, with extremely low compensation ratios, as compared with samples from commercial wafers. This further indicates that dephasing due to HT is not the dominant mechanism, since HT depends strongly on the compensation ratio.

[1] M. Römer et al.; *Phys. Rev. B*, **81**, 075216 (2010).
[2] G.A. Intronati et al.; *Phys. Rev. Lett.*, **108**, 016601 (2012).

TT 62.2 Wed 10:30 POT 006

Nanomechanical read-out and manipulation of a single spin — •Heng Wang and Guido Burkard — University of Konstanz, Department of Physics

The single electron spin in quantum dot is a promising candidate as a qubit for quantum computation and quantum information. We investigate detection as well as manipulation of the single spin in a suspended carbon nanotube quantum dot. The detection and the manipulation are based on the spin-mechanical coupling induced from the intrinsic spin-orbit coupling. We use a Jaynes-Cummings model with a quantized flexural mode of the resonator to describe the system. An external electric field is used to drive the resonator and to induce an the interaction between the single electron in the quantum dot and the external driving field. The spin states can be identified by measuring the mechanical motion of the nanotube, which is detected by observing the current through a nearby charge sensor. Arbitrary-angle rotations about arbitrary axes of the single electron spin can be achieved by varying the frequency and the strength of the external electric driving field.

TT 62.3 Wed 10:45 POT 006

Time-resolved electrical detection of the inverse spin Hall Effect after ps optical excitation — •Manfred Ersfeld[1], Ivan Stepanov[1], Sammy Pissinger[1], Christopher Franzen[1], Sebastian Kuhlen[1], Mihail Lepsa[2], and Bernd Beschoten[1] — [1]2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH, Germany

Electrical detection of spin currents give an insight into the microscopic mechanisms of spin transport and play an important role in spin electronics. In previous experiments spin currents due to spin Hall effect have been imaged in optical measurements as spin accumulation.[1]

Here we report on the first time-resolved electrical detection of spin precession in n-InGaAs in time-resolved measurements of the inverse spin Hall effect. Net spin currents are achieved by applying electric fields and by polarization of the electrons with circularly polarized picosecond laser pulses. Electron spin precession in an external magnetic field can be monitored using a phase-triggered sampling oscilloscope as an oscillating voltage perpendicular to the applied electric field. Temperature dependent measurements of the spin Hall effect are presented. Time-resolved Faraday rotation measurements on the same sample under identical experimental conditions show good agreement between the measured spin dephasing times and the g-factor in the spin Hall measurements.

This Work has been supported by DFG through FOR 912

[1] Y. K. Kato et al., Science 306, 1910 (2004)

TT 62.4 Wed 11:00 POT 006

Terahertz out-of-plane resonances due to spin-orbit coupling — •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

A microscopic kinetic theory is developed which allows to investigate non-Abelian SU(2) systems interacting with mean fields and spin-orbit coupling under magnetic fields in one, two, and three dimensions. The coupled kinetic equations for the scalar and spin components are presented and linearized with respect to an external electric field. The dynamical classical and quantum Hall effect are described in this way as well as the anomalous Hall effect for which a new symmetric dynamical contribution to the conductivity is presented. The coupled density and spin response functions to an electric field are derived including arbitrary magnetic fields. The magnetic field induces a staircase structure at frequencies of the Landau levels. It is found that for linear Dresselhaus and Rashba spin-orbit coupling a dynamical out-of-plane spin response appears at these Landau level frequencies establishing terahertz resonances. (EPL, 104 (2013) 2700)

TT 62.5 Wed 11:15 POT 006

Resonant spin amplification in intrinsic bulk germanium — •Jan Lohrenz, Timo Paschen, and Markus Betz — Experimentelle Physik 2, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund

Recent experiments have revealed the possibility to optically orient electron spins in bulk germanium via indirect optical transitions. However, the temporal limitations to both the spin lifetime and the coherence of photogenerated electrons have remained unexplored so far. Here we demonstrate resonant spin amplification in intrinsic bulk germanium using a 90 MHz femtosecond pulse train at 0.8 eV central photon energy. Most importantly, we find remarkably long spin lifetimes exceeding 50 ns at temperatures of up to 60 K, limited by Elliott Yafet type processes. Consistent with model simulations we also find pronounced signatures of the g-factor anisotropy in germanium in the resonant spin amplification data.

TT 62.6 Wed 11:30 POT 006

Ultrahigh Bandwidth Spin Noise Spectroscopy — •Fabian Berski, Hendrik Kuhn, Jan G. Lonnemann, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

We advance all optical spin noise spectroscopy (SNS) in semiconductors to detection bandwidths of several hundred gigahertz by employing a sophisticated scheme of pulse trains from ultrafast laser oscillators as an optical probe [1]. The ultrafast SNS technique avoids the need for optical pumping and enables nearly perturbation free measurements of extremely short spin dephasing times. We apply the technique to highly-n-doped bulk GaAs where magnetic field dependent measurements show unexpected large g-factor fluctuations. Calculations suggest that such large g-factor fluctuations do not necessarily result from extrinsic sample variations but are intrinsically present in every doped semiconductor due to the stochastic nature of the dopant distribution.

[1] Berski, F., et al., Phys. Rev. Lett. **111**, 186602 (2013).

TT 62.7 Wed 11:45 POT 006

Effect of Nuclear Quadrupole Moments on Electron Spin Coherence in Semiconductor Quantum Dots — •Erik Welander[1], Evgeny Chekhovich[2], Alexander Tartakovskii[2], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Department of Physics and Astronomy, University of Sheffield, United Kingdom

We theoretically investigate the influence of the fluctuating Overhauser field on the spin of an electron confined to a quantum dot. The fluctuations arise from nuclear spin being exchanged between different nuclei via the nuclear magnetic dipole coupling. We focus on the role of the nuclear interaction from electric quadrupole moments (QPM), which generally cause a reduction in internuclear spin transfer efficiency. By dividing the nuclear problem into subcells we are able to describe $10^4 - 10^5$ nuclei, which are realistic numbers for a quantum dot. The effects on the electron spin coherence time are studied by

modeling an electron spin echo experiment. We find that the QPM cause an increase in the electron spin coherence time and that an inhomogeneous distribution, where different nuclei have different QPM, causes an even larger increase than a homogeneous distribution.

TT 63: Topological Insulators: Theory (organized by HL)

Time: Wednesday 9:30–11:15 Location: POT 151

TT 63.1 Wed 9:30 POT 151

Stabilizing Chern and fractional Chern insulators — •Adolfo G. Grushin, Johannes Motruk, and Frank Pollmann — Max Planck Institute for the Physics of Complex Systems, Dresden

The experimental realization of Chern insulators (CI) and fractional Chern insulators (FCI), zero field lattice analogues of the integer and fractional Hall effects respectively, is still a major open problem in condensed matter. For the former, it was proposed that short range interactions at the mean-field level can drive a trivial insulator into a CI. For the latter, the effect of band dispersion and sizes of the single-particle gaps with respect to the interaction strength have been argued to be important to stabilize an FCI state. In this talk we will examine the robustness and fate of these statements both with exact diagonalization and infinite density matrix renormalization group (iDMRG).

TT 63.2 Wed 9:45 POT 151

Point contacts and localization in generic helical liquids — •Christoph P. Orth, Grégory Strübi, and Thomas L. Schmidt — University of Basel, Switzerland

We consider two helical liquids on opposite edges of a two-dimensional topological insulator, which are connected by one or several local tunnel junctions. In the presence of spatially inhomogeneous Rashba spin-orbit coupling, the spin of the helical edge states is momentum dependent, and this spin texture can be different on opposite edges. We demonstrate that this has a strong impact on the electron transport between the edges. In particular, in the case of many random tunnel contacts, the localization length depends strongly on the spin textures of the edge states.

TT 63.3 Wed 10:00 POT 151

***ab-initio* investigation of topological states and symmetry inversion in HgTe-CdTe Quantum wells** — •Sebastian Kuefner, Juergen Furthmueller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

Topological insulators (TIs) recently attracted a high level of attention in solid state physics due to their unique physical properties. Generally, a TI is a material that is insulating in the bulk but exhibits metallic surface or edge states. These states are topologically protected which means that they are independent of surface orientation and passivation. The edge states usually have linear band dispersion forming Dirac cones.

The electromagnetic properties of the edge states might be used for the realisation of topological superconducting phases. In two dimensions the edge states build the quantum spin Hall state (QSH). In 2006, Bernevig et al. predicted the occurence of the QSH in HgTe-CdTe superlattices theoretically by an **kp**-approch which was later verified by König et al. experimentally.

However, these results have not yet been discussed in the framework of a reasonable electronic structure theory based on *ab-initio* methods but account for quasiparticle effects and spin-orbit coupling. Using density-functional theory together with the Tran-Blaha approximation we discuss the occurence of topological quantum-well states and investigate the topological transition in atomic structures.

TT 63.4 Wed 10:15 POT 151

Nontrivial Interface States Confined Between Two Topological Insulators — •Tomáš Rauch[1], Markus Flieger[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle (Saale), Germany

By *ab initio*-based tight-binding calculations, we show that nontrivial electronic states exist at an interface of a $\mathcal{Z}_2$ topological insulator and a topological crystalline insulator. At the exemplary (111) interface between Bi_2Te_3 and SnTe, the two Dirac surface states at the Brillouin zone center $\bar{\Gamma}$ annihilate upon approaching the semi-infinite subsystems but one topologically protected Dirac surface state remains at each time-reversal invariant momentum $\bar{\mathrm{M}}$. This leads to a highly conducting spin-momentum-locked channel at the interface but insulating bulk regions. For the Sb_2Te_3/Bi_2Te_3 interface we find complete annihilation of Dirac states because both subsystems belong to the same topology class.

TT 63.5 Wed 10:30 POT 151

Natural three-dimensional topological insulators in Tl_4PbTe_3 and Tl_4SnTe_3 — •Chengwang Niu[1,2], Ying Dai[1], Baibiao Huang[1], Gustav Bihlmayer[2], Yuriy Mokrousov[2], Daniel Wortmann[2], and Stefan Blügel[2] — [1]School of Physics, Shandong University, Jinan, China — [2]Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The recently discovered three-dimensional topological insulators have attracted much interest due to their exceptional properties of possessing insulating bulk but time-reversal symmetry protected metallic surfaces with Dirac-like band structure [1,2]. The search for new topological insulators is critical for both fundamental and practical interests. Based on first-principles calculations, we reveal that both Tl_4PbTe_3 and Tl_4SnTe_3 are strong topological insulators with different band inversion behaviors at Γ point [3]. The mechanisms of band inversion in Tl_4PbTe_3 and Tl_4SnTe_3, as well as in Bi_2Se_3 and Sb_2Se_3, are investigated and classified. The Z_2 topological invariants and topological surface states are investigated to confirm the topologically non-trivial phase. Our calculations further indicate that the electron- or hole-type Dirac fermion can be effectively engineered by hole doping, which is necessary for device applications of topological insulators.

[1] M. Hasan and C. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
[2] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).
[3] C. Niu et al., in preparation.

TT 63.6 Wed 10:45 POT 151

Electronic properties of the topological crystalline insulator SnTe and its (001) and (111) surfaces: an ab-initio study — •Matthias Drüppel, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster

The insulator SnTe belongs to the recently discovered class of materials in which a crystalline symmetry ensures the existence of topologically protected surface states. We report on the properties of these states at the (001) and (111) surfaces. To this end, we have employed density-functional theory.

The bulk band structure of SnTe is characterized by inversion at the four equivalent L points giving rise to a mirror Chern number $n_m = -2$. The (001) surface exhibits two mirror planes and shows four Dirac cones at non-time-reversal-invariant points along the $\pm\bar{\Gamma}\bar{\mathrm{X}}$ and $\pm\bar{\Gamma}\bar{\mathrm{X}}'$ lines, respectively. Here we explore the influence of lattice deformations on the stability of the surface states. Our results reveal that distortions of the topmost layers which break a mirror symmetry locally at the surface do *not* lead to an opening of the surface band gap. We find that only *bulk* lattice deformations, e.g. rhombohedrial distortions, that break one or both mirror symmetries also in the bulk part of the system give rise to a surface band gap. Our calculations show that the Sn terminated (111) surface exhibits Dirac cones centered at $\bar{\Gamma}$ and $\bar{\mathrm{M}}$. In particular at the $\bar{\mathrm{M}}$ point, these topologically protected states are distinctly extended into the bulk. Interestingly, we observe for the Te terminated (111) surface a gap-closing Dirac state only at the $\bar{\Gamma}$ point

TT 63.7 Wed 11:00 POT 151

Adsorbate- and vacancy-induced band bending in Bi_2Se_3: ab-initio calculations — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Bi_2Se_3 is one of the first topological insulators ever discovered. It has been widely studied both experimentally und theoretically, due to its

simple electronic structure with only one Dirac point at $\bar{\Gamma}$. In experiments, a downward band bending and an ageing effect are frequently observed. This has been attributed to an intrinsic n-doping and to coverage with adsorbates. Models for the band bending mostly focussed on the intrinsic doping.

Using DFT calculations, we show that a long-ranged potential also occurs for an adsorbate-covered surface, even without intrinsic doping. As a prototype adsorbate, we have investigated potassium at various coverages. The resulting changes in the charge density, the potential, and the band structure can be attributed to two distinct origins: short-ranged adsorbate-specific changes and the formation of a long-ranged potential (which is independent of the specific adatom). We will explain how the band bending is related to the layered structure of Bi_2Se_3. Similar effects result from our calculations for different types of adsorbates as well as for selenium vacancies in the surface layer.

TT 64: Quantum Dots: Optical Properties I (organized by HL)

Time: Wednesday 9:30–11:15 Location: POT 251

TT 64.1 Wed 9:30 POT 251

Single line emission of InGaN quantum dots grown on AlGaN templates — •Elahe Zakizadeh, Carsten Laurus, Stephan Figge, Timo Aschenbrenner, Kathrin Sebald, Jürgen Gutowski, and Detlef Hommel — Institute of Solid State Physics, University of Bremen, Germany

InGaN quantum dots (QDs) are a good candidates for realizing single-photon emission in the blue to green spectral region at elevated temperatures, because of the large bandgap and high exciton binding energies of the nitrides. Up to now, temperature dependent measurements demonstrate thermal stability up to 150 K of the emission of a single InGaN quantum dot grown on GaN template.

In order to achieve single-line emission at even higher temperatures, an enhancement of the carrier confinement in the quantum dots is needed. This can be realized by growing InGaN quantum dots on AlGaN templates by metal organic vaper phase epitaxy.

In this contribution we present the optical properties of single InGaN quantum dots achieved by the micro-photoluminescence measurements. The thermal stability of the emission lines and their dependance on the excitation density will be discussed.

TT 64.2 Wed 9:45 POT 251

Electronic coupling and luminescence dynamics of hybrid inorganic core/organic shell nanostructures — •Stephanie Bley, Michael Diez, Angelina Vogt, Jürgen Gutowski, and Tobias Voss — Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen, Germany

Hybrid core/shell nanostructures allow for spectral tuning of light emission and absorption processes what is of substantial interest for light-sensing and energy harvesting applications. Here, we study the luminescence decay dynamics of colloidal CdSe quantum dots (QDs) in different solvents and on different semiconducting and insulating surfaces. The QDs are optically excited with light from an optical parametric amplifier pumped by a Ti:Sapphire laser system. The time resolved luminescence signal is detected using a streak camera. The radiative recombination processes in the quantum dots attached to different three-dimensional nanostructure surfaces can be strongly influenced by different electron tunneling processes from excited states of the quantum dots into the conduction band of the nanostructures. In this context the experimental results show that different solvents and materials significantly change the decay process of the QDs. Possible reasons for decay time variations, including different polarities of solvents and dielectric constants of the solids, will be discussed.

TT 64.3 Wed 10:00 POT 251

Cubic GaN/AlN quantum dots - Characterization of individual emission lines — •Dmitrij Bostanjoglo[1], Gordon Callsen[1], Stefan Kalinowski[1], Gerald Hönig[1], Matthias Bürger[2], Donat As[2], Toni Markurt[3], Martin Albrecht[3], Andrei Schliwa[1], Stephan Reitzenstein[1], and Axel Hoffmann[1] — [1]TU Berlin, Germany — [2]Universität Paderborn, Germany — [3]Leibniz Institut für Kristallzüchtung, Germany

Group III-nitride quantum dots (QDs) with a wurtzite crystal structure (WZ) are plagued by a large spatial electron-hole separation, due to built-in pyro- and piezoelectric fields. As a consequence, one observes large excitonic lifetimes from the ns- up to the us-range in such QDs accompanied by a strong reduction of the overall light output. As most natural alternative to the WZ QDs one can examine their zincblende (ZB) counterparts. By growing nitride QDs onto ZB substrates such as 3C-SiC, the metastable ZB structure can be stabilized leading to the absence of spontaneous and a reduced piezoelectric polarization. Hence, a drastic reduction of the excitonic lifetime down to the 100 ps regime is observed. However, prior studies lack an interpretation of the physical origin of the observed emission lines. We examined the ZB GaN/AlN QDs in a time-resolved micro-photoluminescence setup. The measured decay times of all occurring excitonic complexes yield values from 100 ps up to 5 ns. This observation clearly demonstrates an enhanced charge carrier overlap. Our conclusive identification of the emission lines is supported by an analysis of the power- and polarization-dependence of all occurring emission lines.

TT 64.4 Wed 10:15 POT 251

Observation of carrier relaxation dynamics in Quantum Dot Excited State Laser — Holger Schmeckebier[1], Dejan Arsenijevic[1], Dieter Bimberg[1], •Bastian Herzog[2], Yücel Kaptan[2], Nina Owschimikow[2], Ulrike Woggon[2], Vissarion Mikhelashvili[3], and Gadi Eisenstein[3] — [1]Institute of Solid-State Physics, Technical University Berlin, Germany — [2]Institute of Optics and Atomic Physics, Technical University Berlin, Germany — [3]Electrical Engineering Dept. Technion - Israel Institute of Technology, Haifa, Israel

Single- and two-color Heterodyne pump-probe measurements were used to investigate the carrier dynamics of an InAs/InGaAs quantum dot based excited state laser at room temperature. Our main attention has been attracted by the excitonic ground state relaxation dynamics before and after the onset of excited state lasing, giving information about possible carrier relaxation paths. We found an ultrafast recovery with higher device currents, showing no change at and above the excited state lasing threshold. This could be an indication for a decoupling of the ground state gain recovery from the excited state gain dynamics. Two-color pump-probe experiments were performed to identify the excited state and ground state sub-ensemble belonging to the equal dot sub-ensemble.

TT 64.5 Wed 10:30 POT 251

Deterministic fabrication of quantum-dot microlenses for enhanced photon extraction efficiencies — •Manuel Gschrey, Marc Seifried, Luzy Krüger, Jan-Hindrik Schulze, Tobias Heindel, Sven Rodt, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623, Germany

The realization of building blocks for long-distance quantum communication is a major driving force for the development of advanced nanophotonic devices, like efficient quantum-dot-based single-photon sources. One major challenge of a deterministic device fabrication using self-assembled quantum dots (QDs) results from their random growth, which reduces the yield of usable nanophotonic devices. Another issue is the low extraction efficiency (EE), due to the high refractive index of the surrounding semiconductor material, where total internal reflection at the surface occurs already for very small angles. To overcome these obstacles we apply a recently developed cathodoluminescence (CL) lithography technique [1] to fabricate and position microlenses on top of preselected single InGaAs QDs. This in-situ lithography technique is based on low-temperature CL spectroscopy, to identify the spectral features and spatial positions of the statistically grown QDs, prior to the lithography step. To obtain optimum EE, the position and shape of the lens is directly taylored in the CL-system by means of 3D electron-beam lithography. By using this technique we fabricated microlenses that allow for a sixfold increase in EE as compared to plain surfaces - [1] M. Gschrey et al., APL 102, 251113 (2013).

TT 64.6 Wed 10:45 POT 251

Non-resonant and resonant optical spectroscopy of single self-assembled quantum dots, weakly coupled to a two dimensional electron gas — •Annika Kurzmann[1], Benjamin Merkel[1], Arne Ludwig[2], Andreas Wieck[2], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CeNIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Chair of Applied Solid State Physics, Ruhr-Universitaet Bochum, Universitaetsstr. 150, 44780 Bochum, Germany

Self-assembled quantum dots (QDs) are promising candidates for single-photon sources and as hosts for spin qubits. For such applications, the QDs are often embedded in a diode structure which allows controlled charging by tunneling of electrons from a 3D, n-doped reservoir, with fast tunneling times in the order of nanoseconds. Here we show results from photoluminescence, differential reflection, resonant fluorescence, and correlation measurements on a single InAs QD, coupled weakly (tunneling times in the order of milliseconds) to a two-dimensional electron gas (2DEG).

By tuning the electrical field, we are able to occupy the QDs with single charge resolution and observe different excitonic emission lines simultaneously over a large voltage range under non-resonant excitation. This unusual behavior can be explained by auto- and cross-correlation measurements of the exciton and trion recombination line and resonant optical measurements, which give in sight into the capture rates of electrons and holes into the dot states.

TT 64.7 Wed 11:00 POT 251

Charge noise and spin noise in a semiconductor quantum device — •Andreas Kuhlmann[1], Jonathan Prechtel[1], Julien Houel[1], Arne Ludwig[1,2], Dirk Reuter[2], Andreas Wieck[2], Martino Poggio[1], and Richard Warburton[1] — [1]University of Basel, Switzerland — [2]Ruhr-Universität Bochum, Germany

Self-assembled QDs are potentially excellent single-photon sources. The linewidths are in the best case a factor of two larger than the transform-limit. Optimizing performance demands an understanding of noise and a strategy to circumvent its deleterious effects.

There are two sources of noise inherent to the semiconductor: charge noise and spin noise[1]. We present an investigation of noise in an ultra-clean semiconductor quantum device, using a minimally-invasive, ultra-sensitive, local probe: resonance fluorescence from a single QD. We present noise spectra with 6 decades of resolution in the noise power over 6 decades of frequency, from 0.1 Hz to 100 kHz. Significantly, we have discovered a spectroscopic way to distinguish charge noise from spin noise. We present a dynamic feedback technique to remove charge noise from the device[2]. We show that nuclear spin noise is the dominant dephasing mechanism that limits performance as a single-photon source. For the charged exciton, we demonstrate a significant decrease in the spin noise with resonant laser excitation. This noise reduction for the charged exciton is exploited to demonstrate transform-limited optical linewidths even when the measurement is performed very slowly.

[1] A. V. Kuhlmann et al., Nature Phys. 9, 570 (2013). [2] J. H. Prechtel et al., Phys. Rev. X 3, 041006 (2013).

TT 65: Quantum Dots: Optical Properties II (organized by HL)

Time: Wednesday 11:30–13:00 Location: POT 251

TT 65.1 Wed 11:30 POT 251

Revealing the local environment noise of a quantum dot through resonance fluorescence intensity statistics — •Megan Stanley, Clemens Matthiesen, and Mete Atatüre — Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge CB3 0HE, UK

The electronic level structure and optical transitions of quantum dots are subject to fluctuating electric fields from nearby charge traps and a noisy Overhauser field from local nuclear spins [1]. The resultant inhomogeneous electron spin dephasing and reduced photon spectral purity are detrimental to the use of dots in quantum information processing [2]. We combine the intensity autocorrelation of resonance fluorescence (RF) and full photon counting statistics to capture the amplitudes and timescales of environment-induced fluctuations. Full counting statistics offer a robust and technically undemanding method to quantify steady-state spectral diffusion. In particular, it allows us to distinguish blinking or switching from continuous spectral shifts when this is not obvious from RF timetraces. Charge and nuclear spin contributions to noise are distinguished in autocorrelations via a detailed exploration of detuning and excitation power dependent sensitivities in comparison to a theoretical model. We find electric field noise to dominate down to timescales of 100us. Finally, we expose nuclear spin noise exclusively by decoupling the fluorescence from the electric field fluctuations using a two-colour noise compensation technique. [1] A. V. Kuhlmann et al., Nature Phys. 9, 570-575 (2013) [2] C. Santori et al., Nature 419, 594-597 (2002)

TT 65.2 Wed 11:45 POT 251

cQED-controlled anticorrelation between axial and lateral emission of quantum dot - micropillar cavities — •Caspar Hopfmann[1], Micha Strauss[2], Christian Schneider[2], Sven Höfling[2,3], Martin Kamp[2], Alfred Forchel[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Technische Physik, Universität Würzburg, D-97074 Würzburg, Germany — [3]University of St Andrews, North Haugh, KY16 9SS United Kingdom

Cavity quantum electrodynamics (cQED) in high quality quantum dot (QD) microcavities has been subject of extensive research interest in recent years. This includes the study of fundamental cavity effects in the weak and strong coupling regime as well as their application in non-classical light sources. Here, we present an advanced optical characterization method to obtain comprehensive insight into the relevant cQED effects in QD-micropillar cavities. In contrast to conventional approaches in which the micropillar is addressed only in axial direction via its top facet, we implement additionally an in-plane excitation and detection scheme. In this unique configuration, excitation and detection capabilities are available synchronously in the axial and in-plane direction which opens up appealing opportunities for a broad study of cQED effects. For instance, it allows one to investigate the interplay between coupling emission from the QDs into resonator modes and leaky modes, respectively. Indeed, we demonstrate a cQED-controlled anti-correlation between single-QD emission through the top facet via resonator modes and emission through the side-walls via leaky modes.

TT 65.3 Wed 12:00 POT 251

Stark shifts in single and vertically stacked GaAs QDs — •Arne Ungeheuer, Achim Küster, Andreas Graf, David Sonnenberg, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

We study the optical properties of single GaAs quantum dots (QDs) and quantum dot molecules (QDMs) in vertical electrical fields. The QDs and QDMs are fabricated using molecular beam epitaxy in combination with the local droplet etching (LDE) technique [1]. Using Al-droplets on AlGaAs substrates, nanoholes of some ten nanometers depth are drilled and subsequently filled with GaAs to form QDs or with a GaAs/AlGaAs/GaAs sequence to form QDMs. Here, we report on the electric field-dependent energy-shift of the excitonic states due to the quantum-confined Stark-effect. Using a Schottky-diode structure and a micro-photoluminescence setup we observe a red-shift up to 25 meV.

[1] D. Sonnenberg et al., Appl. Phys. Let. **101**, 183113 (2012)

TT 65.4 Wed 12:15 POT 251

Robust population inversion using an excitonic V-type three level system in a single InGaAs quantum dot — •Dirk Mantei[1], Jens Förstner[1], Simon Gordon[1], Yves Alexander Leier[1], Ashish Kumar Rai[2], Dirk Reuter[1], Andreas D. Wieck[2], and Artur Zrenner[1] — [1]Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, Warburger Straße 100, 33098 Paderborn, Germany — [2]Ruhr-Universität Bochum, Universitätsstraße 150, Gebäude NB, 44780 Bochum, Germany

For the optical manipulation of a single quantum system, diverse approaches such as Rabi Oscillations and the Adiabatic Rapid Passage are well established techniques. For instance they are used to realize quantum gates or single photon sources. To achieve an inversion

as complete as possible we present a new possibility by examining a single quantum system with V-type three level scheme, a common ground state and two distinguishable and separately excitable transitions. Their sequential, pulsed excitation allows for the preparation of a robust, fault-tolerant and phase-insensitive inversion. We experimentally demonstrate and theoretically describe this concept, which is based on the polarization-selective excitation of a fine structure split exciton ground state in a single InGaAs quantum.

TT 65.5 Wed 12:30 POT 251

Photocurrent spectroscopy of single InAs quantum dots at 1500 nm — •Simon Gordon[1], Matusala Yacob[2], Yves Alexander Leier[1], Dirk Mantei[1], Mohamed Benyoucef[2], Johann Peter Reithmaier[2], and Artur Zrenner[1] — [1]CeOPP, Universität Paderborn, Paderborn, Germany — [2]INA, Universität Kassel, Kassel, Germany

For long distance quantum communication it is essential to use flying qubits in the telecom wavelength bands. Quantum emitters or detectors in this wavelength regime can be realized with InAs quantum dots on InP substrate. In this work, such InAs quantum dots are investigated by low-temperature high resolution photocurrent spectroscopy. Suitable p-i-n diode structures with self-assembled quantum dots have been grown by molecular beam epitaxy on InP(100) substrates. The layer sequence of the diodes consists of an n-InP back contact, an intrinsic region of lattice-matched InAlGaAs, which contains the quantum dots, and a p-InP front contact. The quantum dots are resonantly excited by a tunable single-frequency diode laser. By changing the applied reverse voltage the resonance energy of the quantum dot is tuned by the quantum confined Stark effect with respect to the laser line. We observe clear ground state absorption of single dots over a large tuning range in the photocurrent response. The highly resolved absorption lines show for the investigated samples no fine-structure splitting. This behavior could be caused by single electron charging, which leads to the decay of trions.

TT 65.6 Wed 12:45 POT 251

Excitons in InAs-quantum dots measured by capacitance-voltage spectroscopy — Patrick Labud, •Arne Ludwig, Andreas D. Wieck, and Dirk Reuter — Ruhr-Universität Bochum, Lehrstuhl für Angewandte Festkörperphysik

Electron-electron and hole-hole interaction has been studied intensively on self-assembled quantum dot (QD) samples using capacitance-voltage spectroscopy (C-V) since two decades. The energetic positions of the charging peaks are considerably affected by the Coulomb interaction energies and in standard C-V spectra only the Coulomb repulsion is seen.

In this contribution, we present C-V data obtained under nonresonant illumination from a light emitting diode. Under these conditions, additional charging peaks appear due to attractive Coulomb interaction between illumination induced holes and electrons, tunnelling into the QD.

We are able to resolve up to five additional charging peaks belonging to an X^0, X^{1+}, X^{2+}, X^{3+}, X^{4+}-complex, formed upon electron charging. The individual Coulomb energies are calculated from the charging gate voltage and the charging dynamics is discussed.

TT 66: Focus Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale IV (organized by O)

Time: Wednesday 10:30–13:15 Location: TRE Ma

Topical Talk TT 66.1 Wed 10:30 TRE Ma

From Rydberg Crystals to Bound Magnons - Probing the Non-Equilibrium Dynamics of Ultracold Atoms in Optical Lattices — •Immanuel Bloch — Max-Planck Institut für Quantenoptik, Garching, Germany — Ludwig-Maximilians-Universität, Munich, Germany

Ultracold atoms in optical lattice form an ideal testbed to probe the non-equilibrium dynamics of quantum many-body systems. In particular recent high-resolution imaging and control techniques allow to probe dynamically evolving non-local correlations in an unprecedented way. As an example, I will focus in my talk on the dynamical excitation of spatially ordered Rydberg structures that are formed through laser exctiation from ground state Mott insulating atoms. In addition, I will show how single-spin and spin-pair impuritites can be used to directly reveal polaron dynamics in a strongy interacting superfluid or the bound state of two magnons in a Heisenberg ferromagnet - a problem discussed first theoretically more than 80 years ago by H.A. Bethe. New atom interferometric schemes to directly probe the Green's function of a many-body system through the impurity dynamics will be discussed.

TT 66.2 Wed 11:00 TRE Ma

Correlated Light-Matter Interactions in Cavity QED — •Johannes Flick[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

In the electronic structure community, the quantized nature of the electrons is usually (approximately) incorporated, whereas the electromagnetic field is mostly treated classically. In contrast, in quantum optics, matter is typically simplified to models with a few levels, while the quantized nature of light is fully explored. In this work, we aim at treating both, matter and light, on an equal quantized footing.
We present exact solutions for fully quantized prototype systems consisting of atoms or molecules placed in optical one- or two-dimensional high-Q cavities and coupled to the quantized electromagnetic modes in the dipole or quadrupole coupling regime. We focus on spontaneous emission, strong-coupling phenomena, dipole-dipole couplings including van-der-Waals interactions, and Förster resonance energy transfer (FRET), all beyond the rotating-wave approximation.
This work has implications for a future development of a time-dependent density functional theory formulation of QED [1,2] for correlated multi-photon configurations.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).
[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

TT 66.3 Wed 11:15 TRE Ma

Optimized effective potential approach to time-dependent density functional theory for many-electron systems interacting with cavity photons — •Camilla Pellegrini[1], Johannes Flick[2], Heiko Appel[2], Ilya V. Tokatly[1,3], and Angel Rubio[1,2] — [1]Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, E-20018 San Sebastían, Spain — [2]Fritz-Haber Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — [3]IKERBASQUE, Bilbao, Spain

In a recent paper [1] time dependent density functional theory has been generalized to many-electron systems strongly coupled to quantum electromagnetic modes of a microcavity. Here we construct an approximation for the corresponding exchange-correlation (xc) potential by extending the optimized effective potential (OEP) method to the electron-photon system. The derivation of the OEP equation employing the non-equilibrium Green's function formalism, and the first order approximation for the electronic self-energy is presented. Beyond the mean field level, the electron-photon coupling generates a time non-local photon-mediated interaction between the electrons, whose propagator enters the exchange-like diagram. We further show the approximated xc-potential for a model two-level diatomic molecule with one electron coupled to photon modes. The comparison between the obtained results and the exact numerical ones in the different coupling regimes (from weak up to ultra-strong) is discussed. [1] I.V. Tokatly, Phys. Rev. Lett. 110, 233001(2013)

TT 66.4 Wed 11:30 TRE Ma

Correlated photon-electron wavefunctions in cavity Quantum Electrodynamics — •Heiko Appel[1], Johannes Flick[1], Rene Jestaedt[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Experimental progress in recent years has enabled the fabrication of Fabry-Perot resonators with high optical quality factors (high-Q). Such cavities allow to study the interaction of matter with a quantized light field at the single-photon level (Nobel prize 2012). In this talk we present the real-time evolution of correlated photon-electron wavefunctions in optical one- and two-dimensional high-Q cavities. We discuss implications for a multi-component density functional theory for Quantum Electrodynamics [1,2] based on the time-dependent electron density and the photon energy density.

[1] M. Ruggenthaler, F. Mackenroth, and D. Bauer, Phys. Rev. A **84**, 042107 (2011).
[2] I. Tolkatly, Phys. Rev. Lett. **110**, 233001 (2013).

TT 66.5 Wed 11:45 TRE Ma

Photoelectron driven plasmaron excitations in (2x2)K/Graphite — •Bo Hellsing — Department of Physics, Gothenburg University, Sweden

A new type of plasmarons formed by the compound of photoelec- trons and acoustic surface plasmon (ASP) excitations is investigated in the system p(2 * 2)-K/Graphite. The physics behind these types of plasmarons, e-plasmarons, is different from the ones re- cently found in graphene and quantum well systems, where the loss features results from the photohole-plasmon interaction in the material, h-plasmarons. Based on the first principles scheme, Time dependent density functional (TDDFT), we calculated the linear response due to the presence of the escaping photo-electron and determine the ASP dispersion. The coupling between the photoelectron and the ASP gives rise to excitation of the e- plasmarons manifested by a broad dispersive feature shifted about 0.5 eV below parabolic K induced quantum well band (QWB) in agreement with the ARPES experiment by Agdal et al. The e-plasmarons should be considered as a source of the loss satellite structure in ARPES for 2D systems. In addition they are important to take into account in theoretical studies of different compounds as they reflect an additional channel for excitations of plasmons. This could then increase the photon-plasmon conversion yield which obviously is of interest in the field of plasmonics.

TT 66.6 Wed 12:00 TRE Ma

Charge-transfer excitations in organic systems from many-body perturbation theory — •Xavier Blase[1], Carina Faber[1,2], Paul Boulanger[1], Claudio Attaccalite[1], and Ivan Duchemin[2] — [1]Institut Néel, CNRS and UJF, Grenoble, France — [2]L_SIM/INAC, CEA, Grenoble, France

Charge-transfer excitations in organic systems lies at the heart of a large variety of physical phenomena, from photosynthesis to photovoltaics, photocatalysis or DNA denaturation. From a theoretical point of view, such nonlocal excitations are well known to lead to difficulties within the TDDFT framework, leading to the development of range-separated hybrids. We present here the merits of the Bethe-Salpeter formalism and demonstrate its ability to reproduce *cold* and *hot* Frenkel or charge-transfer excitations with remarkable accuracy [1-3]. Our calculations are based on a recent Gaussian basis implementation of the GW and Bethe-Salpeter formalism, the Fiesta initiative [1-4], allowing all-electron or pseudopotential excited states calculations for systems comprising several hundred atoms. Recent developments towards discrete and continuous embedding techniques within the many-body perturbation framework will be presented.

References: [1] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, 86, 155315 (2012). [2] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012). [3] I. Duchemin and X. Blase, Phys. Rev. B 87, 245412 (2013). [4] X. Blase, C. Attaccalite, V. Olevano, Phys. Rev. B 83, 115103 (2011).

TT 66.7 Wed 12:15 TRE Ma

Charge transfer from first principles: self-consistent *GW* applied to donor-acceptor systems — •Fabio Caruso[1,2], Viktor Atalla[1], Angel Rubio[1,3], Matthias Scheffler[1], and Patrick Rinke[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Oxford, UK — [3]Universidad del País Vasco, San Sebastián, Spain

Charge transfer in donor-acceptor systems (DAS) is determined by the relative alignment between the frontier orbitals of the donor and the acceptor. Semi-local approximations to density functional theory (DFT) may give a qualitatively wrong level alignment in DAS, if the ionisation potential of one molecule erroneously ends up above the electron affinity of the other. An unphysical fractional electron transfer will then result in weakly interacting DAS [1]. *GW* calculations based on first-order perturbation theory (G_0W_0) correct the level alignment. However, the ground state is unaffected by the G_0W_0 approach, and the charge-transfer properties remain on the level of the initial DFT calculation [1]. We demonstrate that self-consistent *GW* (sc*GW*) – based on the iterative solution of the Dyson's equation – provides an ideal framework for the description of charge transfer in DAS. The sc*GW* level alignment is in agreement with experimental reference data. In addition ground- and excited-state properties are described at the same level of theory. As a result, the electron density in DAS is consistent with the level alignment between donor and acceptor, leading to a qualitatively correct description of charge-transfer properties.

[1] V. Atalla, M. Yoon, F. Caruso, P. Rinke, and M. Scheffler, Phys. Rev. B **88**, 165122 (2013).

TT 66.8 Wed 12:30 TRE Ma

What Koopmans' compliant orbital-density dependent functionals can do for you: a comprehensive benchmark of the G2-set — •Giovanni Borghi[1], Ngoc Linh Nguyen[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]École Polytechnique Fédérale de Lausanne, Lausanne (VD), CH — [2]Centro S3, CNR–NANO, Modena, IT — [3]Department of Materials Science and Engineering, Penn State University, University Park (PA), USA

In this talk we present the results of benchmark calculations of the structure and electronic-structure of all molecules in the g2 set, using different flavours for Koopmans' compliant (KC) functionals. Results are compared not only to LDA and PBE, but also to orbital-density dependent calculations with the Perdew-Zunger self-interaction correction.

Our results assess the accuracy of Koopmans' compliant functionals in improving semilocal functionals to predict electronic eigenvalues and in particular ionization energies, with an accuracy that for molecules seems to be comparable or superior to that of many-body (GW) approaches. We also highlight how the Koopmans' condition tends to preserve the potential energy surface of the underlying functional, with higher reliability than e.g. PBE in structural predictions, while also providing good estimates of atomization energies.

The talk will also provide a general introduction to the theory of Koopmans' compliant functionals and their implementation in existing electronic structure codes.

Ref. Dabo *et al.*, PRB 82, 115121 (2010), and Psik highlight (2012).

TT 66.9 Wed 12:45 TRE Ma

The electronic structure of quinacridone: Optimally tuned range-separated hybrid functional versus GW results — Daniel Lüftner[1], Sivan Refaely-Abramson[2], Michael Pachler[1], Michael G. Ramsey[1], Leeor Kronik[2], and •Peter Puschnig[1] — [1]Institut für Physik, Karl-Franzens-Universität Graz, Austria — [2]Department of Materials and Interfaces, Weizmann Institute of Science, Israel

Quinacridone is an organic molecule (C20H12N2O2) utilized in the formation of organic pigments. It has also been discussed for usage in organic electronics particularly due to its stability under ambient conditions and its tendency to form self-assembled supramolecular networks. Here, we report on its electronic structure, both, for the isolated molecule as well as for the alpha- and beta- bulk molecular crystal polymorphs. We employ an optimally tuned range-separated hybrid functional (OT-RSH) within density functional theory as well as GW corrections within a many-body perturbation theory framework. A comparison of the theoretical results obtained with the different levels of theory and a subsequent comparison with experimental data from angle-resolved photoemission spectroscopy emphasize the need for going beyond simple semi-local DFT-functionals in order to obtain the correct orbital ordering. Furthermore the comparison indicates that the results obtained with OT-RSH greatly improve those of standard DFT functionals and achieve an agreement with experiment at the level of GW calculations, thus making the OT-RSH an alternative to the computationally more expensive GW approach.

TT 66.10 Wed 13:00 TRE Ma

GW many-body perturbation theory for electron-phonon coupling calculations — •Carina Faber[1,2], Paul Boulanger[1], Ivan Duchemin[1,2], and Xavier Blase[1] — [1]Institut Néel, CNRS, Grenoble, France — [2]INAC, CEA, Grenoble, France

We study within many-body perturbation theory the electron-phonon coupling in organic systems, taking as paradigmatic examples the fullerene molecule and the pentacene crystal [1,2]. We show that the

strength of the electron-phonon coupling potential is dramatically underestimated at the LDA level, while GW calculations offer an excellent agreement with experiments [1]. Further, combining GW calculations of the electronic band structure and of the electron-phonon coupling in crystalline pentacene, we show that the hole bands dispersion can be reconciled with photoemission experiments, by solving non-perturbatively (DMFT) the effect of electron-phonon coupling on the electronic self-energy [2]. We finally explore various approximations that may allow to combine the GW formalism with convenient linear response formalisms beyond the frozen-phonon techniques. Our calculations are performed with the Fiesta package, a Gaussian based GW and Bethe-Salpeter code allowing all-electron or pseudopotential calculations with various resolution of the identity techniques and without any plasmon pole approximation [3,4].

[1] C. Faber et al., Phys. Rev. B 84, 155104 (2011) [2] S. Ciuchi et al., Phys. Rev. Lett. 108, 256401 (2012) [3] C. Faber, I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. B, 86, 155315 (2012). [4] I. Duchemin, T. Deutsch, X. Blase, Phys. Rev. Lett. 109, 167801 (2012).

TT 67: Gaede Prize Talk (organized by VA; with DS, O, TT)

Time: Wednesday 12:30–13:00 Location: HSZ 02

TT 67.1 Wed 12:30 HSZ 02

Spectroscopy and microscopy of graphene on metals — •Yuriy Dedkov — SPECS Surface Nano Analysis GmbH, Berlin, Germany

Graphene on metals, which structure can vary from simple lattice matched to commensurate moiré structures, is an ideal system for different kinds of surface science experiments allowing to study many fascinating phenomena. Here we present several examples on the application of electron spectroscopy (NEXAFS, XMCD, XPS, ARPES) and scanning probe methods (STM and AFM) for the investigation of the electronic structure of these systems. These combined approaches allow to understand the bonding mechanism at the graphene-metal interface, the main features of the graphene-derived electronic structure as well as the imaging contrasts in the scanning probe experiments. All experimental data are compared with the state-of-the-art DFT calculations that lead to the deep understanding of the observed phenomena.

TT 68: Superconductivity: Fe-based Superconductors - Theory I

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

Invited Talk TT 68.1 Wed 15:00 HSZ 201

Novel Effects of Disorder in Multiband Unconventional Superconductors — •Peter J Hirschfeld — Phys. Dept.. U. Florida, Gainesville FL 32611, USA — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main

Impurities been studied in superconductors for many years because, depending on the type of impurity and on the symmetry of the superconducting state, they may break Cooper pairs. They thus play an important diagnostic role in deducing the type of superconductivity one has in a newly discovered material. I focus here on the Fe-based superconductors, which are multiband in character and probably exhibit unconventional pairing states, including so-called "s+/-" states which change sign of the order parameter between bands. Impurity scattering in such states depends sensitively on the ratio of intra- to interband scattering, giving rise to novel effects of disorder, including possible transitions to conventional "s++" states and lifting of gap nodes. I propose that one can uniquely identify an s+/- state by a sequence of transitions with controlled disorder, observable in bulk quasiparticle transport or NMR. I next focus on STM experiments, and the inability of current lattice-based theories to capture not only the fine structure of STM conductance maps, but also certain local symmetries. I propose to remedy this by using a Wannier-function based extension of the BdG equations of inhomogenous superconductivity. Finally, I discuss the role of correlations in creating C4 symmetry-broken emergent defect states, which may have important consequences for the ubiquitous electronic nematicity observed in these materials.

TT 68.2 Wed 15:30 HSZ 201

Suppression of T_c due to impurity scattering with a phase — •Mareike Hoyer[1], Sergey Syzranov[1,2], and Jörg Schmalian[1,3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Department of Physics, University of Colorado, Boulder, Colorado, USA — [3]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany

We consider weak disorder in a two-band superconductor and investigate the effect of a finite phase of the off-diagonal matrix element of the impurity potential in band representation. In particular, we analyze the impact on the superconducting transition temperature T_c. We concentrate on s^{++} and s^{+-} symmetries of the superconducting order parameter which are widely discussed as possible candidates in iron pnictides.

We argue that the effect of impurity scattering on the transition temperature in complex materials such as iron pnictides cannot be reduced to the consideration of single-particle scattering rates. Depending on the phase ϕ, we find that nonmagnetic impurities can act as pair-breakers for the s^{++} state while such impurities can leave T_c for the s^{+-} state unchanged.

TT 68.3 Wed 15:45 HSZ 201

Electronic and Magnetic Properties of $Ba(Fe_{1-x}Co_x)_2As_2$ — •Gerald Derondeau, Sergiy Mankovsky, Hubert Ebert, and Ján Minár — Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany

Characteristic for most iron arsenides is an antiferromagnetic ordering in form of a commensurate spin-density wave (SDW) at low temperatures, often coupled with a structural phase transition. Superconductivity emerges when these transitions are suppressed, e.g. by chemical doping. As many DFT calculations have still problems to accurately describe the magnetic state [1] further investigations on this issue are needed.

We investigated the low-temperature orthorhombic phase of $Ba(Fe_{1-x}Co_x)_2As_2$ using the Korringa-Kohn-Rostoker-Green function (KKR-GF) [2] approach which allows inclusion of chemical disorder via the coherent potential approximation (CPA). To examine the magnetic structure with different spin states we used a full magnetic unit cell with 8 Fe atoms and antiferromagnetic ordering. In addition spin-spiral calculations for the $\boldsymbol{q}$-dependent induced magnetization were performed to account for the SDW state. Furthermore, the doping dependent evolution of the strong in-plane anisotropy of the electronic structure as observed in ARPES measurements [3] was investigated and connected to the magnetic behavior.

[1] I. I. Mazin, M. D. Johannes, Nature Phys. *5*, 141 (2009)
[2] H. Ebert, D. Ködderitzsch, J. Minár, Rep. Prog. Phys. *74*, 96501 (2011)
[3] M. Yi, D. Lu, J.-H. Chu, *et al.*, PNAS *108*, 6878 (2011)

TT 68.4 Wed 16:00 HSZ 201

Electronic structure modification and ultrafast SDW generation due to coherent oscillation of the A_{1g} phonon mode in $BaFe_2As_2$ — •Bhaskar Kamble and Ilya Eremin — Institut für Theoretische Physik III, Ruhr Universität Bochum, 44801 Bochum, Germany

Time-resolved ARPES experiments on $BaFe_2As_2$ demonstrate an in-phase oscillation of the ARPES spectral function at the Γ and M points [1], while time-resolved (tr) optical conductivity measurements on normal $BaFe_2As_2$ detect a periodic Spin Density Wave (SDW) at ultrafast time scales [2]. The period of oscillation in both cases equals the A_{1g} phonon frequency in which the As atoms oscillate perpendicular to the Fe-planes. With a 5-orbital tight-binding (TB) model with the TB parameters dependent on the As-Fe-Fe angle α, and assuming that the

electrons react adiabatically to the α oscillation in the A_{1g} phonon, our calculations for changes in the electronic spectral function match well with tr-ARPES results if (i) α oscillates around a value slightly greater than its equilibrium value, and (ii) the electronic spectral function in the photoexcited state is calculated at a temperature higher than in the absence of the laser pulse. The mean-field magnetic order parameter for the (π,0) SDW state shows that the magnetization increases with α. This, coupled with the enhanced mean-α value in the photo-induced A_{1g} phonon, offers a simple explanation for the ultrafast SDW-generation observed in normal $BaFe_2As_2$.

[1] L. Rettig, Ph.D. thesis (Freie-Universität Berlin) (2012)
[2] K. W. Kim et al., Nature Mat. 11, 497 (2012)

TT 68.5 Wed 16:15 HSZ 201

LDA+DMFT study of the iron-pnictide superconductor KFe_2As_2 — •Steffen Backes, Daniel Guterding, Harald Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität, Frankfurt

We study the electronic structure of the iron pnictide superconductor KFe_2As_2, including electronic correlations within dynamical mean field theory. The recent theoretical studies based on density functional calculations (DFT) turned out to be unable to satisfactorily describe experimental observed properties of the electronic band structure. However, treating electronic correlations beyond the local density approximation within an LDA+DMFT (dynamical mean field theory) approach has shown to be a very effective method to overcome some of these discrepancies. Therefore, we perform a comprehensive LDA+DMFT investigation focused on features of the KFe_2As_2 compound that have not been dealt with in existing studies. We also benchmark our findings with ARPES measurements. Our results indicate that KFe_2As_2 is a moderately correlated metal, where the Fe $3d$ orbitals show an electron mass enhancement of a factor of about 2. We find that only when including correlations beyond DFT the shape and size of the hole Fermi surface in experiment can satisfactorily be described. Furthermore, due to correlations a topological change in the Fermi surface is induced, where compared to DFT the hole pocket at the Z point vanishes in LDA+DMFT in agreement with experiments. We also observe a strong k_z-dispersion of the middle hole cylinder around Γ along the k_z-axis , which is not seen in DFT.

15 min. break.

TT 68.6 Wed 16:45 HSZ 201

de Haas-van Alphen effect and effective masses in KFe_2As_2 from LDA+DMFT — •Daniel Guterding, Steffen Backes, Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

We investigate changes in de Haas-van Alphen (dHvA) frequencies and effective masses in the iron-based superconductor KFe_2As_2 upon inclusion of correlation effects beyond the local density approximation (LDA). Quantitative comparison of our findings to dHvA measurements shows that a combination of density functional theory with dynamical mean-field theory (LDA+DMFT) solves the disagreement between previous *ab-initio* calculations and experiment. We also show how to numerically extract de Haas-van Alphen frequencies and effective masses from band structure calculations.

TT 68.7 Wed 17:00 HSZ 201

Wannier orbitals via the projector method for LAPW and effects of correlation in the (collapsed) tetragonal phases of $CaFe_2As_2$ — •Jean Diehl and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

We present a scheme for constructing Wannier orbitals from a (linear) augmented plane wave basis set via projection. This method shows strong sensitivity on the chosen energy window as we discuss. On this projector method we build our code to implement dynamical mean field theory based on density functional theory.

The former introduced method is then used to study the effects of correlation by means of Hubbard U and Hund's rule J in one of the iron pnictides $CaFe_2As_2$. We present results for the band structure, Fermi surface and mass enhancements of the room-temperature ambient-pressure tetragonal and the high-pressure low-temperature collapsed tetragonal phase.

TT 68.8 Wed 17:15 HSZ 201

Using Space Group Representations to Unfold the Bandstructures of Iron Pnictides — •Milan Tomic, Roser Valentí, and Harald Jeschke — Institut für Theoretische Physik, Goethe-Universität, Frankfurt am Main, Germany

We present a general method for unfolding bandstructures beyond the limit of translational symmetry, utilizing irreducible representations of space groups. We demonstrate the method on the representative materials of 11 and 122 iron-pnictide family and discuss the result in context of ARPES experiments.

TT 68.9 Wed 17:30 HSZ 201

Topological Surface States in Paramagnetic, Antiferromagnetic, and Superconducting Iron Pnictides — •Alexander Lau — Institute of Theoretical Physics, Technische Universität Dresden, Dresden, Germany

Motivated by the topologically nontrivial electronic structure of iron pnictides, we study surface states in various strip geometries. For the paramagnetic phase, the existence of these states can be understood from a topological argument. If we go to the antiferromagnetic phase, the surface bands split, depending on the geometry of the strip. In the superconducting phase, assuming an $s_{\pm}$-wave gap structure, the topological surface states under certain conditions remain in the gap. Interestingly, they exist side by side with Andreev bound states for small superconducting gaps and even merge with them for increasing gap amplitude. The bulk and surface dispersions are obtained from exact diagonalisation of two- and five-orbital models.

TT 68.10 Wed 17:45 HSZ 201

Negative transport times in Fe-based superconductors — •Maxim Breitkreiz[1], Philip M. R. Brydon[2], and Carsten Timm[1] — [1]Institute of Theoretical Physics, Technische Universität Dresden, Dresden, Germany — [2]Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, USA

Negative transport times lead to unexpected transport behavior such as negative magnetoresistance, strongly enhanced Hall coefficient, and reduced resistivity. Within a semiclassical Boltzmann approach beyond the relaxation-time approximation, we demonstrate that negative transport times can arise in iron pnictides due to scattering of charge carriers at spin fluctuations. To explore this effect, we consider the temperature dependence of transport coefficients for a phenomenological two-band model relevant for iron pnictides.

TT 69: Correlated Electrons: Spin Systems and Itinerant Magnets - Chiral Magnets

Time: Wednesday 15:00–16:15 Location: HSZ 204

TT 69.1 Wed 15:00 HSZ 204

Effective mass of skyrmions in chiral magnets — •Christoph Schütte, Markus Garst, and Achim Rosch — Universität zu Köln, Zülpicher Straße 77, D-50937 Köln

A single skyrmion in a ferromagnetic background is due to its topological protection a long-lived, large-amplitude excitation. It can be described by a collective coordinate and interpreted as a quasi-particle. To understand its dynamics, it is not sufficient to consider only a rigid skyrmion but also the effects of fluctuations have to be included. We calculate the numerically exact fluctuation spectrum and scattering wavefunctions taking both thermal and quantum fluctuations into account. We show that this gives rise to additional terms in the effective action for the collective coordinate and determine the angle-resolved scattering amplitude and the mass of the skyrmion.

TT 69.2 Wed 15:15 HSZ 204

Small Angle Neutron Scattering of the Skyrmion Lattice Decay in Chiral Magnets — •Jonas Kindervater[1], Alfonso Chacon[1], Andreas Bauer[1], Sebastian Mühlbauer[2], and Christian Pfleiderer[1] — [1]Physik-Department E21, Technische Universität München, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany

Skyrmion lattices in chiral magnets differ from conventional magnetic order in terms of their non-trivial topology. In turn the phase transition between conventional magnetic order and the skyrmion lattice phase is always first order. An open question concerns thereby the specific microscopic mechanisms by which this first order phase transition takes place, i.e., by which the non-trivial topology unwinds. Using small angle neutron scattering we report detailed measurements of the time-dependence of the skyrmion lattice decay in $Fe_{1-x}Co_xSi$ after quenching the skyrmion lattice phase into a metastable state. As our main result we find pronounced differences for the decay into the helical and the conical phase as a function of temperature and magnetic field. We discuss our results in the context of recent magnetic force magnetometry of the skyrmion lattice to helical transition in the same material under similar conditions [1].

TT 69.3 Wed 15:30 HSZ 204

Spin chirality flips in transition-metal monogermanides — •Sven-Arne Siegfried[1], Evgeny.V. Altenbayev[2,3], Nadezhda M. Chubova[2], Vadim Dyadkin[4,2], Evgeny V. Moskvin[2,3], Vladimir Dimitriev[4], Dirk Menzel[5], Charles D. Dewhurst[6], Andre Heinemann[1], Dimitry Chernyshov[4], Ravil A. Sadykov[7,8], Sergey N. Axenov[7], Ludmila N. Formicheva[8], Anatoly V. Tsvyshchenko[8,9], Dieter Lott[1], Andreas Schreyer[1], and Sergey V. Grigoriev[2,3] — [1]Helmholtz-Zentrum Geesthacht, Germany — [2]Petersburg Nuclear Physics Institute, Russia — [3]Saint-Petersburg State University, Russia — [4]Swiss Norwegian Beamlines at ESRF, France — [5]TU Braunschweig, Germany — [6]Institute Laue-Langevin, France — [7]Institute for Nuclear Research, Russia — [8]Institute for High Pressure Physics, Russia — [9]Moscow State University, Russia

The $Mn_{1-x}Fe_xGe$ compounds are helimagnetically ordered within the full concentration range. Small-angle neutron diffraction measurements show a change of the helical wavevector from $|\mathbf{k}| = 2.23$ nm^{-1} for pure MnGe passing through a minimum at $x \approx 0.75$ (with $|\mathbf{k}| \to 0$) to a value of $|\mathbf{k}| = 0.09$ nm^{-1} for pure FeGe. The helical structure transforms to a ferromagnetic-like one for $x \to x_c$, along with a change of the magnetic chirality for $x < x_c$ and $x > x_c$. Further studies reveal similar behaviour for $Fe_{1-x}Co_xGe$ compounds [2]. We argue that this behaviour is caused not by the different signs of the Dzyaloshinskii-Moriya interaction but rather by the complex multi-shell exchange interaction.

[1] S.V. Grigoriev et al.,Phys. Rev. Lett. 110, 207201 (2013)
[2] S.V. Grigoriev et al., to be published.

TT 69.4 Wed 15:45 HSZ 204

Anisotropies in the phase transition between helical and conical state in MnSi — •Alfonso Chacon Roldan[1,3], Felix Rucker[1], Michael Wagner[1], Andreas Bauer[1], Tim Adams[1], Markus Garst[2], and Christian Pfleiderer[1] — [1]Physik Department E21, Technische Universität München, München, Deutschland — [2]Institut für Theoretische Physik, Universität zu Köln, Köln, Deutschland — [3]Heinz Maier-Leibnitz Zentrum, Garching b. München, Deutschland

We report a comprehensive study of the crystalline anisotropies of the cubic chiral helimagnet MnSi, in which we focus on the transition between the multi-domain helical state at low fields and the single-domain conical state at higher fields. Careful measurements of the magnetization and the transverse susceptibility as well as small-angle neutron scattering were carried out on a spherical sample in order to account for the effects of demagnetization fields. In combiniation with high-precision specific heat data, we establish a consistant picture and determine the cubic anisotropy terms of the free energy quantitatively.

TT 69.5 Wed 16:00 HSZ 204

Excitations in magnetoelectric Cu_2OSeO_3 — •Steffen Harms[1], Maria Belesi[2], Helmuth Berger[3], Jean-Philippe Ansermet[3], Daniel Niermann[1], Christoph Grams[1], and 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

The magnetoelectric helimagnetic insulator Cu_2OSeO_3 shows a multiplicity of magnetic phases due to the interplay of ferrimagnetic and Dzyaloshinkii-Moriya interaction. It was recently shown, that the excitations of these phases can be seen in the microwave absorption spectra where an AC magnetic field was coupled to the sample[1].
Additionally, topologically protected spin textures called skyrmions have been identified in these spectra. Since their discovery in MnSi, skyrmions have been of specialy interest because of their high potential for applications in spintronics[2].
We present the results of our broadband dielectric spectroscopy measurements up to 5 GHz, in which we measured the excitations created by coupling electric and magnetic AC-fields to the sample for different magnetic DC-fields at fixed temperatures of 57.5 K and 40 K.

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

[1] Y. Onose et al., Phys. Rev. Lett. 109, 037603 (2012)
[2] C. Pfleiderer and A. Rosch., Nature 465, 880 (2010)

TT 70: Transport: Topological Insulators II (organized by TT)

Time: Wednesday 16:30–18:30 Location: HSZ 204

TT 70.1 Wed 16:30 HSZ 204

Rashba spin orbit coupling in the Kane-Mele-Hubbard model — •Stephan Rachel — Institut für Theoretische Physik, TU Dresden

Spin-orbit (SO) coupling is the crucial ingredient for topological insulating phases. In particular, the generic emergence of SO coupling involves the Rashba term which fully breaks the SU(2) spin symmetry. As soon as interactions are taken into account, however, many theoretical studies have to content themselves with the analysis of a simplified U(1) conserving SO term without Rashba coupling. We intend to fill this gap by studying the Kane-Mele-Hubbard model in the presence of Rashba SO coupling. We apply the variational cluster approach to determine the interacting phase diagram by computing local density of states, magnetization, single particle spectral function, and edge states.

We find that the Rashba SO coupling drives new electronic phases such as a metallic regime and a "gapless topological insulator phase" which persist in the presence of interactions.

TT 70.2 Wed 16:45 HSZ 204

Conductivity of a generic helical liquid — •Nikolaos Kainaris[1], Igor Gornyi[1,2,4], Sam Carr[3], and Alexander Mirlin[1,2,5] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]School of physical sciences, University of Kent, Canterbury, UK — [4]A.F. Ioffe Physico-Technical Institute, St. Petersburg, Russia — [5]Petersburg Nuclear Physics Institute, St. Petersburg, Russia

We study the transport properties of a helical Luttinger liquid without S_z symmetry. We focus on the case of long edges of 2D topological insulators and calculate the conductivity in the presence of both interactions and disorder. In the regime where temperature is larger than the frequency of the external field we use a kinetic equation approach to calculate the AC and DC conductivity for weakly interacting fermions. The opposite regime of the AC conductivity is discussed via full bosonization that allows us to treat certain interactions exactly. We find the dependence of the conductivity on temperature, frequency and Fermi energy for different scattering mechanisms and discuss their relevance to transport.

TT 70.3 Wed 17:00 HSZ 204

Influence of a random Rashba spin-orbit coupling on the transport properties of helical liquids — •Florian Geissler, Francois Crepin, and Björn Trauzettel — Theoretische Physik IV, Universität Würzburg, Germany

In a quantum spin Hall system, the edge states are one-dimensional and helical, i.e. their (pseudo) spin degree of freedom and their direction of motion are strongly coupled to each other. This coupling gives rise to protection against elastic backscattering off non-magnetic impurities. Here, we analyze inelastic (two-particle) backscattering in interacting helical liquids in presence of random Rashba spin-orbit coupling. To study this peculiar type of disorder, we bosonize the Hamiltonian and employ a combination of operator product expansion and renormalization group calculations. Thereby, we obtain a consistent set of flow equations for the renormalization of the Luttinger liquid parameters, the disorder strength, and the two-particle backscattering. Finally, we discuss the corrections to the conductance at finite temperature stemming from this type of disorder.

TT 70.4 Wed 17:15 HSZ 204

Generic Helical Liquids: the effect of rotation of the spin-quantization axis — •Alexia Rod[1], Thomas L. Schmidt[2], and Stephan Rachel[1] — [1]Institut für Theoretische Physik, TU Dresden — [2]Department of Physics, University of Basel

The generic helical liquid is the most general model of a time-reversal invariant helical liquid without axial spin symmetry. This symmetry is usually broken in experimental realizations, and it has been shown that its absence changes the transport properties significantly [1]. For a translation invariant system, the breaking of axial spin symmetry manifests itself in a rotation of the spin quantization axis with momentum. Its manifestation in real space has, however, remained elusive. Here we consider topological insulator sheets and discs and investigate the non-trivial spin structure of the helical edge states. We further propose how to measure this spin structure and discuss potential applications. [1] T.L. Schmidt, S. Rachel, F. von Oppen, L. Glazman, Phys. Rev. Lett. 108, (2012).

TT 70.5 Wed 17:30 HSZ 204

Hanbury Brown-Twiss and Aharonov-Casher effects in a quantum spin Hall Corbino ring — •Anders Ström[1], Henrik Johannesson[2], and Patrik Recher[1] — [1]Institute for Mathematical Physics, TU Braunschweig, Germany — [2]Department of Physics, University of Gothenburg, Sweden

We study the entanglement production in a quantum spin Hall ring where electrons of different spins are emitted from a biased source and detected in two different grounded detectors. The fermionic Hanbury-Brown Twiss effect gives rise to entanglement in the system, measurable via the current-current correlations between the detectors. The production of entanglement is electrically controlled via the Aharonov-Casher phases arising from the Rashba coupling in the system.

TT 70.6 Wed 17:45 HSZ 204

Proximity induced perfectly conducting channel in 2D-metal topological insulator heterostructures — •Sven Essert, Viktor Krueckl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Two-dimensional topological insulators have attracted much attention because of their peculiar edge-state transport features. We investigate how these properties carry over to heterostructures made of topological insulators and materials with extended states which are not topologically classifiable (metallic systems).

We find that the proximity of a topological insulator induces a perfectly conducting channel in the metal which is however not localized along the edge but spanning the whole extended state region. This resembles the perfectly conducting channels predicted in graphene nanoribbons and carbon nanotubes. However, the proximity induced channel is expected to be stable even with short-range disorder which should simplify its observation.

We propose experiments to detect this effect by conductance and shot-noise measurements and also show how the proximity of a topological insulator can be understood in terms of an effective boundary condition.

TT 70.7 Wed 18:00 HSZ 204

Majorana fermions on a hexagonally warped 3D topological insulator in proximity to a superconductor — •Daniel Mendler, Panagiotis Kotetes, and Gerd Schön — Institut für theoretische Festkörperphysik, KIT, Karlsruhe

The recent discovery of topological insulators (TIs) opened new perspectives in the field of topological quantum computing (TQC), in terms of Majorana fermions (MFs). The latter are expected to appear in the vortex cores of artificial topological superconductors (TSCs), engineered from the surface states of a 3D-TI in proximity to a conventional SC. Nonetheless, if time-reversal symmetry is spontaneously broken on the TI surface, the hybrid system supports Majorana fermions without the requirement of vortices. The latter property can be advantageous for the experimental realization of TSCs and facilitate the implementation of TQC protocols. In this work, we investigate the above scenario for the hexagonally warped Dirac itinerant surface states of Bi2Te3, which demonstrate enhanced tendency towards the spontaneous formation of magnetism due to Fermi surface nesting. We perform a complete classification of the accessible spin density wave order parameters in the presence of a repulsive Hubbard-like interaction and retrieve the hierarchy of magnetic phase transitions which can occur in the particular system. For the dominant magnetic instability, we investigate the conditions which favor proximity induced SC on the magnetic TI surface. We explicitly demonstrate the emergence of MFs in this system and propose methods for their manipulation.

TT 70.8 Wed 18:15 HSZ 204

Unconventional s- and p-wave proximity effect in topological insulator/superconductor structures — •Tkachov Grigory — University of Wuerzburg

Currently, much effort is being put into understanding unconventional superconductivity in topological insulators (TIs). This contri-

bution addresses a microscopic theory of the proximity effect in three-dimensional TIs coupled to an s-wave superconductor. In agreement with earlier results [1] we demonstrate that the induced superconductivity is a mixture of singlet s-wave and triplet p-wave components [2]. Their interplay depends on several factors, such as the position of the Fermi level, excitation energy, and external magnetic fields, among others. We also discuss the role of disorder and applications of the theory to recent experiments on HgTe-based TIs [3,4].

This work was supported by the German Research Foundation (DFG), Grant No TK60/1-1.

[1] T. D. Stanescu, J. D. Sau, R. M. Lutchyn, and S. Das Sarma, Phys. Rev. B **81**, 241310(R) (2010).
[2] G. Tkachov, Phys. Rev. B **87**, 245422 (2013).
[3] L. Maier, J. B. Oostinga, D. Knott, C. Brüne, P. Virtanen, G. Tkachov, E. M. Hankiewicz, C. Gould, H. Buhmann, and L. W. Molenkamp, Phys. Rev. Lett. 109, 186806 (2012).
[4] J. B. Oostinga, L. Maier, P. Schüffelgen, D. Knott, P. Leubner, C. Brüne, G. Tkachov, H. Buhmann, and L. W. Molenkamp, Phys. Rev. X **2**, 021007 (2013)

TT 71: Transport: Majorana Fermions (organized by TT)

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

TT 71.1 Wed 15:00 HSZ 03

Majorana spin liquid and dimensional reduction in Cs_2CuCl_4 — •Tim Herfurth, Simon Streib, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany

The low-temperature behavior of the magnetic insulator Cs_2CuCl_4 can be modeled by an anisotropic triangular lattice spin 1/2 Heisenberg antiferromagnet with two different exchange couplings J and $J' \approx J/3$. We show that in a wide range of magnetic fields the experimentally observed field dependence of the crossover temperature T_c for spin-liquid behavior can be explained within a mean-field theory based on the representation of spin operators in terms of Majorana fermions. We also show that for small magnetic fields the specific heat and the spin susceptibility both exhibit a maximum as a function of temperature at $T_c = J/2$. In the spin-liquid regime, the Majorana fermions can only propagate along the direction of the strongest bond, in agreement with the dimensional reduction scenario advanced by Balents[1].
[1] Nature **464**, 199 (2010)

TT 71.2 Wed 15:15 HSZ 03

Supersymmetry in the Majorana Cooper pair box — •Jascha Ulrich and Fabian Hassler — Institut für Quanteninformation, RWTH Aachen

Over the years, supersymmetric quantum mechanics (SUSY QM) has evolved from a toy model of high energy physics to a research direction of its own. Although many examples of SUSY QM systems have been found, systems that can be naturally realized are generally scarce. In this work, we argue that the interaction of fermionic subgap Majorana bound states with the underlying Cooper pair condensate provides a natural setting for SUSY QM. We show that the extension of the conventional Cooper pair box by an anomalous Majorana-Josephson coupling realizes SUSY QM for certain values of gate voltage and Josephon/Majorana-Josephson coupling ratio. We show that the resulting degeneracy of all subgap energy levels can be probed directly in a tunneling experiment and discuss the various transport signatures. An observation of the predicted level degeneracy would provide evidence for the presence of a Majorana-induced anomalous Josephson coupling.

TT 71.3 Wed 15:30 HSZ 03

Robustness of exchange protocols of Majorana fermions in quantum wire networks — •Rolf W. Reinthaler[1], Chao Lei[2], Allan H. MacDonald[2], and Ewelina M. Hankiewicz[1] — [1]Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Department of Physics, University of Texas at Austin, USA

The ends of one-dimensional spinless p-wave superconductors support Majorana bound states [1], whose non-trivial exchange statistics makes them promising candidates for topological quantum computation [2]. The huge advantage of using networks of 1D nano wires is that the Majorana fermions can be manipulated and exchanged by purely electrical means [3]. By applying a tight binding approach we solve the time dependent Bogoliubov-de Gennes equations for the Kitaev chain model [1]. We analyze how the robustness of the exchange protocols is affected by non-adiabatic effects as well as by a finite overlap of the Majorana bound states.

We acknowledge financial support by the DFG grant HA 5893/3-1.
[1] A. Y. Kitaev, Physics-Uspekhi **44** (2001) 131
[2] D. A. Ivanov, PRL **86** (2001) 268
[3] J. Alicea et al., Nature Physics **7** (2011) 412

TT 71.4 Wed 15:45 HSZ 03

Absence of Aharonov-Bohm effect of chiral Majorana fermion edge states — •Sunghun Park[1,4], Joel Moore[2,3], and Heung-Sun Sim[1] — [1]Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Korea — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA — [4]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

Majorana fermions in a superconductor hybrid system are charge neutral zero-energy states. For the detection of this unique feature, we propose an interferometry of a chiral Majorana edge channel, formed along the interface between a superconductor and a topological insulator under an external magnetic field perpendicular to the surface of the topological insulator. The superconductor is of a ring shape and has a Josephson junction that allows the Majorana state to enclose continuously tunable magnetic flux. Zero-bias differential electron conductance between the Majorana state and a normal lead is found to be independent of the flux at zero temperature, manifesting the Majorana feature of a charge neutral zero-energy state. To compare with a non-Majorana case, we consider the same setup on graphene. In this case, the setup has no Majorana states and shows Aharonov-Bohm effects.

TT 71.5 Wed 16:00 HSZ 03

Fractional Josephson effect in a quadruple quantum dot — •Björn Sothmann, Jian Li, and Markus Büttiker — Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland

A double quantum dot coupled to an s-wave superconductor and subject to an inhomogenous magnetic field can host a pair of zero-energy Majorana fermions when the dot properties are tuned appropriately [1]. Here, we demonstrate the possibility to generate a fractional 4π Josephson effect in two such double dots tunnel-coupled to each other. We discuss the robustness of this effect with respect to perturbations away from the special point in parameter space where the uncoupled doube dots host Majorana fermions. We point out the possibility to generate Josephson effects with a period of 8π and 12π in strongly-coupled double dots.
[1] M. Leijnse and K. Flensberg, Phys. Rev. B **86**, 134528 (2012)
[2] B. Sothmann, J. Li, M. Büttiker, New J. Phys. **15**, 085018 (2013)

15 min. break.

Invited Talk TT 71.6 Wed 16:30 HSZ 03

Majorana Fermions in Chains of Magnetic Atoms on the Surface of a Superconductor — •Ali Yazdani — Princeton University

In this talk, I will describe a proposal and related experiments for realization of Majorana fermions in chains of magnetic atoms on the surface of a conventional superconductors. I will describe model calculations that motivate the experimental studies, which show that a spiral spin textured chain of atoms give rise to a topological superconducting phase when place in contact with a s-wave superconductor. Remarkably, only chains of as long as few tens of atoms is required to realize this phase in the calculations. I will also describe experiments in which we use in situ assembly of magnetic atoms on the surface of an s-wave superconductor and spectroscopic mapping with a scanning tunneling microscope (STM) to search for signatures of Majorana fermions at the end of such chains. Spin-polarized STM experiments in which we probe the spin texture of such chains will also be described.

[1] S. Nadj-Perge, I.K. Drozdov, B.A. Bernevig, and A. Yazdani, Phys. Rev. B 88, 020407 (2013)
[2]J. Klinovaja, P. Stano, A. Yazdani, and D. Loss, Phys. Rev. Lett. 111, 186805 (2013)

TT 71.7 Wed 17:00 HSZ 03

Disordered one-dimensional topological superconductors — •Michael Wimmer[1,2], Inanc Adagideli[3], and Aykut Teker[3] — [1]Universiteit Leiden, The Netherlands — [2]TU Delft, The Netherlands — [3]Sabanci University, Istanbul, Turkey

It is well-established that disorder is harmful to a topological phase in p-wave superconductors [1]. Recently, it has been proposed to engineer ap-wave superconductor using conventional materials: a nanowire with strong spin-obrit coupling in proximity to a s-wave superconductor and in a magnetic field ("s-wave Rashba wires"), and first experimental results have been obtained [2].

We present a simple and intuitive method to link topological properties of superconducting wires to their normal state properties. This allows to describe ensemble-averaged topological properties as well as individual systems. In particular, we show that the effect of disorder is quite different in p-wave superconductors and s-wave Rahsba wires: While disorder is always harmful for the former, topology can be created by disorder in the latter [3].

[1] P. Brouwer *et al.* Phys. Rev. B **84**, 144526 (2011)
[2] V. Mourik *et al.* Science **336**, 1003 (2012)
[3] I. Adagideli, M. Wimmer, A. Teker. arXiv:1302.2612 (2013)

TT 71.8 Wed 17:15 HSZ 03

Majorana Fermions in Antiferromagnetically doped Superconductors — •Andreas Heimes, Panagiotis Kotetes, and Gerd Schön — Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

Recently the field of Majorana fermions (MFs) in solid state physics has attracted great attention. Among the many existing proposals for their experimental realization and detection, one can distinguish a class of self-tuned MF systems, consisting of spiral spin chains on s-wave superconductors. We propose an alternative MF platform based on a chain of antiferromagnetically (AFM) ordered magnetic impurities on top of a conventional superconductor, which has the advantage that it allows for an external tunability by experimental parameters: The transition to the MF regime is achieved and controlled by the combination of a supercurrent flow and a Zeeman field. In fact, the latter can be considerably weak since the presence of the AFM order relaxes the requirement of a large Zeeman energy. Evenmore, the currently existing STM technology renders our proposal directly experimentally accessible.

TT 71.9 Wed 17:30 HSZ 03

Majorana fermions in quasi-1d Rashba semiconductor/superconductor heterostructures without the requirement of a Zeeman field — •Panagiotis Kotetes, Alexander Shnirman, and Gerd Schön — Karlsruhe Institute of Technology

Recent experiments have provided the first promising indications of Majorana fermions (MFs) in heterostructures consisting of Rashba semiconducting wires and superconductors in the presence of a Zeeman field. By performing a complete classification of engineered topological superconductors (TSCs) [1] we predict that MFs are accessible in quasi-1d Rashba semiconductors with proximity induced superconductivity, even in the absence of magnetism. The only requirement is the presence of a Josephson current, flowing transversely to the principal axis of the quasi-1d structure. Here, we demonstrate how MFs emerge within our proposal when multi-wire or multi-channnel semiconductors are involved. The crucial effect of the supercurrent flow is to convert the inter-wire/channel spin-orbit coupling into an effective Zeeman term. Our results can motivate a new set of experiments using the already developed devices but in different configurations, providing in this way an accessible and irrefutable method for confirming the emergence of MFs.

[1] P. Kotetes, New J. Phys. 15, 105027 (2013)

TT 71.10 Wed 17:45 HSZ 03

Quantum spin liquid with a Majorana Fermi surface on the three-dimensional hyperoctagon lattice — •Maria Hermanns and Simon Trebst — Institut für Theoretische Physik, Universität zu Köln

Motivated by the recent synthesis of β-Li_2IrO_3 – a spin-orbit entangled $j = 1/2$ Mott insulator with a three-dimensional lattice structure of the Ir^{4+} ions – we consider generalizations of the Kitaev model, believed to capture some of the microscopic interactions between the Iridium moments, on various trivalent lattice structures in three spatial dimensions. Of particular interest is the so-called hyperoctagon lattice – a cubic non-Bravais lattice, which is probably best described as the premedial lattice of the hyperkagome lattice – for which the ground state is a gapless quantum spin liquid where the gapless Majorana modes form an extended Majorana Fermi surface. We demonstrate that this Majorana Fermi surface is inherently protected by lattice symmetries and discuss possible instabilities when allowing for a reduction in lattice symmetries. We discuss these findings also in light of recent results obtained for the hyperhoneycomb lattice.

TT 72: Transport: Molecular Electronics II

Time: Wednesday 15:00–16:15 Location: HSZ 304

TT 72.1 Wed 15:00 HSZ 304

Conductance and thermopower of long molecular wires — •F. Rochau[1], M. Kotiuga[2,3], T. J. Hellmuth[4], J. B. Neaton[2,3], and F. Pauly[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Molecular Foundry, Lawrence Berkeley National Laboratory, California, USA — [3]Department of Physics, University of California, Berkeley, USA — [4]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Germany

We study the transition from coherent tunneling to incoherent hopping for the conductance G and the thermopower S of long molecular wires [1]. Using a tight-binding model for the electronic structure combined with Green's function techniques to describe transport, we include dephasing by means of Büttiker probes. We discuss the one-dimensional chain as well as several benzene-based molecular junctions (oligophenylenes, polyacenes and polyphenanthrenes). For the one-dimensional chain we derive analytical formulas for the length dependence of the phase-coherent G and S, distinguishing off-resonant, band-edge, and on-resonant transport. Irrespective of the regime and the system considered, we find an ohmic inverse length dependence of G and a saturating S for long molecular wires, when dephasing is included. The power factor S^2G of long wires is therefore determined by G. Finally, we study the huge thermopower resulting from transmission nodes for the polyphenanthrenes and observe how they disappear when decoherence is added.

[1] F. Rochau, M. Kotiuga, T. Hellmuth, J. B. Neaton, and F. Pauly, in preparation

TT 72.2 Wed 15:15 HSZ 304

Noncollinear electronic transport through star-shaped Fe_4 nanomagnet — •Volodymyr V. Maslyuk[1], Leonid Sandratskii[2], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

During the last decade single molecular magnets have attracted huge interest because of their spectacular magnetic properties. Here we present a theoretical investigation of the star-shaped $Fe_4(OMe)_6(dpm)_6$ nanomagnets placed between ferromagnetic Co(100) electrodes. We use the combination of the NEGF method and the density-functional theory realized in the TranSIESTA code [1] and adapted for the investigation of the magnetic systems with non-collinear magnetic order. We take into account electron-correlations effects via a Hubbard-like term that was added to our DFT functional. We found that the Fe_4 molecule has a magnetic moment of 10 μ_B in the ground state. We also obtain that the magnetic anisotropy barrier of the molecule is small, 0.33 meV, that allows us to neglect the spin-orbit interaction in the transport properties calculations. The molecule placed between electrodes tends to be antiferromagnetically alined with the magnetization of the leads. We show that the direc-

tion of the magnetization of the molecule changes with the variation of the relative directions of the magnetization of the leads. This has an impact on the transmission spectra of the system.
[1] M. Brandbyge, *et al*, Phys. Rev. B 65, 165401 (2002)

TT 72.3 Wed 15:30 HSZ 304

Localization under the effect of randomly distributed decoherence — •Thomas Stegmann[1], Orsolya Ujsághy[2], and Dietrich E. Wolf[1] — [1]Department of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary

Electron transport through disordered quasi one-dimensional quantum systems is studied. Decoherence is taken into account by a spatial distribution of virtual reservoirs, which represent local interactions of the conduction electrons with their environment.

We show that the decoherence distribution has observable effects on the transport. If the decoherence reservoirs are distributed randomly without spatial correlations, a minimal degree of decoherence is necessary to obtain Ohmic conduction. Below this threshold the system is localized and thus, a decoherence driven metal-insulator transition is found. In contrast, for homogenously distributed decoherence, any finite degree of decoherence is sufficient to destroy localization. Thus, the presence or absence of localization in a disordered one-dimensional system may give important insight about how the electron phase is randomized.
[1] arXiv:1308.4328

TT 72.4 Wed 15:45 HSZ 304

Electronic and Structural Properties of Functionalized Nanoparticle Networks: A Multi-Scale Approach — •Tahereh Ghane[1], Daijiro Nozaki[1], Arezoo Dianat[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [2]Center of Advancing Electronics Dresden, TU Dresden, Germany — [3]Dresden Center for Computational Materials Science, TU Dresden, Germany

Functionalized nanoparticle networks offer a model system for the study of charge transport in low-dimensional systems as well as a potential platform to implement electronic functionalities. The electrical response of a nanoparticle network is expected to sensitively depend on the molecular inter-connects, i.e. on the linker chemistry. If these linkers have complex charge transport properties as is the case of molecular switches with conformational dependent electronic properties or molecular memristors showing hysteretic behavior, then phenomenological models addressing the large scale properties of the network need to be complemented with microscopic calculations of the network building blocks. In this study we investigate the electronic, structural and charge transport properties of functionalized nanoparticle by employing a multi-scale method in which we combine density-functional based approaches, classical molecular dynamics, and charge transport calculations.

This work has been funded by the European Union through the project "Synaptic Molecular Networks for Bio-inspired Information Processing".

TT 72.5 Wed 16:00 HSZ 304

Influence of structural distortions on the polarization function in molecular-based quantum cellular automata: a minimal model approach — •Alejandro Santana[1,2], Rafael Gutierrez[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, 01062 Dresden, Germany. — [2]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany.

Molecular Quantum Cellular Automata (m-QCA) offers a new paradigm in which information can be encoded using special geometrical arrangements of charges within one of the m-QCA cell and transmitted by cell-cell interaction between nearest neighbors. In fact, m-QCA implementation relies on three basic assumptions (a) charge localization within the molecule, (b) switching between two possible electronic states and (c) electrostatic coupling between nearest-neighbors. Therefore, under those conditions, functionality of m-QCA implies a complex relationship between quantum mechanical effects, such as electron transfer (ET) processes within the molecule, and electrostatic interactions between cells. Fundamental questions about the impact of structural distortions of individual m-QCA are addressed and allowing us to formulate a response function in which the geometry of the system and the ET coupling are used as effective parameters. Our study indicates that even small changes in the original geometry of the system have a dramatic impact on the cell response and, therefore, changing the idea of the QCA-network implementation when is compared with the classical paradigm.

TT 73: Transport: Carbon Nanotubes (organized by TT)

Time: Wednesday 16:30–18:30 Location: HSZ 304

TT 73.1 Wed 16:30 HSZ 304

Revealing the carbon nanotube quantum dot fine structure by transport spectroscopy — •Daniel R. Schmid[1], Alois Dirnaichner[1,2], Magdalena Marganska[2], Peter L. Stiller[1], Milena Grifoni[2], Andreas K. Hüttel[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Transport spectroscopy on an ultra-clean carbon nanotube quantum dot allows us to measure the level spectrum of the very first electron above the band gap, which can be understood by an underlying minimal Hamiltonian. This includes curvature induced spin-orbit coupling and KK'-mixing terms. The sample orientation in an external magnetic field can be adjusted from perpendicular to parallel alignment with the nanotube axis. Magnetic fields up to 17 T enable us to get an insight on the full dispersion of the first longitudinal modes.

TT 73.2 Wed 16:45 HSZ 304

Valley-mixed states and energy splitting as a finite size effect in chiral carbon nanotubes — •Magdalena Marganska, Piotr Chudzinski, and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

The two main degrees of freedom of an electron in a carbon nanotube (CNT) are valley and spin. The electronic spectra obtained in transport experiments on CNT quantum dots in parallel magnetic field often show an anticrossing of spectral lines assigned to the opposite valleys. One source of this phenomenon could be the disorder, with impurity induced scattering. However, we show that this effect can be reproduced also in ultraclean CNTs, where it is caused solely by the presence of the boundaries. It is therefore a finite size effect, not an inherent property of the CNT. We identify the nanotube chirality class which supports this phenomenon and analyze its dependence on the CNT parameters and on the distance from the charge neutrality point.

TT 73.3 Wed 17:00 HSZ 304

Large scale *ab initio* study of extended metal-CNT contacts — •Artem Fediai[1,2,3], Dmitry Ryndyk[1,2,3], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Center for Advancing Electronics Dresden, TU Dresden, Germany — [3]Dresden Center for Computational Materials Science, TU Dresden, Germany

In experimental samples of carbon nanotube transistors (CNT-FETs) the electrical contact and current inflow occur along relatively long portion of a CNT embedded into a metal. Only very few theoretical studies were done with geometries and materials close to realistic ones. The most common simplified approaches are using the models of point-like or very slightly embedded contacts.We perform large-scale modeling of extended metal-CNT contacts by density functional theory accompanied by Green function method in order to elucidate electrical properties of realistic metal-CNT contacts. We have obtained smooth shrinking of the band gap inside embedded portion of a semiconductor nanotube and induced by the metal doping of the embedded and free-standing part of a CNT. It causes geometry and material dependent behavior of the transmission coefficient and density of states along a CNT. We also analyze the electrostatic potential and charge redistribution and formulate an ab initio based effective transport model to calculate the current-voltage characteristics of large scale CNT-FETs.

TT 73.4 Wed 17:15 HSZ 304

A carbon nanotube in the strong coupling regime: Fabry-Perot interference in a ballistic electron wave guide. — •Alois Dirnaichner[1], Miriam del Valle[2], Andreas Hüttel[1], Christoph Strunk[1], and Milena Grifoni[2] — [1]Institute of Experimental and Applied Physics Regensburg — [2]Institute for Theoretical Physics Regensburg

We present low-temperature measurements of transport through a ultra clean suspended carbon nanotube with strong coupling to the leads. The sample exhibits strikingly high conductance and little reflection at the interfaces between tube and metal, as can be seen from pronounced Fabry-Perot interference patterns in the conductance. The measurements are compared to theoretical results obtained from a scattering matrix calculation where the reflection at the contacts is treated as a perturbation. Furthermore, we discuss the evolution of the patterns in a magnetic field perpendicular to the nanotube axis.

TT 73.5 Wed 17:30 HSZ 304

Signatures of quanta of 1D collective modes in inelastic co-tunneling through a metallic carbon nanotube. — Daniel Steininger[1], •Piotr Chudzinski[2], Amit Kumar[1], Martin Gaim[1], Milena Grifoni[2], Andreas K. Hüttel[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We report low temperature transport properties of an individual single wall carbon nanotube contacted to superconducting leads. Coulomb diamonds with sharp elastic and inelastic co-tunneling features at applied bias voltages of $2\Delta/e$ and $(2\Delta + \delta)/e$ (with the BCS gap Δ), respectively, are observed. Higher order transport processes generate subgap features at bias voltage Δ/e via the Andreev reflection process. In contrast to previously reported co-tunneling spectra [1], the elastic/in-elastic co-tunneling features we observe are horizontal lines on the bias-gate voltage plane (no bending effect) and do not display any effect related to even and odd electron occupancy of the quantum dot. The in-elastic part has a rich internal structure consisting of several equidistant sub peaks. We analyze various possibilities for the occurrence of such harmonic spectrum. Among these are vibrational excitations of the carbon lattice or the many body bosonic modes that are expected from the Tomonaga-Luttinger liquid description of single wall carbon nanotubes.

[1] Phys. Rev. B 79, 134518

TT 73.6 Wed 17:45 HSZ 304

Fingerprints of thermal quasiparticle excitations in CNT-superconductor hybrid junctions — •Sebastian Pfaller[1], Andrea Donarini[1], Markus Gaass[2], Andreas K. Hüttel[2], Thomas Geiger[2], Christoph Strunk[2], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Exp. and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We present a study of a electronic transport through a carbon nanotube quantum dot coupled to superconducting contacts. By increasing the temperature above 300mK additional transport features are observed in the stability diagrams. They appear as lines in the Coulomb blockade region, and are attributed to sequential tunneling of thermally excited quasiparticles. Whenever two of these lines cross at zero bias, a conductance peak is observed. In particular, we observe two of these peaks in the vicinity of the charge degeneracy point. The nature of these lines as well as their temperature dependence can be explained by a transport theory based on a generalized master equation approach to lowest order in the tunnel coupling [1].

[1] S. Pfaller *et al.* Phys. Rev. B **87**, 155439 (2013)

TT 73.7 Wed 18:00 HSZ 304

Fine structure of the Kondo resonance in carbon nanotube quantum dots — Daniel R. Schmid[1], Sergey Smirnov[2], Magdalena Margańska[2], Alois Dirnaichner[1], Peter L. Stiller[1], Milena Grifoni[2], •Andreas K. Hüttel[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Ultraclean carbon nanotubes enable spectroscopy of the unperturbed quantum mechanical properties of electronic states in transport experiments with a high degree of precision. This applies to the case of opaque tunnel barriers between nanotube and leads and, e.g., the excitation spectrum of one or two electrons trapped in the quantum dot as well as to the case of many electrons and strong coupling to the leads.

Manybody correlations in carbon nanotubes with a quadruplet of both spin and valley (K-K') degenerate quantum states can give rise to the so-called SU(4) Kondo effect. We demonstrate a highly regular carbon nanotube quantum dot, where SU(4) symmetry is broken by intrinsic both spin-orbit interaction and valley mixing. This leads to a characteristic Kondo peak in differential conductance at zero bias along with satellite peaks at finite bias. The evolution of these peaks is strikingly different at finite perpendicular and parallel magnetic fields. We demonstrate how their combined spin and orbital origin and their evolution at finite magnetic fields can be understood in detail in terms of the discrete symmetries of the carbon nanotube Hamiltonian.

TT 73.8 Wed 18:15 HSZ 304

Theory of the Kondo effect in carbon nanotube quantum dots with broken SU(4) symmetry — •Sergey Smirnov[1], Magdalena Margańska[1], Daniel R. Schmid[2], Alois Dirnaichner[2], Peter L. Stiller[2], Andreas K. Hüttel[2], Christoph Strunk[2], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We develop an effective low energy field theory for the Kondo effect in a quantum dot where the original four-fold degeneracy of the dot level is partially removed. The SU(2) Keldysh effective action approach [1,2] is generalized to the case of the broken SU(4) Anderson model with spin and orbital degrees of freedom. The theory is valid in the strong and weak coupling regimes as well as in the crossover. It provides universal differential conductance with the scale having the correct limiting behavior for the SU(2) and SU(4) cases. As an application to a physical system, we explore the Kondo effect in a quantum dot made of a carbon nanotube with strong spin-orbit interaction and valley mixing. The symmetry properties of the carbon nanotube Hamiltonian are exploited to identify the structure of the Keldysh effective action. We further investigate in detail the Kondo resonance and its behavior in perpendicular and parallel magnetic fields and compare it with recent experiments on the Kondo effect in ultraclean carbon nanotubes.

[1] S. Smirnov and M. Grifoni, Phys. Rev. B 87, 121302(R) (2013).
[2] S. Smirnov and M. Grifoni, New. J. Phys. 15, 073047 (2013).

TT 74: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Wednesday 15:00–18:45 Location: BEY 81

TT 74.1 Wed 15:00 BEY 81

The Kondo model in nonequilibrium: Interplay between voltage and temperature and crossover from weak to strong coupling — Frank Reininghaus, Mikhail Pletyukhov, and •Herbert Schoeller — Institut für Theorie der Statistischen Physik, RWTH Aachen

We analyze the 1-channel spin-1/2 nonequilibrium Kondo model at finite voltage and temperature by using a new formulation of real-time renormalization group with the Laplace variable E as flow parameter [1,3]. If the effective Liouvillian in Laplace space is analytic around E=0 (corresponding to the stationary state), we present convincing arguments that the method is capable of describing reliably the crossover from weak to strong coupling for the stationary conductance as function of voltage and temperature. Besides universal line shapes, we propose an elegant way to determine the Kondo temperature from the voltage dependence of the conductance. Furthermore, for a fixed finite voltage, we find that the temperature-dependence of the differential conductance exhibits non-monotonic behavior. We compare our results with recent experiments and find good agreement [2,3]. For the N-channel Kondo model with N¿¿1, we calculate the transient dynamics and find a pure power-law decay typical for non-Fermi liquid behaviour.
[1] M. Pletyukhov and H. Schoeller, Phys. Rev. Lett. 108, 260601 (2012)
[2] A.V. Kretinin, H. Shtrikman, and D. Mahalu, Phys. Rev. B 85, 201301(R) (2012)
[3] O. Klochan et al., Phys. Rev. B 87, 201104(R) (2013)

TT 74.2 Wed 15:15 BEY 81

Transport properties of fully screened Kondo models — •Christoph B. M. Hörig[1,3], Christophe Mora[2], and Dirk Schuricht[3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University and JARA-Fundamentals of Future Information Technology, Germany — [2]Laboratoire Pierre Aigrain, École Normale Supérieure, France — [3]Institute for Theoretical Physics, Utrecht University, The Netherlands

We study the crossover from strong to weak coupling in two fully screened Kondo quantum dots, the spin-1/2 and the spin-1 model coupled to one or two screening channels respectively. The quantum dots are subject to either a finite bias voltage or a finite temperature. Using a real-time renormalisation group method we calculate the static susceptibility, dynamical spin-spin correlation functions, and the differential conductance. We extract the various Kondo scales and Fermi liquid coefficients at low energies and compare with exact known and newly derived Fermi liquid results.

TT 74.3 Wed 15:30 BEY 81

Spatial and temporal propagation of Kondo correlations — •Benedikt Lechtenberg and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

While the equilibrium properties of the Kondo problem are theoretically well understood, its non-equilibrium properties are subject to recent research. To set the stage, we present the spatial correlation function $\langle \vec{S}_{\rm imp} \vec{s}(r) \rangle$ between the impurity spin $\vec{S}_{\rm imp}$ and the spin density of the conduction electrons in thermodynamic equilibrium using the numerical renormalization group (NRG). Then, we will address the key question, how this spatial correlation function builds up as function of time starting from an initially decoupled impurity spin. We will show that the spatial and temporal Kondo correlations propagate along a light-cone determined by the Fermi-velocity. Surprisingly, we find that $\langle \vec{S}_{\rm imp} \vec{s}(r) \rangle(t)$ contains significant non-exponential contributions outside of the light-cone. Augmenting our time-dependent NRG calculation with perturbative expansion of the density operator we can explicitly trace the origin of these correlations to the intrinsic spin-density correlations of the initial Fermi see. Contributions outside of the light-cone only vanish in a true linear response function.

TT 74.4 Wed 15:45 BEY 81

Spin-noise in the anisotropic central spin model — •Johannes Hackmann and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

We have investigated the spin noise in an ensemble of semiconductor quantum dots (QDs) using the anisotropic central spin model. This model describes the dynamics of both electron and/or hole doped QDs. First, we have computed the spectral correlation function $\langle S^z(\omega) S^z \rangle$ for a single QD to reveal the influence of the external magnetic field and the anisotropy factor on the spin dynamics. Second, we have performed an ensemble average to compare our results to recent experiments. We will show that the measurement of spin noise on an ensemble of hole doped QDs reveals more about the distribution function of the QD parameters than on the dynamics of a single QD spin.

TT 74.5 Wed 16:00 BEY 81

Finite-Temperature Studies of Inverse Indirect Magnetic Exchange — •Maximilian Aulbach, Irakli Titvinidze, Andrej Schwabe, and Michael Potthoff — Universität Hamburg, Hamburg, Deutschland

The standard Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction emerges as an effective low-energy coupling in systems where the magnetic moments of impurities are coupled via a weak local exchange J to the spins of a system of itinerant conduction electrons. Contrary, in the case of antiferromagnetic and strong J, the impurity spins are screened individually by the formation of almost local Kondo singlets. In confined magnetic nanostructures, this results in a localization of conduction electrons and a corresponding formation of local magnetic moments which are indirectly coupled via virtual excitations of the Kondo singlets. This new "inverse" indirect magnetic exchange (IIME) [1] can also be studied in Anderson-lattice models with diluted impurities and results in a ferromagnetic ground state.

Here we focus on the finite-temperature properties. Using dynamical mean-field theory and a continuous-time quantum Monte-Carlo impurity solver, we calculate the temperature-dependent magnetization at the different inequivalent sites as well as the Curie temperature. The QMC results are compared with the predictions of static mean-field theory applied to an effective low-energy spin-only Hamiltonian that is derived in fourth-order strong-coupling perturbation theory.
[1] A. Schwabe, I. Titvinidze and M. Potthoff, Phys. Rev. B 88, 121107(R) (2013)

TT 74.6 Wed 16:15 BEY 81

Continuous-time Quantum Monte Carlo approach for quantum impurity problems in Tomonaga-Luttinger liquids — •Kazumasa Hattori[1,2] and Achim Rosch[1] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]Institute for Solid State Physics, University of Tokyo, Japan

We have developed a continuous-time quantum monte carlo method [1] for single-impurity problems in Tomonaga-Luttinger (TL) liquid in one-dimension. The method is negative-sign free and applicable to varieties of models. In this contribution, we will show results for a potential barrier problem in one-channel TL liquid [2] as a benchmark and also discuss an anisotropic Kondo problem in a helical TL liquid on the edge of two-dimensional topological insulator. Various correlation functions are calculated and we discuss the crossover functions from high- to very low-temperature fixed points and their critical behaviors.
[1] E. Gull, et al., Rev. Mod. Phys. 83, 349 (2011)
[2] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. 68, 1220 (1992)

TT 74.7 Wed 16:30 BEY 81

Time Evolution of a Quantum Impurity System following a Quantum Quench at Finite Temperatures - a td-NRG Study — •Hoa Nghiem and Theodoulos A. Costi — Peter Grünberg Institut and Institute for Advanced Simulation, Research Centre Jülich, 52425 Jülich, Germany

To study the time evolution of an observable of a quantum impurity system after a sudden quench at an arbitrary temperature, we apply the recently developed time-dependent numerical renormalization group approach (td-NRG) to the Anderson model [1]. The quenches studied include switching from mixed valence to Kondo regime or vice versa, and from a uncorrelated to a correlated system or vice versa. We quantify the results in the short and long time limits by comparing them to the thermodynamic values in the initial and final states. We also present the time evolution due to general continuous pulses, acting in a finite time interval. The study is based on the general-

ization of td-NRG to a general pulse [1], where we consider the pulse as a sequence of smaller quenches, and formulate the time evolution following an arbitrary number of quenches.
[1] H. Nghiem and T. A. Costi, Preprint (2013).

15 min. break.

TT 74.8 Wed 17:00 BEY 81

The Kondo effect in atomic chains — •Deung-Jang Choi[1,2], Shichao Yan[1,2], Jacob Burgess[1,2], Steffen Rolf-Pissarczyk[1,2], and Sebastian Loth[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

We can construct atomic model structures to engineer Spin Hamiltonians using a sub-Kelvin scanning tunneling microscope (STM). For that, different kinds of transition metal atoms were manipulated and construction of atomic chains was performed. The chains composed of transition metal atoms form a highly correlated spin singlet ground state exhibiting a Kondo resonance. We studied temperature and magnetic field dependence to confirm the Kondo effect in this composite magnetic system. It is revealed that the occurrence of the Kondo resonance sensitively depends on the length of the atomic chain and the spin anisotropy energy of each atom. We build chains with different elemental composition and obtain various spin ground states. In this way, we can tailor the singlet ground state on and off. Such composite magnetic chains present a fruitful experimental model spin system and make it possible to engineer prototypical correlated spin states at atomic dimensions.

TT 74.9 Wed 17:15 BEY 81

Nonequilibrium evolution of the Kondo screening cloud — •Martin Nuss, Martin Ganahl, Hans Gerd Evertz, Enrico Arrigoni, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, Graz University of Technology

Quantum impurity models feature nonperturbative physics at low temperatures, manifest in the Kondo effect. In equilibrium, the Kondo effect is accompanied by a diverging length scale for increasing interaction strength. While elusive in experiment this "Kondo length" has been observed in the spin-spin correlation functions in theoretical work. We extend these studies to the nonequilibrium regime by studying the interacting single impurity Anderson model after a quantum quench. Making use of Density Matrix Renormalization Group techniques, we present high accuracy numerical results for time dependent correlation functions and discuss the spatio-temporal evolution of the Kondo cloud. We furthermore present results for a system under bias, its temporal evolution as well as steady state characteristics [1].
[1] Phys. Rev. B 88, 045132 (2013)

TT 74.10 Wed 17:30 BEY 81

Local susceptibility and Kondo scaling — Markus Hanl and •Andreas Weichselbaum — Ludwig Maximilians University, Munich

The Kondo scale T_K for quantum impurity systems is typically assumed to guarantee universal scaling of physical quantities. In practice, however, not every definition of T_K necessarily supports this notion away from the strict scaling limit for finite bandwidth D. Various theoretical definitions of T_K are analyzed based on the inverse magnetic impurity susceptibility at zero temperature. While conventional definitions in that respect quickly fail to ensure universal Kondo scaling for all D, an altered definition of T_K^{sc} is presented which allows universal scaling of dynamical or thermal quantities for a given fixed Hamiltonian. If the scaling is performed with respect to an external parameter which directly enters the Hamiltonian, such as magnetic field, the corresponding $T_K^{\mathrm{sc,B}}$ for universal scaling may differ, yet becomes equivalent to T_K^{sc} in the scaling limit. The only requirement for universal scaling in the full Kondo parameter regime with a residual error of less than 1% is a well-defined isolated Kondo feature with $T_K \leq 0.01\,D$. In particular, by varying D over a wide range relative to the bare energies of the impurity, this allows a smooth transition from the Anderson to the Kondo model.

TT 74.11 Wed 17:45 BEY 81

π Fluxes near the Edge of a Topological Insulator: Kondo Screening of a Soliton — •Manuel Weber, Martin Hohenadler, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The insertion of a π flux into a quantum spin Hall insulator creates four spin-charge separated states: the two chargeons with $Q = \pm 1$ and the two spinons with $S_z = \pm 1/2$. In the presence of repulsive Coulomb interactions the charged states are gapped out and a local moment is formed. For both free and interacting systems the fluxons lead to a characteristic Curie law in the magnetic susceptibility. We consider the Kane-Mele-Hubbard model on a ribbon with zigzag edges to show that the spinon can be screened by the edge states of a quantum spin Hall insulator. At $U = 0$ their hybridization is dominated by the extent of the edge states, which becomes larger with increasing spin-orbit coupling λ. As the fluxons are exponentially localized, it is sufficient to include Hubbard interactions only at lattice sites directly around the π flux. We have extended the CTQMC method by global susceptibility measurements that reproduce the Curie law of a free π flux even for this reduced interacting system. When the spinon is screened by the edge states, we observe deviations from the Curie law for different U and λ that follow the universal behavior obtained from a data collapse. Moreover, at low temperatures a Kondo resonance arises in the spectral function between two low-lying Hubbard peaks.

TT 74.12 Wed 18:00 BEY 81

Kondo effect in Transition Metal Phthalocyanine Molecules on metal surfaces — •Michael Karolak and Giorgio Sangiovanni — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We study the impact of strong electronic correlations on the electronic structure of Phthalocyanine (PC) molecules with 3d transition metal centers, adsorbed on different surfaces. Specifically, we investigate MnPC and CuPC adsorberd on Au(111), Ag(100), as well as Cu(100) surfaces. To this end we employ a first principles DFT++ method (density functional theory combined with an impurity solver) for calculating the electronic structure, explicitly taking into account the dynamic correlations arising from the strongly interacting 3d shell of the transition metal center. We compare our calculations with new scanning tunnelling microscopy experiments. Depending on the chemical valence of the transition metal center and the geometry of the molecule in contact with the different surfaces very different spectra are observed in the experiment. Our first principles calculations provide explanations of the observed data in terms of multi-orbital Kondo physics.

TT 74.13 Wed 18:15 BEY 81

Double Kondo effect induced by combining two non-Kondo systems: Fe atoms and polyphenyl molecules on Cu(111) — •Giulia Pacchioni, Marina Pivetta, Luca Gragnaniello, Fabio Donati, Stefano Rusponi, and Harald Brune — Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

We use scanning tunneling spectroscopy and X-ray magnetic circular dichroism to investigate the Kondo effect for a system formed by individual Fe atoms adsorbed under polyphenyl-dicarbonitrile molecules on Cu(111).

Neither the molecules nor the Fe atoms adsorbed on the substrate display the Kondo effect. Combining them by burying the Fe adatoms below a phenyl ring of the organic molecules induces a Kondo effect in the Fe atoms as well as in the molecules. For the molecules this is inferred from scanning tunneling spectroscopy showing an intense Kondo peak above the phenyl ring. A Fano dip with twice the Kondo temperature is detected above the buried Fe atoms. X-ray magnetic circular dichroism reveals the screening of the magnetic moment for the buried Fe atoms, confirming the Kondo effect also for Fe.

TT 74.14 Wed 18:30 BEY 81

Irregular $4f^1$ spin-orbit splitting in collapsed α-cerium — •Jürgen Röhler — Universität zu Köln, 50937 Köln

The $J_{5/2} - J_{7/2}$ spin-orbit splitting of the $4f^1$ groundstate manifold in solid cerium systems is generally close to the value of free ions, $\Delta_{\mathrm{SO}} \simeq 3100$ K. Inelastic neutron scattering confirmed this for elemental γ-Ce, but not for the collapsed α-phase with strongly increased $\Delta_{\mathrm{SO}} \simeq 5300$ K [1]. Also α-type Ce-compounds exhibit significantly increased Δ_{SO}. Renormalization of Δ_{SO} in strongly correlated $4f$-systems is usually attributed to $4f$-c.e. hybridization increasing slightly the mean orbital expectation value $< r_{4f} >$, hence decreasing Δ_{SO}. In fact in most Kondo-type and mixed valent systems Δ_{SO} is decreased by $\simeq -10\%$, but not in collapsed α-type Ce systems. The apparent deficiency of the Kondo volume collapse model will be adressed. In particular we discuss the significance of $4f^n$ occupation numbers in the framework of a Mott transition within the $4f$ configuration.
[1] A.P. Murani et al., Phys. Rev. B**48**, 13981 (1993).

TT 75: Focus Session: Spin-Orbit Torque at Surfaces and Interfaces (organized by MA)

Organizer: Y. Mokrousov (RWTH Aachen)

The phenomenon of the spin-orbit torque (SOT) is rapidly moving to the center of attention both in theoretical as well as applied spintronics. The principle of SOT relies on the spin-orbit interaction in combination with ferromagnetic magnetization and broken inversion symmetry, and it can be used to successfully switch the magnetization of a deposited collinear ferromagnetic layer with strong perpendicular anisotropy in an in-plane current geometry. Despite extensive experimental evidence of this effect, its origins are still intensively debated. In this session we want to focus on the foremost experimental achievements in the field of SOT, and on theoretical progress in understanding of the SOT and its description based on microscopic material theory.

Time: Wednesday 15:00–17:45 Location: BEY 118

Topical Talk TT 75.1 Wed 15:00 BEY 118
Magnetization switching and spin-orbit torques in AlOx/Co/Pt and MgO/CoFeB/Ta layers — •Pietro Gambardella — Department of Materials, ETH Zurich

Spin-orbit torques induced by spin Hall and Rashba-like effects in heavy metal/ferromagnetic bilayers allow for magnetization switching based on in-plane current injection. Using this geometry, we demonstrate deterministic magnetization reversal induced by sub-ns current pulses in 100 to 200 nm sized dots and discuss the switching efficiency as a function of pulse duration. Further, we present vector measurements of the longitudinal and transverse spin-orbit torques in AlOx/Co/Pt and MgO/CoFeB/Ta trilayers using harmonic analysis of the anomalous and planar Hall effects, providing evidence for strongly anisotropic field-like and spin transfer-like components that are compatible with the symmetry of the trilayers. The switching efficiency and relative magnitude of the longitudinal and transverse torques are analyzed in annealed MgO/CoFeB/Ta trilayers as a function of magnetization, magnetic anisotropy, and resistivity.

Topical Talk TT 75.2 Wed 15:30 BEY 118
Recent Theoretical Progress in Spin-orbit Torques — •Aurelien Manchon — Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal 23955, Saudi Arabia

Utilizing spin-orbit coupling to enable the electrical manipulation of ferromagnets and magnetic textures has attracted a considerable amount of interest in the past few years. In a first part, I will introduce the most striking experimental achievements to date in bulk or interfacial inversion asymmetric systems. In a second part, I will present the most recent theoretical progress in the field, spanning from the role of intrinsic contributions to the spin-orbit torque to the impact of the newly predicted spin swapping effect. In a third part, I will introduce a new paradigm, coined spin-orbit caloritronics. Indeed, we recently demonstrated that even in the absence of magnetic texture, a magnon flow generates torques if magnons are subject to Dzyaloshinskii-Moriya interaction (DMI) just as an electron flow generates torques when submitted to Rashba interaction. We show that merging the spin-orbit torques with spin caloritronics is rendered possible by the emergence of DMI in magnetic materials and opens promising avenues in the development of chargeless information technology.

Topical Talk TT 75.3 Wed 16:00 BEY 118
Domain-wall depinning governed by the spin Hall effect — •Reinoud Lavrijsen, Bert Koopmans, Henk Swagten, Elena Mure, Jeroen Franken, and Pascal Haazen — Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

Current induced domain wall motion (CIDWM) in perpendicular materials has caused much excitement over the last few year years due to the discovery of unexpected DW driving mechanisms. Recently, we have shown that the Spin Hall Effect (SHE) [1,2] provides a radically new mechanism for CIDWM in these systems [3]. Essential for this work was the ability to create and pin DWs at well-defined positions in a Pt/Co/Pt nanowire. By studying the depinning of these DW*s as function of applied field directions and current we were able to disentangle different contributions. This allows us to unambiguously identify the SHE as the driving mechanism.

In the first part of this talk we will discuss the SHE mechanism and introduce an DW depinning experiment that allows us to disentangle different contributions to CIDWM. In the second part of this talk we will discuss potential applications of the SHE for magnetization manipulation in gated heterostructures. Furthermore, we will discuss preliminary experiments where we study the effect of growth conditions on the SHE efficiency.

[1] I. M. Miron et al., Nature 476, 189 (2011) [2] L. Liu et al., Science 336, 555 (2012) [3] P.P.J. Haazen et al., Nature Materials, 12, 299-303 (2013

15 min. break

Topical Talk TT 75.4 Wed 16:45 BEY 118
The Spin Hall Effect and Spin Orbit Torques in Ferromagnetic/Normal Metal Nanostructures — •Robert Buhrman — Cornell University, Ithaca NY USA

In the spin Hall effect (SHE) the passage of a charge current through a non-ferromagnetic metal (NM) film generates a transverse spin current that when it impinges onto an adjacent ferromagnetic (FM) film will exert both a damping-like torque and a field-like torque on the FM, with the former arising from the absorption of the transverse component of the incident spin current and the latter due to spin rotation during the reflection of a portion of the incident spin current. Certain NMs (e.g. Pt, Ta, and W) have been found to exhibit a strong SHE and the damping-like torque that can be exerted in this manner on thin film magnetic materials has significant potential for spintronics in that it has been demonstrated to be capable of reversibly switching the magnetization direction of both in-plane and out-of-plane magnetized nanomagnets, to induce persistent microwave magnetic oscillations, and to facilitate the high-speed manipulation of domain walls in magnetic nanostrips. I will report some recent results from our SHE studies, including investigations into the fundamental role that the interfacial spin-mixing conductance plays in determining the effectiveness of the SHE for exerting strong anti-damping spin torques on the adjacent ferromagnet and experiments which demonstrate that both the damping-like torque and the field-like torque arise from the *bulk* SHE.

Topical Talk TT 75.5 Wed 17:15 BEY 118
Spin-orbit torques from first principles — •Frank Freimuth — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Under application of electric currents, ferromagnetic (FM) layers asymmetrically sandwiched between nonmagnets (NM1, NM2) in NM1/FM/NM2 films are subject to spin-orbit torques (SOTs), which can serve to switch magnetization. Using density-functional theory calculations we study SOTs within the Kubo linear response formalism [1]. Comparing SOTs in NM1/FM films for different choices of NM1 (Pt, W, Ta, Ir, Ru, Au) we show that the sign of the spin Hall effect in these transition metals correlates with the even ("damping-like") component of SOT. Resolving torques and spin-fluxes on the atomic scale allows us to elucidate further the role of spin-currents in mediating the SOTs and to identify an additional spin-current independent component. Varying the thickness of Co and the choice of NM2 in NM2/Co/Pt(111) films we find a strong sensitivity of the odd ("field-like") component of SOT, while the even component is less sensitive. Estimating extrinsic contributions from a scalar disorder model [2] we argue that intrinsic effects prevail. We relate the intrinsic even SOT to the Dzyaloshinskii-Moriya interaction [3,4] and show that the intrinsic even SOT can be driven also by temperature gradients instead of electric currents.

[1] F. Freimuth et al., arXiv:1305.4873 [2] J. Weischenberg et al.,

PRL **107**, 106601 (2011) [3] F. Freimuth et al., arXiv:1308.5983 [4] F. Freimuth et al., arXiv:1307.8085

TT 76: Quantum Information Systems I (organized by HL)

Time: Wednesday 15:00–16:30 Location: POT 006

TT 76.1 Wed 15:00 POT 006

Improving the efficiency of passive Hall effect circulator — •Giovanni Viola[1] and David DiVincenzo[1,2] — [1]Institute for Quantum Information , RWTH Aachen — [2]Department of Theoretical Nanoelectronics, Peter Gruenberg Institute, Forschungszentrum Juelich

Low temperature microwave technology and the implementation of quantum computation require circulators as building blocks. Three-port circulators are examples of non-reciprocal devices; they should be passive, low noise and must operate at and below microwave frequencies. It is known that the Hall effect in the quantum regime shows non reciprocal behavior, and it can be utilized in a straightforward way in the realization of highly lossy circulators as well as gyrators. We have analyzed the physical origin of this lossy behaviour and, based on this understanding, developed a novel device that improves efficiency by dealing with the galvanic loss of the earlier designs. These novel circulators and gyrators are particularly suitable for current experiments: they are characterized by low loss and should be suitable for low temperature operation.

TT 76.2 Wed 15:15 POT 006

Large-scale density functional theory study of localization of donor electrons in phosphorus-doped silicon — •Pengxiang Xu[1], Elias Rabel[2], Wei Zhang[1], Riccardo Mazzarello[1], Rudolf Zeller[2], and Stefan Blügel[2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen, 52074 Aachen, Germany — [2]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The spin of an electron bound to a Phosphorus impurity in lightly Phosphorus-doped Silicon is a promising system for the realization of a spin quantum bit. By using two highly scalable density functional theory codes, KKRnano and QUICKSTEP, we investigate the structural and electronic properties of large models of P-doped Si containing up to 10^4 atoms, focusing in particular on those properties which are relevant to their application as spin qubits.

Computation of the electronic structure of a P impurity as a function of the isotropic doping fraction enable us to determine the doping potential, the doping density and the exchange interaction between donor electrons up to inter-impurity distances of approximately six nanometers.

Our density functional calculations reveal details in the density and potential distribution of the dopants, which are not evident in calculations that do not include explicit treatment of the P donor atom and the relaxation of the crystal lattice.

TT 76.3 Wed 15:30 POT 006

Deterministic Entanglement of Distant Nitrogen Vacancy Centers on an Integrated Photonic Platform — •Janik Wolters[1], Julia Kabuss[2], Andreas Knorr[2], and Oliver Benson[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, AG Nano-Optik, Newtonstraße 15, 12489 Berlin — [2]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

The nitrogen vacancy (NV) defect center in diamond has emerged as one of the most promising candidates for future solid state quantum technology. In particular recent progress on the integration of NV centers into photonic hybrid platforms attracted attention [1]. We explore the prospects of such an integrated quantum hybrid platform. The applicability of a robust, fast and deterministic entanglement scheme [2] is evaluated. Using realistic conditions and parameters (cavity quality factors, radiative dephasing and spectral diffusion) we find that significant entanglement can be generated between medium distant NV centers via a shared cavity mode. These studies outline a route towards deterministic quantum information processing on a realistic solid state platform.

[1] Wolters, J. et al. Enhancement of the zero phonon line emission from a single nitrogen vacancy center in a nanodiamond via coupling to a photonic crystal cavity. Appl. Phys. Lett. 97, 141108 (2010).

[2] Imamoglu, A. et al. Quantum Information Processing Using Quantum Dot Spins and Cavity QED. Phys. Rev. Lett. 83, 4204 (1999).

TT 76.4 Wed 15:45 POT 006

Interaction between differently charged states of the nitrogen vacancy in diamond — •Dion Braukmann[1], J. Debus[1], D. Dunker[1], V. Yu. Ivanov[2], D. R. Yakovlev[1], and M. Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland

The nitrogen vacancy (NV) in diamond is studied on account of its possible applications in spin-electronics. Temperature-stable properties are ranked among the main advantages of the NV center: Even at room temperature spin coherence times exceed one second.[1] The NV center appears in differently charged states. About 70% are negatively charged (NV^-), the rest are neutral (NV^0) centers. In contrast to the NV^-, the NV^0 is poorly investigated. For single NV centers it was shown that both charge states can transform into each other. In that context, an ensemble of NV centers has not been studied yet. We report on polarization-dependent optical characterization of ensembles of NV^- and NV^0 centers in diamond subjected to high magnetic fields, thus providing insight into their level structures. The talk will be focused on interactions between both charged states. We observe a strong increase in NV^- ZPL intensity and a characteristic resonance of the NV^- ZPL energy when the NV^0 center is excited resonantly. This behavior can either be explained by a change in the charge state or by a Förster resonant energy transfer. Both possibilities will be discussed in detail.

[1] P. C. Maurer et al., Science, 336, 1283 (2012).

TT 76.5 Wed 16:00 POT 006

Few spin NMR of external spins using a strongly coupled sensor in diamond — •Christoph Müller[1], Xi Kong[2], Jiangming Cai[3], Kristina Melentijević[1], Alastair Stacey[4], Matthew Markham[4], Daniel Twitchen[4], Junichi Isoya[5], Sébastien Pezzagna[6], Jan Meijer[6], Jiangfeng Du[2], Martin Plenio[3], Boris Naydenov[1], Liam McGuinness[1], and Fedor Jelezko[1] — [1]Institute for Quantum Optics, University Ulm, Germany — [2]Hefei National Laboratory for Physics Sciences at Microscale and Depatment of Modern Physics, University of Science and Technology of China, Hefei, China — [3]Institute for Theoretical Physics, University Ulm, Germany — [4]Element Six, Ltd, Ascot, Berkshire, United Kingdom — [5]Research Center for Knowledge Communities, University of Tsukuba, Ibakiri, Japan — [6]Experimental Physics II, University Leipzig, Germany

Negatively charged nitrogen-vacancy (NV^-) centres in diamond, located around 2 nm below the diamond surface were used as a NMR sensor at room-temperature. Strong coupling between the electron spin of the NV^- centre and external nuclear ^{29}Si spins on the diamond surface made it possible to measure the NMR signal aroused by four nuclear spins. With the achieved signal to noise ratio, single spin sensitivity within seconds is possible. In addition, the field gradient created by the NV^- centre itself combined with compressed sensing enables to locate the detected individual nuclei with Angstrom resolution.

TT 76.6 Wed 16:15 POT 006

Increasing the creation yield of shallow nitrogen-vacancy centers by surface plasma termination — •Christian Osterkamp[1], Jochen Scharpf[1], Sebastien Pezzagna[2], Jan Meijer[2], Thomas Diemant[3], Rolf Jürgen Behm[3], Boris Naydenov[1], and Fedor Jelezko[1] — [1]Institut für Quantenoptik, Ulm University, Albert Einstein Allee 11, 89081 Ulm, Germany. — [2]Institut für Experimentelle Physik II, Abteilung Nukleare Festkörperphysik, Universität Leipzig, Linnestraße 5, 04103 Leipzig, Germany. — [3]Institut für Oberflächenchemie und Katalyse, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany.

Single nitrogen-vacancy (NV) centers in diamond close to the crystal surface are very promising magnetic field sensors with very high sensitivity and nanometer spacial resolution. The fluorescence of single

NVs can be detected and its electron spin can be polarized, read-out and manipulated at ambient conditions. Here we report the enhanced creation of very shallow (less than 3 nm below the diamond surface) NVs by using fluorine and oxygen plasma treatment. We observe a four fold increase - from 0.11 % to about 0.45 % in the production yield when the sample surface is terminated with fluorine or oxygen atoms [1]. This effect is explained by the stabilization of the NV's negative charge state which is influenced by the various impurities present on the diamond surface.

[1]: Osterkamp et al., Appl. Phys. Lett. 103 (19), S.193118. (2013)

TT 77: Focus Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale V (organized by O)

Time: Wednesday 16:00–19:15 Location: TRE Ma

Topical Talk TT 77.1 Wed 16:00 TRE Ma

Theory of nonlinear phononics for coherent light-control of solids — •Antoine Georges[1,2,3], Alaska Subedi[2], and Andrea Cavalleri[4] — [1]College de France, Paris, France — [2]Ecole Polytechnique - CPHT, Palaiseau, France — [3]University of Geneva, DPMC, Switzerland — [4]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The use of light to control the structural and electronic properties of solids is an area of great current interest. We present a microscopic theory [arXiv:1311.0544] for ultrafast control of solids with high-intensity Tera-Hertz frequency optical pulses. When resonant with selected infrared-active vibrations, these pulses transiently modify the crystal structure and lead to new collective electronic properties. The theory predicts the dynamical path taken by the crystal lattice using first-principles calculations of the energy surface and classical equations of motion, as well as symmetry considerations. Two classes of dynamics are identified. In the perturbative regime, displacements along the normal mode coordinate of symmetry-preserving Raman-active mode can be achieved by cubic anharmonicities. This validates the mechanism proposed by Först et al. [Nature Physics 7, 854 (2011)] and explains the light-induced insulator-to-metal transition of manganites reported experimentally by Rini et al. [Rini et al. Nature 449, 72 (2007)]. We also predict a new non-perturbative regime in which ultra-fast instabilities that break crystal symmetry can be induced.

TT 77.2 Wed 16:30 TRE Ma

DFT+Frontier Orbital U — •Emine Kucukbenli and Nicola Marzari — Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH)

Piecewise linearity of the total energy with respect to occupations is not only a fundamental property that should be obeyed by any exact energy functional, but also a starting point to improve approximate functionals that are used in practical applications.

DFT+U enforces piecewise linearity on the Hubbard manifold [1], and it has been shown to greatly improve the accuracy of density-functional theory for transition-metal complexes, thanks to its correction of self-interaction errors [2]. However, it still performs poorly in complexes where significant covalency is present, and intersite corrections (so-called DFT+U+V) have been introduced to improve these challenging cases [3].

Here, we revisit piecewise linearity within the DFT+U and DFT+U+V correction schemes, and explore a novel approach where self-interaction corrections are applied directly to the frontier orbitals. We test this approach on model transition metal complexes, where highly accurate reference results can be established, and on small molecules with varying degrees of covalency.

References: [1] M. Coccoccioni and S. de Gironcoli, Phys. Rev. B 71, 35105 (2005). [2] H. J. Kulik, M. Cococcioni, D. A. Scherlis and N. Marzari, Phys. Rev. Lett. 97, 103001 (2006). [3] V. Leiria Campo Jr and M. Cococcioni, J. Phys. Cond. Matt. 22, 055602 (2010); H. J. Kulik and N. Marzari, J. Chem. Phys. 134, 094103 (2011).

TT 77.3 Wed 16:45 TRE Ma

Quasiparticle self-consistent *GW* method with spin-orbit coupling applied to Bi and HgTe — •Christoph Friedrich, Irene Aguilera, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present an implementation of the quasiparticle self-consistent (QS) *GW* method where the spin-orbit coupling (SOC) is fully taken into account in each iteration rather than being added *a posteriori*. The implementation is based on the FLAPW method. The SOC gives rise to spin off-diagonal blocks in the Green function G^{SOC} and the self-energy $\Sigma^{\mathrm{SOC}} = iG^{\mathrm{SOC}}W^{\mathrm{SOC}}$. We applied the QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ method to the semimetal Bi, which presents in experiment small electron and hole pockets and a tiny band gap (11-15 meV) at the L point, all of them largely overestimated by LDA (e.g., the gap is 86 meV). The QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ approach predicts a value of the band gap of 8 meV and electron and hole pockets in very good agreement with experiment. The *a posteriori* treatment of the SOC (QSGW+SOC), on the other hand, yields an unphysical result for Bi, predicting it to be a topological insulator with a very large gap at L (260 meV) instead of a trivial semimetal. Similarly, for HgTe, QSGW+SOC reorders the bands in a wrong way and opens a gap at the Γ point in disagreement with experiment. In contrast, the QS$G^{\mathrm{SOC}}W^{\mathrm{SOC}}$ approach yields a qualitatively and quantitatively correct description of the electronic band structure. We acknowledge support from the Helmholtz Association through the Virtual Institute for Topological Insulators (VITI).

TT 77.4 Wed 17:00 TRE Ma

Studies of semiconducting pyrite and marcasite compounds using many-body perturbation theory in the *GW* approximation — •Timo Schena, Gustav Bihlmayer, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

FeS_2 pyrite and marcasite have recently gained renewed interest as materials for photovoltaic applications, due to their large optical absorption and abundance. Therefore, a reliable description of the fundamental band gap of these compounds within first-principles calculations is desirable. However, common density functional theory (DFT) often suffers from an underestimation of band gaps. This calls for beyond-DFT methods, *e.g.*, the *GW* approximation, which is known to yield gaps in much better agreement with experiment. Although this is widely accepted for "simple" semiconductors, the situation is not well understood for more complicated cases, where the band edges differ in atomic and orbital character. In fact, we observe an uncommon band gap reduction in FeS_2 when applying single-shot *GW* on top of DFT, which might be problematic for photovoltaic applications [1]. In this work, we investigate the effects of the *GW* approximation on a couple of pyrite and marcasite compounds, employing the FLAPW code `FLEUR` and the *GW* code `SPEX` (www.flapw.de). In addition to single-shot *GW*, we also compare to the results of the recently implemented quasi-particle self-consistent *GW* approximation. We gratefully acknowledge funding from BMBF of the NADNuM project 03SF0402A.

[1] T. Schena *et al.* Physical Review B (accepted 2013)

15 min. break

TT 77.5 Wed 17:30 TRE Ma

Probing d-band Quantum Well States in Palladium Nanofilms — •Srijan Kumar Saha[1], Sujit Manna[1], Marek Przybylski[1,2], Valeri Stepanyuk[1], and Jurgen Kirschener[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, 30-059 Kraków, Poland — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

We present the results of our new study which probes the d-bands quantum well (QW) states in Pd nanofilms grown on Cu(001) using first-principles density functional theory (DFT) calculations combined with scanning tunneling spectroscopy (STS) experiments. This study reveals that QW states occur in the overlayer films of Pd over a strikingly large film thickness (up to 17 monolayers) and in a large binding energy range (from 0.1 to 3.0 eV below Fermi level), thanks to its distinct and broad 4d-bands. The orbital characters of these states are unambiguously identified by our DFT calculations. Calculations also

demonstrate oscillatory multilayer relaxations and d-derived quantum size oscillations in Pd films. The pseudomorphic growth, well-defined interface, and spatially resolved STS allows us to probe individual occupied QW states and extract the accurate dispersion of the (Δ_5-like) d electronic band, as these states are laterally highly localized and give rise to distinct and sharp feature in the tunneling spectra.

TT 77.6 Wed 17:45 TRE Ma

Implementation and analysis of a plane wave and real space pseudopotential method including an efficient spin-orbit coupling treatment tailored to calculate the electronic structure of large-scale semiconductor nanostructures — •Frank Zirkelbach, Pierre-Yves Prodhomme, Jerome Jackson, and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The implementation of the *large-scale atomic effective pseudopotential program* to solve the Schrödinger equation of an electronic system is discussed. *Atomic effective pseudopotentials* that are derived from screened local effective crystal potentials of self-consistent density functional theory (DFT) calculations are utilized, which ensure an accurate treatment at reduced computational costs. The capability of describing relevant electronic eigenstates of a quantum dot structure consisting of hundred thousand atoms at an atomistic *ab initio* level comparable to DFT is demonstrated. The possibility to represent the wavefunction and to evaluate parts of the Hamiltonian either in a plane wave or real space basis allows for a coherent analysis of various different approaches. In the fully real space treatment, linear scaling with respect to the system size is achieved. The convergence behavior of the different methods and utilized approximations is shown. Furthermore, an efficient spin-orbit treatment different to previously existing implementations within the pseudopotential formalism is outlined. The accuracy of the method is demonstrated via direct comparison to standard DFT codes.

TT 77.7 Wed 18:00 TRE Ma

Strong Parallelization of Real-Space DFT Calculations — •Andrea Nobile[1,2], Paul Baumeister[1,2], Daniel Wortmann[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungzentrum Jülich and JARA, 52425 Jülich, Germany — [2]Jülich Supercomputing Center, Forschungzentrum Jülich, 52425 Jülich, Germany

The rapid change in modern supercomputing architectures poses a challenge to well established DFT codes. In particular, the increase in raw floating point power obtained through parallelism at different levels is not easily exploitable by using the traditional direct diagonalization methods. We will present our new real-space Projector Augmented Wave (PAW) implementation. The real-space representation of the wave functions, densities and potentials, enables the usage of very flexible boundary conditions and naturally adapts to massively parallel architectures. Parallelism can be exploited in the form of domain decomposition of the three dimensional grid, k-point sampling and bands. The kinetic energy operator, realized as a finite difference stencil, is localized. As a consequence the real-space representation of the Hamiltonian is sparse. This limits the amount of necessary communications and allows an application of the operator to a trial vector in order(N) operations. We will present results about the efficiency of the most numerical intensive parts of the code and we will compare the accuracy of the calculations for reference systems with other established DFT methods.

TT 77.8 Wed 18:15 TRE Ma

Rare Earth Metals in Density-Functional Theory — •Marco Casadei[1], Xinguo Ren[2], Patrick Rinke[1], Angel Rubio[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Technology, Hefei, China — [3]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

The presence of f electrons in the rare earths and their interaction with the s and p electrons give rise to several physical phenomena. One prominent example is the isostructural α-γ phase transition in cerium (Ce). We have shown that density-functional theory (DFT) captures the volume collapse associated with the transition, but only if advanced functionals such as exact exchange plus correlation in the random-phase approximation (EX+cRPA) are used [1]. The volume collapse is understood in terms of a *localization/delocalization* of the f electrons. We then addressed the question: *is the isostructural volume collapse in cerium unique*? By applying DFT, we studied lanthanum (La), praseodymium (Pr) and neodymium (Nd), which undergo several structural changes with pressure. We find that the transitions are already captured at a lower level of DFT (i.e. with (semi)-local functionals) and therefore conclude that f-electrons are not the driving force in this case. Within hybrid functionals, we find only one phase in lanthanum, which has no f-electrons, and more than one stable solution in the fcc crystal for Pr and Nd, as found for Ce. Unlike in Ce, however, there is always one solution that is the most stable, thus no isostructural volume collapse emerges in agreement with experiments.
[1] M. Casadei *et al.*, Phys. Rev. Lett. **109**, 14642 (2012).

TT 77.9 Wed 18:30 TRE Ma

Electronic Structure and van der Waals Interactions in the Stability and Mobility of Point Defects in Semiconductors — •Wang Gao and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Point defects are abundant in materials, and significantly affect the electronic, optical, and magnetic properties of solids. However, our understanding of the stability and mobility of point defects remains incomplete, despite decades of intensive work on the subject. In the framework of density-functional theory, Perdew-Burke-Ernzerhof functional underestimates formation energies by 0.7 eV due to the electron self-interaction error, while Heyd-Scuseria-Ernzerhof (HSE) functional yields formation energies in better agreement with high-level many-body methods, but often overestimates migration barriers by up to 0.4 eV.

Using HSE coupled with screened long-range vdW interactions [1], we demonstrate that HSE+vdW can simultaneously and accurately describe the formation energies and migration barriers of point defects. The inclusion of vdW interactions significantly changes the transition state geometries, and brings migration barrier into close agreement with experimental values for six different defects. For multiatom vacancies and point defects in heavier semiconductors, vdW interactions play an increasingly larger role [2].

[1] G. X. Zhang, *et al.*, PRL **107**, 245501 (2011); A. Tkatchenko, *et al.*, PRL **108**, 236402 (2012).

[2] W. Gao and A. Tkatchenko, PRL **111**, 045501 (2013).

TT 77.10 Wed 18:45 TRE Ma

Scaling Laws for van der Waals Interactions in Nanostructured Materials — •Vivekanand Gobre and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Berlin

Accurate description of van der Waals (vdW) interactions is crucial for precise prediction of structure and stability of complex materials. VdW forces originate from interactions between fluctuating multipoles in matter and play a significant role in the self-assembly of nanostructured materials. Many models used to describe vdW interactions in nanomaterials are based on a simple pairwise-additive approximation, neglecting the strong electrodynamic response effects caused by long-range fluctuations in matter. We develop and utilize an efficient microscopic method [1,2] to demonstrate that vdW interactions in nanomaterials act at distances greater than typically assumed, and can be characterized by different scaling laws depending on the dimensionality and size of the system. Specifically, we study the behaviour of vdW interactions in single-layer and multilayer graphene, fullerenes of varying size, single-wall carbon nanotubes and graphene nanoribbons. As a function of nanostructure size, the van der Waals coefficients follow unusual trends for all of the considered systems, and deviate significantly from the conventionally employed pairwise-additive picture. We propose that the peculiar van der Waals interactions in nanostructured materials could be exploited to control their self-assembly.
[1] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012); [2] Gobre, Tkatchenko, Nat. Commun. (2013).

TT 77.11 Wed 19:00 TRE Ma

2D nanopatterns of shape-persistent molecular polygons on HOPG — •Stefan-S. Jester, Nina Schönfelder, Eva Sigmund, and Sigurd Höger — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Shape-persistent organic molecules with flexible side chains self-assemble at the solution/solid interface to form 2D nanoarchitectures. Scanning tunneling microscopy yields a submolecularly resolved insight into the adsorbate structures. A key issue is how the shape and symmetry of the backbones and their alkyl chain substitution pattern determine the shape and symmetry of the adsorbate patterns. Recently we focused on molecular polygons (triangles, squares, pentagons, and hexagons) with dithiophene corners and phenylene-alkynylene sides.[1]

In my talk I will give insight into the relation between Archimedean surface patterns and supramolecular 2D adlayers. [1] S.-S. Jester, E. Sigmund, S. Höger *J. Am. Chem. Soc.* **2011**, *133*, 11062.

TT 78: Graphene: Electronic Properties (organized by O)

Time: Wednesday 16:00–19:15 Location: WIL C107

TT 78.1 Wed 16:00 WIL C107

Monomer Doping of Self-Assembled Graphene Nanoribbons for Band Gap Alignment — •Christopher Bronner[1,3], Stephan Stremlau[1,3], Marie Gille[2], Felix Brausse[2], Anton Haase[1], Stefan Hecht[2], and Petra Tegeder[1,3] — [1]Freie Universität Berlin — [2]Humboldt-Universität zu Berlin — [3]Ruprecht-Karls-Universität Heidelberg

In order to exploit the technologically interesting electronic properties of graphene, several concepts have been discussed which would lead to the opening of a band gap. One approach is spatial confinement of the charge carriers in quasi-one-dimensional graphene nanoribbons (GNRs). The band gap of a GNR scales inversely with its width and particularly nanometer-scale widths are desirable for application e.g. in transistor devices. Since the electronic properties of GNRs depend critically on their structure, precise synthesis is necessary but challenging for conventional methods such as lithography. In contrast, self-assembly from molecular precursors is an intriguing approach which has been employed to fabricate defect-free GNRs with well-defined widths and edge structures. Only this high level of structural precision allows introduction of dopant atoms at specific doping sites and concentrations in the graphene lattice. Nitrogen doping has been known to shift the band structure of GNRs with respect to the Fermi level which is interesting for GNRs in contact with electrodes and other device materials. Using surface-sensitive electron spectroscopies we demonstrate a continuous down-shift of the band structure with increased nitrogen doping of the monomers.

TT 78.2 Wed 16:15 WIL C107

Transport in chemically gated graphene p-n junctions — •Jens Baringhaus[1], Alexander Stöhr[2], Ulrich Starke[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Max-Planck Institut für Festkörperforschung, 70569 Stuttgart, Germany

The chirality of charge carriers in graphene allows them to get through potential barriers without any reflection (known as Klein tunneling). To study this effect the fabrication of well-defined p-n junctions is necessary. We use the intercalation of Ge to convert the buffer layer on the SiC(0001) surface into graphene with local p-type or n-type doping depending on the local Ge coverage. The buffer layer is initially patterned using optical lithography, to fabricate isolated n-p, n-p-n and p-n-p structures. The n- and p-type doping (340 meV, -290 meV) is confirmed by STS which also reveals very narrow p-n junctions with a length below 5 nm. The corresponding electric fields are as high as 10^6 V/cm and therefore significantly higher than those induced by field effects, providing a perfect environment to study Klein tunneling. Transport experiments are carried out by means of a 4-tip STM system, on n-p-n as well as p-n-p structures. Their resistance was found to be strongly dependent on temperature and the inner barrier length. While short barriers (< 200 nm) appear almost transparent, the resistance increases rapidly for barrier widths exceeding the coherence length (> 600 nm). The resistance of a single p-n junction fits to the theoretically predicted value for a Klein tunneling junction.

TT 78.3 Wed 16:30 WIL C107

Exceptional ballistic transport in epitaxial graphene nanoribbons — Jens Baringhaus[1], Frederik Edler[1], Claire Berger[2], Walter A. de Heer[2], and •Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Georgia Institute of Technology, Atlanta, Georgia 30332-0430, USA

The patterning of graphene into graphene nanoribbons is an essential task for the development of graphene based devices. For such ribbons with a well-ordered edge geometry the presence of one-dimensional edge states has been predicted. We use a selective graphitization process on SiC-mesa structures to produce graphene nanoribbons with a width of 40 nm. The local electronic properties of the ribbons are investigated by means of a 4-tip STM. In combination with a SEM, the precise positioning of all four tips on the nanometer range is possible to perform local transport measurements. Additionally, local tunneling spectroscopy reveals characteristic features of ferromagnetic zig-zag graphene nanoribbons. Transport experiments carried out on the very same ribbon show a conductance close to e^2/h for a wide temperature range from 30 K up to room temperature and probe spacings between 1 μm and 10 μm. Description within the Landauer formalism is possible assuming ballistic transport dominated by a single channel. Transport in the second zeroth subband is only detectable for probe spacings smaller than 1 μm due to the short localization length of carriers in this subband manifesting in the increase of the conductance to 2 e^2/h at probe spacings below 200 nm.

TT 78.4 Wed 16:45 WIL C107

Electrical Transport in Freestanding Epitaxial Graphene: Evidence of an AB-Stacked Bilayer — •Johannes Jobst[1,2], Shriram Shivaraman[3], Michael G. Spencer[3], and Heiko B. Weber[2] — [1]Leiden University, Kamerlingh Onnes Laboratorium, P.O. Box 9504, NL-2300 RA Leiden, Netherlands — [2]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]School of Electrical and Computer Engineering, Cornell University, Ithaca, NY 14853, USA

We investigate the properties of freestanding epitaxial graphene devices, which are created using a photo-electrochemical etching technique. This technique allows to selectively remove the silicon carbide (SiC) substrate on which the graphene was grown by thermal decomposition of SiC. We focus on completely freestanding devices of various geometries and devoid of any graphene-substrate interactions. We prepare freestanding Hall bars in order to study the low-temperature transport and Shubnikov-de Haas oscillations. We find evidence that the buffer layer is transformed to an additional graphene layer upon the etching process, and that the formed bilayer is AB stacked. Inhomogeneities in the buffer layer or introduced during the etching process are discussed.

TT 78.5 Wed 17:00 WIL C107

Scattering mechanisms in Tl-doped epitaxial graphene — •Carola Strasser[1], Bart Ludbrook[2], Andrea Damascelli[2], Christian R. Ast[1], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Quantum Matter Institute, UBC, Vancouver, BC V6T 1Z4, Canada — [3]Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Since the charge carrier density in graphene can very easily be tuned by means of chemical doping this approach counts as a promising way to design graphene-based future electronic devices. It was shown [1] that the Fermi level can be shifted over a wide range in either direction. But one has to consider that the dopants do not just donate or take the electrons but they have an impact on the electronic structure: they act as scattering centres and change the charge carrier mobility.

We investigated small amounts of Thallium atoms on a monolayer of epitaxial graphene by angular resolved photoemission spectroscopy and did a careful analysis of the line width. Although Tl is very weakly bound and at first sight a paradigm long-range scatterer, we found that it introduces a sizeable short-range contribution. Only by using a model which combines both, long-range and short-range scattering we were able to describe our observations. This allowed us to put an upper limit on the dielectric constant for Tl-doped epitaxial graphene.

[1] H. Liu et al., *J. Mater. Chem.* **21**, 3335 (2011)

TT 78.6 Wed 17:15 WIL C107

Excited electron dynamics in spatially aligned 7a-graphene nanoribbons on Au(788) — •Nils Fabian Kleimeier[1], Alexander Timmer[1], Harry Mönig[1], Xinliang Feng[2], Klaus Müllen[2], Harald Fuchs[1], and Helmut Zacharias[1] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Max-Planck-Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Photoelectron spectroscopy of spatially aligned straight 7-armchair

graphene nanoribbons (7-aGNRs) on Au(788) was carried out under ultra high vacuum conditions utilizing a time-of-flight spectrometer and a multi-anode detector. We found two unoccupied states at energies of E_1=3.6 eV and E_2=3.9 eV above the Fermi energy by exciting the sample with different photon energies (3.94 eV to 4.35 eV) from a femtosecond OPA. When exciting the sample with ultrashort pules (20 fs) at λ=390 nm ($h\nu$=3.15 eV) by frequency- doubling the output of a femtosecond Ti:sapphire laser amplifier, these states can further be investigated by 3-photon photoemission using a third state at an energy of E_3-E_F=0.6 eV as intermediate. All three states are in agreement with IPE measurements we performed previously on this system [1]. Thus the electronic dynamics of the state can be measured by time-resolved 3-photon photoemission spectroscopy with cross-polarized laser pulses. Preliminary evaluation of these measurements indicates electronic lifetimes of the unoccupied states of τ ∼110 fs and 85 fs for the states at E-E_F 3.9 eV and 3.6 eV, respectively.

References: [1] S. Linden et al., Phys. Rev. Lett. 108 (2012) 216801

TT 78.7 Wed 17:30 WIL C107

Optical characterization of atomically precise graphene nanoribbons — •Richard Denk[1], Michael Hohage[1], Jinming Cai[2], Pascal Ruffieux[2], Roman Fasel[2], and Peter Zeppenfeld[1] — [1]Experimental Physics, JKU Linz, Altenbergerstrasse 69, 4040 Linz, Austria — [2]nanotech@surfaces, EMPA, Überlandstasse 129, 6800 Dübendorf, Switzerland

Graphene nanoribbons (GNRs) promise high potential for future nanoscale electronic devices. While 2-dimensional graphene is semimetallic, electron confinement and edge effects in narrow (<10nm) GNRs can result in the opening of a band gap. The electronic and optical properties, however, strongly depend on the structural details of the GNRs. Only recent advances in the bottom-up fabrication of atomically precise GNRs [1] have enabled reliable experimental investigations of well-defined GNRs.

We have studied the fabrication process and the optical properties of GNRs on Au(788) using reflectance difference spectroscopy (RDS), taking advantage of the optical anisotropy due to the uniaxial alignment of the GNRs parallel to the step edges of the vicinal Au(788) surface. We find that the optical properties of the GNRs are highly anisotropic and dominated by three excitonic transitions, in excellent agreement with theoretical calculations.

[1] J. Cai at el, Nature, 466 (2010) 470.

TT 78.8 Wed 17:45 WIL C107

Electronic and transport properties of BNC heterostructures, a first-principles investigation. — •Simon Dubois and Jean-Christophe Charlier — Institute of Condensed Matter and Nanosciences, UCL, Louvain-La-Neuve, Belgium

Two dimensional hexagonal BN (h-BN), an isomorph of graphene with a lattice mismatch of only 1 .7%, is a wide gap insulator as its bulk counterpart. Advances in the synthesis of hybrid BNC heterostructures offer new opportunities to engineer the electronic properties of low-dimensional systems. Recently, it has been shown that the introduction of h-BN nanodomains into graphene enables to induce a tunable band gap in the honeycomb lattice. Lateral junctions between electrically conductive graphene and insulating h-BN provide new ways to embed electrically isolated elements within single atomic layers. Not only the two-dimensional BNC heterostructures hold promises for new applications but also the corresponding quasi-1D nanoribbons as well as the few layers structures obtained by plane stacking.

We report on the properties of low energy carriers in various kind of BNC heterostructures investigated by means of first-principles calculations: quasi one dimensional junctions made of h-BN and graphene ribbons, two-dimensional atomic layers made of hybridized domains, as well as few-layers stacks.

TT 78.9 Wed 18:00 WIL C107

Time- and Angle-Resolved Photoemission Studies of Epitaxial Graphene — •Søren Ulstrup[1], Jens C. Johannsen[2], Federico Cilento[3], Alberto Crepaldi[3], Michele Zacchigna[3], Jill A. Miwa[1], Philip D. C. King[4], Cephise Cacho[5], Edmond Turcu[5], Emma Springate[5], Felix Fromm[6], Christian Raidel[6], Thomas Seyller[6], Fulvio Parmigiani[3], Marco Grioni[2], and Philip Hofmann[1] — [1]Aarhus University, Aarhus, Denmark — [2]EPFL, Lausanne, Switzerland — [3]Sincrotrone Trieste, Trieste, Italy — [4]University of St. Andrews, St. Andrews, United Kingdom — [5]STFC Rutherford Appleton Laboratory, Didcot, United Kingdom — [6]Technical University of Chemnitz, Chemnitz, Germany

Understanding of the ultrafast carrier dynamics in graphene is of central importance for many electronic and optoelectronic applications. With the advent of high harmonic laser-based time- and angle-resolved photoemission (TR-ARPES) it is possible to gain a direct view of the non-equilibrium electronic structure around the Dirac point in graphene with femtosecond time resolution. Here, we characterize the dynamic processes around the Dirac point in epitaxial graphene using TR-ARPES measurements. In particular, we study the time-scales and significance of hot electron thermalization processes and electron-phonon coupling, and address the possibility of carrier multiplication.

TT 78.10 Wed 18:15 WIL C107

Electronic and Transport Properties of Epitaxial Graphene on the Atomic Scale — •Philip Willke[1], Thomas Druga[1], Alexander Schneider[2], Rainer Ulbrich[1], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Lehrstuhl für Festkörperphysik, FAU Erlangen, D-91058, Germany

The application of graphene in future devices requires a thorough understanding of its transport properties on the nanometer scale. We present a scanning tunneling potentiometry study at 6 K of electron scattering in mono- and bilayer graphene on n-doped SiC. Using STP we combine the imaging of local transport fields and sample topography. By probing simultaneously the thermovoltage signal [1] created due to slightly different temperatures of sample and tip, we can moreover obtain sensitive information on the electronic structure at the Fermi energy. We demonstrate how both transport and electronic information can be disentangled from STP measurements. We identify substrate steps and monolayer-bilayer junctions as local scattering centers which impede the electronic current and create local voltage drops that we compare to recent measurements at 72 K. [2] Moreover, wrinkles and substrate inhomogeinities have been identified as further sources of scattering. We acknowledge the financial support by the SPP 1459 "Graphene".

[1] K. J. Engel, M. Wenderoth, N. Quaas, T. Reusch, K. Sauthoff and R.Ulbrich, Phys. Rev. B 63, 165402 (2001)

[2] S. H. Ji et al., Nature Materials 11, 114-119 (2012)

TT 78.11 Wed 18:30 WIL C107

Exchange coupling between 3*d*-transition metal adatoms and Ni(111) mediated by graphene — •Simon Fichtner, Paolo Ferriani, and Stefan Heinze — Institut für Theoretische Physik und Astrophysik, Christian-Albrecht-Universität zu Kiel, D-24098 Kiel, Germany

Recently, 3*d*-transition metal (TM) adatoms on graphene have been intensively studied both experimentally (e.g. [1]) and theoretically (e.g. [2]). However, the possibility to stabilize their magnetic moment by exchange coupling to an underlying magnetic substrate has received little attention so far. Graphene on Ni(111) is a very good candidate in this respect as it has been experimentally shown to grow pseudomorphically. Here, we determine the electronic and magnetic properties of 3*d*-TM adatoms adsorbed on graphene on Ni(111) based on density functional theory as implemented in the VASP code. We perform a systematic study on the dependence of the exchange interaction across the 3*d*-TM series and take local correlations into account using the DFT+U formalism. We demonstrate the essential influence of the alignment of the adatoms 3d-states with the spin-polarized graphene states on the magnetic coupling with the Ni surface.

[1] Eelbo et al., Phys. Rev. Lett. **110**, 136804, 2013

[2] Wehling et al., Phys. Rev. B **84**, 235110, 2011

TT 78.12 Wed 18:45 WIL C107

Highly spin-polarized Dirac fermions at the graphene-Co interface — •Dmitry Marchenko[1,2], Andrei Varykhalov[1], Jaime Sánchez- Barriga[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, Berlin, Germany

The interface of graphene with ferromagnets is very interesting for spintronics due to possible use of peculiar graphene electronic structure in transport and spin-filter applications when graphene is used together with nickel or cobalt as ferromagnetic contacts for spin injection and detection [1]. Despite a strong hybridization between graphene and ferromagnetic substrate states the graphene Dirac cone was observed by angle-resolved photoemission without gap between pi and pi* parts [2]. Here we report strong spin polarization of the Dirac cone measured by spin- and angle-resolved photoemission. Wave-vector dependent measurements exclude a Rashba-type spin-orbit contribution to the spin

polarization; ferromagnetic origin is verified by reversal of the remanent magnetization. The importance of the spin polarization at the interface for spin filtering is pointed out.

[1] V. M. Karpan et al., Phys. Rev. Lett. 99, 176602 (2007) [2] A. Varykhalov et al., Phys. Rev. X 2, 041017 (2012)

TT 78.13 Wed 19:00 WIL C107

Controlling and understanding the non-linear photoluminescence in graphene on a femtosecond time scale — •Richard Ciesielski[1], Alberto Comin[1], Matthias Handloser[1], Kevin Donkers[1], Torben Winzer[2], Ermin Malic[2], and Achim Hartschuh[1] — [1]Ludwig Maximilians Universität München & CeNS — [2]TU Berlin

Upon excitation, graphene exhibits nonlinear photoluminescence [1-3] that reflects the charge-carrier population and relaxation around the K-point. We present microscopic measurements on high quality exfoliated graphene samples with a pulsed laser system of ca. 18fs and a broad spectrum centred at 800nm.

Using a pulse shaping setup we can measure and manipulate the incident pulse in amplitude and phase. We find that the PL intensity depends sensitively on the temporal shape of the laser pulse, which we use to study and control the charge-carrier relaxation processes of graphene. Our findings are compared to numerical calculations.

[1] Stöhr, Wachtrup, Phys. Rev. B 82, 121408(R) (2010)
[2] Malic, Winzer, Bobkin, Knorr, Phys. Rev. B 84, 205404 (2011)
[3] Malic, Knorr, John Wiley & Sons (2013)

TT 79: Correlated Electrons - Poster Session

Time: Wednesday 15:00–19:00 Location: P2

TT 79.1 Wed 15:00 P2

Electron Spin Resonance in $Yb(Rh_{0.73}Co_{0.27})_2Si_2$ below 1 K — Ilshat Fazlishanov[1,4], •Zakir Seidov[1,5], Jörg Sichelschmidt[2], Hans-Albrecht Krug von Nidda[1], Cornelius Krellner[3], Christoph Geibel[2], Frank Steglich[2], and Manuel Brando[2] — [1]Experimental Physics V, EKM, University of Augsburg, 86159 Augsburg — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden — [3]Institute of Physics, Goethe University Frankfurt, 60438 Frankfurt am Main — [4]E.K.Zavoisky Physical Technical Institute, Russian Academy of Sciences, 420029 Kazan, Russia — [5]Institute of Physics, Azerbaijan National Academy of Sciences, AZ-1143 Baku, Azerbaijan

We report Electron Spin Resonance (ESR) experiments on the heavy-fermion metal $Yb(Rh_{0.73}Co_{0.27})_2Si_2$ in the temperature range $0.75K \leq T \leq 4K$. The ESR measurements were performed at X-band frequencies using a home-built 3He cryostat. We found that below 1.3K the ESR spectra of $Yb(Rh_{0.73}Co_{0.27})_2Si_2$ split into two lines. Such a behavior can be explained by the strong anisotropy of the ferromagnetic ground state in agreement with magnetization measurements [1].

[1] S. Lausberg, A. Hannaske, A. Steppke, L. Steinke, T. Gruner, L. Pedrero, C. Krellner, C. Klingner, M. Brando, C. Geibel, F. Steglich, Phys. Rev. Lett. **110**, 256402 (2013)

TT 79.2 Wed 15:00 P2

Heavy fermion behaviour and structural change in high pressure $CeSb_2$ — Zhuo Feng[1], •Yang Zou[1], Terence Giles[2], Philipp Niklowitz[2], Heribert Wilhelm[3], Giulio I. Lampronti[4], and F. Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [2]Dep. of Physics, Royal Holloway, University of London, Egham TW20 0EX, UK — [3]Beamline I15, Diamond Light Source, Didcot OX11 0DE, UK — [4]Department of Earth Sciences, University of Cambridge, Cambridge CB2 3EQ, UK

The Kondo lattice system $CeSb_2$ crystallises in the orthorhombic $SmSb_2$ structure and exhibits a series of magnetic phase transition at low temperature. It has been reported to become ferromagnetic below 15 K, with the ordered moment oriented within the basal plane, and to undergo two further transitions at 9 K and 12 K [1]. These transition are suppressed above a hydrostatic pressure $p_c \simeq 16$ kbar. We present high pressure transport and x-ray diffraction results, which examine the high pressure state of $CeSb_2$. Our findings suggest that $CeSb_2$ undergoes a drastic structural change at p_c. Whereas in the low pressure structure, $CeSb_2$ is local moment magnet, in the high pressure structure it exhibits tranport properties characteristic of a heavy fermion material with a low Kondo temperature scale of the order of 10 K.

[1] Bud'ko et al. PRB **57,21 (1998)**

TT 79.3 Wed 15:00 P2

de Haas-van Alphen oscillations in (La,Ce)$TiGe_3$ — R. Seerig[1,5], •M. Uhlarz[1], W. Kittler[2], V. Fritsch[2], O. Stockert[3], T. Förster[1], P. Canfield[4], J. Wosnitza[1,5], and H. v. Löhneysen[2] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Karlsruher Institut für Technologie, 76049 Karlsruhe, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [4]Ames Laboratory, US DOE, and Dept. of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA — [5]Institut für Festkörperphysik, TU Dresden, 01062 Dresden, Germany

$CeTiGe_3$ is one of the few Kondo-lattice compounds which order ferromagnetically ($T_C \approx 14$ K); $LaTiGe_3$ may be used as its nonmagnetic reference, since both compounds crystallize in the hexagonal perovskite structure [1, 2]. We report on de Haas-van Alphen (dHvA) oscillations in single crystals grown from Ge flux, measured in magnetic fields up to 13 T in a cantilever-type torque magnetometer. We found four dHvA frequencies ranging from 60 T to 4300 T, with effective masses between $0.31\,m_0$ and $1.31\,m_0$, featuring a comparatively weak angular dependence. Further, we give an interpretation of our results on the basis of DFT calculations of the electronic bandstructure of $LaTiGe_3$.

[1] P. Manfrinetti et al., Solid State Commun. **135** (2005) 444
[2] W. Kittler et al., Phys. Rev. B **88** (2013) 165123

TT 79.4 Wed 15:00 P2

Evolution of ferromagnetic correlations in $FeGa_{3-x}Ge_x$ probed by ^{69,71}Ga nuclear quadrupolar resonance — •M. Majumder, M. Wagner-Reetz, P. Khuntia, Yu. Grin, and M. Baenitz — Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany

Binary Fe based semimetals like FeSi, $FeSb_2$ and $FeGa_3$ earned great attention because of their unconventional ground state (possible Kondo insulators) and good thermoelectric performance. Metallic behavior and Fe based magnetism can be introduced by various substitutions. In contrast to $FeSb_2$ (where Te substitution results in a disorder dominated Griffiths phase) [1], the system $FeGa_3$ seems to be an ideal candidate to study the evolution of ferromagnetic quantum criticality (FMQC) by magnetic resonance. Recently it was shown that Fe(Ga, $Ge)_3$ develops FMQC behavior without strong disorder effects [2,3]. The nuclear quadrupolar resonance (NQR) spectra provide direct information about the degree of local disorder (line width) and the critical fluctuations at the verge of FM ordering (spin lattice relaxation at zero field). In $FeGa_3$ four NQR lines have been found, of which two lines are from the two Ga sites in the crystal structure and other two are due to the two Ga isotopes [4]. ^{69,71}Ga NQR investigation have been performed in $FeGa_{3-x}Ge_x$ polycrystalline sample with x=0.1 (absent magnetic order), 0.2 ($T_C \simeq 6$ K) and $x_c \approx 0.15$ (critical concentration for FMQC).

[1] Phys. Rev. Lett. **109**, 256401 (2012)
[2] Phys. Rev.B **86**, 144421, (2012)
[3] arXiv: 1304.1897 (2013)
[4] arXiv: 1311.1501 (2013)

TT 79.5 Wed 15:00 P2

NMR on the quantum critical ferromagnet $YbNi_4P_2$: Evidence for a large basal plane local anisotropy — •Rajib Sarkar[1], Marco Günter[1], Cornelius Krellner[3], Christoph Geibel[2], and Hans-Henning Klauss[1] — [1]IFP, TU Dresden, D-01069 Dresden, Germany — [2]MPI-CPFS, D-01187 Dresden, Germany — [3]Goethe University Frankfurt, D-60438 Frankfurt am Main, Germany

In the last 10 years there was growing evidence both from theoretical work and experimental observations that a ferromagnetic (FM) quantum critical point (QCP) cannot exist in a pure system, because the transition becomes first order before reaching the QCP. Therefore the recent report of clear evidence for a FM-QCP in the heavy fermion compound $YbNi_4P_2$ attracted considerable attention. While the Bra-

vais lattice of this compound is tetragonal, resulting in isotropic in-plane macroscopic magnetic properties, the local symmetry on the Yb site (and on the P-site) is lower, orthorhombic. Therefore some in-plane anisotropy of local magnetic properties is expected, which could however not yet been studied because of the absence of related effects on macroscopic properties. We performed ^{31}P NMR investigations on a grain aligned polycrystalline sample of $YbNi_4P_2$. We observed three structures in the NMR spectra, which present quite different T-dependence of the respective Knight shifts. An analysis of these results provides a clear evidence for strong local in-plane anisotropy of the Yb-moment due to the orthorhombic crystal electric field. Implication for the magnetic ordered state shall be discussed.

TT 79.6 Wed 15:00 P2

Phase diagram of the effective Ising spin-1/2 chain system $CoNb_2O_6$ in transverse magnetic field and comparison with the 1D Ising model — •Victoria Cho[1], Simon Scharffe[1], Oliver Breunig[1], Martin Valldor[1], Markus Garst[2], Eran Sela[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Insitut für Theoretische Physik, 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 79.7 Wed 15:00 P2

Magnetic excitations in quantum-critical $Ce(Pd_{0.86}Ni_{0.14})Al$ — •O. Stockert[1], K. Schmalzl[2], V. Fritsch[3], and H. v. Löhneysen[3] — [1]Max-Planck-Institut CPfS, Dresden, Germany — [2]Forschungszentrum Jülich, Jülich Centre for Neutron Science at Institut Laue-Langevin, Grenoble, France — [3]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany

The heavy-fermion compound CePdAl offers the opportunity to study quantum criticality in the presence of geometrical frustration. The antiferromagnetic order in CePdAl decreases strongly when substituting nickel for palladium and a quantum critical point is approached in $CePd_{1-x}Ni_xAl$ for $x = 0.14$. We performed extensive inelastic neutron scattering to study the low-energy magnetic excitations in $Ce(Pd_{0.86}Ni_{0.14})Al$, i.e., the alloy where magnetic order is just suppressed. We find spin fluctuations being broad in q-space indicating only short-range dynamic spin correlations. We discuss their q-space and temperature dependence and will compare the results to the spin excitations in the magnetically ordered parent compound CePdAl.

TT 79.8 Wed 15:00 P2

Hidden energy scale in CePdAl — Chien-Lung Huang[1], Kai Grube[1], •Christian Taubenheim[1], Veronika Fritsch[1], Sarah Woitschach[2], Zita Huesges[2], Oliver Stockert[2], and Hilbert v. Löhneysen[1] — [1]Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

CePdAl is a partially geometrically-frustrated heavy-fermion antiferromagnet with a Néel temperature $T_N = 2.7$ K crystallizing in the hexagonal ZrNiAl structure. We measured the thermal expansion $\alpha_{a,c}$ and the magnetostriction $\lambda_{a,c}$ along both crystallographic axes in the temperature range of $0.02\,\mathrm{K} \leq T \leq 10\,\mathrm{K}$ and magnetic fields of up to 14 T. From $\alpha_{a,c}$ and $\lambda_{a,c}$ we derive the T-B phase diagram below 1 K. Across the magnetic phase boundaries into the paramagnetic state $\alpha_{a,c}/T$ shows a peak moving to $T \to 0$ at $B^* = 3.5$ T, which is concomitant with maxima in $\lambda(B)$, entropy $S(B)$, and magnetic susceptibility $\chi(B)$. This suggests a possible hidden energy scale in CePdAl, which might be tuned by applying pressure. To this end, we investigated the pressure dependence of the magnetization and performed magnetoresistivity measurements between $1.8\,\mathrm{K} \leq T \leq 10\,\mathrm{K}$ and $B \leq 5$ T. As a first result the pressure dependence is found to be very weak, since α_a and α_c have opposite signs. This explains the different values for T_N found in literature.

TT 79.9 Wed 15:00 P2

Effect of Ni-doping on the geometrically frustrated heavy-fermion system CePdAl — •Stefan Lucas[1], Zita Huesges[1], Sarah Woitschach[1], Oliver Stockert[1], Veronika Fritsch[2], and Hilbert von Löhneysen[2] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany

The heavy-fermion compound CePdAl is an interesting system for investigations of quantum criticality in combination with geometric magnetic frustration, which arises from the hexagonal crystal structure of the system. In zero magnetic field, the Néel temperature of 2.7 K can be reduced by doping nickel on the palladium sites. At a doping level of about 14 %, the Néel temperature becomes zero and a quantum critical point is reached. To follow the magnetic order upon nickel doping and investigate the effect of magnetic frustration closer to the quantum critical point, we performed extensive heat capacity measurements on a 5 % Ni-doped single crystal. $CePd_{0.95}Ni_{0.05}Al$ orders below $T_N \approx 1.85$ K via a second-order phase transition in contrast to the weakly first-order transition in pure CePdAl. Our measurements reveal for $CePd_{0.95}Ni_{0.05}Al$ a critical magnetic field $B_C \approx 3$ T ($B \parallel c$, $T \to 0$) to fully suppress the antiferromagnetic phase. We will discuss the resulting magnetic $B-T$ phase diagram and compare it with the parent compound CePdAl.

TT 79.10 Wed 15:00 P2

QPI in singlet, triplet and non-centrosymmetric unconventional superconductors — •Alireza Akbari[1] and Peter Thalmeier[2] — [1]MPI for Solid State Research, Stuttgart, Germany — [2]MPI for the Chemical Physics of Solids, Dresden, Germany

The technique of quasiparticle interference (QPI) has recently been successfully applied to heavy fermion compounds to determine the unconventional superconducting gap symmetry. It was proposed [1] and proven [2,3] that QPI can distinguish between the d-wave singlet candidates of superconducting $CeCoIn_5$. The QPI theory has now also been developed for non-centrosymmetric (NCS) superconductors [4] with mixed singlet-triplet gap function. Qualitatively new effects in the QPI pattern originate from Rashba spin-orbit coupling: Distinct differences between charge- and spin QPI and anisotropies appear due to additional Rashba coherence factors. We use Born approximation and full t-matrix theory to calculate the QPI spectrum and apply it to a 2D model for the NCS heavy fermion unconventional superconductor $CePt_3Si$. We discuss the new QPI features for a gap model with accidental node lines due to its composite singlet-triplet nature. Furthermore we predict the quasiparticle interference spectrum for the multiband chiral p-wave superconductor Sr_2RuO_4 [5] and the possible chiral d-wave superconductor SrPtAs.

[1] A. Akbari et al, PRB 84 , 134505 (2011)
[2] M. P. Allan et al, Nat. Phys. 9, 468 (2013)
[3] B. B. Zhou et al, Nat. Phys. 9, 474 (2013)
[4] A. Akbari and P. Thalmeier, EPL, 102, 57008 (2013)
[5] A. Akbari and P. Thalmeier, PRB 88, 134519 (2013)

TT 79.11 Wed 15:00 P2

Theory of Magnetic Excitations in Van Vleck-type Mott insulator on Square Lattice — •Alireza Akbari and Giniyat Khaliullin — Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

We study magnetism in Van Vleck-type d^4 Mott insulators with square lattice symmetry. A theory includes the exchange interactions, tetragonal crystal field splitting, and spin orbit coupling. We found two different magnetic phases, with in-plane and out-of-plane magnetization for the higher and lower values of the crystal field splitting, respectively. We calculated the excitation spectra for paramagnetic and two magnetically ordered phases. The results are discussed in the context of d^4 Mott insulator Ca_2RuO_4.

TT 79.12 Wed 15:00 P2

Magnetostriction and thermal expansion of the triple-layered $Sr_4Ru_3O_{10}$ System — •W. Schottenhamel[1], R. Fittipaldi[2], A. Vecchione[2], A.U.B. Wolter[1], and B. Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01171 Dresden, Germany — [2]Univ. Salerno, Dipartimento Fis ER Caian-

iello, I-84084 Fisciano, Italy

$Sr_4Ru_3O_{10}$ is a member of the $(Sr,Ca)_{n+1}Ru_nO_{3n+1}$ Ruddlesden Popper series and displays spontaneous ferromagnetism at $T_c \sim 102\,K$ along the c axis coexisting with orbital-dependent intralayer metamagnetism around $T^* \sim 50\,K$ [1]. Since a strong spin-phonon coupling has been proposed in this material, we performed detailed thermodynamic investigations by means of dilatometry as well as by SQUID magnetometry under pressure. Measurements of magnetostriction, thermal expansion and magnetization were performed on single crystalline samples in the temperature range $T = 2$–$200\,K$ at magnetic fields up to 15 T. The crystal expansion exhibits a highly anisotropic behavior. Signatures of the ferromagnetic phase-transition were found for both directions. Further distinct anomalies are visible in the lower temperature region, which could be correlated to the metamagnetic transition at T^*. By combining the changes of the thermal expansion and the heat-capacity at the ferromagnetic transition, a strong volumetric pressure dependence of $dTc/dp \sim$ -8 K/ GPa has been revealed. Additional measurements of magnetization under hydrostatic pressure have been done in order to verify this big negative value.
[1] V. Granata et. al., J. Phys.: Cond. Mat. 25 (2013) 056004

TT 79.13 Wed 15:00 P2

Realistic Calculation of Optical Spectra of Layered Ruthenates — •Esmaeel Sarvestani, Guoren Zhang, Evgeny Gorelov, and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Juelich, D-52425 Juelich, Germany

Within the LDA + dynamical mean field theory, the optical conductivity of layered ruthenates is investigated for various temperatures, in the framework of linear response theory and Kubo's formalism. The anisotropic properties of charge dynamics and temperature dependence of in-plane and out-of-plane conductivity are studied. The effect of spin-orbit coupling in the spectrum is considered.

TT 79.14 Wed 15:00 P2

Ab initio study of electronic correlation in $SrRuO_3$ — •Liang Si, Zhicheng Zhong, and Karsten Held — Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria

4d ferromagnetic oxide $SrRuO_3$ (SRO) has a great potential for future oxide electronic device applications, so the deep understanding and masterful control are important to its development and application. The ferromagnetic-to-nonmagnetic and metal-to-insulator transitions in SRO thin film, which depend on film thickness, are fancy properties, whereas there is no conclusion whether such two transitions are intrinsic properties because both DFT and DFT+U methods fail in simulation of such experimentally observed ferromagnetic-to-nonmagnetic and metal-to-insulator transitions. We employed DFT+DMFT method to study the electronic structures of SRO in bulk and thin film systems in order to explain the experimentally observed transitions at thin film. According to our calculations we suggest the following two conclusions regarding the experimentally observed transitions: firstly, both transitions in SRO thin films are intrinsic properties due to strongly electronic correlation rather than surface relaxation and defects effect, secondly, dynamic mean filed theory is necessary in studying of transition metal oxides especially for interface or thin film systems.

TT 79.15 Wed 15:00 P2

Critical scaling analysis of the itinerant ferromagnet $Sr_{1-x}Ca_xRuO_3$ — •Dirk Fuchs, Markus Wissinger, Jörg Schmalian, Chien-Lung Huang, Rudolf Schneider, and Hilbert von Löhneysen — Karlsruhe Institute of Technology, Karlsruhe, Germany

The critical behavior of $Sr_{1-x}Ca_xRuO_3$ was investigated by a scaling analysis based on the Arrott-Noakes equation of state. The critical exponents β, γ, and δ of the magnetic critical behavior were extracted for samples with $0 \leq x \leq 0.6$. The ferromagnetic system exhibits a smooth suppression of the Curie temperature T_C to zero at a critical concentration $x_c \approx 0.7$. For $x = 0$, mean-field like exponents are observed. With increasing x the critical exponents β, γ, and δ change nearly linearly from $\beta \approx 0.5$, $\gamma \approx 1$ and $\delta \approx 3$ for $x = 0$ to $\beta \approx 1$, $\gamma \approx 0.9$ and $\delta \approx 1.6$ for $x \approx 0.6$. Despite the systematic evolution of the critical exponents as a function of x the exponents can not be described by a universality class of known classical standard models.

TT 79.16 Wed 15:00 P2

Doping Induced Spin State Transition in $LaCoO_3$: Dynamical Mean-Field study — •Pavel Augustinsky[1], Vlastimil Krapek[1,2], and Jan Kunes[1] — [1]Institute of Physics, ASCR, Prague, Czech Republic — [2]CEITEC, Brno Univesity of Technology, Czech Republic

Hole and electron doped $LaCoO_3$ is studied using dynamical mean-field theory. The one-particle spectra are analyzed and compared to the available experimental data, in particular the x-ray absorption spectra. Analyzing the temporal spin-spin correlation functions we find the atomic intermediate spin state is not important for the observed Curie-Weiss susceptibility. Contrary to the commonly held view about the roles played by the t_{2g} and e_g electrons we find narrow quasiparticle bands of t_{2g} character crossing the Fermi level accompanied by strongly damped e_g excitations.

TT 79.17 Wed 15:00 P2

Excitonic instability in Two-Band Hubbard Model — •Pavel Augustinsky and Jan Kunes — Institute of Physics, ASCR, Prague, Czech Republic

We report a newly observed instability in the two-band Hubbard model close to the spin-state transition [1]. Using unbiased search for the particle-hole instabilities in DMFT, we found that the earlier observed high-spin low-spin checker-board order is competing with the excitonic phase characterized by condensed spinful excitons. We present both numerical results and an analytic description in the strong-coupling limit.
[1] arXiv:1310.0669

TT 79.18 Wed 15:00 P2

Signatures of electronic correlations in half-metals — •Markus Dutschke[1], Liviu Chioncel[1,2], and Junya Otsuki[1,3] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [3]Department of Physics, Tohoku University, Sendai 980-8578, Japan

The distinctive feature of the electronic correlations in half-metals is the existence of Non-quasiparticle states, within the half-metallic gap, predicted previously in model as well as realistic LDA+DMFT calculations. We revisit this problem considering a simplified Hubbard model solved in DMFT using the CT-QMC impurity solver. In the same time we present an implementation of the hybridization expansion quantum impurity solver, based on the segment representation.

TT 79.19 Wed 15:00 P2

Bulk and interface half-metallicity in heterostructures based on Co_2MnAl — •Andreas Held[1], Kathrin Garb[1], Igor Di Marco[2], Stanislav Chadov[3], and Liviu Chioncel[1,4] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [4]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany

We study electronic correlation effects in bulk Co_2MnAl and (Co_2MnAl/CoMnVAl) heterostructures within a combined density functional and Dynamical Mean Field Theory. We analyze the changes in the topology of the bulk Fermi surface as well as in the electronic properties by approaching the interface via a function of temperature and the strength of the local Coulomb interaction U.

TT 79.20 Wed 15:00 P2

Importance of electronic correlations for the phase stability of V_2O_3 — •Ivan Leonov and Dieter Vollhardt — Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

We report results for V_2O_3 obtained by a novel implementation of the LDA+DMFT approach for the computation of the total energy of materials with strongly interacting electrons. It includes a fully self-consistent calculation of the charge density, whereby correlation-induced changes in the effective Kohn-Sham Hamiltonian are taken into account. This scheme is employed to study the electronic structure and phase stability of V_2O_3 near a pressure-induced Mott-Hubbard metal-insulator transition. To explore structural transformations as a function of pressure, we use the experimentally determined atomic positions for the metallic and insulating phases, respectively, and cal-

culate the total energy as a function of volume. We find that the structural stability depends very sensitively on changes of the lattice volume. In agreement with experiment, we observe that the metal-insulator transition is accompanied by a remarkable change of the c/a ratio. Full charge self-consistency is shown to be important to understand the phase stability of V_2O_3 near the Mott-Hubbard metal-insulator phase transition.

TT 79.21 Wed 15:00 P2

The correlated semiconductor $CrSb_2$ — •Anna Galler, Jan Tomczak, and Karsten Held — Institut für Festkörperphysik, Technische Universität Wien

Intermetallic-based correlated semiconductors display an intriguing temperature dependence in their physical properties: while at high temperatures a Curie-Weiss-like susceptibility develops, a regime of notably large thermopower is found at low temperatures. Between the two regimes optical spectra exhibit large transfers of spectral weight.

Here, we present a theoretical many-body study for a member of this class of materials: $CrSb_2$. We compute interaction matrix elements from first principles using the constrained random-phase-approximation (cRPA) and study many-body spectra and response functions within LDA+DMFT (local density approximation combined with dynamical mean field theory).

TT 79.22 Wed 15:00 P2

Real-Time Dynamics in Bose-Fermi Impurity Models — •Christian Kleine and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

We consider the real-time dynamics in a nano-device coupled to a fermionic lead and subject to additional charge noise or coupling to a phononic bath. We have extended the recently adopted numerical renormalisation group (NRG) to Bose-Fermi models in equilibrium to non-equilibrium quenches by employing the time-dependent NRG. It is known that such Bose-Fermi models show very rich physics in equilibrium manifested in a variety of different fixed points governing the phase transitions between different ground states. We present relaxation rates of different physical properties such as the local occupancy or spin polarisation across the quantum phase transition between the localised/delocalised phases in the Bose-Fermi Kondo model as well as in the more general Bose-Fermi Anderson model.

TT 79.23 Wed 15:00 P2

Magnetic phase-diagram of the spin-diluted Kondo-lattice model — •Matthias Peschke, Maximilian Aulbach, and Michael Potthoff — Universität Hamburg I. Institut für Theoretische Physik, Hamburg , Germany

We analyze the magnetic phase diagram of the spin-diluted Kondo-lattice model for strong antiferromagnetic Kondo couplings J and fillings ranging from quarter filling down to the magnetic-polaron limit with a single conduction electron. This range of electron densities permits to employ the Lanczos method for systems consisting of a moderate number of lattice sites and local spins. At quarter filling, and for a "diluted" system where every second site of the conduction-electron system couples to a local quantum spin $s = 1/2$, the formation of almost local Kondo singlets results in a non-magnetic ground state. For low densities we expect a state with magnetic long-range order of the local spins mediated by extremely heavy polarons. In the single conduction-electron limit, an almost fully polarized ferromagnet is enforced by a generalized Lieb-Mattis theorem. While the size of the Kondo clouds is predominantly controlled by J, the polaron size is additionally determined by the degree of spin dilution. We study the crossover from polaron-mediated magnetism to a non-magnetic state with local spins screened individually for different degrees of dilution and for different J in the strong-coupling regime.

TT 79.24 Wed 15:00 P2

Multi-Fermi Points in the Kondo-vs.-RKKY Quantum Box — •Mirek Hänsel, Andrej Schwabe, and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg, Germany

The competition between the Kondo effect and the indirect (RKKY) magnetic exchange is studied for nanoscale systems where, besides the Kondo temperature and the RKKY coupling, the finite-size gap represents a third relevant energy scale.

As has been shown recently [1] for the typical "on resonance" case with a single electron at the non-degenerate Fermi level, a Kondo-type screening of an impurity spin is possible, depending on the system's geometry. This leads to an unconventional Kondo-vs.-RKKY competition with a re-entrant behavior that manifests itself in an unusual J dependence of spin correlations and a total ground-state spin deviating from the predictions of standard RKKY theory.

Here, we extend our studies by applying the density-matrix renormalization group as well as weak-coupling perturbation theory to multi-impurity Kondo models on confined one- and two-dimensional lattices where the conduction-electron system has a degenerate Fermi level. In this case and for weak J, the system is perturbatively mapped onto an effective central-spin model where typically each impurity spin couples to a different itinerant spin in the central region. We discuss the geometry dependence of the effective couplings and the resulting magnetic structure.

[1] A. Schwabe, D. Gütersloh and M. Potthoff, Phys. Rev. Lett. 109, 257202 (2012).

TT 79.25 Wed 15:00 P2

Kondo regime of the non-equilibrium time evolution of an Anderson quantum dot — •Sebastian Bock[1,2], Alexander Liluashvili[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 79.26 Wed 15:00 P2

Exact diagonalization techniques for strongly correlated systems — •Sareh Motahari and David Jacob — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Gaining an understanding of strongly correlated electron materials and nanoscale devices is one of the main challenges of condensed matter physics. One of the most important models in this context is the Anderson impurity model which is central to the understanding of the Kondo effect [1] and is at the heart of the Dynamical Mean-Field Theory [2]. Here we explore different techniques based on exact diagonalization of finite Anderson models for the description of strong correlations in nanoscale systems and molecules with transition metal centers. In particular, we explore the use of the novel Distributional Exact Diagonalization [3] method for the description of the Kondo effect in realistic systems.

[1] Hewson, The Kondo Problem to Heavy Fermions, Cambridge University Press, Cambridge (1997)
[2] Kotliar et al., Rev. Mod. Phys. 78, 865 (2006)
[3] Granth and Strand, Phys. Rev. B 86, 115111 (2012)

TT 79.27 Wed 15:00 P2

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]Faculty of Physics, Adam Mickiewicz University, Poznań

Wilson's Numerical Renormalization Group (NRG) allows to describe many quantum impurity problems in equilibrium. But it remains a challenge to extend the use of NRG to situations of steady-state non-equilibrium, such as current through a quantum dot at finite bias. In our approach we consider additional baths coupled to the fermionic leads of the given impurity problem. The effect of these additional baths on the leads can be described by using Lindblad operators [1,2] in the Liouville equation for the density matrix of the dot and the leads. To efficiently solve the Liouville equation we use the stochastic

quantum trajectory method [2].

Here we present first results how the Lindblad operators could be chosen to hold the leads in thermal equilibrium at a specific chemical potential and temperature and how the quantum trajectory method can be implemented in terms of time-dependent NRG based on complete basis sets.

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TT 79.28 Wed 15:00 P2

The Numerical Renormalization Group as impurity solver within the Dynamical Mean-Field - Theory for multi-band lattice models — •Katharina Stadler, Andreas Weichselbaum, and Jan von Delft — Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center of NanoScience, Ludwig-Maximilians-Universität, Munich, Germany

Dynamical Mean-Field Theory (DMFT) provides a non-perturbative many-body approach to describe the local dynamics of strongly correlated materials by mapping a lattice model self-consistently onto an effective quantum impurity model, which is then solved by a non-perturbative method, such as Quantum Monte Carlo simulations (QMC) or the Numerical Renormalization Group (NRG) approach.

Here, we use NRG as DMFT impurity solver to treat multi-band models. Typically, the application of NRG in this context is strongly limited since the numerical cost increases exponentially with the number of bands. To deal with this limitation, we investigate two strategies: First, for multi-band models with intrinsic symmetries, we implement these explicitly in our numerical code using non-abelian channel symmetries [1] where applicable. Second, for models without symmetries we investigate the feasibility of using interleaved Wilson chains, as recently proposed [2]. We also test the reliability of the latter method by applying it to models with symmetries and comparing the results to those obtained by the explicit treatment of the non-abelian channel symmetry.

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TT 79.29 Wed 15:00 P2

Charge order and frustration in two-dimensional Falicov-Kimball models — •younes javanmard, andrey antipov, pedro ribeiro, and stefan kirchner — Max Planck Institute for Physics of Complex Systems, Nöthnitzer Str 38, 01187 Dresden, Germany

The Falicov-Kimball model is frequently employed in a number of contexts ranging from the melting of charge order to the metal-insulator transition. Its popularity is in part due to its solvability in the limit of infinite coordination number, i.e. within the Dynamical Mean Field Theory (DMFT).

At sufficiently large interaction strength the Falicov-Kimball model can be mapped to an Ising model on the same lattice. On the square lattice at half-filling, the DMFT fails to capture the interacting nature of the charge-ordering transition and predicts a continuous transition of mean-field character for all coupling strengths. In contrast, a recent study suggest the transition of the two-dimensional square lattice to be of first order at small interaction strength [1].

We set up a Monte Carlo algorithm for the two-and three-dimensional Falicov-Kimball model and study the nature of the transition in the half-filled Falicov-Kimball model on the square lattice and extend the study to lattice types allowing for geometrical frustration, like the triangular lattice [2].

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TT 79.30 Wed 15:00 P2

Optimizing Matrix Product State Codes Using SciPAL: Parallelisation and GPU Portability — •Thomas Köhler[1], Johannes Hagemann[2], Salvatore R. Manmana[1], and Stephan C. Kramer[3] — [1]Institut f. Theoretische Physik, Universität Göttingen — [2]Institut f. Röntgenphysik, Universität Göttingen — [3]Max-Planck-Institut f. biophysikalische Chemie, Göttingen

We apply the SciPAL library [1] to matrix product states (MPS), as used in the context of density-matrix renormalization group (DMRG) methods, which are important tools for treating low-dimensional strongly correlated quantum systems as realized in certain materials like quantum magnets (e.g. Azurite) and typically described by Hubbard-like or Heisenberg models. SciPAL (scientific parallel algorithms library) is a C++-based, hardware-independent open-source library, compatible with the widely used finite element library deal.II. By its link to CUDA, it provides the flexibility to extend existing codes to work on graphics processors. SciPAL's core asset is a user-friendly API to BLAS and NVidia's CUBLAS which allows to use an operator-based formulation of typical linear algebra operations. We discuss the extension of SciPAL to a domain-specific formulation of the numerical methods for computing the properties of MPS and their performance on graphics cards. A. K. Mitchell et al. [1] SciPAL: Expression Templates and Composition Closure Objects for High Performance Computational Physics with CUDA and OpenMP, S. C. Kramer and J. Hagemann, submitted to ACM TOPC.

TT 79.31 Wed 15:00 P2

Accelerations of Diagrammatic Determinantal Quantum Monte Carlo Calculations using GPUs — •Markus Schmitt[1], Iain Bethune[2], and Thomas Pruschke[3] — [1]Georg-August-Universität, Göttingen, Germany — [2]EPCC (University of Edinburgh), Edinburgh, UK — [3]Georg-August-Universität, Göttingen, Germany

Diagrammatic Determinantal Quantum Monte Carlo (DDQMC) algorithms are used to solve quantum impurity models such as the Anderson model. The calculation of acceptance rates and observables during the Monte Carlo walk involves linear algebra operations whose computational expense increases with decreasing temperature. Thus, the lower boundary of the treatable temperature range is limited by the available compute capacity. In order to make use of GPUs as cheap and powerful accelerators parts of a DDQMC code were ported to CUDA. The measurement of the observables turned out to be well suited for acceleration on GPUs and a speedup of more than 100 times over the unaccelerated version was obtained for the largest problem size under consideration.

TT 79.32 Wed 15:00 P2

Superconducting gap at a ferromagnetic quantum critical point — •Matthias Einenkel[1], Hendrik Meier[2], Catherine Pépin[3], and Konstantin B. Efetov[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Department of Physics, Yale University, New Haven, CT 06520, USA — [3]IPhT, CEA-Saclay, L'Orme des Merisiers, 91191 Gif-sur-Yvette, France

We discuss the quantum critical behaviour of a two-dimensional quantum ferromagnet in the context of the spin-fermion model. In this system fermions interact with critical bosonic excitations. We investigate the system by first performing a mean-field analysis, and show that close to the quantum critical point a superconducting gap appears which has spin triplet symmetry. Further, we calculate the action of the Goldstone modes associated with this symmetry breaking and derive a non-linear sigma model. These fluctuations turn out to be not suppressed by any small parameter and therefore eventually destroy the order. This reveals the failure of the large N expansion which was reported by previous works.

TT 79.33 Wed 15:00 P2

Disorder-driven Coulomb gas transitions — •Stefan Wolff and Simon Trebst — Institut for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Coulomb gases with power-law correlations emerge as effective low-temperature description of various frustrated magnets where the low-temperature states obey certain local constraints. An even more direct realization of a Coulomb phase is provided by close-packed dimer models on bipartite lattices. Here we report results from extensive numerical simulations of such dimer models, where we study the characteristics of the phase transition induced by static disorder of the lattice, i.e. site and/or bond percolation.

TT 79.34 Wed 15:00 P2

LDA+Slave-Boson Mean-Field Theory: itinerant electrons, magnetism and dynamics in realistic materials with multi-orbital degrees of freedom — •Christoph Piefke, Malte Behrmann, and Frank Lechermann — Uni Hamburg

The rotationally invariant slave-boson mean-field theory (RISB) in combination with the LDA framework is used to investigate strongly interacting systems [2]. In a tailored correlated subspace the multi-orbital Hubbard Hamiltonian is mapped onto an itinerant quasiparticle part and localized bosonic degrees of freedom. This decouples complex interactions (e.g. spin-flip, pair-hopping, spin-orbit coupling), quartic

in the original electron operators, at the cost of a set of constraints. At saddle-point, a self-consistent mean-field solution is obtained. With rigorous derivation of the slave-boson formalism by matrix calculus over complex numbers and group theory, we show how to reduce the number of parameters in our functional. The connection to similar approaches within the Gutzwiller formalism [2] will be discussed. Finally, we also investigate the dynamical behaviour of quasiparticles and multiplets after sudden changes of interaction parameters via the time-dependent extension of the RISB method [3].

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TT 79.35 Wed 15:00 P2

ESR studies of $CoCr_2O_4$ — •Alexey Ponomaryov[1], Mykhaylo Ozerov[1], Joachim Woznitza[1], Vladimir Tsurkan[2,3], Alois Loidl[2], and Sergei Zvyagin[1] — [1]High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [3]Institute of Applied Physics, Academy of Science of Moldova, Chisinau, Republic of Moldova

$CoCr_2O_4$ is a ferrimagnet ($T_C \sim 97K$) with cubic spinel structure and two magnetic ions (Co^{2+} and Cr^{3+}) in the elementary cell. Significant spin-lattice coupling and magnetic frustration are important features of $CoCr_2O_4$, defining its very unusual phase diagram [1]. Here, we report on high-field electron spin resonance (ESR) studies of single-crystalline samples of $CoCr_2O_4$ performed in the frequency range from 90 to 1000 GHz in magnetic fields up to 16 T. Two modes were observed. Peculiarities of the ESR excitation spectra are discussed.

This work was partly supported by the DFG.

[1] Tsurkan et al., Phys. Rev. Lett. 110, 115502 (2013)

TT 79.36 Wed 15:00 P2

Magnetic ground state and low-energy spin dynamics in single crystals of the frustrated magnet $CoAl_2O_4$ — •S. Zimmermann[1,2], A. Alfonsov[1], M. Iakovleva[3], E. Vavilova[3], H.-J. Grafe[1], H. Luetkens[4], O. Zaharko[4], H.-H. Klauss[2], A. Maljuk[1], S. Wurmehl[1], T. Dey[1], V. Kataev[1], and B. Büchner[1,2] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany — [3]Zavoisky Phys.-Tech. Inst., RAS, Kazan, Russia — [4]PSI Villigen, Switzerland

Frustrated magnetic systems are of special interest because they can exhibit exotic magnetic ground states like spin ice or spin liquid. The compound $CoAl_2O_4$ belongs to the A-site spinels, where the Co ions form a diamond lattice and the frustration originates from competing nearest- and next-nearest neighbor interactions. Thus the frustration tends to suppress long-range magnetic ordering and favors short-range spin correlations. This effect can be supported by disorder, e.g., site inversion. Due to the recent breakthrough in the growth of high-quality single crystals [1], it has become possible to study the magnetic ground state of $CoAl_2O_4$ in detail. Recent neutron scattering results give strong indications that a spin liquid like magnetic ground state is realized in such $CoAl_2O_4$ single crystals [2]. To further clarify this question, we have studied these crystals with high field high frequency ESR, NMR and μ-SR techniques. The experimental results have enabled to obtain important insights into the properties of the ground state, spin dynamics and magnetic interactions in this compound which will be discussed in this presentation.

[1] A. Maljuk et al., J. Cryst. Growth **311**, 3997 (2009)
[2] O.Zaharko et al., Phys. Rev. B **84**, 094403 (2011)

TT 79.37 Wed 15:00 P2

Thermal expansion and magnetostriction measurements at sub Kelvin temperatures - experiments on the frustrated quantum magnet Cs_2CuCl_4 — •satya krishna Thallapaka, Bernd Wolf, and Michael Lang — Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TR49, D-60438 Frankfurt (M), Germany.

We describe the device suitable for high-resolution thermal expansion and magnetostriction measurements using a capacitive dilatometer [1] which measures length changes with a sensitivity of $\Delta l \geq 10^{-2}$ Å, corresponding to a relative resolution of $\Delta l/l \sim 10^{-10}$. The system operates down to 40 mK and in magnetic fields up to 18 T. We report measurements on the spin S = 1/2 triangular-lattice Heisenberg antiferromagnet Cs_2CuCl_4 aiming at exploring its field-induced quantum critical point.

[1] R. Pott and R. Schefzyk, J. Phys. E **16**, 444 (1983)

TT 79.38 Wed 15:00 P2

Localized states on triangular traps and low-temperature properties of the antiferromagnetic Heisenberg and repulsive Hubbard models — •Mykola Maksymenko[1,3], Johannes Richter[2], and Oleg Derzhko[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38 01187 Dresden — [2]Institut für theoretische Physik, Universität Magdeburg, D-39016 Magdeburg, Germany — [3]Institute for Condensed Matter Physics of NAS of Ukraine

We consider the antiferromagnetic Heisenberg and the repulsive Hubbard model on two N-site one-dimensional lattices, which support dispersionless one-particle states corresponding to localized states on triangular trapping cells. We calculate the degeneracy of the ground states in the subspaces with low number of magnons or electrons as well as the contribution of these states (independent localized states) to thermodynamic quantities. Moreover, we discuss another class of low-lying eigenstates (so-called interacting localized states) and calculate their contribution to the partition function. We also discuss the effect of extra interactions, which lift the degeneracy present due to the chirality of the localized states on triangles.

TT 79.39 Wed 15:00 P2

1/d expansion for coupled dimer magnets — •Darshan G. Joshi[1], Kris Coester[2], Kai P. Schmidt[2], and Matthias Vojta[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Theoretische Physik, Technische Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

Using bond operators we develop a systematic expansion in 1/d, where d is spatial dimension, for coupled-dimer Heisenberg magnets. We apply this technique to a model of dimers on a hypercubic lattice, a generalization of the square-lattice bilayer Heisenberg model to arbitrary d. The method covers both the quantum paramagnetic and antiferromagnetic phases including the quantum critical point. Physical observables such as the phase boundary, mode dispersions and ground-state energy are shown to have a systematic expansion in powers of 1/d and are calculated to next-to-leading order. In the paramagnetic phase, an expansion in ratio of inter-dimer and intra-dimer coupling for arbitrary d is shown to be consistent with the results of the 1/d expansion.

TT 79.40 Wed 15:00 P2

Bond randomness in Kitaev's honeycomb spin-liquid model — •Fabian Zschocke and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

The Kitaev model on the honeycomb lattice realizes a spin liquid whose emergent excitations are gapless Majorana fermions and static Z2 gauge fluxes. Upon introduction of bond randomness the model remains exactly solvable, via an equivalent tight-binding model of canonical fermions. We use this to study a number of observables as function of disorder strength, paying particular attention to properly selecting physical states within the canonical-fermion description. Specifically, we calculate the distribution of local susceptibilities, extract the NMR lineshape, and make contact with known results on the problem of disordered Dirac fermions.

TT 79.41 Wed 15:00 P2

NMR as a local probe for 5d and 4d magnetism in honeycomb lattices A_2TO_3; (A=Na,Li; T=Ir,Rh) — •Panchanana Khuntia[1], Mayukh Majumder[1], Soham Manni[2], Philipp Gegenwart[2], and Michael Baenitz[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]I. Physikalisches Institut, Georg-August-Universitaet Goettingen, Goettingen, Germany

Recently, 5d iridates like the honeycomb lattices $(Na,Li)_2IrO_3$ and 4d analog Li_2RhO_3 display unconventioal magnetic properties which are driven by spin orbit coupling and frustration. There is a cross-over from Néel (zig-zag) type magnetic ordering to a spin-liquid state in the Heisenberg-Kitaev model. We report temperature (T) and field (H) dependent NMR study on Na_2IrO_3, Li_2IrO_3, and Li_2RhO_3. ^{23}Na NMR in Na_2IrO_3 enable us to disentangle three Na sites and deduce the magnetic order parameter.The T and H dependent NMR spectra and spin lattice relaxation rate (SLR) reveal that Na_2IrO_3 and Li_2IrO_3

are magnetically ordered with T_N = 15 K, additionally, Li_2IrO_3 exhibits features reminiscent of a spin-liquid.In Li_2RhO_3, magnetization and specific heat data exhibit no sign of long range ordering down to 0.3 K but a spin glass transition is observed at T_g=8 K. ^{7}Li NMR line width and SLR in Li_2RhO_3, display signatures of spin correlation and emergence of slowing down of spin fluctuations on approaching the freezing temperature. The specific heat and SLR show power law behavior below T_g reflecting the persistence of low lying excitations pointing towards a spin liquid state.

TT 79.42 Wed 15:00 P2

Energy dynamics in the Heisenberg-Kitaev chain — •Robin Steinigeweg and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

Spin liquids are realized by the Kitaev model and by the Heisenberg model in one dimension, with a finite-temperature dynamics only partially resolved despite the integrability of both models. We make an essential step forward by studying the dynamics in the Heisenberg-Kitaev chain as a model of two competing spin liquids. Using analytical and numerical approaches within linear response, we show the emergence of purely ballistic energy transport at all integrable points, which manifests as pronounced Drude weights and low-frequency suppression of regular contributions. Varying several model parameters including exchange-coupling strength, ratio, and anisotropy as well as magnetic field, we find extended quantum chaotic regions with vanishing Drude weights and well-defined DC contributions. In the vicinity of the Kitaev model, we find clear signatures of the topological gap in the response function.

TT 79.43 Wed 15:00 P2

Magnetic properties of antiferromagnetic Heisenberg chains with spin-S boundary defects in magnetic fields — •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 anisotropic S=1/2 Heisenberg chains with spin-S boundary defects with an impurity coupling beyond simple superexchange. We employ finite temperature Quantum Monte-Carlo methods based on Stochastic Series Expansion. For particular choices of parameters and at zero temperature the models we investigate are exactly solvable by means of Bethe Ansatz techniques. Results will be presented for magnetic properties as functions of uniform and edge magnetic fields, exchange-coupling constants, anisotropy, temperature, and system size. Properties include the susceptiblity and magnetization. Of special interest are bulk and boundary properties which are expressed in orders of 1/L and the magnetization with respect to the corresponding magnetic fields. We will compare our findings from both methods in the zero temperature limit.

TT 79.44 Wed 15:00 P2

Optical absorption of a spin-1/2 Heisenberg antiferromagnet on a triangular lattice — •Boris Celan and Wolfram Brenig — Institute for theoretical Physics, Technische Universität Braunschweig

We investigate the optical absorption in a spin-1/2 antiferromagnetic Heisenberg model on the anisotropic triangular lattice coupled to lattice degrees of freedom. We describe the scattering of light from the system via a simple model of magneto-elastic coupling to nearest neighbor bond dipoles, assuming a monoatomic unit cell. The magnetic excitations are described using linear spin wave theory including interaction to $O(1/S^2)$. The absorption cross section is evaluated in terms of two-magnon-one-phonon Greens functions. Results will be presented for the conductivity versus frequency and temperature, with and without final state interactions. The impact of anisotropy will be analyzed. The role of different phonon density of states will be considered.

TT 79.45 Wed 15:00 P2

Magnetic phase diagram of the metallic triangular-lattice antiferromagnet $PdCrO_2$ — Jong Mok Ok[1], •M. Dietterle[2], J. Wosnitza[2], and Jun Sung Kim[1] — [1]Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea — [2]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany

Due to geometrical frustration, two-dimensional triangular-lattice antiferromagnets (TAFM) exhibit a variety of magnetic phases and transitions in an applied magnetic field [1]. The phase diagram becomes fantastically rich if magnetic anisotropy and competing first- and second-neighbor interactions come into play, as it is the case in many magnetic materials [2]. $PdCrO_2$ is a rare example of a metallic TAFM consisting of stacked layers of Pd and Cr triangular lattices in a delafossite structure. The localized $S = 3/2$ spins of the Cr^{3+} ions in the CrO_2 layer are expected to be AFM ordered in the 120-degree helical spin structure at $T_N = 37.5$ K. Previous de Haas-van Alphen experiments reveal a Fermi-surface reconstruction due to the AFM ordering, confirming the strong coupling between the itinerant electrons and the localized spins [3]. With torque magnetometry on single crystals in high pulsed magnetic fields up to 70 Tesla we investigate the phase diagram of $PdCrO_2$ and the influence of meta-magnetic transitions on the nature of coupled itinerant electrons.

[1] L. Seabra *et al.*, Phys. Rev. B **84**, 214418 (2011)
[2] L. Seabra *et al.*, Phys. Rev. B **83**, 134412 (2011)
[3] Jong Mok Ok *et al.*, Phys. Rev. Lett. **111**, 176405 (2013)

TT 79.46 Wed 15:00 P2

Fermi condensation near Van Hove singularities in the triangular lattice — •Daniel Hirschmeier[1], Dmitry Yudin[2], Hartmut Hafermann[3], Olle Eriksson[2], Alexander I. Lichtenstein[1], and Mikhail I. Katsnelson[4] — [1]Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Department of Physics and Astronomy, Uppsala University, Box 516, SE-751 20 Uppsala, Sweden — [3]Institut de Physique Théorique (IPhT), CEA, CNRS, 91191 Gif-sur-Yvette, France — [4]Radboud University Nijmegen, Institute for Molecules and Materials, NL-6525, AJ Nijmegen, The Netherlands

The proximity of the Fermi surface to Van Hove singularities drastically enhances interaction effects and leads to essentially new physics. In this work we address the formation of flat bands ("Fermi condensation") within the Hubbard model on the triangular lattice and provide a detailed analysis from an analytical and numerical perspective. To describe the effect we consider both weak-coupling and strong-coupling approaches, namely the renormalization group and dual fermion methods. It is shown that the band flattening is driven by correlations and is well pronounced even at sufficiently high temperatures, of the order of 0.1-0.2 of the hopping parameter. The effect can therefore be probed in experiments with ultra cold fermions in optical lattices.

TT 79.47 Wed 15:00 P2

Magnetic Ordering and Superconductivity in Triangular Lattices in the Hubbard Model — Maria Daghofer and •André Fischer — IFW Dresden, Dresden, Germany

The 2D triangular lattice provides a simple model with intrinsic geometric frustration and is therefore well suited to study effects induced by electronic interactions. The aim of this work is to find possible ground state scenarios at the van-Hove filling within the Hubbard model, taking various magnetically ordered states and superconducting states into account. Using cluster perturbation theory allows us to tread the system on a level beyond mean field theory. We find a superconducting phase with unconventional symmetry to be the supported ground state in a wide parameter regime. A comparison of selected magnetically ordered states does not show a support of a previously proposed chiral phase.

TT 79.48 Wed 15:00 P2

Strongly correlated system on frustrated lattices: Beyond the flat-band scenario — •J. Richter[1], O. Derzhko[2], O. Krupnitska[2], and T. Krokhmalskii[2] — [1]University Magdeburg, Germany — [2]Institute for Condensed Matter Physics, Ukraine

We consider the spin-1/2 antiferromagnetic Heisenberg model at high magnetic fields as well as the Hubbard model at low electron density on some frustrated lattices with almost dispersionless lowest one-particle band. Eliminating high-energy degrees of freedom we construct low-energy effective Hamiltonians which are much simpler than the initial ones. Based on the effective-model description we examine the low-temperature properties of the considered frustrated quantum Heisenberg antiferromagnets in the high-field regime. We also apply our approach to describe azurite. Interesting features of these highly frustrated spin models consist in a steep increase of the entropy at very small temperatures T and a characteristic extra low-T peak in the specific heat. The most prominent effect for spin models is the existence of a magnetic-field driven Berezinskii-Kosterlitz-Thouless phase transition occurring in the two-dimensional model [1]. For the Hubbard

model we discuss the existence of ground-state ferromagnetism. While for the considered model for a completely flat band the ground state is paramagnetic, we find a transition to ground-state ferromagnetism driven by the on-site repulsion in case that the band becomes dispersive. We present the ground-state phase diagram for the Hubbard model on the frustrated diamond chain at 1/6 electron filling.
[1] O.Derzhko et al., Phys. Rev. B 88, 094426 (2013)

TT 79.49 Wed 15:00 P2

Magnetocrystalline anisotropy in low dimensional systems — •Kira Riedl, Harald O. Jeschke, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

We study the magnetic and electronic properties of low dimensional systems with focus on consequences of spin-orbit coupling. On the basis of density functional theory (DFT) calculations we analyze several materials regarding if effects of the magnetocrystalline anisotropy or the Dzyaloshinskii-Moriya interaction can be observed. We investigate recent reports of a significant magnetic anisotropy in the copper compound $CuBr_2$ and the pyrochlore $R_2V_2O_7$ with DFT+U+SOC calculations. As a member of another class of materials with dominant effects of spin-orbit coupling we also study the magnetic properties of the hexagonal iridate Na_2IrO_3. It is of high physical interest since there is no general agreement yet whether it is a realization of the Heisenberg-Kitaev model or it can rather be described with quasi-molecular orbitals.

TT 79.50 Wed 15:00 P2

Magnetic anisotropy of azurite probed by high-field electron resonance — •Mykhaylo Ozerov, Jochen Wosnitza, and Sergei Zvyagin — Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Electron spin resonance (ESR) studies of single crystals of the natural mineral azurite $Cu_3(CO_3)_2(OH)_2$, a spin-chain compound with a distorted diamond structure, in magnetic fields up to 16 T are reported. Two ESR modes were observed below $T_N = 1.8$ K. The ESR angular dependence measured at 248 GHz revealed an extremum at a direction of $42^o \pm 3^o$, tilted from the a axis towards to the c axis. Field dependence of the resonance frequencies was measured with magnetic fields applied parallel, as well as perpendicular, to this direction. Two gaps in the ESR excitation spectrum were found at 84 and 145 GHz (0.35 and 0.6 meV), which is consistent with results of inelastic neutron scattering measurements [Rule *et al.*, PRB 84, 184419 (2011)]. Peculiarities of the obtained frequency-field diagram evidence essential role of the Dzyaloshinskii-Moriya interaction in the microscopic picture of the magnetic interactions in this compound.

This work was partly supported by the DFG.

TT 79.51 Wed 15:00 P2

Crystal growth and analysis of $BaCuSi_2O_6$ — •Pascal Puphal, Natalija van Well, Franz Ritter, Cornelius Krellner, and Wolf Assmus — Physikalisches Institut, Goethe-Universität Frankfurt, Deutschland

$BaCuSi_2O_6$ is of interest since it has a two dimensional BEC-Phase at low temperature from 23,2 to 49,3 T. Crystal growth of this crystal is difficult, but was achieved using oxygen partial pressure or flux-method($LiBO_2$). However, the system tends to glaze especially using $LiBO_2$ as flux. We found $NaBO_2$ to work as flux as well and KBO_2 to be the best. Also we could prove with an electron microscope that the flux is not incorporated in the structure. We have investigated that an alloy of platinum and gold as crucible material improves the growth since it interacts less with the material.
$BaCuSi_2O_6$ has a structural phase transition from tetragonal to orthorhombic, which we explore with low temperature powder diffraction, magnetic, and specific heat measurements. Furthermore, we investigated strontium substitution on the barium side, which we proved to be possible up to 30%. It leads to a reduction of the unit cell, which suppresses the structural phase transition already at 5% strontium. Calcium substitution behaves differently: it only leads to defects in the crystal, which also suppress the phase transition but with increasing calcium, it even destroys the dimer-coupling of cupper.

TT 79.52 Wed 15:00 P2

Specific heat studies of the $Cs_2CuCl_{4-x}Br_x$-system — •Markus Kuhnt, Natalija van Well, Franz Ritter, Pham Thanh Cong, Bernd Wolf, Michael Lang, Cornelius Krellner, and Wolf Assmus — Institute of Physics, Goethe-University Frankfurt, Max-von-Laue-Straße 1, D-60438 Frankfurt (M), Germany

In this contribution, we report on a systematic study of the magnetic properties on single crystals of the $Cs_2CuCl_{4-x}Br_x$-system ($0 \leq x \leq 4$), which include the well studied end components Cs_2CuCl_4 and Cs_2CuBr_4. Both are $S = \frac{1}{2}$ quasi-two-dimensional-quantum antiferromagnets, but whereas Cs_2CuCl_4 exhibits field-induced Bose-Einstein-condensation, in Cs_2CuBr_4 triplet crystallization is found. In 2011 Cong et al. studied the magnetic susceptibility of the $Cs_2CuCl_{4-x}Br_x$-system ($0 \leq x \leq 4$) above 2 K and found that the transition from Cs_2CuCl_4 to Cs_2CuBr_4 evolves discontinuously[1].

This discontinuous evolution motivates to study the magnetic properties of this system more thoroughly. Thus, we measured the specific heat at various x in the temperature range $1.8 \leq T \leq 20$ K. We will discuss the magnetic part of the specific heat as well as the ratio between the maximum temperatures of magnetic specific heat and magnetic susceptibility as a function of x. These data will also be compared to theoretical calculations for Heisenberg antiferromagnetic chains and 2D Heisenberg triangular antiferromagnets.
[1] P.T. Cong et al., Phys. Rev. B **83**, 064425

TT 79.53 Wed 15:00 P2

Magnetic Properties of Cu_2OSeO_3 under weak doping — Markus Strobl[1], •Marco Halder[1], Tim Adams[1], Sebastian Mühlbauer[2], Michael Wagner[1], Andreas Bauer[1], Helmut Berger[3], 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

The magnetoelectric Cu_2OSeO_3 is the first established insulator within the class of cubic chiral helimagnets crystallizing with space group $P2_13$. Perhaps most fascinating, these compounds give rise to a regular lattice of topologically non-trivial spin whirls, the so-called Skyrmion lattice. The magnetoelectric coupling in Cu_2OSeO_3 thereby promises novel phenomena compared to itinerant magnets such as MnSi, $Fe_{1-x}Co_xSi$, or FeGe. While in the latter systems the influence of doping on the magnetic properties was already investigated in detail, no corresponding data are available for Cu_2OSeO_3. Here, we report a comprehensive study by means of magnetization and small-angle neutron scattering focusing on the determination of the magnetic phase diagram of vapor-transport-grown samples of Cu_2OSeO_3 substitutionally doped with various transition metals.

TT 79.54 Wed 15:00 P2

Phase-space Berry phases in chiral magnets: Skyrmion charge, Dzyaloshinskii-Moriya interaction and Hall effect — •Robert Bamler[1], Frank Freimuth[2], Yuriy Mokrousov[2], and Achim Rosch[1] — [1]Universität zu Köln, Cologne, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present a theory for electronic properties of systems with spin-orbit coupling and smooth magnetic textures, such as chiral magnets. We show that Berry phases in mixed position/momentum space play an important role for both equilibrium and non-equilibrium properties.

In magnetic materials without inversion symmetry (chiral magnets) the spin-orbit coupling can lead to smooth whirls (skyrmions) in the magnetization. They give rise to a strong Hall signal due to the Berry phase an electron picks up when it moves in position space. At the same time, spin-orbit interactions in chiral magnets lead to Berry-phase effects in momentum space, such as the anomalous Hall effect.

In our work we show that the combination of spin-orbit coupling and a magnetic texture leads to new effects due to Berry phases picked up on closed loops in mixed position/momentum space. Using a gradient expansion of the Green's function we identify mixed phase-space Berry phases as the cause of Dzyaloshinskii-Moriya interactions and the charge of skyrmions in metals. By applying the gradient expansion to the Kubo formula we recover the known contributions to the Hall conductivity due to Berry phases in position and momentum space and discuss new contributions due to mixed phase-space Berry phases.

TT 79.55 Wed 15:00 P2

Large lattice distortions associated with the magnetic transition in $La_{0.7}Sr_{0.3}MnO_3$ — •Frank Weber[1], Dimitri Argyriou[2,3], Oleksandr Prokhnenko[4], and Dmitry Reznik[5] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, D-76021 Karlsruhe, Germany — [2]European Spallation Source ESS AB, PO Box 176, SE-221 00 Lund, Sweden — [3]Department of Synchrotron Radiation

Research, Lund University, Box 118, Lund, Sweden — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany — [5]Department of Physics, University of Colorado - Boulder, Boulder, CO 80309

Colossal magnetoresistance (CMR) is associated with the phase transition from a metallic ferromagnetic to insulating paramagnetic phase, which can be controlled by an applied magnetic field. The insulating phase occurs due to trapping of the charge carriers by polaronic lattice distortions, which raise the resistivity. Theories based on local physics predict that the magnitude of the resistivity jump at T_C is determined by how much, on average, the amplitude of these distortions increases at the phase transition. Using neutron scattering, we measured the average distortion amplitude in $La_{0.7}Sr_{0.3}MnO_3$. Surprisingly, its increase from below to above T_C is just as large as in other manganites, which have a much larger resistivity jump. This result suggests that the strength of CMR is determined not by the size of distortions, but by their cooperative nature, specific to each compound. Existing theories need to be extended to include correlations between different unit cells to explain and predict the strength of CMR.

TT 79.56 Wed 15:00 P2

Crystal growth and physical properties of doped honeycomb lattice systems A_2IrO_3 (A=Na, Li) — •Friedrich Freund, Soham Manni, and Philipp Gegenwart — I. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

Honeycomb-lattice iridates have recently attracted interest in the context of novel electronic and magnetic states like spin-orbit Mott or quasi-molecular orbital insulators, Kitaev-Heisenberg magnets or correlated topological insulators. Starting from Na_2IrO_3 and Li_2IrO_3, which display insulating antiferromagnetic ground states, we investigate the influence of various dopings on the magnetic interaction and electronic properties. Single and polycrystals are synthesized using solid state reactions under appropriate conditions.

TT 79.57 Wed 15:00 P2

Interplay of Spin-Orbit Coupling and Electron Correlations in Iridate Compounds — •Alexander Hampel and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg, Germany

This work deals with the investigation of the electronic structure of perovskite iridates, such as Ba_2IrO_4. Recent experiments exploring different iridate compounds found out that the cooperation of strong electron correlations and spin-orbit coupling plays an important role in the correct description of their physical behaviour. The reason for this are large spin-orbit interaction energies in the 5d transition metal oxides, which have the same order of magnitude as the local Coulomb interaction.
We apply a combination of density functional theory (DFT) with explicit many-body methods to handle the realistic electronic correlations within the relativistic environment. More explicitly, the mixed-basis pseudopotential approach is allied with rotational-invariant slave bosons in order to address the intriguing correlated spin-orbit physics.

TT 79.58 Wed 15:00 P2

Electronic structure of Sr_2IrO_4 polycrystals and PLD grown thin films — •Ozan Kirilmaz[1], Atsushi Yamasaki[2], Michael Sing[1], Akira Sekiyama[3,4], Masaaki Isobe[5], Shigemasa Suga[3,4], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Faculty of Science and Engineering, Konan University, Kobe 658-8501, Japan — [3]Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan — [4]RIKEN SPring-8 Center, Sayo, Hyogo 679-5148, Japan — [5]National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan

Novel physics induced by strong spin-orbit coupling has attracted strong attention from both theory and experiment in recent years. Sr_2IrO_4 has an insulating ground state which seems to be driven by the strong spin-orbit coupling and relatively weak Coulomb interaction. The electronic structure near the Fermi level in Sr_2IrO_4 is characterized by $J_{eff} = \frac{1}{2}$ states. In order to provide deeper insight into these states, we have carried out high energy-resolution photoemission spectroscopy on both polycrystalline and thin film 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.

TT 79.59 Wed 15:00 P2

Effect of Gd doping and O deficiency on the Curie temperature of EuO — •Nuttachai Jutong[1], Thomas Mairoser[2], Ulrich Eckern[1], and Udo Schwingenschlögl[3] — [1]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg, 86159 Augsburg, Germany — [3]KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

The effect of Gd doping and O deficiency on the electronic structure, exchange interaction, and Curie temperature of EuO in the cubic and tetragonal phases is modeled by means of density functional theory. We observe a maximum in the Curie temperature around 6.25% Gd doping, originating from a combination of f-d hopping and indirect exchange. However, the effect is suppressed at high doping. An increased Curie temperature is found in the case of O deficiency and is attributed to a double exchange mechanism, which is suppressed in the tetragonal phase due to Jahn-Teller distortions.

TT 79.60 Wed 15:00 P2

Investigations on the Fermi surface of $SrCo_2P_2$ — •K. Götze[1,2], J. Klotz[1,2], C. Geibel[3], C. Bergmann[3], H. Rosner[3], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor (HLD), Helmholtz-Zentrum Dresden-Rossendorf — [2]Institut für Festkörperphysik, TU Dresden — [3]Max-Planck-Institut CPfS, Dresden

$SrCo_2P_2$ is a non-superconducting member of the 122 pnictides with $ThCr_2Si_2$ tetragonal structure type. Although band-structure calculations predict ferromagnetic ordering in this compound, it only exhibits Stoner-enhanced paramagnetism [1]. However, peculiarities of the electronic structure depend on details of the crystal structure (like the P z coordinate) which are not known precisely enough. Therefore, an experimental determination of the Fermi surface is desirable to explain this discrepancy. Probing the de Haas-van Alphen effect by use of a capacitive torque magnetometer setup, we measured the full angular dependence of quantum oscillations and effective masses of $SrCo_2P_2$. Our experiments were carried out in a top-loading dilution refrigerator and a ^{3}He system at temperatures ranging from 25 mK to 4.2 K, and in magnetic fields up to 35 T. In combiniation with density-functional band-structure calculations, our results provide detailed information about the Fermi surface of $SrCo_2P_2$.
[1] S. Jia *et al.*, Phys. Rev B. **80**, 165107 (2009).

TT 79.61 Wed 15:00 P2

Algebraic-diagrammatic algorithm for the high-order perturbation expansion of the Green's function in the Mott-Hubbard insulator in high dimensions — Eva Kalinowski[1], Walter Apel[2,3], •Martin Paech[3,1], and Eric Jeckelmann[3] — [1]Academy of Computer Science and Management, Bielsko-Biała, Poland — [2]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [3]Leibniz Universität, Hannover, Germany

One of the open problems in the theory of Mott-Hubbard insulators is the shape of the Hubbard bands in the single-particle density of states (DOS). In particular, for the Hubbard model on a Bethe lattice in the limit of an infinite coordination number, dynamical mean-field theory (DMFT) calculations reveal some unexplained sharp structures at the low-energy edges of the Hubbard bands in both the Mott insulating phase and the metallic phase in the critical region. Previous analytical expansions (up to second order for the Hubbard model and up to third order by solving the DMFT self-consistency equation) cannot fully explain the observed structures.

We show that the calculation of the DOS can also be formulated in a form, which is amenable to an algebraic-diagrammatic approach. We prove this procedure for the case of the Falicov-Kimball model and determine manually the DOS and the gap up to the fourth order for the Hubbard model. Additionally, we outline the generalization of an algorithm [1], which is well established for the ground-state energy and related critical properties up to the 15th order, for the computation of higher orders of the Green's function and the gap.
[1] PRB 85, 045105

TT 79.62 Wed 15:00 P2

Generalization of the Time-Dependent Numerical Renormalization Group Method to Finite Temperatures and General Pulses — •Hoa Nghiem and Theodoulos A. Costi — Peter Grünberg Institut and Institute for Advanced Simulation, Research Centre Jülich, 52425 Jülich, Germany

We generalize the time-dependent numerical renormalization group

method (td-NRG)[1] to study the time evolution of an observable of an interacting quantum impurity system after a sudden quench at an arbitrary temperature without truncating the length of the Wilson chain [2]. This generalization requires the use of the full density matrix [3], and determining all the terms of the projected density matrix appearing in the time evolution. To evaluate these terms, we introduce efficient recursion relations. The numerical results are shown to be exact in the short time limit, while, in the long time limit, they strongly depend on the discretization parameter of NRG. We also consider the time evolution due to general continuous pulses, acting in a finite time interval. The calculation is done by discretizing the pulse into a sequence of small quenches, and generalizing the td-NRG to an arbitrary number of quenches.

[1] F. B. Anders and A. Schiller, Phys. Rev. Lett. 95, 196801 (2005).
[2] H. Nghiem and T. A. Costi, Preprint (2013).
[3] A. Weichselbaum and J. von Delft, Phys. Rev. Lett. 99, 076402 (2007).

TT 79.63 Wed 15:00 P2

Self-energy and analytic continuation for multi-orbital quantum impurity models — •Andreas Hausoel, Nicolaus Parragh, and Giorgio Sangiovanni — University of Würzburg, Germany

Continuous-time quantum Monte Carlo (CTQMC) allows us to treat quantum-impurity problems with several orbitals and general interactions. We present strategies to reduce the computational effort exploiting conserved quantities of the local Hamiltonian. In order to perform the analytic continuation of the self-energy from the Matsubara to the real axis the high frequency behavior is needed. We discuss how the necessary measurements can be implemented in hybridization-expansion CTQMC for multi-orbital problems and show first applications.

TT 79.64 Wed 15:00 P2

Hierarchical Master Equation Approach to Nonequilibrium Green's Functions: From Transport through Interacting Quantum Dots to Dynamical Mean Field Theory — •Rainer Härtle[1,2], Guy Cohen[3], David R. Reichman[3], and Andrew J. Millis[2] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Physics, Columbia Universtiy, New York, USA — [3]Department of Chemistry, Columbia Universtiy, New York, USA

We extend the hierarchical quantum master equation methodology [1,2,3] to the computation of the Green's function of an impurity system that can be driven out of equilibrium. We employ an auxiliary lead method [4], which involves a smearing over a certain energy range, and a direct method, where besides the reduced density matrix correlations between the impurity and its environment have to be included [5]. We compare both methods, studying nonequilibrium quantum transport through an interacting double quantum dot [3] and discuss applications to nonequilibrium dynamical mean field theory.

[1] Y. Tanimura, J. Phys. Soc. Jpn. 75, 082001 (2006).
[2] J. Jin *et al.*, J. Chem. Phys. 128, 234703 (2008).
[3] R. Härtle *et al.*, arXiv:1309.1170 (2013).
[4] G. Cohen *et al.*, arXiv:1310.4151 (2013).
[5] S. Wang *et al.*, arXiv:1301.6850 (2013).

TT 79.65 Wed 15:00 P2

Electronic structure of substitutionally disordered systems within a pseudopotential approach — •Alexander Herbig and Rolf Heid — Institut for solid state physics, Karlsruhe Institute of Technology

The study of the electronic structure of substitutionally disordered systems (e.g. doped compounds) via density functional-based methods is a challenge. A common approach based on supercells is limited to special impurity concentrations. Green's function based methods seem to be more promising to deal with arbitrary impurity concentrations where interesting physics can emerge. One of these methods, the coherent potential approximation (CPA), has already been successfully applied in the KKR-DFT-framework. In this work we discuss the development and first results of a CPA-like treatment of disorder based on a mixed-basis-pseudopotential DFT-code. After projection of the Kohn-Sham-orbitals onto a nonorthogonal localized basis we apply an extension of CPA based on the formalism of Blackman, Esterling and Berk (BEB) [1]. This method on the one hand allows to handle off-diagonal disorder and on the other hand can be implemented in a very natural way within an LCAO-framework [2]. Finally charge self-consistency will be achieved by feeding the BEB-CPA-results back into the DFT-calculation.

[1] J.A. Blackman et. al., Phys. Rev. B 4, 2412 (1971)
[2] K. Koerpenik et. al. Phys. Rev. B 55, 5729 (1997)

TT 79.66 Wed 15:00 P2

Green functions approach to Hubbard nano-clusters with the GKBA and T-matrix approximation — •Niclas Schlünzen, Sebastian Hermanns, and Michael Bonitz — ITAP, Christian-Albrechts-Universität Kiel, Leibnizstraße 15, 24098 Kiel

The Hubbard model describes narrow-band solid state systems in terms of sites, on which the electrons can interact, and hopping amplitudes between these sites. It exhibits the quantum characteristics of solids and recently can also be experimentally realized in finite systems, e.g., ultracold atoms in optical lattices. To describe the out-of-equilibrium dynamics of those systems, the theoretical framework of non-equilibrium Green functions is well suited [1]. It provides a controlled way to apply different many-body approximations. The equations of motion for the Green function can be solved very efficiently by using the generalized Kadanoff–Baym ansatz (GKBA), which has shown accurate results for weak coupling [2]. To describe strongly interacting systems, the T-matrix many-body approximation is a convenient choice [3]. In this contribution, we show first benchmark results for the non-equilibrium dynamics of Hubbard nano-clusters with T-matrix+GKBA comparing them with exact solutions as well as results from different many-body approximations.

[1] K. Balzer, and M. Bonitz, *Nonequilibrium Green's Functions Approach to Inhomogeneous Systems*, Springer (2013)
[2] K. Balzer et al., J. Phys. Conf. Ser. **427**, 012006 (2013)
[3] M. Puig von Friesen et al., Phys. Rev. Lett. **103**, 17 (2009)

TT 79.67 Wed 15:00 P2

Thermalization dynamics of finite Hubbard nano-clusters with non-equilibrium Green functions — •Sebastian Hermanns and Michael Bonitz — ITAP, Christian-Albrechts-Universität Kiel, Leibnizstraße 15, 24098 Kiel

The Hubbard model is widely used for the description of narrow-band solid state systems in terms of sites, on which the electrons interact, and hopping amplitudes between these sites. Recently, the Hubbard model has attracted new experimental interest with the ability to perform measurements on only a few ultracold atoms in an optical trap [1]. To describe these processes theoretically, the framework of non-equilibrium Green functions is very well suited, since it provides a controlled way of approximations, is non–perturbative in the exciting field and has shown good results for 1D and 2D Hubbard nano-clusters [2]. In this contribution, we focus on the thermalization dynamics in finite Hubbard systems analyzing the free evolution from strong non-equilibrium initial conditions. We examine the occurence of different relaxation stages and their dependence on the interaction strength, particle number as well as the dimensionality and filling factor.

[1] D. Jaksch et al., Ann. Phys. (N.Y.) **315**, 1452 (2005)
[2] M. Bonitz et al., Contrib. Plasma Phys. **53**, 778-787 (2013)

TT 79.68 Wed 15:00 P2

Reduced density matrix functional theory via a wave function based approach — •Robert Schade[1], Peter Blöchl[1], and Thomas Pruschke[2] — [1]Clausthal University of Technology, Clausthal, Germany — [2]University of Goettingen, Goettingen, Germany

We propose a new method for the calculation of the electronic and atomic structure of correlated electron systems based on reduced density matrix functional theory (rDMFT). The density matrix functional is evaluated on the fly using Levy's constrained search formalism. The present implementation rests on a local approximation of the interaction reminiscent to that of dynamical mean field theory (DMFT). This wave function based approach can be integrated into the existing DFT framework by making use of natural orbitals.

TT 79.69 Wed 15:00 P2

Time-resolved Auger electron spectroscopy — •Roman Rausch and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg

Motivated by the recent time-resolved measurements of Auger spectra, we develop a theory of time-resolved Auger electron spectroscopy (AES) for strongly correlated many-body systems. The temporal cor-

relation of the two conduction-band holes in the final state is described within the framework of the Hubbard model, extended by core states to account for the dynamics of core-hole screening. Using a numerically exact Chebyshev polynomial expansion technique (kernel polynomial method) in the low hole-density limit, the time-dependent cross section is computed for different setups. We also discuss the time-dependence of correlation-induced satellites, the validity of a two-step description and the effects resulting from a non-perturbative treatment of the Auger process.

TT 79.70 Wed 15:00 P2

Singular-mode functional renormalization group vs. Fermi surface patching: A comparison of two FRG schemes applied to the 2D Hubbard model — •Julian Lichtenstein[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 the capabilities of the singular-mode functional renormalization group (SM-FRG) which was introduced in [1]. The most important dependencies of the two particle vertex on Matsubara frequencies are included in our implementation. Moreover, the role of the self energy feedback has been investigated. We apply this method to the 2D Hubbard model and compare the results to those from previous studies that have used FRG via Fermi surface patching.

[1] W.-S. Wang *et al.*, Phys. Ref. B **85** (2012) 035414

TT 79.71 Wed 15:00 P2

Competing order in correlated electron systems made simple — Jing Wang[1,2], •Andreas Eberlein[1], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

We derive an efficient and unbiased method for computing order parameters in correlated electron systems with competing instabilities. Charge, magnetic and pairing fluctuations above the energy scale of spontaneous symmetry breaking are taken into account by a functional renormalization group flow, while the formation of order below that scale is treated in mean-field theory. The method captures fluctuation driven instabilities such as d-wave superconductivity. As a first application we study the competition between antiferromagnetism and superconductivity in the ground state of the two-dimensional Hubbard model.

TT 79.72 Wed 15:00 P2

Information entropies in Fe and Ni: Numerical evidence for electronic correlation in Momentum space — •Wilhelm Hans Appelt[1,2], Diana Benea[3], and Liviu Chioncel[1,2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Augsburg Center for Innovative Technologies, University of Augsburg — [3]Faculty of Physics, Babes-Bolyai University, Kogalniceanustr 1, Ro-400084 Cluj-Napoca, Romania

Various momentum-space properties are computed for Fe and Ni within the framework of a combined Density Functional and Dynamical Mean Field theory. We asses the effects of electron correlation in momentum space by making a comparison with the results obtained from the Local Density Approximation. We study the information entropy using the one-electron density in momentum space along different directions and as a function of local Coulomb parameter U.

TT 79.73 Wed 15:00 P2

Hydrodynamic long-time tails after a quantum quench — Jonathan Lux[1], •Jan Müller[1], Aditi Mitra[1,2], and Achim Rosch[1] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Department of Physics, New York University

After a quantum quench, a sudden change of parameters, generic many particle quantum systems are expected to equilibrate. While a few collisions of quasi particles are usually sufficient to establish approximately local equilibrium, the eventual global equilibrium is, however, much more difficult to detect: conserved quantities have to be transported for long distances to build up a characteristic pattern of fluctuations, which takes a very long time.

Here we investigate a quantum quench of the one-dimensional bosonic Mott insulator from infinite to finite interaction strength using semiclassical methods for weak, and exact diagonalization for strong quenches. We demonstrate that equilibrium is approached only slowly, as $t^{-1/2}$ with subleading corrections, consistent with predictions from hydrodynamics.

TT 79.74 Wed 15:00 P2

Stochastic mean-field approach to non-equilibrium dynamics of correlated systems — Christopher Hinz, •Sebastian Hermanns, and Michael Bonitz — ITAP, Christian-Albrechts-Universität Kiel, Leibnizstraße 15, 24098 Kiel

One major obstacle for the simulation of strongly interacting many-particle systems is the exponential growth of the state space with the number of particles—the so-called curse of dimensionality. One possibility to mitigate this problem is the application of the stochastic formulation of quantum mechanics. Within this framework, one can impose approximations on the ensemble and the equations of motion. An example for such an approximate treatment is the stochastic mean-field method (SMF) [1,2], which aims at embedding some of the correlations into the initial ensemble, while using the time-dependent Hartree-Fock method to propagate different stochastic realizations of the system independently of each other. As a benchmark system, we use the time evolution of Hubbard nano-clusters in one to three dimensions.

[1] S. Ayik, Phys. Lett. B **658**, 174 (2008)
[2] D. Lacroix et al., Phys. Rev. C **85**, 041602(R) (2012)

TT 79.75 Wed 15:00 P2

Nonlocal quantum kinetic theory — •Klaus Morawetz[1,2,3] and Pavel Lipavsky[4] — [1]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

A consistent kinetic equation of nonlocal and non-instantaneous character is derived which unifies the achievements of transport in dense gases with the quantum transport of dense Fermi systems. The numerical solution is not more expensive than solving the Boltzmann equation. In order to achieve this, large cancellations in the off-shell motion have been used which are buried usually in non-Markovian behaviors. The remaining effects are: (i) off-shell tails of the Wigner distribution, (ii) renormalization of scattering rates and (iii) of the single-particle energy, (iv) collision delay and (v) related non-local corrections to the scattering integral. The balance equations for the density, momentum and energy now include besides known quasiparticle parts additionally two-particle contributions exceeding the Landau theory. Different aplications are worked out. The collision delay results into the correlated density and consequently the number of quasiparticles is not conserved. In superconductors this leads to a shift of the chemical potential and the compensating electrostatic potential known as Bernoulli potential.

TT 80: Low-Dimensional Systems - Poster Session

Time: Wednesday 15:00–19:00 Location: P2

TT 80.1 Wed 15:00 P2

Engineering of low-energy models for topological insulators with d-electrons — •Martin Edelmann, Michael Karolak, and Giorgio Sangiovanni — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg

We present ab-initio calculations performed on Nickel-based bulk materials and heterostructures via density-functional-theory (DFT). We explore different geometries and heterostructures, focussing on cases with e_g-orbitals. This constitutes the first step for upcoming many-body calculations to possibly realize a topological state with d-orbitals.

In our first DFT-calculations, the in-plane lattice parameters were changed in order to match different substrates and explore the possibility of realizing a band-insulator. Another road to this goal is the introduction of one (or multiple) insulating planes in between the bulk material to create a heterostructure and suppress inter-orbital hopping.

We discuss the Wannier projection procedure to obtain the minimal low-energy one-body Hamiltonian which will serve as an input for the many-body calculations.

TT 80.2 Wed 15:00 P2

Symmetry protection in topological insulators: fundamentals and applications — •Stephan Rachel — Institut für Theoretische Physik, TU Dresden

We consider two-dimensional topological insulators as prototypes of symmetry protected topological phases where spin-orbit coupling gives rise to the topological insulator phase. The appearance of additional non-topological terms might cause quantum phase transitions into trivial phases when this topologically trivial term overweights the spin-orbit coupling. Usually such a phase transition is associated with closing of the bulk gap. In contrast, time-reversal symmetry breaking terms immediately destroy the topological phase without closing of the bulk gap unless the axial spin symmetry remains preserved. These findings pave the way for interesting applications in topological nano-ribbons.

TT 80.3 Wed 15:00 P2

Polaritons in a Quantum Spin Hall Insulator — •Alexander Janot[1], Bernd Rosenow[1], and Gil Refael[2] — [1]Institut für Theoretische Physik, Universität Leipzig, 04009 Leipzig, Germany — [2]Department of Physics, California Institute of Technology, Pasadena, CA 91125, USA

We study the topological properties of mixed matter-light particles, so called polaritons, in a quantum spin hall insulator coupled to photonic cavity modes. Taking into account the spin and polarization structure of electrons and photons, respectively, we find that the electron-photon coupling matrix can be characterized by a non-trivial pseudo-spin vector. For a topological quantum spin hall system this vector wraps around the Bloch sphere twice as the wave vector covers the entire Brillouin zone, while the winding number is zero in the topologically trivial case. We find that the Hilbert space spanned by the two lower polariton branches is no longer degenerate as in the absence of spin-orbit coupling, and exhibits a pseudo-spin vector which is constraint to the x-y plane. This picture changes for the case of a chiral cavity supporting only one polarization. Focusing on the lower polariton branch, the excitonic components of the polaritons are characterized by a non-trivial pseudo-spin vector. This findings suggest a possible variety of new topological phenomena in coupled light-matter systems.

TT 80.4 Wed 15:00 P2

Electronic reconstruction at the isopolar $LaTiO_3/LaFeO_3$ interface — •Judith Gabel[1], Josée E. Kleibeuker[1,2], Zhicheng Zhong[3], Hiroaki Nishikawa[4], Andreas Müller[1], Florian Pfaff[1], Dave H.A. Blank[2], Michael Sing[1], Gertjan Koster[2], Karsten Held[3], Ralph Claessen[1], and Guus Rijnders[2] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg — [2]Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente — [3]Institute of Solid State Physics, Vienna University of Technology — [4]B.O.S.T., Kinki University

We report the formation of a new non-magnetic Mott insulating phase (U =0.5 eV) at the isopolar interface between two insulating antiferromagnets, $LaTiO_3$ and $LaFeO_3$. The formation is driven by the combination of electrochemical energy, which can be described by O band alignment, and crystal field splitting energy of the t_{2g} and e_g bands. As a result of these two driving forces, the Fe 3d bands rearrange and electrons are transferred from Ti to Fe. Using X-ray photoelectron spectroscopy, we find a strong electron transfer of almost $1\,e^-$/interface unit cell. The shown route for interfacial electronic reconstruction opens possibilities to design new functional oxide heterointerfaces.

TT 80.5 Wed 15:00 P2

Probing the eletronic structure of γ-$Al_2O_3/SrTiO_3$ oxide heterostructures by hard x-ray photoelectron spectroscopy — •Philipp Schütz[1], Florian Pfaff[1], Philipp Scheiderer[1], Götz Berner[1], Mihaela Gorgoi[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie (HZB-BESSY II), Albert-Einstein-Strasse 15, 12489 Berlin, Germany

The heterointerface between the band insulators γ-Al_2O_3 and $SrTiO_3$ hosts a two-dimensional electron system (2DES) with exceptionally high electron mobility. The promising spinel/perovskite complex oxide heterostructure has been studied by hard x-ray photoelectron spectroscopy with high interface sensitivity. A detailed core level and valence band analysis yields information about the electronic structure, including band bending and band alignment at the interface. Evidence for the two-dimensional nature of the conducting interface is obtained from the angle dependent chemically shifted Ti^{3+} 2p core level signal, which is generally attributed to Ti ions with electrons hosted in the Ti 3d shell. The 2DES is found to be strongly confined within several unit cells of $SrTiO_3$ in proximity to the interface, with sheet carrier densities in the range of $10^{-14}\,cm^{-2}$.

TT 80.6 Wed 15:00 P2

Magnetization of two-dimensional electron systems in MgZnO/ZnO heterostructures — •Schorsch Michael Sauther[1], Matthias Brasse[1], Stephan Albert[1], Yusuke Kozuka[2], Joseph Falson[2], Atsushi Tsukazaki[2], Christian Heyn[3], Fauzia Jabeen[4], Marc Andreas Wilde[1], Anna Fontcuberta i Morral[4], Masashi Kawasaki[2], and Dirk Grundler[1] — [1]Phys.-Dep. E10, TU München — [2]Dep. of App. Phys. and QPEC, University of Tokyo — [3]Inst. f. Angew. Phys., Universität Hamburg — [4]LMSC, EPF Lausanne

Two-dimensional electron systems (2DESs) in oxide heterostructures have created great interest in the last few years. We study the magnetization M of MgZnO/ZnO heterostructures with 2DESs of small carrier density and high mobility at low temperatures and in high magnetic fields B. We report a sawtooth-like oscillating signal $M(B)$, i.e. the de Haas-van Alphen-effect, from which we extract thermodynamic energy gaps. Furthermore we observe non-equilibrium currents and unexpected overshoots in $M(B)$ that we analyze in terms of the residual disorder. The work is supported by the DFG via TRR 80.

TT 80.7 Wed 15:00 P2

Interface properties of NiMnSb/MgO and NiMnSi/MgO heterostructures — •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, NiMnSi and MgO have been investigated using first-principles density-functional calculations with projector augmented wave potentials generated in the generalized gradient approximation. In the case of the NiMnSb/MgO (100) interface the half-metallicity is lost, whereas the MnSb/MgO contact in the NiMnSb/MgO (100) interface maintains a substantial degree of spin polarization at the Fermi level ($\sim$ 60%). Remarkably, the NiMnSi/MgO (111) interface shows 100% spin polarization at the Fermi level, despite considerable distortions at the interface, as well as rather short Si/O bonds after full structural optimization. This behavior markedly distinguishes NiMnSi/MgO (111) from the corresponding NiMnSb/CdS and NiMnSb/InP interfaces.

TT 80.8 Wed 15:00 P2

MBE-growth of $LaNiO_3$ based heterostructures - From empirical growth to designing new materials — •Friederike Wrobel, Gennady Logvenov, Georg Christiani, Eva Benckiser, and Bernhard Keimer — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

Motivated by predictions of model calculations, which showed that heterostructured nickelates provide the essential ingredients for the occurrence of high T_c-superconductivity [1], we started to investigate these materials. Confinement and strain influence the structure, orbital occupation and electronic as well as magnetic properties [2,3]. Superlattices with 2 unit-cell thick layers of $LaAlO_3$ (LAO) and 2 layers of $LaNiO_3$ (counted in pseudo-cubic unit cells) show a transition to an antiferromagnetically ordered state at low temperatures. In contrast, samples with a periodicity of 4 layers of $LaNiO_3$ remain paramagnetic/metallic at all temperatures. Here, we present first results on how to extend our study on nickelate superlattices. Our goal is to modify the electronic and magnetic structure by charge carrier doping, either via oxygen reduction or chemical doping. Oxide molecular beam epitaxy (oxide MBE) is used to realize new superlattice systems and to improve the sample quality.

[1] J. Chaloupka, G. Khaliullin, Phys. Rev. Lett. **100**, 016404 (2008)
[2] M. Wu *et al.*, Phys. Rev. B **88**, 125124 (2013)
[3] A. Frano *et al.*, Phys. Rev. Lett. **111**, 106804 (2013)

TT 80.9 Wed 15:00 P2

Phase Transitions in Nickelate Thin Films and Superlattices Studied by Raman Light Scattering — •Matthias Hepting, Mathieu Le Tacon, Eva Benckiser, Matteo Minola, Friederike Wrobel, Dmitry Kukuruznyak, Georg Christiani, Gennady Logvenov, and Bernhard Keimer — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Recent work on heterostructures based on rare-earth nickelates revealed that it is possible to control their magnetic and electronic properties by epitaxial strain and spatial confinement [1,2]. To gain a deeper understanding of the correlation between the electronic and the structural phase transitions, we have developed an advanced method of Raman spectroscopy which enables the study of heterostructures as thin as ∼10nm.

Here we present temperature-dependent Raman spectra of $PrNiO_3$ based thin films and superlattices in different strain states and with different periodicities. We will discuss how signatures of a charge ordered ground state are mirrored in the Raman spectrum of tensile strained $PrNiO_3$ and how this observation can give deeper insights on the character of the ground state of rare-earth nickelates [3].

[1] A. Boris *et al.*, Science **332**, 937 (2011)
[2] A. Frano *et al.*, Phys. Rev. Lett. **111**, 106804 (2013)
[3] S. Lee, *et al.*, Phys. Rev. Lett., **106** 016405 (2011)

TT 80.10 Wed 15:00 P2

Under-pressure measurements of resistivity and magnetic susceptibility and the pressure-temperature phase diagram of $(DOEO)_4[HgBr_4]$TCE organic charge-transfer crystals — •Alisa Chernenkaya[1,2], S. Köhler[3], E. Gati[3], V. Ksenofontov[4], K. Medjanik[2], A. Kotov[5], R. Morgunov[5], E. Yagubskii[5], H.-J. Elmers[2], M. Lang[3], and G. Schönhense[2] — [1]Graduate School Materials Science in Mainz, 55128, Mainz, Germany — [2]Inst. für Physik, JGU, 55128, Mainz, Germany — [3]Phys. Inst., J.W. GUF, 60438, Frankfurt am Main, Germany — [4]Inst. für Anorg. und Analyt. Chem., JGU, 55128, Mainz, Germany — [5]Inst. of Probl. of Chem. Phys., RAS, 142432 Chernogolovka, Russia

The asymmetrical molecule DOEO (1,4-(dioxandiil-2,3-dithio) ethylenedithiotetrathiafulvalene)is the essential building block of the cation-radical salt $(DOEO)_4[HgBr_4]$TCE (TCE is 1,1,2-trichloroethane) [1].

It was shown before that the temperature dependence of resistivity of $(DOEO)_4[HgBr_4]$TCE at ambient pressure is non-trivial [1]. There is a maximum at $T = 120$ K and a minimum at $T = 70$ K in resistivity. We found evidence of an antiferromagnetic phase existing below 40 K. $(DOEO)_4[HgBr_4]$TCE is a possible candidate for a superconducting state below 7 K due to the comparability to BEDT-TTF salts. We performed characterization of phases and phase transitions and present a tentative pressure-temperature phase diagram.

Funded by DFG (Transregio TR49).

[1] A. Bardin et. al., Coord. Chem., 32, 88 (2006).

TT 80.11 Wed 15:00 P2

In-plane dependence of the FFLO state in the quasi-2D organic superconductor β''-$(ET)_2SF_5CH_2CF_2SO_3$ — •R. Beyer[1], E. Green[1], J.A. Schlueter[2], R. Zahn[1], S. Jahns[3], G. Zwicknagl[3], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor (HLD), Helmholtz-Zentrum Dresden- Rossendorf (HZDR), Germany — [2]Materials Science Division, Argonne National Laboratory, USA — [3]Institute for Mathematical Physics, TU Braunschweig, Germany

In recent years, clear thermodynamic evidence for FFLO superconductivity in the organic superconductor κ-$(ET)_2Cu(NCS)_2$, where ET stands for bisethylenedithio-tetrathiafulvalene, was found [1]. Performing high-resolution specific-heat measurements, we found as well evidence for the FFLO state in β''-$(ET)_2SF_5CH_2CF_2SO_3$, when the magnetic field is applied parallel to the superconducting ET layers [2]. Theoretical studies predict a strong in-plane critical field anisotropy of the FFLO phase. As a consequence of the low-dimensional character of the electronic structure, the calculations predict pronounced fluctuation effects which are reflected in substantial broadening of the superconducting transition. Therefore, we carried out specific-heat measurements with three different in-plane field orientations. The phase diagram with the pronounced upturn around 9.5 Tesla is independent of the in-plane field orientation. This points to an FFLO wave vector, that is fixed to a certain in-plane direction.

[1] R. Lortz *et al.*, Phys. Rev. Lett. **99**, 187002 (2007)
[2] R. Beyer *et al.*, Phys. Rev. Lett. **109**, 027003 (2012)

TT 80.12 Wed 15:00 P2

Unconventional thermal conductivity of the organic superconductor κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br$ — S. Kühlmorgen[1], J. Wosnitza[1], J. Müller[2], T. Herrmannsdörfer[1], and •R. Schönemann[1] — [1]Hochfeld-Magnetlabor (HLD), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [2]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt, Germany

We have investigated the organic superconductor κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br$ by means of high-resolution thermal-conductivity measurements. The thermal conductivity was measured in a wide temperature range between 0.15 and 17 K. Data were taken at fields up to 14 T in the super- and normal-conducting state of κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br$. In the superconducting state, a strong increase of the thermal conductivity below the transition temperature is observed, passes through a maximum and decreases with further decreasing the temperature. This maximum disappears when higher magnetic fields are applied. From our measurements we can conclude that the phonons are the dominant carriers for thermal transport. In the investigated temperature range the thermal conductivity in the superconducting state is higher than in the normal state. Down to lowest temperatures, this is due to quasi-particle scattering which affects the mean free path of the phonons.

TT 80.13 Wed 15:00 P2

Multiferroicity in the Mott insulating charge-transfer salt κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$ — •E. Gati[1], P. Lunkenheimer[2], J. Müller[1], A. Loidl[2], B. Hartmann[1], N.H. Hoang[1], H. Schubert[1], J.A. Schlueter[3], and M. Lang[1] — [1]Institute of Physics, Goethe University Frankfurt(M), SFB/TR49, Germany — [2]Experimental Physics V, University of Augsburg, Germany — [3]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

Multiferroics are materials which show a coincident electric and magnetic order and have been extensively studied throughout the last years. In a recent work [1], multiferroicity has been found in κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$, a two-dimensional organic charge-transfer salt. In contrast to well-known spin-driven ferroelectricity in helical magnets, a charge-order-driven mechanism has been proposed in this case. To get more insight into this issue, in particular to check for sample-to-sample variations, we performed measurements of the dielectric constant and magnetic susceptibility [2] on the same single crystals. We confirm that magnetic and electric order appear nearly simultaneously. Furthermore, we discuss results on various other, differently prepared single crystals. The results verify an order-disorder-type ferroelectric state and are incompatible with an inhomogenous, short-range-ordered state which has been proposed recently [3].

[1] P. Lunkenheimer et al., Nature Mater. 11, 755 (2012)
[2] M. Lang et al., arXiv: 1311.2715
[3] S. Tomić et al., J. Phys.: Cond. Mat. 25, 436004 (2013)

TT 80.14 Wed 15:00 P2

Dilatometric investigations on the quasi-2D organic charge-

transfer salt κ-(ET)$_2$Cu[N(CN)$_2$]I — •Carola Dietrich[1], Rudra Sekhar Manna[1], John A. Schlueter[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, SFB/TR 49, D-60438, Frankfurt (M), Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

High-resolution thermal expansion measurements have been performed on the quasi-two-dimensional organic charge-transfer salt κ-(ET)$_2$Cu[N(CN)$_2$]I along the in-plane c-axis and the out-of-plane b-axis for temperatures 1.4 K $\leq T \leq$ 200 K. In accordance with previous studies [1], we find a highly anomalous expansivity at high temperatures followed by a pronounced glass-like transition for both axes. The glass-like transition at $\sim$ 84 K is similar to that observed for the related κ-(ET)$_2$X salts with X = Cu[N(CN)$_2$]Br and Cu[N(CN)$_2$]Cl [2], and can be assigned to a freezing of orientational degrees of freedom of the terminal ethylene groups. The expansivity along the c-axis shows a hump-like anomaly at around 20 K, where a pronounced minimum was also observed in thermopower measurements [3]. We attribute the thermal expansion anomaly, which remains unaffected upon applying magnetic fields $B \leq 8$ T, to short-range magnetic correlations. Upon further cooling, a rather small anisotropic anomaly is observed at around 5 K of unknown origin.

[1] M. Kund *et al.*, Synth. Met. **70**, 951 (1995)
[2] J. Müller *et al.*, Phys. Rev. B **65**, 144521 (2002)
[3] M. A. Tanatar *et al.*, Phys. Rev. B **62**, 15561 (2000)

TT 80.15 Wed 15:00 P2

Resistivity measurements on the quasi-two-dimensional organic conductor κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl — •Sebastian Köhler[1], John Schlueter[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt(M), SFB/TR49, D-60438 Frankfurt(M), Germany — [2]Material Science Division, Argonne National Laboratory, Argonne, IL 60439-4831, USA

The organic charge-transfer salt κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl is a member of the family of (BEDT-TTF) or short - (ET)-based organic conductors in which conducting layers formed by ET molecules alternate with insulating anion layers. Notably the κ-type configuration is of high interest as these compounds exhibit a rich phase diagram containing metallic, (Mott-)insulating and even superconducting behaviour which can be easily accessed either by chemical pressure or by applying hydrostatic physical pressure. In contrast to the extensively studied copper-based salts, the monoclinic κ-(ET)$_2$Hg(SCN)$_{3-n}$X$_n$ (X=Cl,Br; n=1,2) compounds use mercury as metallic ion in the anion layer. At ambient pressure and high temperatures κ-(ET)$_2$Hg(SCN)$_2$Cl exhibits metallic behaviour with a metal-to-insulator transition at T_{MI}=34K and an AFM transition at T_{AFM}=27K [1].We present resistivity measurements of κ-(ET)$_2$Hg(SCN)$_2$Cl at various hydrostatic pressure values provided by using ^{4}He as pressure-transmitting medium.We find a significant shift of the metal-to-insulator transition to lower temperatures with a rate $\partial T_{MI}/\partial p \approx$ 0.3K/MPa and an increase in metallicity at lower temperatures similar to the behaviour observed for κ-(ET)$_2$Cu[N(CN)$_2$]Cl.

[1]Yasin et al., Physica B **407** (2012) 1689

TT 80.16 Wed 15:00 P2

Statistical properties of the charge-carrier dynamics at the Mott critical endpoint in κ-(BEDT-TTF)$_2$X-Salts — •David Zielke[1], Benedikt Hartmann[1], Jana Polzin[1], Robert Rommel[1], John A. Schlueter[2], Takahiko Sasaki[3], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL, USA — [3]Institute for Materials Research, Tohoku University, Sendai, Japan

The quasi-2D organic charge-transfer salts κ-(ET)$_2$X are considered as model systems for studying the Mott metal-insulator transition (MIT) in reduced dimensions. We investigated partially deuterated κ-[(H$_8$-ET)$_{0.2}$(D$_8$-ET)$_{0.8}$]$_2$Cu[N(CN)$_2$]Br, which can be reversibly tuned through the critical region in the generalized phase diagram by employing different cooling rates which has a crucial effect on the ratio of bandwith W to on-site Coulomb repulsion U. On this poster, we describe our statistical analysis of the resistance fluctuations by means of time-resolved transport measurements in the vicinity of the finite-T critical endpoint (p_0, T_0). Utilizing a fast data acquisition card in combination with a self-written software we derive the resistance noise power spectral density and higher-order statistical moments (second spectrum). At T_0, we observe a drastic enhancement and slowing down of the low-frequency resistance fluctuations for certain cooling rates together with a frequency dependent signature in the second spectrum. We interpret our observations in terms of a glassy electronic system possibly being universal for MITs.

TT 80.17 Wed 15:00 P2

Antiferromagnetism, superconductivity and quantum oscillations in the bifunctional organic conductor κ-(BETS)$_2$FeBr$_4$ — •Ludwig Scheidhammer[1], Michael Kunz[1], Werner Biberacher[1], Natasha D. Kushch[2], and Mark V. Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Institute of Problems of Chemical Physics, Chernogolovka, Russia

The layered organic metal κ-(BETS)$_2$FeBr$_4$ is a bifunctional material that consists of organic layers containing a metallic π electron system and inorganic layers that carry localized magnetic moments. It shows an antiferromagnetic (AFM) transition with the Néel temperature $T_N \approx 2.5$ K and a superconducting (SC) transition at the critical temperature $T_c \approx 1.1$ K. Shubnikov-de Haas oscillations have been studied in both the normal metallic and AFM states at different magnetic field orientations. From the angle dependence of the oscillation amplitude the exchange field can be obtained. The comparison of the oscillations in AFM and normal metallic state yields information on the Fermi surface reconstruction in the AFM state. We also present the angle dependence of the metamagnetic transition and discuss its influence on superconductivity.

TT 80.18 Wed 15:00 P2

Vibrational infrared spectroscopy of a charge-ordered κ-phase under pressure — Sarika Singh[1], Rebecca Beyer[1], •Tomislav Ivek[1,2], Matija Čulo[2], 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, Chernogolovka, Russia

Dimerized organic conductors from the κ-(BEDT-TTF)$_2X$ family are regarded as prime examples of Mott physics in two dimensions. Due to highly frustrated electron-electron interactions within the half-filled band, their ground states vary from superconducting X = Cu[N(CN)$_2$]Br, over spin liquid insulator of X = Cu$_2$(CN)$_3$, to canted antiferromagnetic insulator X = Cu[N(CN)$_2$]Cl. The related phase diagrams are generally well-described by the Hubbard model with only on-site repulsion U. On the other hand, the recent addition to the family, the X = Hg(SCN)$_2$Cl, undergoes a phase transition into a charge order at 30 K and ambient pressure. This particular ground state is completely unexpected within the Hubbard model.

In order to examine the exotic charge-ordered phase of κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl, we performed vibrational reflectance infrared measurements under hydrostatic pressure up to 11 kbar and at temperatures from 300 down to 10 K. By tracking the charge-sensitive ν_{27}(B$_{1u}$) molecular vibration we are able to map the molecular charges present in the p–T phase diagram. We discuss the effects of pressure on the charge order by taking into account the nearest-neighbor electron repulsion within the paired-electron crystal model.

TT 80.19 Wed 15:00 P2

Photo-induced phase transition in α-(BEDT-TTF)$_2$I$_3$ probed by FTIR and photoconductivity measurements — •Tobias Peterseim, Patricia Haremski, Tomislav Ivek, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Germany

In recent years, the study of nonequilibrium states generated by external stimuli, for instance photo-induced phase transition (PIPT), gained a lot of attention as they shed new light on the physics of the equilibrium state in various materials classes. Furthermore, the observed PIPT show potential routes to build new electronic devices for the application, i.e. optical switches or volatile memories.

The 2D organic salt α-(BEDT-TTF)$_2$I$_3$ is such a candidate in the class of molecular conductors revealing a metal-insulator phase transition at 136 K. It is accompanied by a charge disproportionation between the different molecular sites. We investigated the photoresponse of α-(BEDT-TTF)$_2$I$_3$ in the charged-ordered state. The observed photocurrent shows a non-exponential decay with a residual conductivity. Furthermore, it exhibits a distinct dependency on the laser intensity and the applied electric field including a delayed switching into a high conducting state. Additionally, we performed time-dependent FTIR measurements where traces of a photo-induced metallic phase could be observed. Its decay is in accordance with the photocurrent measurements. However, no indication for the residual conductivity could be found in the time-dependent infrared spectra. We will suggest a possible model which explains the observations.

TT 80.20 Wed 15:00 P2

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. For the sampling of the electric field of the charged molecular orbital on the lattice of polarizabilities we derived an Ewald summation. 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 80.21 Wed 15:00 P2

Leaf-to-leaf distances and their moments in finite and infinite m-ary acyclic graphs — •Andrew M. Goldsborough, S. Alex Rautu, and Rudolf A. Römer — University of Warwick, Coventry, UK

It has recently been shown [1] that two-point correlation functions in tensor network wavefunctions are related to the length of the path through the network that connects the two lattice sites. In reference to a binary tree tensor network (TTN) [2], we analyse the geometry of a complete regular binary tree where the leaves represent the points on a 1-D lattice. We find an analytic expression for the average path length for a given separation in a tree with n levels. This expression is then generalised to give any raw statistical moment for m-ary trees with open and periodic boundary conditions. We also present first results for random binary trees.

[1] G. Evenbly and G. Vidal, J. Stat. Phys. 145, 891 (2011)
[2] Y. Shi, L. Duan, and G. Vidal, Phys. Rev. A 74, 022320 (2006)

TT 80.22 Wed 15:00 P2

Incommensurate insulator and pairing in an asymmetric ladder system — •Anas Abdelwahab[1], Eric Jeckelmann[1], and Martin Hohenadler[2] — [1]Leibniz Universität Hannover — [2]Universität Würzburg

We investigate a ladder system made of two inequivalent legs, a Hubbard chain and a free electron gas. Analytical approximations, density-matrix renormalization group, and continuous-time quantum Monte Carlo are used to determine ground-state properties such as correlation functions, gaps, and spectral functions of this system. At half filling and intermediate Hubbard on-site interaction we observe three different phases as a function of the inter-chain hopping. The system is a Luttinger liquid and a correlated band insulator at weak and strong inter-chain hopping, respectively. For intermediate inter-chain hopping we find an insulating phase with gap minima at incommensurate wave numbers. In this parameter regime and close to half filling doped particles have a significant binding energy but pairing correlations decay rapidly.

TT 81: Superconductivity: Properties and Electronic Structure

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

TT 81.1 Thu 9:30 HSZ 201

Growth of superconducting $LaPd_1-xBi_2$ thin films by molecular beam epitaxy — •Reiner Retzlaff, Niklas van Elten, Jose Kurian, and Lambert Alff — Institute of Materials Science, TU Darmstadt, Germany

We have grown thin films of $LaPdBi_2$ by reactive molecular beam epitaxy on single crystal MgO substrates. Films were grown in a custom designed UHV chamber by the simultaneous evaporation of high purity La, Pd and Bi metals by e-beam evaporaters with in situ rate control. Single phase $LaPdBi_2$ films are stable in a small window of growth temperature. The films were characterised by RHEED, X-ray diffraction and electrical transport measurements. $LaPdBi_2$ films were epitaxial and c-axis oriented as evident from RHEED and XRD analysis. The Pd deficient $LaPdBi_2$ thin films showed superconductivity with a superconducting transition of about 3 K. To best of our knowledge this is the first report of the synthesis and superconductivity of $LaPdBi_2$.

TT 81.2 Thu 9:45 HSZ 201

Strain homogeneity in uniaxial stress and strain measurements — •Mark E. Barber[1], Cliford W. Hicks[1,2], Stephen D. Edkins[1], Daniel O. Brodsky[1], and Andrew P. Mackenzie[1,2] — [1]Scottish Universities Physics Alliance (SUPA), University of St. Andrews, St. Andrews, United Kingdom — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Response to uniaxial distortion can be a powerful probe of the electronic properties of a solid. However, it is not a very commonly applied technique, chiefly because of the technical challenges of obtaining good strain homogeneity while applying significant pressures. In typical uniaxial pressure measurements, thin and wide samples are clamped between two anvils. We have carried out measurements on Sr_2RuO_4 using a different, easier technique: cutting the sample into a long, narrow bar, and securing its two ends with epoxy across a vice. We explain the details of this technique and by using finite element simulations present the guidelines (readily achievable in experiments) that need to be followed in order to achieve high strain homogeneity.

TT 81.3 Thu 10:00 HSZ 201

Large enhancement of the T_c of Sr_2RuO_4 under uni-axial strain — •Daniel O. Brodsky[1], Clifford W. Hicks[1,2], Edward A. Yelland[1], Alexandra S. Gibbs[1,3], Jan A. N. Bruin[1,4], Mark E. Barber[1], Stephen D. Edkins[1], Keigo Nishimura[5], Shingo Yonezawa[5], Yoshiteru Maeno[5], and Andrew P. Mackenzie[1,2] — [1]University of St Andrews, United Kingdom — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]The University of Tokyo, Japan — [4]High Field Magnet Laboratory, Radboud University Nijmegen, Netherlands — [5]Kyoto University, Japan

We present AC magnetic susceptibility data taken on samples of the spin-triplet superconductor Sr_2RuO_4 under uni-axial strain. To do this, we built a probe that enables us to vary the strain applied to our samples continuously from compression to tension, whilst at cryogenic temperatures. We found that T_c changes dramatically with in-plane strain: strain along the crystallographic [100] direction leads to a strong strain-symmetric response of T_c, which is pushed up from 1.35 K to 1.9 K for 0.23% strain. Conversely, the response along the [110] direction is weak and mostly linear in strain. We discuss these results in the context of the predicted $p_x + ip_y$ topological order parameter.

TT 81.4 Thu 10:15 HSZ 201

The high-energy anomaly in ARPES spectra of cuprates– many body or matrix element effect? — •J. Fink[1], E.D.L. Rienks[2], M. Ärrälä[3], M. Lindroos[3], F. Roth[4], W. Tabis[5], G. Yu[5], and M. Greven[5] — [1]Leibnitz-Institute for Solid State and Materials Research, Dresden, Germany — [2]Helmholtz-Zentrum, Berlin, Germany — [3]Tempere University of Technology, Tempere, Finland — [4]Center for Free-Electron Laser Science, Hamburg, Germany — [5]University of Minnesota, Mineapolis, USA

We used angle-resolved and polarization-dependent photoemission spectroscopy (ARPES) and density functional theory calculations to study the high-energy anomaly (HEA) in the dispersion of $Nd_{2-x}Ce_xCuO_4$, $x = 0.123$. We have found that at particular photon energies the anomalous, waterfall-like dispersion gives way to a broad, continuous band. This suggests that the HEA is a matrix element effect: it arises due to a local suppression of the intensity of

the broadened quasiparticle band. We confirm this interpretation experimentally, by showing that a waterfall appears when the matrix element is suppressed deliberately by changing the light polarization. Calculations of the matrix element using atomic wave functions and simulation of the ARPES intensity with one-step calculations provides further proof for this scenario. The possibility to detect the full quasiparticle dispersion further allows us to extract the mass enhancement and the scattering rates at high binding energies at the center and edge of the Brillouin zone.

TT 81.5 Thu 10:30 HSZ 201

Following doped charges in cuprate superconductors by ^{17}O and ^{63}Cu NMR — •Michael Jurkutat[1], Damian Rybicki[1], Grant Williams[2], Andreas Erb[3], and Jürgen Haase[1] — [1]Universität Leipzig, Faculty of Physics and Earth Sciences, 04103 Leipzig, Germany — [2]Victoria University, Wellington, New Zealand — [3]Walther Meissner Institute for Low Temperature Research, 85748 Garching, Germany

We report results of a ^{17}O and ^{63}Cu NMR investigation of aligned powder as well as single crystal samples of electron-doped cuprates $RE_{2-x}Ce_xCuO_4$(with RE=Pr,Nd and x=0.0,..,0.2), a hitherto hardly investigated field of high-T_C research. Employing a range of NMR techniques we show that doped electrons almost exclusively go to planar Cu, while leaving a considerable hole density at planar O largely unchanged. Our results are then compared with findings in hole-doped cuprates shedding new light on the local charge distribution within the CuO_2-plane.

TT 81.6 Thu 10:45 HSZ 201

Spin excitations of ferronematic order in underdoped cuprate superconductors — •Götz Seibold[1], Carlo Di Castro[2], Marco Grilli[2], and Jose Lorenzana[2] — [1]BTU Cottbus-Senftenberg, Germany — [2]University of Rome 'La Sapienza', Italy

The presence of an anisotropic hourglass shaped spectrum for magnetic excitations in underdoped cuprates is explained by a model in which topological defects of the antiferromagnet clump to producing domain wall segments with ferronematic order. This state does not invoke global charge order but breaks C4 rotational and inversion symmetry. The incommensurability of the low doping charge-disordered state is in good agreement with experiment and interpolates smoothly with the incommensurability of the stripe phase at higher doping. Within linear spin-wave theory the dynamic structure factor is in very good agreement with inelastic neutron scattering data and can account for the energy dependent anisotropy observed.

TT 81.7 Thu 11:00 HSZ 201

Tuning the performance of $YBa_2Cu_3O_{7-\delta}$ thin films by a local incorporation of gold nanoparticles — •Christian Katzer[1], Markus Westerhausen[1], Claudia Stahl[2], Joachim Albrecht[3], Evelyn Stilp[4], Andreas Suter[4], and Frank Schmidl[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, 07743 Jena — [2]Max-Planck-Institut für Intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart — [3]Hochschule Aalen, Beethovenstraße 1, 73430 Aalen — [4]Laboratory for Muonspin Spectroscopy, PSI, CH-5232 Villigen PSI, Switzerland

Many superconducting thin film applications require a spatially resolved current carrying capability due to different boundary conditions. On the one hand, the critical current density should be increased for high-current applications or in the antenna structures of sensor devices like gradiometers; on the other hand, the critical current of Josephson Junctions must not be too high to ensure a proper functionality. We report that a local incorporation of crystalline gold nanoparticles in $YBa_2Cu_3O_{7-\delta}$ thin films allows engineering the critical current landscape on the sub-micrometre scale. Meanwhile, as we will show the growth conditions of the YBCO are modified, resulting in less a-axis growth and an improved oxygen stoichiometry. Furthermore, we will present Muon Spin Spectroscopy measurements of the London-penetration depth which indicate a reduced defect density in YBCO thin films modified by Au particles.

[1] C. Katzer, et al., Supercond. Sci. Techn. 26, 125008 (2013)
[2] C. Katzer et al., New J. Phys. 15, 113029 (2013)

15 min. break.

TT 81.8 Thu 11:30 HSZ 201

Electrospun superconducting $La_{1.85}Sr_{0.15}CuO_4$ nanowires and nanoribbons — •XianLin Zeng[1], Michael R. Koblischka[1], Jennifer S. Atchinson[2], Volker Presser[2], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, Campus C 6 3, 66123 Saarbrücken, Germany — [2]INM – Institute of New Materials Saarbrücken, Campus D 2 2, 66123 Saarbrücken, Germany

The synthesis of high-temperature superconducting $La_{1.85}Sr_{0.15}CuO_4$ nanostructures via electrospinning and a subsequent calcination in air and oxygen is reported. Nanowire and nanoribbon structures are obtained in the experiments with a maximum $T_{c,onset}$ of 20 K. According to the morphological characterization via scanning electron microscopy (SEM) and transmission electron microscopy (TEM), the nanowires have average diameters of about 230 nm and the length spans more than 30 μm. The nanowires are polycrystalline with a mean grain size of about 110 nm and 30 nm as determined by TEM and X-ray analysis, respectively. The nanoribbons are about 0.5 to 1 μm wide but show a thickness of only 60 to 80 nm, which indicates that the ribbons have a monolayer crystal structure. A confirmation of the chemical phase and component ratio is given by X-ray diffraction and EDX measurements. Attempts are made to achieve a detailed understanding of the formation of nanowires and -ribbons. Furthermore, additional information concerning the symmetry breaking of two phonon modes is obtained via Raman spectra of the nanowires, confirming the previous results presented in [1].

[1] J. M. Li, X. L. Zeng, et al., Cryst. Eng. Comm. 13, 6964 (2011)

TT 81.9 Thu 11:45 HSZ 201

Magnetic characterization of bulk MgB_2 — Alex Wiederhold[1], •Michael R. Koblischka[1], Miryala Muralidhar[2], Masato Murakami[2], Thomas Hauet[3], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [2]Department of Materials Science and Engineering, Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-ku, Tokyo 135-8548, Japan — [3]Institute Jean Lamour, University of Lorraine, Vandœuvre-les-Nancy, France

A series of disk-shaped, bulk MgB_2 superconductors (sample diameter up to 4 cm) was prepared in order to improve the performance for superconducting super-magnets. Several samples were fabricated using a solid state reaction in pure Ar atmosphere from 750 to 950 °C to obtain the highest critical current density as well as large trapped field values. Microstructural observations obtained from scanning electron microscopy (SEM) and atomic force microscopy (AFM) indicated that the grain size is the crucial parameter to improve the critical currents as well as the trapped field values. The small samples cut from the large bulks were characterized by transport measurements ($R(T,B)$ and I/V characteristics) in magnetic fields up to 8 T and by magnetization loops measured by SQUID magnetometry. The pinning force analysis revealed a well developed scaling of the pinning force $F_p = j_c \times B$ data with $p = 0.65$, $q = 1.35$ and a peak at $h_0 = 0.32$, indicating pinning at normal conducting precipitates. Similar values are obtained in the literature for pure, small MgB_2 samples.

TT 81.10 Thu 12:00 HSZ 201

Effect of Coulomb Interactions on the Disorder-Driven Superconductor-Insulator Transition — Daniel Sherman[1,2], Uwe S. Pracht[1], Boris Gorshunov[1,3,4], Shachaf Poran[2], Nandini Trivedi[5], Pratap Raychaudhuri[6], Aviad Frydman[2], and •Martin Dressel[1] — [1]1. Phys. Inst., Universität Stuttgart, Germany — [2]Dept. Phys., Bar Ilan Univ., Israel — [3]Prokhorov Inst. Gen. Phys., RAS, Moscow, Russia — [4]Moscow Inst. Phys. Techn., Dolgoprudny, Russia — [5]Dept. Phys., Ohio State Univ., Columbus, OH, U.S.A. — [6]Tata Inst. Fund. Res., Mumbai, India

We have studied the evolution of the superconducting energy gap through the disorder-driven superconductor to insulator transition in InO and NbN films using two distinct experimental methods that allow us to test the influence of metallic screening on the electronic interactions. In the case of tunneling spectroscopy a metallic electrode is adjacent to the superconducting film thus screening Coulomb interactions. On the other hand terahertz spectroscopy is a contactless method which probes the sample without affecting the electron-electron interaction. In the presence of screening, a similar superconducting gap is detected on both sides of the superconductor-insulator transition, and at temperatures above and below T_c. Contactless measurements are able to identify the superconducting gap below but not above the critical temperature or in the insulating state. Our study reveals the importance of Coulomb interactions on the energy gap of disordered superconductors.

TT 81.11 Thu 12:15 HSZ 201

Superconducting gap of the noncentrosymmetric superconductor α-BiPd — •Zhixiang Sun[1], Mostafa Enayat[1], Darren Peets[1], Ana Maldonado[1], Andreas P. Schnyder[1], Alexander Yaresko[1], and Peter Wahl[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]SUPA, School of Physics and Astronomy, University of St. Andrews, North Haugh, St. Andrews, Fife, KY16 9SS, United Kingdom

In most known superconductors, inversion symmetry and Pauli exclusion ensure that the Cooper pair wave function can be separated into an orbital component that has either even or odd parity, and a spin component which is then either singlet or triplet, but this does not hold in general. In the absence of an inversion center in the crystal structure, parity is not a good quantum number, and the Cooper pairs will be some mixture of singlet and triplet. We report ultra-low temperature scanning tunneling microscopy/spectroscopy (ULT-STM/STS) measurements at temperatures down to 15 mK on the recently rediscovered non-centrosymmetric superconductor α-BiPd. Tunneling spectra show only a single superconducting gap with $\Delta(0)= 0.6$ meV, the temperature and magnetic field dependence of which are found to be well described by BCS theory and a single s-wave gap. Our results provide an upper limit for a possible triplet component in α-BiPd of 10 μ eV.

TT 81.12 Thu 12:30 HSZ 201

Suppression of superconductivity in a single layer of Pb on Si(111) by insertion of a single layer of Ag — •Hirofumi Oka[1], Augusto A. Leon Vanegas[1], Agnieszka Stepniak[1], Michael Caminale[1], Dirk Sander[1], and Jürgen Kirschner[1,2] — [1]MPI Halle — [2]MLU Halle-Wittenberg

A recent study indicates that even a single atomic layer of Pb on Si(111) is superconducting with a critical temperature of 1.83 K [1]. Here, we investigate effect of insertion of a single layer of Ag on superconductivity (SC) in a single layer of Pb on Si(111) using a ^{3}He-cooled STM with a vector magnetic field. Ag was deposited onto the clean 7×7-Si(111) surface held at 770 K, leading to a formation of a single layer of Ag on Si(111). Subsequently Pb atoms were evaporated at 300 K, followed by annealing at 560 K for 1 min. Our STM study reveals that the Pb/Ag/Si(111) surface has a well-ordered atomic structure. Most of the surface shows a stripe pattern indicative of a $\sqrt{3}\times\sqrt{7}$ structure and small areas show a $\sqrt{3}\times\sqrt{3}$ structure. STS measurements on the Pb/Ag/Si(111) surface show almost the same differential-conductance spectrum with temperature (0.38–6.0 K) or magnetic field (up to 3 T). We do not observe a SC gap in spectroscopy. Our results indicate that the insertion of a Ag layer suppresses SC in a single layer of Pb on Si(111). We speculate that the Ag insertion modifies the bonding situation between Pb and Si, which has been reported to play a crucial role for the SC of the single Pb layer on Si(111) [2].

[1] Zhang et al., Nat. Phys. 6, 104 (2010)
[2] Noffsinger and Cohen, Sol. State Comm. 151, 421 (2011)

TT 81.13 Thu 12:45 HSZ 201

Position-dependent tunneling spectroscopy from a superconducting Pb island towards a normal conducting single layer — •Agnieszka Stepniak[1], Augusto A. Leon Vanegas[1], Michael Caminale[1], Hirofumi Oka[1], Dirk Sander[1], and Jürgen Kirschner[1,2] — [1]Max-Planck-Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

Using scanning tunneling microscopy (STM) and spectroscopy (STS) we study the superconducting properties of Pb islands on a Ag monolayer on Si(111). We use a 3He-cooled STM with a vector magnetic field to characterize the structural and electronic properties of the Pb/Ag-Si system at the temperatures range of 0.38*4.0 K, in dependence of a magnetic field of up to 6 T along the sample normal. We find SC in Pb islands, where the transition temperature is 6 K in a 9 layer high Pb island. The interlayer of Ag suppresses superconductivity (SC) in single layer Pb surrounding the Pb islands. We exploit the spatial resolution of STM/STS to study the position dependent differential conductivity for a transition from a SC Pb island to the surrounding non-superconducting Pb layer on Ag/Si, as a function of temperature and magnetic field. The quantitative analysis of the SC gap in spectroscopy identifies an exponential decay on which SC faints into the normal-metal region with a decay length of 5+/-1 nm at 1.8 K. This length is larger at lower temperature (10 nm at 0.4 K), and smaller at higher temperature (1 nm at 4 K). A magnetic field of up to 0.5 T along the sample normal does not change the decay length.

TT 81.14 Thu 13:00 HSZ 201

Search for superconductivity in differently treated graphite powders — •Pablo Esquinazi, Annette Setzer, Jose Carlos de Moraes Silva, and Winfried Böhlmann — Division of Superconductivity and Magnetism, University of Leipzig, Leipzig, Germany

Hints on the existence of superconductivity at high temperatures were reported recently in water-treated graphite powders [1], graphite TEM lamellae [2], as well as in graphite flakes embedded in alkanes [3]. There is evidence that interfaces between graphite Bernal structure could play a role in the measured response [2,4]. In this contribution we studied the magnetic response of high purity graphite powders treated with water, alkanes as well as with acids. Background independent as well as background dependent methods were used to check for pinned magnetic entities. Clear hysteresis in temperature (between zero-field cooled and field cooled) as well as in field were measured, which survives at very high temperatures. To compare the observed behavior with that expected from ferromagnetic particles, we have also measured ferromagnetic magnetite particles embedded in amorphous carbon. We discuss the obtained evidence in terms of triggered superconductivity and/or magnetic order.

[1] T. Scheike et al., Adv. Mater. 24, 5826 (2012)
[2] A. Ballestar et al., New J. Phys. 15, 023024 (2013)
[3] Y. Kawashima, AIP Advances 3, 052132 (2013)
[4] T. Scheike et al., Carbon 59, 140 (2013)

TT 82: Low-Dimensional Systems: Topological Order (organized by TT)

Time: Thursday 9:30–13:15 Location: HSZ 204

TT 82.1 Thu 9:30 HSZ 204

Silicene and germanene as topological insulators: ab-initio approach — •Lars Matthes and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Silicene is a two-dimensional honeycomb lattice formed by silicon atoms and shares many properties of graphene, e.g. massless Dirac electrons at the Fermi level. In silicene the effect of spin-orbit interaction (SOI) is enhanced due to its buckled structure. Furthermore, by means of tight-binding calculations including SOI the emergence of topologically protected edge states has been predicted in silicene (and also germanene) nanoribbons [1] for zigzag and armchair edges, turning these crystals into topological insulators.

In this talk we study, whether or not silicene and germanene are topological insulators in a real simulation. We employ density-functional theory for the simulation of germanene nanoribbons. The band structures of ribbons of several widths as well as zigzag and armchair edges with hydrogen passivation are presented. The presence of topologically protected states is discussed versus edge shape, edge magnetization, ribbon width, and strength of spin-orbit interaction. The validity of results of the tight-binding model is critically discussed.

[1] M. Ezawa and N. Nagaosa, Phys. Rev. B 88, 121401(R) (2013)

TT 82.2 Thu 9:45 HSZ 204

First-principles Fermi surface characterization of doped PbTe — •Boris Sangiorgio, Michael Fechner, and Nicola Spaldin — ETH Zürich, Department of Materials, CH-8093 Zürich, Switzerland

Doped PbTe has raised increased interest because of its peculiar properties. In particular, it shows enhanced thermoelectricity, topological insulator behaviour and a charge Kondo effect, depending on the dopant atom. Here we investigate the nature of the Fermi surface in hole-doped PbTe using first-principles calculations. We begin by comparing recent experimental characterizations of the Fermi surface by means of effective masses, band offsets and de Haas-van Alphen frequencies with results from density functional theory (DFT). We find

that the values of these properties depend strongly on the choice of exchange-correlation functional and identify functionals that give good agreement with experiment. Our results indicate appropriate methodologies for first-principles studies of doped-PbTe, and give insights into the origin of the charge Kondo effect.

TT 82.3 Thu 10:00 HSZ 204

Conductance of flat bands with long range Coulomb interactions — •Wolfgang Häusler — Institut für Physik, Universität Augsburg, D-86135 Augsburg

Dispersionless ("flat") electronic bands can arise throughout the Brillouin zone in certain multipartite lattices, besides ordinary dispersing bands. In such a flat band, hoppings between atomic orbitals interfere destructively which then leads to localization, a phenomenon denoted as "caging" of carriers. As a consequence, the system is insulating at zero temperature even when this band is partly filled, provided all other bands are either empty or completely filled.

One may ask whether long range Coulomb interactions can alter this situation and cause finite conductivity. In the absence of kinetic energy, flat band carriers tend to Wigner crystallize. Here, this general observation is analyzed for the two-dimensional case specifically for the Sutherland or $\mathcal{T}_3$–lattice where a conductivity is found, depending non-trivially on the carrier density at small flat band fillings.

TT 82.4 Thu 10:15 HSZ 204

Fluctuation-Induced Topological Insulators — •Sebastian Riese and Stephan Rachel — Institut für Theoretische Physik, TU Dresden

We consider interaction-induced topological insulators as paradigms for systems which are dominated by the interplay of a topological band structure and electron-electron correlations. In particular, we extend the previous work about fluctuation-induced topological phases. We show that the fluctuation-induced Chern insulator phase can be reduced to the non-interacting model with an additional mass-term which depends on the parameters of the self-energy. Then we generalize this idea to the spinfull case of time-reversal invariant topological insulators. We show that his phase is stable with respect to spin-mixing in the band structure and in the self-energy. Implications for realistic interacting Hamiltonians are discussed.

TT 82.5 Thu 10:30 HSZ 204

Topological phase transition in the Kitaev-Ising ladder — Amir Mohammad-Aghaie[1], Reza Haghshenas[1], and •Abdollah Langari[1,2] — [1]Department of Physics, Sharif University of Technology, P.O.Box 11155-9161, Tehran, Iran — [2]Max-Planck-Institut fuer Physik komplexer Systeme, 01187 Dresden, Germany

We have studied the Kitaev-Ising model on a ladder geometry using iDMRG algorithm. We find a quantum phase transition between the Kitaev and Ising phases whenever the ratio of Ising to Kitaev coupling is exactly equal to 1/2. The divergence in the von-Neumann entropy and the change of degeneracy in the entanglement spectrum justifies the symmetry protected topological phase (SPT) transition. We investigate the robustness of the SPT phase in the presence of cluster terms which preserve/break the symmetry of the model. We also discuss the effect of Ising terms on the legs of ladder in addition to the rhombic interaction, which leads to frustration for the antiferromagnetic interactions.

TT 82.6 Thu 10:45 HSZ 204

Entanglement Spectra of Interacting Fermions in Quantum Monte Carlo Simulations — Fakher F. Assaad[1], Thomas C. Lang[2], and •Francesco Parisen Toldin[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Department of Physics, Boston University, U.S.A.

In a recent article T. Grover introduced a simple method to compute Renyi entanglement entropies in the realm of the auxiliary field quantum Monte Carlo algorithm [1]. Here, we further develop this approach and provide a stabilization scheme to compute higher order Renyi entropies and an extension to access the entanglement spectrum [2]. The method is tested on systems of correlated topological insulators.

[1] T. Grover, Phys. Rev. Lett. 111, 130402 (2013)
[2] F. F. Assaad, T. C. Lang, F. P. Toldin, arXiv:1311.5851

TT 82.7 Thu 11:00 HSZ 204

Topological insulators with arbitrarily tunable entanglement scaling — •Jan Carl Budich[1], Jens Eisert[2], and Emil Johansson Bergholtz[2] — [1]Department of Physics, Stockholm University, SE-106 91 Stockholm, Sweden — [2]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We elucidate how Chern and topological insulators fulfill an area law for the entanglement entropy. By ex- plicit construction of a family of lattice Hamiltonians, we are able to demonstrate that the area law contribution can be tuned to an arbitrarily small value, but is topologically protected from vanishing exactly. We prove this by introducing novel methods to bound entanglement entropies from correlations using perturbation bounds and complement this approach by an intuitive understanding. These insights have a number of important consequences. The non-universality implies that the entanglement scaling cannot be used as a faithful diagnostic of topological insulators. The existence of arbitrarily weakly entangled topological insulators opens up possibili- ties of devising correlated topological phases in which the entanglement entropy is small and which are thereby numerically tractable, specifically in tensor network approaches.

15 min. break.

Topical Talk TT 82.8 Thu 11:30 HSZ 204

Density Matrix Renormalization Group: Probing the Topology of Quantum States — •Frank Pollmann — Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany

Matter occurs in various phases with different properties. Usually these phases are characterized in terms of symmetry breaking. A major discovery in the 1980s was the quantum Hall effect which forms a new kind of "topological" order. This order represents exotic phases with unusual properties and cannot be understood in terms of symmetry breaking. Since then, a growing number of instances of topological phases has accumulated, and important applications – not least topological quantum computers – have been proposed, but a characterization and classification of these new phenomena has been slow to emerge. In parallel, DMRG has arrived as a powerful numerical method with extensions to two dimensional systems and time-dependent phenomena. I will show how to use DMRG to develop new frameworks that help to understand topologically ordered systems. For example, it is now possible to extract characterizing properties of the anyonic excitations directly from the ground state of fractional quantum Hall systems. This approach further makes contact with "measurable" quantities (Hall viscosity) and field theories (central charge at critical points). Other remarkable examples are symmetry protected topological phases in one-dimensional systems for which DMRG provides a complete characterization.

TT 82.9 Thu 12:00 HSZ 204

Excitation statistics distinguish topologically ordered phases — •Siddhardh Morampudi[1], Curt von Keyserlingk[2], and Frank Pollmann[1] — [1]Affiliation: Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Affiliation: Rudolf Peierls Centre for Theoretical Physics, 1 Keble Road, Oxford, OX1 3NP, United Kingdom

We investigate the characterization of topologically ordered phases and phase transitions between them. Topological order is a kind of order which cannot be characterized by the traditional approach of Landau's symmetry breaking theory and local order parameters. It is known to arise in diverse systems ranging from the well known fractional quantum hall systems to highly frustrated systems like the Heisenberg antiferromagnet on the Kagome lattice. The lack of local order parameters makes it difficult to uniquely identify a topologically ordered phase and to investigate phase transitions between them.

We consider two topologically ordered phases and use exact diagonalization to look at behaviour of various quantities as we move between them. We find that the usual methods of identifying a topologically ordered phase fail to uniquely distinguish these two phases. We then extract the braiding statistics of the excitations in the phases and use it as a non-local order parameter to distinguish the two phases, finding a first-order transition between them. Finally, we discuss how the approach could easily be generalized to other topologically ordered systems.

TT 82.10 Thu 12:15 HSZ 204

Detection of symmetry enriched topological phases — •Ching-Yu Huang[1], Xie Chen[2], and Frank Pollmann[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany —

[2]Department of Physics, University of California, Berkeley, California, USA

Topologically ordered systems in the presence of symmetries can exhibit new structures which are referred to as symmetry enriched topological (SET) phases. We introduce simple methods to detect the SET order directly from a complete set of topologically degenerate ground state wave functions. In particular, we first show how to directly determine the characteristic symmetry fractionalization of the quasiparticles from the reduced density matrix of the minimally entangled states. Second, we show how a simple generalization of a string order parameter can be measured to detect SET. The selection rules will get a characterization of SET. This way is more physical, and can be used by other methods, e.g., quantum Monte Carlo methods or potentially measured experimentally. We demonstrated the usefulness of this approach by considering first a spin-1 model on the honeycomb lattice and the resonating valence bond state on a kagome lattice.

TT 82.11 Thu 12:30 HSZ 204

Persisting topological order via geometric frustration — •Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, Deutschland

We introduce a toric code model on the dice lattice which is exactly solvable and displays topological order at zero temperature. In the presence of a magnetic field, the flux dynamics is mapped to the highly frustrated transverse field Ising model on the kagome lattice. This correspondence suggests an intriguing disorder by disorder phenomenon in a topologically ordered system implying that the topological order is extremely robust due to the geometric frustration. Furthermore, a connection between fully frustrated transverse field Ising models and topologically ordered systems is demonstrated which opens an exciting physical playground due to the interplay of topological quantum order and geometric frustration.

TT 82.12 Thu 12:45 HSZ 204

Kondo holes in topological Kondo insulators — •Pier Paolo Baruselli and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

The interplay between strong correlations and topology is a fast-developing and fascinating subject in the field of condensed matter.

Recently, the existence of topological Kondo insulators has been proposed [1]. In these materials the insulating behavior arises from strong correlations, that is from the Kondo screening of localized moments via conduction electrons, while non-trivial topology emerges from the structure of the hybridization between the local-moment and conduction bands.

We present a study of the physics of Kondo holes, i.e., missing local moments, in such topological Kondo insulators, using a self-consistent real-space mean-field theory. Kondo holes induce in-gap states which, for Kondo holes at or near the surface, hybridize with the topological surface state. In particular, we investigate the surface-state quasiparticle interference (QPI) induced by a dilute concentration of surface Kondo holes. We find that most QPI features can be interpreted by taking into account the shape of two-dimensional Fermi surface, together with the absence of backscattering characterizing Dirac cones in topological insulators. However, deviations from this simple picture arise: for example, the real part of the substrate Green's function and of the scattering matrix cannot be neglected in several cases.

[1] M. Dzero, K. Sun, V. Galitski, and P. Coleman, Phys. Rev. Lett. 104, 106408 (2010)

TT 82.13 Thu 13:00 HSZ 204

Topological entanglement entropy at quantum critical points — •Johannes Helmes and Simon Trebst — Institut für Theoretische Physik, Universität zu Köln, Germany

It is increasingly appreciated that a precise determination of the entanglement entropy of an interacting quantum many-body system can be used to identify the fundamental nature of its ground states. In particular, corrections to the prevalent boundary-law can be used to unambiguously identify topological order – a non-local form of order that eludes a standard characterization via correlation functions.

Here we report results for the entanglement entropy at a family of quantum critical points separating a topologically ordered phase from a conventionally ordered one. In technical terms, we employ large-scale quantum Monte Carlo simulations to study various deformations of the paradigmatic toric code model harboring a Z2 topological quantum spin liquid.

TT 83: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems I

Time: Thursday 9:30–13:00 Location: HSZ 03

Topical Talk TT 83.1 Thu 9:30 HSZ 03

Kinetic Theory for the Relaxation of Quantum Many-Body Systems — •Marcus Kollar — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universit*ät Augsburg

After being forced out of equilibrium, an isolated quantum many-body system is expected to relax to thermal equilibrium, unless it is integrable and retains memory of the initial state due to a large number of constants of motion. For weak interactions a large number of *approximate* constants of motion leads to a short-time prethermalization regime [1], which we discuss for several interacting systems in high and low dimensions. We then use a weak-coupling kinetic theory [2] to describe both the initial prethermalization regime as well as the subequent crossover towards the thermal state.

[1] M. Kollar, F. A. Wolf, and M. Eckstein, PRB 84, 054304 (2011).
[2] M. Stark and M. Kollar, arXiv:1308.1610.

TT 83.2 Thu 10:00 HSZ 03

Quench Dynamics in a Model with Tuneable Integrability Breaking — Fabian H.L. Essler[1], Stefan Kehrein[2], •Salvatore R. Manmana[2], and Neil J. Robinson[1] — [1]The Rudolf Peierls Centre for Theoretical Physics, Oxford University, UK — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

We consider quantum quenches in an integrable quantum chain with tuneable integrability breaking interactions. In the case where these interactions are weak, we demonstrate that at intermediate times after the quench local observables relax to a prethermalized regime, which can be described by a density matrix that can be viewed as a deformation of a generalized Gibbs ensemble. We present explicit expressions for the approximately conserved charges characterizing this ensemble. We do not find evidence for a crossover from the prethermalized to a thermalized regime on the time scales accessible to us. Increasing the integrability-breaking interactions leads to a behaviour that is compatible with eventual thermalization.

TT 83.3 Thu 10:15 HSZ 03

Finite-size scaling of eigenstate thermalization — •Wouter Beugeling, Roderich Moessner, and Masud Haque — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

According to the eigenstate thermalization hypothesis (ETH), even isolated quantum systems can thermalize because the eigenstate-to-eigenstate fluctuations of typical observables vanish in the limit of large systems. Since isolated systems are by nature finite, the finite-size scaling of such fluctuations is a central aspect of the ETH. We propose that for generic non-integrable systems these fluctuations scale with a universal power law in the dimension of the Hilbert space. We present extensive multiple-system numerical evidence for this scaling law and provide supporting arguments. We also show how the scaling changes when approaching integrability.

TT 83.4 Thu 10:30 HSZ 03

Entanglement propagation and typicality of measurements in a quantum version of the Kac ring — •Johannes M. Oberreuter, Ingo Homrighausen, and Stefan Kehrein — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

Time development in quantum many body systems poses serious challenges to our understanding of classical statistical mechanics. Exact results are very rare due to the large Hilbert spaces and the resulting complexity involved. We propose a pedagogical approach with a very tractable toy model, in which questions of entanglement creation, propagation and destruction between a system and an environment can be studied explicitly. Comparing this quantum model with its classi-

cal counterpart [1], we find an intriguing correspondence between the typical result of repeated measurements on a classical ensemble and the repeated measurements of a quantum system in an appropriate superposition.
[1] G. Gottwald and M. Oliver, Boltzmann's Dilemma : An Introduction to Statistical Mechanics via the Kac Ring, SIAM Rev. 51, 613 (2009)

TT 83.5 Thu 10:45 HSZ 03

Excited states above a non-equilibrium steady state (NESS) and approach to NESS — •Mariya Medvedyeva and Stefan Kehrein — Goettingen University

The simplest way to address the evolution of an open quantum system is the Lindblad equation, which describes a quantum system coupled to a classical environment. In the long-time time limit the system reaches a non-equilibrium steady state (NESS). The spectrum of the Liouvillian operator from the Lindblad equation determines the excited states with respect to the NESS. In general, the spectrum consists of complex numbers, whose real parts determine the relaxation speed while the imaginary parts lead to oscillations. The approach of a generic initial state to equilibrium is determined by the longest-living excited states which do not oscillate. If the density of such states shows a power law behavoir close to zero, then the approach to NESS also follows a power-law rather than an exponential behavior. We demonstrate this statement for the example of non-interacting fermions coupled to a Markovian bath, where the solution can be found exactly (up to numerical matrix diagonalization).

TT 83.6 Thu 11:00 HSZ 03

Analysis of the work distribution function after a quench in the transverse field Ising model — •Nils Abeling and Stefan Kehrein — Department of Physics, Georg-August-Universität, Göttingen, Germany

Non-analytic behaviour of the Loschmidt echo in non-equilibrium quantum many-body systems indicates a breakdown of the short time expansion. The analytically calculated work distribution function in the thermodynamic limit was shown to display such non-analytic behaviour at $T = 0$ in Ref. [1] indicating a dynamical phase transition. The result is generalized to non-zero temperature and a suggestive interpretation is given.
[1] M. Heyl, A. Polkovnikov, and S. Kehrein, Phys. Rev. Lett. 110, 135704 (2013)

15 min. break.

TT 83.7 Thu 11:30 HSZ 03

Thermalization timescales in a 1d Hubbard model with slightly broken integrability — •Fabian Biebl and Stefan Kehrein — Univ. Göttingen, Germany

Understanding relaxation in quantum systems is essential to determine whether an experimental setup can be described by equilibrium concepts. For example integrable systems do not thermalize, but develop into non-thermal steady states. By slightly breaking integrability, thermalization of such non-thermal (prethermalized) states becomes possible. An important question is to identify the corresponding timescale for thermalization due to the breaking of integrability.

We investigate this question for a fermionic Hubbard chain. The integrability breaking term is a small next to nearest neighbor hopping term [1,2]. The thermalization timescale is extracted from the quantum Boltzmann equation and depends strongly on temperature.
[1] M. L. R. Fuerst et al., Phys. Rev. E 86, 031122 (2012)
[2] M. L. R. Fuerst et al., Phys. Rev. E 88, 012108 (2013)

TT 83.8 Thu 11:45 HSZ 03

Nonequilibrium Dynamics beyond the Mean Field Approximation — •Ingo Homrighausen and Stefan Kehrein — Universität Göttingen

Mean field type approximations are one of the most accessible methods to study the complexity of quantum many body systems out of equilibrium. However, the validity of such approximations has to be examined in each case. Building on Ref. [1] we investigate three different quantum many particle models on finite fully connected lattices: the transverse field Ising model, the Bose-Hubbard model and the Jaynes Cummings model. In particular, we explore the nonequilibrium dynamics of the order parameter and its variance after a quantum quench. The most intriguing observation is that all three models exhibit the same universal behavior: For quenches within the ordered phase, the variance of the order parameter shows a quasiperiodic breathing behavior. The local maxima of this breathing increase in time whereas the local minima decrease. Applying a semiclassical expansion, we explain these findings and argue why the observations are generic. We also discuss the time scale of validity of our analysis by comparing to numerically exact data.
[1] B. Sciolla, G. Biroli, J. Stat. Mech. (2011) P11003

TT 83.9 Thu 12:00 HSZ 03

Is there Andreev-reflection in 1D Fermi-Hubbard systems? — •Mirco Marahrens[1], Salvatore R. Manmana[1], and Philippe Jacquod[2] — [1]University of Göttingen, Göttingen, Germany — [2]University of Arizona, Tucson, Arizona, USA

We investigate for the possibility of *directly* observing Andreev-reflection in the time evolution of an initial wave packet at a metal/superconductor junction in interacting one-dimensional Fermi-Hubbard systems. We apply the adaptive time-dependent density matrix renormalization group (t-DMRG) method to obtain the behaviour when the wave packet initially prepared in the metallic region (modelled by non-interacting electrons) hits the interface to the superconducting region which we model by an attractive Fermi-Hubbard model. Somewhat surprisingly, and at first sight in contradiction to the findings in [1,2], we do not obtain a clear signal for hole-reflection over a wide range of parameters. This appears to be different for bosonic systems, in which we identify hole-like reflection, in line with the findings of [2]. We discuss ongoing work on this issue and the different aspects of the results obtained so far.
[1] A.E. Feiguin, S.R. White, D.J. Scalapino, PRB 75, 024505 (2007)
[2] A.J. Daley, P. Zoller, B. Trauzettel, PRL 100, 110404 (2008).

TT 83.10 Thu 12:15 HSZ 03

A DMFT approach to dynamical quantum phase transitions. — •Elena Canovi and Martin Eckstein — Max Planck Research Department for Structural Dynamics, University of Hamburg (CFEL), Building 99, Luruper Chaussee 149, 22761 Hamburg, Germany

Recently, dynamical quantum phase transitions have been identified with non-analytic behavior of the Loschmidt echo in the thermodynamic limit (Heyl et al., Phys. Rev. Lett. 110 135704 (2013)), in analogy to non-analytic behavior of the free energy at a thermal phase transition. In this talk, we develop a formalism to obtain the Loschmidt echo within nonequilibrium dynamical mean-field theory, by mapping the lattice model to an impurity problem for which the time evolution is dictated by different Hamiltonians on the upper and lower real branches of the Keldysh contour. This opens the possibility of studying dynamical quantum phase transitions for the Hubbard model and related models in large dimensions.

TT 83.11 Thu 12:30 HSZ 03

Exact solution of polaron dynamics within nonequilibrium dynamical mean-field theory — •Sharareh Sayyad and Martin Eckstein — Max Planck Research Department for structural dynamics, University of Hamburg-CFEL, Hamburg, Germany

Ultra-fast pump-probe experiments have opened promising new avenues to control complex phases in correlated materials on femtosecond timescales. Of particular interest is an understanding of the combined electron lattice dynamics. In this talk we address the fundamental problem of a single electron interacting with the lattice, which is studied within the Holstein model. In equilibrium, this problem has been solved exactly using dynamical mean-field theory (DMFT) [1]. We have generalized this solution to non-equilibrium DMFT, which allows us to investigate the dynamics of photo-excited carriers in the presence of a strong electron-phonon interaction, and thus follow the formation of a polaron in real time.
[1] S. Ciuchi *et al.*, Phy. Rev. B **56**, 8 (1997)

TT 83.12 Thu 12:45 HSZ 03

Auxiliary Hamiltonian representation of the nonequilibrium Dyson equation — •Karsten Balzer and Martin Eckstein — Max Planck Research Department for Structural Dynamics, University of Hamburg (CFEL), Building 99, Luruper Chaussee 149, 22761 Hamburg, Germany

The nonequilibrium Dyson (or Kadanoff-Baym) equation, which is an equation of motion with long-range memory kernel for real-time Green functions, underlies many numerical approaches based on the Keldysh formalism. We show how the problem of solving the Dyson equation

in real-time can be mapped onto a noninteracting auxiliary Hamiltonian with additional bath degrees of freedom [1]. The solution of the auxiliary model does not require the evaluation of a memory kernel and can thus be implemented in a very memory efficient way. The mapping is derived for a self-energy which is local in space and is thus directly applicable within nonequilibrium dynamical mean-field theory (DMFT) [2]. We apply the method to study the interaction quench in the Hubbard model for an optical lattice with a narrow confinement, using inhomogeneous DMFT in combination with second-order weak-coupling perturbation theory. We find that, although the quench excites pronounced density oscillations, signatures of the two-stage relaxation similar to the homogeneous system can be observed by looking at the time-dependent occupations of natural orbitals.

[1] C. Gramsch, K. Balzer, M. Eckstein and M. Kollar, Phys. Rev. B, accepted (2013) [arXiv:1306.6315]
[2] H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka and P. Werner (2013) [arXiv:1310.5329]

TT 84: Correlated Electrons: (General) Theory

Time: Thursday 9:30–13:15 Location: HSZ 304

TT 84.1 Thu 9:30 HSZ 304

Uniform Electron Gas Approximation for the Second Order Screened Exchange Energy — •Felix Hummel and Georg Kresse — University of Vienna, Austria

The second order screened exchange (SOSEX) energy is the leading order correction to the random phase approximation (RPA) of the correlation energy. Computing the SOSEX contribution from the Kohn-Sham or Hartree-Fock orbitals scales like N^5, making it considerably less practical than direct RPA, which can be implemented with an N^4 or even an N^3 scaling.

We approximate the exchange kernel by the respective kernel of the uniform electron gas. This allows for an approximation of the RPA+SOSEX energy with the favourable scaling of RPA. We believe, this captures the dominant part of the SOSEX contribution for many materials and we compare it with full RPA+SOSEX calculations.

TT 84.2 Thu 9:45 HSZ 304

Calculation of screened coulomb interaction in f electron systems: dynamical screening and role of self-consistency. — •Bernard Amadon[1], Thomas Applencourt[1], and Fabien Bruneval[2] — [1]CEA, DAM, DIF, F-91297 Arpajon, France — [2]CEA, DEN, Service de Recherches de Métallurgie Physique , F-91191 Gif-sur-Yvette, France

The combination of density functional theory in the local density approximation (LDA) and dynamical mean field theory (DMFT) [1] has been successful to describe localized or delocalized correlated electrons in condensed matter [2]. However, the accurate calculations of structural or spectral properties relies on the determination of the screened Coulomb interactions between correlated electrons. In the last ten years, the constrained Random Phase Approximation was developed to describe the screening of correlated electrons by non correlated electrons [3]. In this presentation, we will first discuss the calculation of the screened interaction for strongly correlated metals and insulating oxides with correlated f electrons. We will discuss the importance of dynamical screening and self-consistency. Then we show applications to DFT+DMFT calculations with a recent implementation [4].

[1] A. Georges et al., Rev. Mod. Phys. 68, 13 (1996)
[2] G. Kotliar et al., Rev. Mod. Phys. 78, 865 (2006)
[3] F. Aryasetiawan et al Phys. Rev. B 70, 195104 (2004)
[4] B. Amadon, Journal of Phys.: Condens. Matter 24, 075604 (2012)

TT 84.3 Thu 10:00 HSZ 304

First multi-reference correlation treatment of bulk metals — •Elena Voloshina[1] and Beate Paulus[2] — [1]Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Freie Universität Berlin, 14195 Berlin, Germany

Existence of the *sp-d* hybridization of the valence band states of the *fcc* Ca and Sr in the vicinity of the Fermi level indicates that their electronic wave function can have a multi-reference (MR) character. We performed a wave function-based correlation treatment for these materials by means of the method of increments. As oppose to the single-reference correlation treatment (here: coupled cluster), which fails to describe cohesive properties in both cases, employing the MR averaged coupled pair functional one can achieve almost 100 % of the experimental correlation energy.

TT 84.4 Thu 10:15 HSZ 304

The puzzle of the basis-set for realistic calculations of correlated materials: The examples of Ni-heterostructures and Cuprates — •Giorgio Sangiovanni[1], Nicolaus Parragh[1], Philipp Hansmann[2], Stefan Hummel[3], Karsten Held[3], and Alessandro Toschi[3] — [1]Universität Würzburg — [2]Ecole Polytechnique, Paris — [3]Technische Universität Wien

The input for materials calculations done with dynamical mean field theory is a low-energy model defined on a small set of localized wave-functions constructed after the density functional theory step. The larger the energy window of the bands used in such a construction is, the more localized the resulting wave-functions will be. Since the assumption of a local Coulomb interaction is justified only if the orbitals of the minimal basis set considered as correlated are truly localized, the agreement with experiments is expected to improve upon including a higher number of relevant degrees of freedom. In the case of transition-metal oxides this would mean considering both the more correlated *d*- and the less correlated *p*-orbitals. In several cases, however, the agreement is surprisingly much better in the *d*-only case. We have shown that the physics arising from *d*-only and *dp* models for Ni-based heterostructures is indeed very dissimilar due to a different effect of the Hund's rule coupling in the two cases [1]. Analogous issues affect also theoretical predictions for Cuprates, for which the role of the *d-p* hybridization may appear at a first sight less relevant [2].

[1] N. Parragh, *et al.*, Phys. Rev. B **88**, 195116 (2013)
[2] P. Hansmann, *et al.*, *preprint* (2013)

TT 84.5 Thu 10:30 HSZ 304

One-particle irreducible functional approach: A route to diagrammatic extensions of the dynamical mean-field theory — •Georg Rohringer[1], Alessandro Toschi[1], Hartmut Hafermann[2], Karsten Held[1], Vladimir Anisimov[3,4], and Andrey Katanin[3,4] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Centre de Physique Théorique, École Polytechnique, CNRS, 91128 Palaiseau Cedex, France — [3]Institute of Metal Physics, 620990, Ekaterinburg, Russia — [4]Ural Federal University, 620002, Ekaterinburg, Russia

We present an approach[1] which is based on the one-particle irreducible (1PI) generating functional formalism and includes electronic correlations on all length-scales beyond the local correlations of dynamical mean field theory (DMFT). This formalism allows us to unify aspects of the dynamical vertex approximation (DΓA) and the dual fermion (DF) scheme, yielding a consistent formulation of nonlocal correlations at the one- and two-particle level beyond DMFT within the functional integral formalism. In particular, the considered approach includes one-particle reducible contributions from the three- and more-particle vertices in the dual fermion approach, as well as some diagrams not included in the ladder version of DΓA. To demonstrate the applicability and physical content of the 1PI approach, we compare the diagrammatics of 1PI, DF and DΓA, as well as the numerical results of these approaches for the half-filled Hubbard model in two dimensions.

[1] G. Rohringer, A. Toschi, K. Held, V. I. Anisimov, and A. A. Katanin, Phys. Rev. B **88**, 115112 (2013)

TT 84.6 Thu 10:45 HSZ 304

Efficient real frequency solver for dynamical mean field theory — •Yi Lu[1,2] and Maurits W. Haverkort[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Max Planck Institute for Chemical Physics of Solids, Dresden

We present an efficient exact diagonalization (ED) based real frequency solver for the general Anderson impurity problem and dynamical mean field theory (DMFT). It alleviates the exponential increasing Hilbert space encountered by conventional ED algorithms as a function of the

number of bath sites. A specific bath geometry is realized upon which basis set optimization can be applied. The restricted Hilbert space allows calculations including a few hundred bath sites at moderate cost, which solve for spectral functions with energy resolution better than $1/\mathcal{O}(10^2)$ of the bandwidth. Good agreement with other methods including numerical renormalization group and continuous-time quantum Monte Carlo is obtained for model systems over a wide parameter space, with comparable or better accuracy at much lower computation cost. Dynamical quantities can be easily obtained on the real axis. We show several examples of DMFT calculations on transition metal oxides, including nickelates and related heterostructures.

TT 84.7 Thu 11:00 HSZ 304

Quasi-continuous-time impurity solver for the cluster dynamical mean-field theory with linear scaling in the inverse temperature — •Daniel Rost[1,2], Nils Blümer[1], and Fakher F. Assaad[3] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Johannes Gutenberg University, Mainz, Germany — [3]Institute of Theoretical Physics and Astrophysics, University of Würzburg, Germany

We present an extension to cellular dynamical mean-field theory (CDMFT) of an recently developed unbiased quantum Monte Carlo (QMC) impurity solver for single-site DMFT [1]. The novel algorithm is based on a multigrid version of BSS-QMC [2,3], which yields Green functions free of significant Trotter errors, and scales linearly with the inverse temperature $\beta = 1/T$ and cubically in the cluster size N. We use the superior scaling to explore ultra-low temperature regimes at moderate cluster sizes, not reachable with state-of-the-art continuous time QMC impurity solvers that scale cubically in β.

[1] D. Rost, F. Assaad and N. Blümer, PRE 87, 053305 (2013)
[2] E. Khatami et al., PRE 81, 056703 (2010)
[3] R. Blankenbecler, D. Scalapino, R. Sugar, PRD 24, 2278 (1981)

15 min. break.

TT 84.8 Thu 11:30 HSZ 304

Divergent precursors of the Mott metal-insulator transition in dynamical mean field theory and beyond — •T. Schäfer[1], G. Rohringer[1], O. Gunnarsson[2], S. Ciuchi[3], G. Sangiovanni[4], E. Gull[5], J. LeBlanc[6], P. Thunström[1], M. Wallerberger[1], and A. Toschi[1] — [1]Institute of Solid State Physics, Vienna University of Technology, Austria — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Dipartimento di Scienze Fisiche e Chimiche, Università dell'Aquila, Italy — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [5]Department of Physics, University of Michigan, USA — [6]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Bulk electronic correlated systems can be often successfully studied by dynamical mean field theory (DMFT), which is able to properly describe the intrinsically non-perturbative phenomenon of the Mott-Hubbard metal-to-insulator transition (MIT). Recently it has been shown that the first hallmarks of the MIT can already be identified well inside the metallic regime in terms of divergences of the two-particle irreducible vertex [1].

In this talk the non-perturbative region of the Hubbard model's phase diagram beyond the first precursor line towards the MIT is explored in more detail and, eventually, the effects of the inclusion of short-ranged spatial correlations are discussed [2].

[1] T. Schaefer, G. Rohringer, O. Gunnarsson, S. Ciuchi, G. Sangiovanni, and A. Toschi, Phys. Rev. Lett. 110, 246405 (2013)
[2] T. Schaefer et al., in preparation

TT 84.9 Thu 11:45 HSZ 304

Stochastic Mode Sampling (SMS) - An Efficient Approach to the Analytic Continuation Problem — •Khaldoon Ghanem and Erik Koch — Computational Materials Science, German Research School for Simulation Sciences, Jülich, Germany

Stochastic sampling methods (SSMs) provide a promising alternative to the commonly used maximum entropy method (MEM) in solving the analytic continuation problem of non-negative quantities like the spectral function or the optical conductivity. SSMs assume a flat prior probability, which is the appropriate choice in the absence of any prior knowledge, while MEM unjustifiably biases the results toward a default model. On the other hand, SSMs can be exceedingly slow compared to MEM because of the large correlation times.

We present a new stochastic sampling method, *Stochastic Mode Sampling* (SMS). Instead of sampling the components of the solution directly, we sample the singular vectors (modes) of the kernel, which relates the data to the solution. In this basis, the sampled quantities are uncorrelated except for the coupling through the non-negativity constraint. The weaker this coupling, the more efficient the method, so we modify the kernel such that the coupling is minimized, thus reducing correlation times dramatically in comparison to other SSMs. We also show how to make SMS solutions converge as the discretization grid becomes larger and denser.

TT 84.10 Thu 12:00 HSZ 304

Fermionic functional renormalization group flows into antiferromagnetically ordered phases — •Stefan A. Maier and Carsten Honerkamp — Institute for Theoretical Solid State Physics, RWTH Aachen University, 52074 Aachen, Germany and JARA - FIT Fundamentals of Future Information Technology

In this talk, we report on purely fermionic functional renormalization group flows into antiferromagnetically ordered phases. Starting from the fRG one-loop flow equations, a hierarchy of approximations is devised. Interaction terms breaking the discrete time-reversal and translational symmetries are thereby successively neglected, whereas they remain broken on the one-particle level. In the course of these approximations, also an exchange parametrization is employed. For the spin-density wave (SDW) phase of a two-pocket model initially proposed by Chubukov *et al.* in Phys. Rev. B **78** 134512, the flow equations are then integrated numerically at the most approximate level of the hierarchy. This yields a SDW gap that is significantly reduced compared to mean-field theory, and the inclusion of the charge-density wave and singlet-pairing channels turns out to be crucial. The observed violation of the SU(2) Ward identity appears acceptable on a qualitative level, suggesting that the underlying approximations are physically meaningful.

TT 84.11 Thu 12:15 HSZ 304

Impurity solver based on Dynamical Density Matrix Renormalization Group — •Markus Greger and Marcus Kollar — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg

We present a deconvolution-free extension of the dynamical density matrix renormalization group (DDMRG) for impurity problems. Our method is highly accurate in the low-energy sector and yields spectra that are comparable in resolution to the numerical renormalization group (NRG). The method is suitable as an impurity solver for multi-orbital dynamical mean-field theory (DMFT). We present results for the Green function, self-energy, and spin-susceptibility for multi-band Hubbard models, focusing on the effect of the Hund's rule coupling on these spectra at low-energies.

TT 84.12 Thu 12:30 HSZ 304

Low-energy singularities in the ground state of fermionic superfluids — •Benjamin Obert[1], Christoph Husemann[2], and Walter Metzner[1] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Carl Zeiss AG, Carl Zeiss Promenade 10, D-07745 Jena, Germany.

We analyze the effects of order parameter fluctuations on the ground state of fully gapped charge-neutral fermionic superfluids. The Goldstone mode associated with the spontaneously broken symmetry leads to a problem of coupled singularities in $d \leq 3$ dimensions. We derive a minimal set of one-loop renormalization group equations which fully captures the interplay of the singularities. The flow equations are based on a symmetry conserving truncation of a scale dependent effective action. We compute the low energy behavior of longitudinal, transverse and mixed order parameter correlations, and their impact on the fermionic gap. We demonstrate analytically that cancellations protecting the Goldstone mode are respected by the flow, and we present a numerical solution of the flow equations for the two-dimensional attractive Hubbard model.

TT 84.13 Thu 12:45 HSZ 304

Symmetry breaking with Projected Entangled Pair States — •Manuel Rispler and Norbert Schuch — Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

Projected Entangled Pair States (PEPS) have been introduced as a two-dimensional generalization of Matrix Product States and form a part of the larger class of Tensor Network States, which parametrize quantum states according to their entanglement structure. In this

talk, we explain how the mechanism of symmetry breaking can be understood in the framework of PEPS models. We give examples and illustrate how perturbations give rise to the symmetry broken states. We further discuss how this allows to understand the entanglement spectrum as arising from a local Hamiltonian on the boundary of the system.

TT 84.14 Thu 13:00 HSZ 304

Critical Exponents of Strongly Correlated Fermion Systems from Diagrammatic Multi-Scale Methods — Andrey Antipov[1,2], Emanuel Gull[3], and •Stefan Kirchner[1,2] — [1]MPI for Physics of Complex Systems, Dresden — [2]MPI for Chemical Physics of Solids — [3]Department of Physics, University of Michigan

The dynamical mean field theory (DMFT) has become the standard tool in describing strongly correlated electron materials. While it captures the quantum dynamics of local fields, it neglects spatial correlations. To describe e.g. anti-ferromagnetism, unconventional superconductivity or frustration a proper treatment of non-local correlations is necessary. Diagrammatic multi-scale approaches offer an elegant option to accomplish this: the difficult correlated part of the system is solved using a non-perturbative many-body method, whereas 'easier', 'weakly correlated' parts of the problem are tackled using a secondary perturbative scheme. Here we employ such a method, the dual fermion approach, to problems of charge ordering in Falicov-Kimball model [1] by constructing a systematic diagrammatic extension on top of DMFT. Near the critical point of the Falicov-Kimball model we study the interplay between charge excitations and long-range fluctuations. We show that such multi-scale approach is indeed capable of capturing the non mean-field nature of the critical point of the lattice model and correctly describes the transition to mean-field like behavior as the number of spatial dimensions increases.

[1] A. Antipov, E. Gull, S. Kirchner, arXiv:1309.5976(2013).

TT 85: Spincaloric Transport II (organized by MA)

Time: Thursday 9:30–12:15 Location: HSZ 04

TT 85.1 Thu 9:30 HSZ 04

6000 % tunnel magneto-Seebeck effect under applied bias — •Alexander Boehnke[1], Marius Minikel[2], Marvin Walter[2], Vladylsav Zbarsky[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. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

Recently, significantly different values of the tunnel magneto-Seebeck effect (TMS) [1-5] have been reported when the material system of the magnetic tunnel junction (MTJ) is changed. Ab initio calculations shine first light on the origin of these differences, as they propose a strong influence of the lead material on the TMS [6]. We applied an additional bias voltage V_{Bias} to MTJs while measuring the TMS.

This well-defined tuning of the electrodes' Fermi level positions allows to compare the bias voltage dependence of the TMS with the theoretical predictions. We demonstrate drastically changing TMS ratios of up to 6000 % generated by the variation of the bias voltage. At certain values of V_{Bias}, an on/off behavior of the Seebeck voltage is found when the magnetization alignment of an MTJ is reversed. These findings are in good agreement with the ab into calculations [6].

[1] M. Walter et al. (2011). Nat. Mater., 10(10), 742.
[2] N. Liebing et al. (2011). Phys. Rev. Lett., 107(17), 177201.
[3] W. Lin et al. (2012). Nat. Commun., 3, 744.
[4] N. Liebing et al. (2013). Appl. Phys. Lett., 102(24), 242413.
[5] A. Boehnke et al. (2013). Rev. Sci. Instrum., 84(6), 063905.
[6] C. Heiliger et al. (2013). Phys. Rev. B, 87(22), 224412.

TT 85.2 Thu 9:45 HSZ 04

Thin film studies of the spin Seebeck effect in insulating ferrimagnets — •Andreas Kehlberger[1], Gerhard Jakob[1], Ulrike Ritzmann[2], Denise Hinzke[2], Ulrich Nowak[2], Mehmet Onbasil[3], Dong Hun Kim[3], Caroline A. Ross[3], Matthias Benjamin Jungfleisch[4], Burkard Hillebrands[4], and Mathias Kläui[1] — [1]University of Mainz, D-55099 Mainz — [2]University of Konstanz, D-78457 Konstanz — [3]Massachusetts Institute of Technology, USA MA-02139 — [4]Technische Universität Kaiserslautern, D-67663 Kaiserslautern

One of the most basic and still unresolved questions is the origin of the spin-Seebeck effect (SSE) in magnetic insulators. Recent studies focused on the investigation of the dependence of the SSE on material parameters in bulk material [1], while for applications thin films are more appropriated. We study the longitudinal SSE (LSSE) in thin film garnets grown by PLD, which allows us to probe the dependence of the SSE on magnetic material parameters as well as on the thickness of the ferromagnetic material, revealing a relevant length scale for the LSSE in the order of 100 nm in YIG. A comparison with the magnetoresistance allows us to estimate its contributions and to identify the genuine origin of the SSE in the bulk of the YIG [2]. Beyond YIG, we study other garnets at variable temperatures to determine the SSE dependence on the dominating sub-lattice that governs the effective magnetic moment in a ferrimagnet [3]. [1] K. Uchida et al., Phys. Rev. B 87, 104412 (2013) [2] A. Kehlberger et al., arXiv:1306.0784 (2013) [3] Y. Ohnuma et al., Phys. Rev. B 87, 014423 (2013)

TT 85.3 Thu 10:00 HSZ 04

Magnonic spin currents and the spin Seebeck effect — •Ulrike Ritzmann, Denise Hinzke, and Ulrich Nowak — Universität Konstanz

In ferromagnetic insulators spatial temperature gradients can lead to a magnon accumulation [1]. Furthermore, it was shown that the measured voltage of the longitudinal spin Seebeck effect increases with film thicknes, saturating on a characteristic length scale [2].

We perform atomistic spin model simulation with the stochastic Landau-Lifshitz-Gilbert equation to investigate the relevant length scales for magnon accumulation. Supported by an analytical description we first calculate the characteristic length scale of magnon propagation in the vicinity of a temperature step [3]. Then we explore magnon propagation in a linear temperature gradient and determine the mean propagation length of the magnons [2]. Our main finding is that the magnon accumulation at the cold end of the temperature gradient first increases with the the length scale of the temperature gradient and then saturates when reaching the length scale of the magnon propagation. These results can explain the saturation of the longitudinal spin Seebeck effect [2] and can help to understand recent measurements regarding the temporal evolution of the spin Seebeck effect [4].

[1] K. Uchida et al, Nat. Mater. 9, 894 (2010)
[2] A. Kehlberger et al.,arXiv:1306.0784
[3] U. Ritzmann et al., submitted
[4] M. Agrawal et al., arXiv:1309.2164

TT 85.4 Thu 10:15 HSZ 04

Temporal evolution of the longitudinal spin Seebeck effect — •Vitaliy Vasyuchka[1], Milan Agrawal[1,2], Alexander Serga[1], Akihiro Kirihara[1,3], Philipp Pirro[1], Thomas Langner[1], Frank Heussner[1], Benjamin Jungfleisch[1], Andrii Chumak[1], Evangelos Papaioannou[1], and Burkard Hillebrands[1] — [1]FB Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz — [3]Smart Energy Research Laboratories, NEC Corporation, Tsukuba, Japan

The spin Seebeck effect (SSE) is one of the most fascinating phenomena in the contemporary period of spin caloritronics. Further advancements in industrial applications like temperature gradient sensors and thermal spin-current generators require an in-depth understanding of this effect. We developed an experimental approach where we studied the temporal evolution of the SSE in YIG/Pt bilayer structures in the longitudinal configuration. Our findings reveal that this effect is a submicrosecond fast phenomenon governed by the temperature gradient and the thermal magnons diffusion in the magnetic material. A comparison of our experimental results with the thermal-driven magnon-diffusion model shows that the temporal behavior of the SSE depends on the time development of the temperature gradient in the vicinity of the YIG/Pt interface. The effective thermal-magnon diffusion length for our YIG/Pt system is estimated to be around 500 nm.

Financial support by the Deutsche Forschungsgemeinschaft (SE 1771/4-1) within Priority Program 1538 "Spin Caloric Transport" is gratefully acknowledged.

TT 85.5 Thu 10:30 HSZ 04

Thermally driven domain wall motion — •Frank Schlickeiser, Ulrike Ritzmann, Denise Hinzke, and Ulrich Nowak — University Konstanz, 78457 Konstanz, Germany

The existence of thermally driven domain wall (DW) motion caused solely by magnonic spin currents was forecast on the basis of computer simulations [1]. Recently, this effect has been measured in a magnetic insulator [2]. A deeper understanding of this effect is of great interest, since it potentially opens the door for new ways to control and manipulate domain structures in spintronic devices.

We present an analytical calculation of the DW velocity as well as the Walker threshold within the framework of the Landau Lifshitz Bloch equation [3] describing the dynamics of the thermally averaged spin polarization on micromagnetic length scales. We demonstrate analytically that the temperature gradient leads effectively to a spin transfer torque where the domain wall is mainly driven by the temperature dependence of the exchange stiffness, or — in a more general picture — by the maximization of entropy. We find a linear dependence of the averaged DW velocity on the temperature gradient in agreement with the experiment [2]. The approximations in our analytical calculation are verified by numerical simulations.

We acknowledge financial support by the DFG through SFB 767.

References: [1] D. Hinzke and U. Nowak, Phys. Rev. Lett. 107, 027205 (2011), [2] W. Jiang et al., Phys. Rev. Lett. 110, 177202 (2013), [3] D. A. Garanin, Phys. Rev. B 55, 3050 (1997).

15 min. break

TT 85.6 Thu 11:00 HSZ 04

Spin disorder effect on the spin-caloric transport properties in magnetic nanostructures from first principles — •Roman Kováčik, Phivos Mavropoulos, Daniel Wortmann, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

An important contribution to the thermoelectric and spin-caloric transport properties in magnetic materials at elevated temperatures is the formation of a spin-disordered state due to the local moment fluctuations. This effect has not been largely investigated so far. We focus on various magnetic nanostructures, motivated by the miniaturization of spintronics devices and by recent suggestions that magnetic nanostructures can lead to extraordinary thermoelectric effects due to quantum confinement [1]. The electronic structure of the studied systems is calculated within the multiple scattering screened Korringa-Kohn-Rostoker Green function (KKR-GF) framework [2]. The Monte-Carlo methodology is used to simulate the effect of temperature induced spin disorder and the transport properties are evaluated from the transmission probability obtained using the Landauer-Büttiker approach for the ballistic transport within the KKR-GF framework [3]. We find qualitative and quantitative changes in the thermoelectric and spin-caloric coefficients in the case that spin-disorder is included in the calculation.
Support from the DFG (SPP 1538) is gratefully acknowledged.
[1] N. Vu *et al.*, APEX 4, 015203 (2011).
[2] N. Papanikolaou *et al.*, JPCM 14, 2799 (2002), also see: kkr-gf.org.
[3] Ph. Mavropoulos *et al.*, PRB 69, 125104 (2004).

TT 85.7 Thu 11:15 HSZ 04

Spin caloric transport in alloys from first-principles — •Sebastian Wimmer, Diemo Ködderitzsch, Kristina Chadova, and Hubert Ebert — Ludwig-Maximilians-Universität, München, Deutschland

A fully relativistic implementation of the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) band structure method [1] in conjunction with Kubo's linear response theory is employed to investigate various transport properties of bulk transition metal alloys. Special emphasis is put on spin-orbit coupling induced phenomena of thermo(-magneto)-electric transport in para- as well as ferromagnetic systems such as spin and anomalous Nernst effects and the anisotropy of the Seebeck effect [2,3]. These transverse and longitudinal responses to a temperature gradient are compared to their respective (magneto-)electric counterparts, the spin and anomalous Hall effects and the anisotropic magnetoresistance. For the transverse effects a decomposition into intrinsic and extrinsic (skew scattering and side-jump) contributions is performed, based on vertex corrections and scaling laws.

[1] H. Ebert, D. Ködderitzsch, and J. Minár, Rep. Prog. Phys. **74**, 096501 (2011).
[2] S. Wimmer, D. Ködderitzsch, K. Chadova, and H. Ebert, PRB **88**, 201108(R) (2013).
[3] S. Wimmer, D. Ködderitzsch, and H. Ebert, arXiv:1311.2498 [cond-mat.mtrl-sci] (2013).

TT 85.8 Thu 11:30 HSZ 04

Static proximity investigations on Pt/$NiFe_2O_4$ and Pt/Fe bilayers using x-ray resonant magnetic reflectivity — •Timo Kuschel[1], Christoph Klewe[1], Jan-Michael Schmalhorst[1], Florian Bertram[2], Olga Schuckmann[3], Tobias Schemme[3], Joachim Wollschläger[3], Arunava Gupta[4], Gerhard Götz[1], Daniel Meier[1], and Günter Reiss[1] — [1]Bielefeld University, Germany — [2]Lund University, Sweden — [3]Osnabrück University, Germany — [4]University of Alabama, Tuscaloosa Alabama, USA

When Pt is used to detect spin currents in an attached magnetic film via the inverse spin Hall effect, parasitic charge based effects can be induced due to spin polarization in Pt generated by static proximity. For example, in spin caloritronics the anomalous Nernst effect (ANE) can contribute to the longitudinal spin Seebeck effect (LSSE) signal when an out-of-plane temperature gradient is applied. In case of Pt/YIG Lu et al. [1] observed a spin polarization in Pt via XMCD, while Geprägs et al. [2] found no evidence for static proximity in Pt/YIG. Recently, we have observed the LSSE in $NiFe_2O_4$ (NFO) thin films [3]. Now, we used x-ray resonant magnetic reflectivity (XRMR) to exclude the ANE. XRMR is interface sensitive and therefore, mainly independent of the Pt thickness, which makes it preferable over XMCD. For Pt/Fe we clearly detect an XRMR signal of some %, while for Pt/NFO we can exclude any effect within our detection limit of $< 0.05\,\%$.
[1] Y. M. Lu et al., Phys. Rev. Lett. 110, 147207 (2013)
[2] S. Geprägs et al., Appl. Phys. Lett. 101, 262407 (2012)
[3] D. Meier et al., Phys. Rev. B. 87, 054421 (2013)

TT 85.9 Thu 11:45 HSZ 04

Thermally induced spin accumulation at Al/Co_2TiSi and Al/Co_2TiGe contacts — •Voicu Popescu, Benjamin Geisler, and Peter Kratzer — Faculty of Physics, University Duisburg-Essen, Duisburg, Germany

Spin injection from a ferromagnet in a semiconductor subtrate can be accomplished either by applying an external voltage or a temperature gradient. In the latter case, one exploits the Seebeck effect, with the temperature gradient across the contact directly resulting in a difference in chemical potentials in the two spin channels due to the spin-dependence of the Seebeck coefficient.

The magnetic Heusler alloys Co_2TiSi or Co_2TiGe exhibit half-metallic ferromagnetism in their ideal $L2_1$ crystal structure, with a potentially high degree of spin polarization of the injected current. As such, they recommend themselves for integrated spin injectors in combination with the closely lattice-matched Al contact layer.

We investigate the possibility of employing Al/Co_2TiX/Al (X=Si,Ge) trilayers as thermally driven spin injectors by means of first-principles calculations of the electronic structure and of the thermoelectric transport properties. Our results show that the spin-dependent Seebeck effect is sensitive to the atomic structure of the Heusler/Al interface. In particular, for a thin Co_2TiSi or Co_2TiGe layer terminated by a TiSi or TiGe atomic plane, the thermal spin accumulation is found to be of the same order of magnitude as the conventional, effective Seebeck coefficent.

TT 85.10 Thu 12:00 HSZ 04

Influence of heat flow directions on Nernst effects in Py/Pt bilayers — •Daniel Meier[1], Daniel Reinhardt[1], Maximilian Schmid[2], Christian H. Back[2], Jan-Michael Schmalhorst[1], Timo Kuschel[1], and Günter Reiss[1] — [1]University of Bielefeld, D-33501 Germany — [2]University of Regensburg, D-93040 Germany

We investigated the voltages obtained in a thin Pt strip on a Permalloy film which was subject to in-plane temperature gradients and magnetic fields. The voltages detected by thin W-tips or bond wires showed a purely symmetric effect with respect to the external magnetic field which can be fully explained by the planar Nernst effect (PNE). To verify the influence of the contacts measurements in vacuum and atmosphere were compared and gave similar results. We explain that a slightly in-plane tilted temperature gradient only shifts the field direction dependence but does not cancel out the observed effects. Additionally, the anomalous Nernst effect (ANE) could be induced by using thick Au-tips which generated a heat current perpendicular to the sample plane. The effect can be manipulated by varying the tem-

perature of the Au-tips. These measurements are discussed concerning their relevance in transverse spin Seebeck effect measurements.

TT 86: Correlated Electrons: Other Materials

Time: Thursday 9:30–12:45 Location: BEY 81

TT 86.1 Thu 9:30 BEY 81

Metal-insulator transition in $LiVS_2$ through correlation-induced orbital-spin ordering — Lewin Boehnke, Alexander I. Lichtenstein, and •Frank Lechermann — I. Institute for Theoretical Physics, University of Hamburg

The investigation of nature's various mechanisms to localize electrons within a material that undergoes a metal-insulator transition (MIT) is a salient research endeavour in condensed matter physics. Prominent localization driving forces in the chemically ordered states are either dominant exchange processes, giving rise to a Slater insulator, or strong correlations, leading to an insulator of Mott type. However in complex compounds with manifest multi-orbital character and apparent geometrical frustration the many-body physics underlying the competition between metallic and insulating state may even be more intricate. Here the advanced combination of density functional theory with dynamical mean-field theory including multi-orbital vertex contributions to determine (dynamic) lattice susceptibilities in the strong correlation regime is used to study the nebulous MIT in quasi-twodimensional $LiVS_2$. Entangled orbital-spin ordering tendencies originating in the high-temperature metallic phase are revealed. Those lead to a transition into a challenging insulating phase close to room temperature.

TT 86.2 Thu 9:45 BEY 81

The insulating phases of Vanadium Sesquioxide (V_2O_3) — •Daniel Grieger[1], Frank Lechermann[2], and Michele Fabrizio[1] — [1]SISSA - Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy — [2]1. Institut für Theoretische Physik, Universität Hamburg, Germany

Vanadium Sesquioxide (V_2O_3) has attracted large attention mainly because of its prototypical Mott insulating behaviour with negative (chemical) pressure/Chromium doping. Besides trying to shed some light on the actual difference between doping and pressure in view of electronic correlations modelled by the charge self-consistent LDA+DMFT approach, this contribution is primarily aimed at the low-temperature (T<140K) antiferromagnetic insulating phase, which has not been properly understood for the last 40 years. It shows a peculiar magnetic ordering involving ferromagnetic out-of-plane bonds and two antiferromagnetic/one ferromagnetic in-plane bond per Vanadium atom, at the additional energetic cost of a monoclinic structural distortion. Arguments about why this complicated structure turns out to be stable are given from a combination of traditional electronic structure formalisms and DFT+-like approaches.

TT 86.3 Thu 10:00 BEY 81

May the character of the metal-insulator transition of disordered materials be determined by how one looks at it? — •Arnulf Möbius — Institute for Theoretical Solid State Physics, IFW Dresden

In a recent experiment, Siegrist et al. studied the metal-insulator transition (MIT) of phase-change materials [1]. They conclude that these substances exhibit a finite minimum metallic conductivity. The striking contrast to reports on other disordered substances motivates the present study of the influence of the MIT criterion used on the character of the MIT obtained [2]. First, we discuss inherent biases of various approaches to locating the MIT. Second, reanalyzing $GeSb_2Te_4$ data from [1], we show that this solid strongly resembles other disordered materials: The data may also be interpreted in terms of a continuous MIT. Checking the justification of these fits, however, uncovers data inconsistencies preventing an unambiguous interpretation. Third, comparing with previous experiments on crystalline Si:As, Si:P, Si:B, Ge:Ga, disordered Gd, and nano-granular Pt-C, we show that such an inconclusive behavior occurs frequently: The logarithmic temperature derivative of the conductivity highlights serious inconsistencies in the original interpretations in terms of a continuous MIT. Thus, the question for the character of the MIT of these materials has to be considered as yet open. The primary challenge lies in improving the measurement precision rather than extending the temperature range.
[1] T. Siegrist et al., Nature Materials 10 (2011) 202.
[2] A. Möbius, arxiv.org/abs/1308.1538.

TT 86.4 Thu 10:15 BEY 81

Non-magnetic ground state of PuO_2 — •Jindrich Kolorenc[1], Alexander B. Shick[1], Ladislav Havela[2], Thomas Gouder[3], and Roberto Caciuffo[3] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [2]Charles University, Prague, Czech Republic — [3]European Commission, Joint Research Centre, Institute for Transuranium Elements, Karlsruhe, Germany

The correlated band theory implemented as a combination of the local density approximation with the exact diagonalization of the Anderson impurity model is applied to PuO_2. We obtain an insulating electronic structure consistent with the experimental photoemission spectra. The calculations yield the band gap of 1.8 eV and a non-magnetic singlet ground state that is characterized by a non-integer filling of the plutonium f shell ($n_f \approx 4.5$). Due to sizeable hybridization of the f shell with the p states of oxygen, the ground state is more complex than the four-electron Russell–Saunders $^5I_4$ manifold split by the crystal field. The inclusion of hybridization improves the agreement between the theory and experiment for the magnetic susceptibility.

TT 86.5 Thu 10:30 BEY 81

The origin of orbital and magnetic order in K_2CuF_4 — •Guoren Zhang[1], Erik Koch[2], and Eva Pavarini[1] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]German Research School for Simulation Sciences, 52425 Jülich, Germany

In this work, we investigate the origin of magnetic and orbital order in K_2CuF_4. We first construct Wannier functions from the Bloch states obtained by local-density approximation calculations with the full-potential linearized augmented plane-wave method. Then, by perturbative theory, we calculate magnetic couplings which are in good agreement with experimental results both for the ambient and high pressure structures. To investigate the origin of orbital order, we perform calculations with local-density approximation+dynamical mean-field theory method. We discuss the roles of crystal-field[1], superexchange and the charge-transfer effects[2] on the orbital ordering.
[1] K. I. Kugel and D. I. Khomskii, Zh. Eksp. Teor. Fiz. **64**, 1429 (1973) [Sov. Phys. JETP **37**, 725 (1973)].
[2] M.V. Mostovoy and D. I. Khomskii, Phys. Rev. Lett. **92**, 167201 (2004).

TT 86.6 Thu 10:45 BEY 81

On the orbital-ordering transition in $KCuF_3$ — •Hunter Sims[1], Eva Pavarini[2], and Erik Koch[1] — [1]German Research School for Simulation Sciences, 52428 Jülich, Germany — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

The Mott insulating perovskite $KCuF_3$ is considered the paradigmatic system with long-ranged orbital order and a cooperative Jahn-Teller distortion of the F-octahedra. This broken symmetry state is usually understood as the result of the destabilization of the symmetric structure due to crystal-field splitting (Jahn-Teller effect) or to superexchange between the orbitals (Kugel-Khomskii mechanism), which leads to a gain in energy with increasing distortion. This is counteracted by the quadratic deformation energy of the lattice. In this picture it is expected that, as a consequence of the lattice entropy, the distortions will be gradually reduced with increasing temperature until they finally vanish at the ordering temperature T_c. Such a transition is, however, not found experimentally. We explain why.

15 min. break.

TT 86.7 Thu 11:15 BEY 81

Fermi surface of $Sr_{n+1}Ru_nO_{3n-1}$ ruthenates: LDA+DMFT study — •Evgeny Gorelov, Guoren Zhang, and Eva Pavarini — IAS, 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 tran-

sition metal compounds. Because kinetic and Coulomb energy are of the same order for Ru 4*d* electrons, these compounds have a very rich phase diagram. Furthermore, the spin-orbit coupling (SOC) is comparable with crystal-field splitting of t_{2g} levels and it is thus crucial for the description of the Fermi surface.

In the present work we focus on three compounds of the $Sr_{n+1}Ru_nO_{3n+1}$ family: single-layered Sr_2RuO_4, double layered $Sr_3Ru_2O_7$, and triple-layered $Sr_4Ru_3O_{10}$. We study the shape of the Fermi surface and the electron mass renormalization in the presence of correlation effects and SOC. In our LDA+DMFT (local-density approximation + dynamical mean-field theory) scheme we use maximally-localized Wannier orbitals obtained from Linearized Augmented Plane Wave (LAPW) ab-initio calculations to build a low-energy Hubbard model for the Ru 4*d* bands; we use the weak-coupling 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 spin-orbital space. For $Sr_4Ru_3O_{10}$ we use the cluster DMFT scheme to account for the inequivalent Ru atoms.

TT 86.8 Thu 11:30 BEY 81

Metal-insulator and magnetic transitions of Ca_2RuO_4 observed by hard x-ray photoemission spectroscopy — •Yuki Utsumi[1], Stefano Agrestini[1], Zhiwei Hu[1], Kyung-Tae Ko[1], Ku-Ding Tsuei[2], Yen-Fa Liao[2], Yu-Han Wu[2], Komarek C. Alexander[1], and Liu Hao Tjeng[1] — [1]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan

Layered perovskite Ca_2RuO_4 has been attracting a great interest as much as the spin triplet superconductor Sr_2RuO_4 because of its rich properties. Isovalent Ca substitution for Sr changes the system from superconductor to Mott insulator. Ca_2RuO_4 is an antiferromagnetic insulator below T_N=110 K and exhibits a metal-insulator transition (MIT) at ∼357 K accompanied by a crystal structure distortion. The MIT temperature continuously decreases with increase in Sr content. For the case of $Ca_{1.91}Sr_{0.09}RuO_4$, the MIT temperature becomes almost equal to T_N. Despite a large number of experimental and theoretical studies, the mechanism of the MIT in Ca_2RuO_4 is still hotly debated. Here we report a hard x-ray photoemission spectroscopy (HAXPES) study of the electronic structure of this layered system as a function of temperature. The valence-band spectrum of Ca_2RuO_4 shows dramatic changes across the MIT. The valence band spectrum of $Ca_{1.91}Sr_{0.09}RuO_4$ displays similar temperature evolution across the MIT. These HAXPES results indicate not only a rearrangement in t_{2g} orbital occupation but also the importance of electronic correlations for the MIT.

TT 86.9 Thu 11:45 BEY 81

HAXPES study of the spectral weight distribution of d^1 Mott insulators $LaTiO_3$ — •Jonas Weinen[1], Stefano Agrestini[1], Alexander C. Komarek[1], Zhiwei Hu[1], Thomas Koethe[2], Maurits W. Haverkort[1], Yen-Fa Liao[3], Ku-Ding Tsuei[3], and Liu H. Tjeng[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [2]II. Physikalisches Institut der Universität zu Köln — [3]National Synchrotron Radiation Research Centre, Hsinchu, Taiwan

Using hard x-ray photoelectron spectroscopy (HAXPES) we have obtained bulk-sensitive valence band spectra of the d^1 Mott insulators $LaTiO_3$ and $YTiO_3$. The experiment was performed in the *s* polarization, thus suppressing the *s* orbitals spectral weight which hide the *d* orbitals when using the more common *p* polarization.

We observed appreciable differences between the spectra of the two compounds, reflecting the difference in the one-electron band width. We also found that the Ti 3*d* spectra of both materials are much broader than the occupied 3*d* bands calculated by band theories. The mean-field inclusion of the Hubbard *U* explains the band gap but produces even narrower bands, indicating the complete breakdown of standard meanfield theories in describing excitation spectra. We associate the observed spectra with the propagation of a hole in a system with surprisingly well suppressed charge fluctuations thereby showing characteristics of a *t*-*J* model.

TT 86.10 Thu 12:00 BEY 81

Topological superconducting phases in the doped Kitaev-Heisenberg model — •Daniel Scherer[1], Michael Scherer[2], Giniyat Khaliullin[3], Carsten Honerkamp[4,5], and Bernd Rosenow[1] — [1]Institute for Theoretical Physics, University of Leipzig, D-04103 Leipzig, Germany — [2]Institute for Theoretical Physics, University of Heidelberg, D-69120 Heidelberg, Germany — [3]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [4]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52056 Aachen, Germany — [5]JARA Fundamentals of Future Information Technologies

The Kitaev-Heisenberg model can describe the magnetic ground-state of the spin-orbit Mott insulator Na2IrO3. Here, we present our analysis of the quantum many-body instabilities found in the doped system within the framework of a t-J model. We determine ordering tendencies by the functional renormalization group (fRG) method for correlated fermionic systems in an unbiased way. To this end, we derived fRG flow-equations and Ward identities adapted to the lack of full spin-rotational invariance in the fermionic interactions caused by the highly anisotropic and frustrated Kitaev exchange. The solution of the flow equations suggests a rich phase diagram emerging upon doping charge carriers into the ground-state manifold (quantum spin liquids, magnetically ordered phases) of the Kitaev-Heisenberg Hamiltonian. We confirm superconducting triplet p-wave instabilities driven by ferromagnetic exchange. These p-wave phases turn topological upon increasing doping-level and support Majorana edge-modes.

TT 86.11 Thu 12:15 BEY 81

Investigation of the Verwey transition in Fe_3O_4 thin films — •Xionghua Liu, Diana Rata, Chun Fu Chang, Alexander Komarek, and Liu Hao Tjeng — Max Planck Institute for Chemical Physics of Solids, Dresden

Magnetite Fe_3O_4 is one of the most investigated materials from the class of correlated transition metal oxides. It shows a first-order anomaly in the temperature dependence of the electrical conductivity at $T_V = 125$ 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. Having found the optimum conditions for the growth of fully stoichiometric Fe_3O_4 thin films, we vary the substrate and study the influence of the microstructure on the Verwey transition. We are now able to obtain Fe_3O_4 thin films with T_V higher than the bulk value.

TT 86.12 Thu 12:30 BEY 81

Hund's and lattice coupling as origin of the insulating state in $BaCrO_3$ — •Markus Aichhorn[1], Gianluca Giovannetti[2], and Massimo Capone[2] — [1]Institute of Theoretical and Computational Physics, TU Graz, Austria — [2]SISSA, Trieste, Italy

Strong correlations play an important role for the physical properties in many oxide materials. Since most of these materials are multi-band systems, the Hunds rule coupling turns out to be a key player for the occurence of sizeable electron correlations. Recently, insulating behavior has been found in layered $BaCrO_3$, which cannot be explained by density-functional theory calculations. Here, we will show that Hund's coupling, orbital, and lattice degrees of freedom cooperate in turning this system with 2 electrons in 3 bands to an insulator. The orbital degrees of freedom are also strongly coupled to spins leading to a magnetic transition with large magnetic moments. We argue that the so-called Hund's correlated metals are very unstable towards perturbations such as Jahn-Teller distortions and orbital ordering.

TT 87: Focus Session: Unconventional Spin Structures (organized by MA)

Organizer: J. Fassbender (HZDR)

Time: Thursday 9:30–12:45 Location: BEY 118

Topical Talk TT 87.1 Thu 9:30 BEY 118

Topological Effects in Nanomagnetism - From Perpendicular Recording to Monopoles — •Hans-Benjamin Braun — University College Dublin

Similar to knots in a rope, the magnetization in a material can form particularly robust configurations. Such topologically stable structures include domain walls, vortices and skyrmions which are not just attractive candidates for future data storage applications but are also of fundamental importance to current memory technology. For example, the creation of soliton pairs of opposite chirality delimits the thermal stability of bits in current high anisotropy perpendicular recording media. After an introduction into various types of topological defects and their implications for current data storage it will be discussed how vortices can be robustly implemented in a system of nanoislands, a system that is in principle scaleable to the smallest length scales. It will then be shown how magnetic monopoles emerge as topological defects in densely packed arrays of nanoislands, a system also known as artificial spin ice. In contrast to conventional thin films, where magnetization reversal occurs via nucleation and extensive domain growth, magnetization reversal in 2D artificial spin ice is restricted to an avalanche-type formation of 1D strings. These objects can be viewed as classical versions of Dirac strings that feed magnetic flux into the emergent magnetic monopoles. It is demonstrated how the motion of these magnetic charges can be individually controlled experimentally and used to perform simple logic operations.

Topical Talk TT 87.2 Thu 10:00 BEY 118

Topology and Origin of Effective Spin Meron Pairs in Ferromagnetic Multilayer Elements — •Sebastian Wintz — Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Topological spin textures, such as vortices or skyrmions, are attracting significant attention because of their intriguing fundamental properties as well as their promising applicability in memory devices or spin torque oscillators. A particular topological texture that was theoretically predicted is the two-dimensional hedgehog state, also known as a 'Spin Meron'. It had been unclear, however, whether this kind of highly divergent magnetization structure can exist in real continuum systems. Only recently, evidence for the occurrence of meron-like states was reported for trilayer elements consisting of two ferromagnetic layers and a non-ferromagnetic interlayer [1]. On this background we now present a direct proof for the existence of meron-like states in trilayer elements via direct magnetic imaging. We also show that in the presence of biquadratic interlayer exchange coupling, such meron-like pair states may even represent the magnetic ground state of the system. Interestingly, the highly divergent magnetization distribution induces an additional, three-dimensional torus vortex that in-turn causes a symmetry break for the allowed topological pair configurations. [1] C. Phatak et al., Phys. Rev. Lett. 108, 067205 (2012). [2] S. Wintz et al., Phys. Rev. Lett. 110, 177201 (2013).

Topical Talk TT 87.3 Thu 10:30 BEY 118

Symmetry breaking in the formation of magnetic vortex states in a permalloy nanodisk — •Peter Fischer[1], Mi-Young Im[1], Keisuke Yamada[2], Tomonori Sato[3], Shinya Kasai[4], Yoshinobu Nakatani[3], and Teruo Ono[2] — [1]CXRO, LBNL, Berkeley CA USA — [2]Inst. f.Chem. Res., Kyoto University Japan — [3]U of Electro-Comm., Chofu, Japan — [4]Spintronics Group, Magn. Mat Center, NIMS, Tsukuba, Japan

Mesoscale phenomena will transform nanomagnetism research to the next level [1], as they add complexity and functionality, which are essential to meet future challenges of spin driven devices.

A priori, one would assume that the formation of magnetic vortex states should exhibit a perfect symmetry, because the magnetic vortex has four degenerate states. We report on the direct observation of an asymmetric phenomenon in the formation process of vortex states in a permalloy nanodisk by magnetic full field transmission soft x-ray microscopy [2]. Micromagnetic simulations confirm that an intrinsic Dzyaloshinskii*Moriya interaction is decisive for the asymmetric formation of vortex states.

Supported by the U.S. Department of Energy (# DE-AC02-05-CH11231) and by the Leading Foreign Research Institute Recruitment Program (# 2012K1A4A3053565) through the NRF of Korea funded by the Ministry of Education, Science and Technology.

[1] R. Service, Science 335 1167 (2012) [2] M.-Y. Im, P. Fischer, Y. Keisuke, T. Sato, S. Kasai, Y. Nakatani, T. Ono, Nature Communications 3 983 (2012)

15 min. break

Topical Talk TT 87.4 Thu 11:15 BEY 118

Commensurability and chaos in magnetic vortex oscillations — •Joo-Von Kim[1], Sébastien Petit-Watelot[1], Antonio Ruotolo[2,3], Rubén Otxoa[1], Karim Bouzehouane[2], Julie Grollier[2], Arne Vansteenkiste[4], Ben Van de Wiele[5], Vincent Cros[2], and Thibaut Devolder[1] — [1]Institut d'Electronique Fondamentale, UMR CNRS 8622, Univ. Paris-Sud, 91405 Orsay, France — [2]Unité Mixte de Physique CNRS/Thales and Univ. Paris-Sud, 1 av. A. Fresnel, 91767 Palaiseau, France — [3]Department of Physics and Materials Science, City University of Hong Kong, Kowloon, Hong Kong — [4]Department of Solid State Sciences, Ghent University, Krijgslaan 281-S1, B-9000 Ghent, Belgium — [5]Department of Electrical Energy, Systems and Automation, Ghent University, Sint-Pietersnieuwstraat 41, B-9000 Ghent, Belgium

In spin-torque driven vortex oscillations in small nanocontacts, periodic reversal of the vortex core appear above a critical current and results in a self-modulation phenomenon involving gyration and relaxation oscillations. By tuning the ratio between the gyration frequency and the rate of core reversal, we show that commensurate phase-locked and incommensurate chaotic states are possible, resulting in Devil's staircases with driving currents. This represents a novel dynamical regime for vortex dynamics in which the gyrotropic dynamics is self-modulated by the periodic core reversal.

Topical Talk TT 87.5 Thu 11:45 BEY 118

Dynamic ordering of vortex cores in interacting mesomagnets — •Valentyn Novosad — Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

Manipulation of the magnetization is a key problem in applied magnetism. In this talk a novel method of controlling the ground state using two interacting vortices as a model system will be presented. A spin vortex consists of an in-plane and out-of-plane (core) regions of magnetization. Control of an in-plane magnetization has been demonstrated previously, whereas manipulation of the vortex cores remain challenging. In our work this is achieved by driving the system from the linear regime of constant vortex gyrations to the non-linear regime of vortex-core reversals at a fixed excitation frequency of one of the coupled modes. Subsequently reducing the excitation field to the linear regime, stabilizes the system to a polarity combination whose resonant frequency is decoupled from the initialization frequency [2]. The transition of the state from one polarity combination to the other is clearly evident from the contrast in the microwave absorption amplitude obtained by gradually increasing the rf-field to higher magnitudes at the resonant frequency of one of the modes and subsequently decreasing it. The results of this work may benefit future advancement of dynamically controlled spintronic devices, such as magnonic crystals, spin-torque oscillators, and magnetic memories.

[1] S. Jain, et al., Applied Physics Letters, 102, 052401 (2013).
[2] S. Jain et al., Nature Comm., DOI: 10.1038/ncomms2331 (2012).

Topical Talk TT 87.6 Thu 12:15 BEY 118

Magnetic Vortex Core Reversal by Excitation of Spin Waves — •Hermann Stoll[1], Matthias Kammerer[1], Matthias Noske[1], Markus Sproll[1], Georg Dieterle[1], Ajay Gangwar[1,2], Markus Weigand[1], Manfred Fähnle[1], Georg Woltersdorf[2], Christian H. Back[2], and Gisela Schütz[1] — [1]MPI for Intelligent Systems, Stuttgart, Germany — [2]University of Regensburg, Germany

Essential progress in the understanding of nonlinear magnetic vortex dynamics was achieved when low-field vortex core reversal by (sub-GHz) excitation of the vortex gyromode was observed using time-resolved scanning transmission X-ray microscopy [1]. This switching

scheme, based on the creation and subsequent annihilation of a vortex-antivortex pair [1,2], has been proved to be universal and independent of the type of excitation, e.g., pulsed magnetic fields or spin transfer torque (STT).

Magnetic vortex structures possess azimuthal spin wave modes showing eigenfrequencies in the multi-GHz range. We could demonstrate [3-5] by experiments and micromagnetic simulations that even much faster unidirectional vortex core reversal can be achieved by exciting these spin wave modes with (multi-GHz) rotating magnetic fields. In that way we have been able to switch vortex cores selectively within less than 100 ps.

[1] B. Van Waeyenberge et al., Nature 444, 462 (2006) [2] A. Vansteenkiste et al., Nature Physics 5, 332 (2009) [3] M. Kammerer et al., Nature Communications 2, 279 (2011) [4] M. Kammerer et al., PRB 86, 134426 (2012) [5] M. Kammerer et al., APL 102, 012404 (2013)

TT 88: Invited Talk - Tobias Korn (organized by HL)

Time: Thursday 9:30–10:00 Location: POT 081

Invited Talk TT 88.1 Thu 9:30 POT 081

Time-resolved optical spectroscopy of 2D dichalcogenides — •Tobias Korn, Gerd Plechinger, Philipp Nagler, and Christian Schüller — Institut für Experimentelle und Angewandte Physik, Universität Regensburg

Recently, atomically thin layers of transition-metal dichalcogenides, such as MoS_2 and WS_2, have attracted a lot of attention. Like graphene, they can be prepared from bulk crystals by mechanical exfoliation. Unlike graphene, these materials are semiconductors with large bandgaps, and a transition from indirect to direct gap occurs for single layers. Spin and valley degrees of freedom in these structures are coupled, and can be directly addressed via optical excitation. We will demonstrate preparation and optical characterization of single-layer dichalcogenides, heterostructures built from different two-dimensional crystals, and large-area MoS_2 films. Deposition of single-layer MoS_2 on viscoelastic substrates allows us to apply local biaxial strain and subsequently vary the bandgap. We observe large valley polarization effects in our structures in photoluminescence experiments under near-resonant excitation. Photocarrier dynamics are investigated using time-resolved photoluminescence and picosecond pump-probe spectroscopy techniques.

TT 89: Graphene-Like Materials: Silicene, MoS_2 and Relatives (organized by HL)

Time: Thursday 10:00–12:30 Location: POT 081

TT 89.1 Thu 10:00 POT 081

Many-body effects in 2D hexagonal semimetals and semiconductors — •Tineke Stroucken, Johanna Grönqvist, and Stephan W. Koch — Department of Physics and Material Sciences Center, Philipps University Marburg, Renthof 5, D-35032 Marburg, Germany

Recently, a variety of graphene-analogues materials like h-BN, silicene or transition-metal dichalcogenides have been fabricated. Similar to graphene, these novel material systems display exciting new physical properties, distinct from their bulk counterparts.

Owing to the symmetry of the hexagonal lattice, band edge carriers are described by massive Dirac Fermions. Typically, the Fermi-velocity is in the range of $c/300$ or below. This yields effective fine structure constants $\alpha = e^2/\epsilon\hbar v_F \gtrsim 2/\epsilon$, implying prominent Coulomb interaction and relativistic effects. Particularly, $\alpha \gtrsim 1$ indicates an excitonic instability of the noninteracting ground state.

In this presentation, we discuss conditions for strong Coulomb coupling in 2D hexagonal crystals and identify experimentally observable signatures signaling an excitonic ground state. To this end, the gap equations are solved self consistently with the polarization function, which depends on the interacting band structure.

[1] T. Stroucken *et al.*, Phys. Rev. B 84, 205445 (2011)
[2] J. H. Grönqvist *et al.*, EPJ B 85, 12 (2012)
[3] T. Stroucken *et al.*, Phys. Rev. B. 87, 245428(2013)
[4] T. Stroucken *et al.*, Appl. Phys. Lett. 103, 163103 (2013)

TT 89.2 Thu 10:15 POT 081

Single and Multi-Layer Silicene: Growth, Properties and Perspectives — •Patrick Vogt[1], Thomas Bruhn[1], Andrea Resta[2], Paola De Padova[3], and Guy Le Lay[2] — [1]Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Aix-Marseille University, CNRS- PIIM UMR 7345, F-13397 Marseille Cedex 20, France — [3]Instituto di Struttura della Materia, Consiglio Nazionale delle Ricerche -ISM, via Fosso del Cavaliere, 00133 Roma, Italy

Silicene, a new silicon allotrope with a graphene-like honeycomb structure, has recently attracted considerable interest, because its topology confers to it the same remarkable electronic properties as those of graphene, with the potential advantage of being easily integrated in current Si-based nano/micro-electronics offering novel technological applications.

We will discuss the epitaxial formation of single layer silicene on Ag substrates and its structural and electronic properties [1-2]. Based on these results we will look at the growth of silicene multi-layers which can be explained by stacking of single silicene sheets [3-4]. Different experimental techniques are used to investigate atomic structure and electronic properties of this layered system and to discuss its similarities to graphite.

1) Vogt, P. et al., Phys. Rev. Lett. 108, 155501 (2012).
2) Avila, J. et al., J. Phys.: Condens. Matter 25, 262001 (2013).
3) De Padova, P.; Vogt, et al. Appl. Phys. Lett. 102, 163106 (2013).
4) Resta, A. et al., Sci. Rep. 3, 2399 (2013).

TT 89.3 Thu 10:30 POT 081

Optical and vibrational properties of MoS2 — •Ludger Wirtz[1], Alejandro Molina-Sanchez[1], and Kerstin Hummer[2] — [1]Physics and Materials Science Research Unit, University of Luxembourg — [2]Faculty of Physics, University of Vienna, Austria

Monolayer MoS2 is currently receiving a lot of attention as a potential alternative to graphene. Its band gap of about 2eV (depending on the dielectric environment) makes it a suitable candidate for thin-film electronics. The optical and vibrational properties of mono-layer, few-layer, and bulk are seemingly straightforward to calculate. Nevertheless some surprises occur: the phonon dispersion displays an anomalous Davydov splitting and the optical absorption spectra display a rich structure of excitonic peaks in the band-gap and in the continuum of interband transitions. We give a short review of the state-of-the art and discuss recent advances in the understanding of the influence of the substrate on the vibrations and electronic excitations.

TT 89.4 Thu 10:45 POT 081

Carrier- and valley dynamics of singlelayer MoS_2 — •Gerd Plechinger[1], John Mann[2], Christian Schüller[1], Ludwig Bartels[2], and Tobias Korn[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Chemistry, Physics, and Materials Science and Engineering, University of California, CA 92521 Riverside, USA

Consisting of an only 0.7 nm thin S-Mo-S sheet and offering a direct bandgap at the K-points in the Brillouin zone, singlelayer MoS_2 represents a promising semiconductor material for flexible and transparent optoelectronic applications. By means of chemical vapor deposition (CVD), large-area films (several mm^2) of singlelayer MoS_2 can be produced. These were characterised by photoluminescence and Raman spectroscopy. In order to investigate the carrier dynamics, we performed pump-probe measurements in the spectral range of the optical transitions in singelayer MoS_2. Helicity-resolved PL measurements have demonstrated an efficient valley polarisation of the K^+ or K^- valley at near-resonant excitation. We probe these valley dynamics with Kerr spectroscopy and find a biexponential decay of the valley

polarisation with decay times of a few tens of ps and a few hundreds of ps at low temperatures.

Coffee break (15 min.)

TT 89.5 Thu 11:15 POT 081

Photocurrent studies on semiconducting MoS2 — Marina Hoheneder, •Eric Parzinger, Alexander Holleitner, and Ursula Wurstbauer — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching

The current interest in transition metal dichalcogenides is stimulated by their peculiar electrical and optoelectrical properties and their potential for novel device applications. We investigate the semiconductor MoS2, which shows a crossover from an indirect to a direct bandgap semiconductor by thinning it down to a monolayer. We prepare MoS2 samples through micromechanical exfoliation and characterize the thin flakes with Raman spectroscopy. We further study photocurrent generation of single and few layer MoS2 in dependence of wavelength and power of the exciting light. We gratefully acknowledge financial support by BaCaTec.

TT 89.6 Thu 11:30 POT 081

Resonant Inelastic Light Scattering on MoS_2 — •Bastian Miller, Eric Parzinger, Alexander Holleitner, and Ursula Wurstbauer — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching (Germany)

Two-dimensional layered 'van-der Waals' materials are of increasing interest for fundamental research due to their peculiar band-structure.

We utilize inelastic light scattering - a contactless and extremely versatile tool - to study phonon excitation spectra of mono- and fewlayer MoS_2. The phonon modes are unique fingerprints of the material properties and are sensitive to defects, strain, doping and the number of MoS_2 -layers.

We observe signatures of multistep scattering processes involving phonon-phonon, electron-phonon as well as electronic excitations under resonant conditions, where the incoming or outgoing light meets the energy of a fundamental optical transition of the system.

TT 89.7 Thu 11:45 POT 081

The effect of substrate and environment on the elementary excitations of MoS_2 — •Eric Parzinger[1], Marina Hoheneder[1], Bastian Miller[1], Anna Cattani-Scholz[1], Alexander Holleitner[1], Joel W. Ager[2], and Ursula Wurstbauer[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching (Germany) — [2]Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, California 94702 (United States)

The novel two-dimensional layered 'van-der Waals' material Molybdenum disulfide (MoS_2) is investigated using inelastic and resonant light scattering - a contactless and extremely versatile tool - to study phonon and electronic excitations. In particular, we focus on the influence of different supporting materials (SiO_2, sapphire and SAMs of organic molecules) as well as various environmental conditions (ambient, vacuum and water) on the low energy excitations of MoS_2. We find that both, different substrate and environment give rise to a significant modification of the most prominent Raman modes, whereas a monolayer is most effected by the environmental conditions. We gratefully acknowledge financial support by BaCaTec.

TT 89.8 Thu 12:00 POT 081

Spin-orbit coupling, quantum dots, and qubits in transition metal dichalcogenides — •Andor Kormanyos[1], Viktor Zolyomi[2], Neil Drummond[2], and Guido Burkard[1] — [1]Universität Konstanz — [2]Lancaster University

We derive an effective Hamiltonian describing the dynamics of electrons in the conduction band of transition metal dichalcogenides (TMDC) in the presence of perpendicular electric and magnetic fields. We discuss both the intrinsic and Bychkov-Rashba spin-orbit coupling (SOC) induced by an external electric field. We identify a new term in the Hamiltonian of the Bychkov-Rashba SOC which does not exist in III-V semiconductors. We point out important differences in the spin-split conduction band between different TMDC compounds. A significant consequence of the strong intrinsic SOC is an effective out-of-plane g-factor for the electrons which differs from the free-electron g-factor $g \simeq 2$. Using first-principles calculations, we give estimates of the various parameters appearing in the theory. Finally, we consider quantum dots (QDs) formed in TMDC materials and derive an effective Hamiltonian allowing us to calculate the magnetic field dependence of the bound states in the QDs. We find that all states are both valley and spin split, which suggests that these QDs could be used as valley-spin filters. We explore the possibility of using spin and valley states in TMDCs as quantum bits, and conclude that, due to the relatively strong intrinsic SOC in the conduction band, the most realistic option appears to be a combined spin-valley (Kramers) qubit at low B fields.

TT 89.9 Thu 12:15 POT 081

Analytical approach to excitonic properties of MoS2 — •Gunnar Berghäuser and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We present an analytical investigation of the optical absorption spectrum of monolayer molybdenum disulfide (MoS2). Based on the density matrix formalism [1], our approach gives insights into the microscopic origin of excitonic transitions, their relative oscillator strength, and binding energy [2]. We show analytical expressions for the carrier-light coupling element, which contains the optical selection rules and well describes the valley- selective polarization in MoS2 . In agreement with experimental results, we find the formation of strongly bound electron-hole pairs due to the efficient Coulomb interaction. The absorption spectrum of MoS2 on a silicon substrate features two pronounced peaks at 1.91 eV and 2.05 eV corresponding to the A and B exciton, which are characterized by binding energies of 420 meV and 440 meV, respectively. Our calculations reveal their relative oscillator strength and predict the appearance of further low-intensity excitonic transitions at higher energies. The presented approach is applicable to other transition metal dichalcogenides and can be extended to investigations of trion and biexcitonic effects.

[1] E. Malic and A. Knorr, Graphene and Carbon Nanotubes: Ultrafast Optics and Relaxation Dynamics, 1st ed. (Wiley-VCH, Berlin, 2013).

[2] Gunnar Berghäuser and Ermin Malic, arXiv:1311.1045 (2013)

TT 90: Spintronics II (organized by HL)

Time: Thursday 10:00–12:15 Location: POT 151

TT 90.1 Thu 10:00 POT 151

Magnetotransport in nanostructured InAs-based Heterostructures — •Olivio Chiatti[1], Sven S. Buchholz[1], Wolfgang Hansen[2], Mehdi Pakmehr[3], Bruce D. McCombe[3], and Saskia F. Fischer[1] — [1]Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, D-10099 Berlin — [2]FG Wachstum, Institut für Angewandte Physik, Universität Hamburg, D-20148 Hamburg — [3]Dept. of Physics, University at Buffalo, the State University of New York, Buffalo, NY 14260-1500 USA

The control of spin-polarized currents entirely by electrical fields is of great interest in the field of spintronics. The spin-orbit coupling in narrow-gap semiconductors has been identified as a possible tool to this end, because it couples the momentum of an electron to its spin. Nanostructures can be used to filter specific momentum modes and offer the possibility to create and detect spin-polarized currents. [1] Quantum point contacts (QPCs) in nominally symmetric InAs quantum well structures have been reported to generate spin-polarized currents, when asymmetric gate voltages are applied. [2]

We have fabricated Hall-bars and QPCs with in-plane gates in InAs quantum well structures, and performed transport measurements at low temperatures and in high magnetic fields. We investigate the effects of symmetric and asymmetric gate voltages. Here, we present the results of our measurements and discuss their implications for investigations of the spin-orbit coupling in InAs.

[1] Silsbee, *J. Phys.: Condens. Matter* **16**, R179 (2004)
[2] Debray *et al.*, *Nature Nanotech.* **4**, 759 (2009)

TT 90.2 Thu 10:15 POT 151

Acoustic charge and spin transport in GaAs (111)B quantum wells — •Alberto Hernández-Mínguez, Klaus Biermann, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The special properties of electron spin dynamics in GaAs (111) quantum wells (QWs) have been subject of study during the last years. Recently, it has been experimentally shown that, to first order in the electron wavevector, the in-plane component of the spin-orbit interaction can be suppressed simultaneously for all electrons in the QW just by applying an electric field of a certain amplitude perpendicularly to the QW plane. As a consequence, by tuning the amplitude of the electric field, the spin polarization lifetime of an electron ensemble is varied from a few hundred picoseconds to tens of nanoseconds.

In addition, surface acoustic waves (SAWs) have proved to be an useful tool for the controlled transport and manipulation of electron spins in GaAs QWs: the piezoelectric field accompanying the SAW allows the spatial confinement of electrons and their transport, with the well defined SAW velocity, over distances of several tens of micrometers. In this contribution, we explore the generation of SAWs in GaAs (111) QWs, as well as their combination with vertical electric fields for the acoustic transport of long living electron spins. In this way, we observe acoustic charge transport along 40μm distance, and spin transport around 15 μm.

TT 90.3 Thu 10:30 POT 151

Indirect Excitons Spin manipulation in GaAs/$Al_xGa_{1-x}As$ double quantum wells — •Adriano Violante[1], Snežana Lazić[2], Klaus Biermann[1], Rudolph Hey[1], Paulo Santos[1], Kobi Kohen[3], and Ronen Rapaport[3] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Departamento de Física de Materiales, Universidad Autónoma de Madrid, Madrid, Spain — [3]Racah Institute of Physics, Hebrew University of Jerusalem, Jerusalem, Israel

A spatially indirect exciton (IX) is a bound state of an electron and a hole localized in different quantum wells (QWs) of a double quantum well structure (DQW). In an IX, the spatial separation of electrons and holes reduces the exchange interaction, thus significantly enhancing the spin lifetime with respect to the direct QW excitons. [1] In this contribution, we show that spin-polarized IXs created using a circularly polarized laser beam diffuse up to distances 15 μm away from the generation point, revealing spatial oscillations of the polarization degree ρ_z. The latter are attributed to the precession of the spin vector in the spin-orbit effective magnetic field B_{SO} as they move away from the excitation spot, which can be modulated both with electric and magnetic fields. The IXs spin transport using acoustic fields is also discussed.

[1] J. R. Leonard, Y. Y. Kuznetsova, S. Yang, L. V. Butov, T. Ostatnick, A. Kavokin, and A. C. Gossard. Nano Lett. 9, 4204-4208 (2009)

TT 90.4 Thu 10:45 POT 151

Time- and space-resolved measurements of spin diffusion in high-mobility GaAs-based 2D electron systems — •Markus Schwemmer[1], Roland Voelkl[1], Tobias Korn[1], Sergey Tarasenko[2], Dieter Schuh[1], Werner Wegscheider[3], and Christian Schüller[1] — [1]Institute of Experimental and Applied Physics, Faculty of Physics,University of Regensburg, Germany — [2]A. F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia — [3]ETH Zurich, Switzerland

Two-dimensional electron systems embedded in (110)-grown, symmetrically doped GaAs/AlGaAs QWs are highly interesting for spintronics. They combine high carrier mobility with long spin dephasing times. Previously, we have studied these systems in different experiments, which either gave temporal or spatial resolution. By using a two-beam Hanle-MOKE method we could observe diffusion lengths of more than 125 μm at low temperatures. As a next step, the experimental setup was modified in order to achieve temporal and spatial resolution with the help of a single pulsed TiSa laser. The main issue is the spectral separation of the pump and the probe beams, which are collinearly focused onto the sample. Due to the broad spectrum of the femtosecond laser pulse, this can be realized using bandpass filters. Besides the mapping of the temporal propagation of the spins via diffusion, this experimental setup should also allow to visualize the evolution of a drifting spin packet. Financial support by the DFG via SFB 689 and SPP 1285 is gratefully acknowledged.

TT 90.5 Thu 11:00 POT 151

Direct measurement of the spin splitting in GaAs quantum wells — •Christoph Schönhuber[1], Matthias Walser[2], Christian Reichl[3], Werner Wegscheider[3], Gian Salis[2], Tobias Korn[1], and Christian Schüller[1] — [1]Universität Regensburg, 93040 Regensburg, Germany — [2]IBM Research-Zurich, 8803 Rüschlikon, Switzerland — [3]ETH Zurich, 8093 Zurich, Switzerland

We investigate the spin splitting in the conduction band of GaAs quantum wells employing Raman scattering experiments. The investigated system consists of a 12-nm-wide (001)-oriented GaAs/AlGaAs QW, which is asymmetrically Si modulation doped to reach a balanced Rashba and Dresselhaus SOI contribution.

The performed measurements on intrasubband transitions reveal a double peak structure for the [11] direction, while in [1-1] direction there is only a single peak. This anisotropic behavior in the spin splitting is probed for a wide range of transfered wavevectors and in good agreement with the prediction for a system with comparable magnitudes of Rashba and Dresselhaus SOI.

TT 90.6 Thu 11:15 POT 151

Hole g-factor anisotropy in coupled GaAs/AlAs quantum wells — •Christian Gradl, Michael Kempf, Dieter Schuh, Dominique Bougeard, Christian Schüller, and Tobias Korn — Universität Regensburg, D-93040 Regensburg, Germany

We performed time-resolved Kerr rotation measurements on undoped [110]- and [113]-grown double quantum well (QW) structures to resolve the spin dynamics of hole ensembles at low temperatures. For these growth directions, a strong anisotropy of the hole g-factor with respect to the in-plane magnetic field direction is theoretically predicted.

Our gated system consists of two QWs with different well widths, which we use for the spatial separation of the optically excited electron-hole pairs. Thus, we are able to create hole ensembles with spin lifetimes of several hundreds of picoseconds in the broader QW without any doping. This also allowed an observation of a strong hole g-factor anisotropy by varying the magnetic field direction in the QW plane. Moreover, our extracted values are in a very good agreement with theoretical predictions.

TT 90.7 Thu 11:30 POT 151

Polarization oscillations in spin-polarized vertical-cavity

surface-emitting lasers controlled by multiple excitation pulses — •Henning Höpfner, Markus Lindemann, Nils C. Gerhardt, and Martin R. Hofmann — Photonics and Terahertz Technology, Ruhr-University Bochum, D-44780 Bochum, Germany

Spin-polarized lasers offer many potential advantages over their conventional counterparts, including threshold reduction, polarization control and ultrafast dynamics for increased modulation bandwidth [1].

Upon excitation with circularly polarized light that creates spin-polarized carrier in a vertical-cavity surface-emitting laser (VCSEL), the VCSEL shows oscillations of the circular polarization degree. These polarization oscillations can be much faster than the relaxation oscillations of the carrier-photon system. From calculations based on a rate-equation model we show that these oscillations can be switched on and off in a controlled manner using multiple circularly polarized optical excitation pulses. The results are verified experimentally, showing spin-induced polarization oscillation in conventional, electrically biased VCSELs subject to optical spin injection. We show polarization oscillation bursts with possible modulation frequencies far beyond the device's electrical modulation bandwidth.

[1] Gerhardt et al., Applied Physics Letters 99 (15), 151107 (2011)

TT 90.8 Thu 11:45 POT 151

Spin polarization of electron states in GaAs quantum wells — •Pavel Streda — Institute of Physics ASCR, Praha, Czech Republic

The standard method to establish the spin orientation of electron states, for zinc-blende semiconductors like GaAs, is based on the effective medium approach represented by the Luttinger Hamiltonian. For a two-dimensional electron gas, confined within a potential well, the real eigenfunctions of bound states across the well has been approximated by an envelope function. It leads to the conclusion that along main crystallographic axis, $[1,0,0]$ and $[0,1,0]$, the spin orientation is parallel or antiparallel with velocity directions. This contradicts to the tendency of the spin to be perpendicular to the velocity direction, observed in bulk structures.

The question arises if an envelope function approach, which suppresses the effect of local environment, is not too crude approach for real quantum wells, which are usually wider than ten lattice constants. To answer this question the empirical pseudopotential method has been used to establish energy dispersions and spin expectation values for two-dimensional electron gas confined within quantum wells of the different width. In all cases the tendency of the spin to be perpendicular to the velocity direction has been observed. For wide enough wells the obtained spin structure approaches that given by the bulk GaAs crystal with $k_z = 0$.

TT 90.9 Thu 12:00 POT 151

Spin injection efficiency dependence on MgO tunnel barrier thickness — •Lennart-Knud Liefeith, Tomotsugu Ishikura, Zhixin Cui, and Kanji Yoh — Research Center for Integrated Quantum Electronics, Japan

We study non-local spin valves in inverted InAlAs/InGaAs high-electron mobility transistors on InP(001). On the ferromagnet (FM) side, permalloy electrodes are employed. On the semiconductor (SC) side the electron system resides in a two-dimensional InAs channel. It has been argued that direct FM/SC contacts provide negligible spin polarization in the SC if the transport is diffusive, known as the conductivity mismatch problem[1]. In the ballistic transport regime efficient spin injection is predicted[2]. For devices basing on ballistic transport, a low contact resistance between FM and SC is essential. An strategy to tackle the conductivity mismatch problem is the insertion of a tunnel barrier at the FM/SC interface. We thus study ballistic structures with MgO tunnel barriers of varied thickness. Here we will compare spin injection efficiencies in non-local spin valve structures with either no or a 2 nm-thick MgO tunnel barrier at the FM/SC interface.

[1] G. Schmidt, „Fundamental obstacle for electrical spin injection from a ferromagnetic metal into a diffusive semiconductor“, Physical Review B 62, R4790 (2000)

[2] M. Zwierzycki, „Spin-injection through an Fe/InAs interface“, Physica Status Solidi A: Applications and Materials Science 1, 25-28 (2003)

TT 91: Focus Session: Frontiers of Electronic Structure Theory - Non-Equilibrium Phenomena at the Nano-Scale VI (organized by O)

Time: Thursday 10:30–13:15 Location: TRE Ma

Topical Talk TT 91.1 Thu 10:30 TRE Ma

Localization at the edge of 2D topological insulator by Kondo impurities — •Boris Altshuler[1], Igor Aleiner[1], and Vladimir Yudson[2] — [1]Physics Department, Columbia University, New York, NY 10027, USA — [2]Institute for Spectroscopy, Russian Academy of Sciences,Troitsk, Moscow 142190, Russia

Recent interest to the topological insulators [1] is inspired by the fact that their boundaries host gapless electronic excitations, which are extended and make the system conductive even in the presence of a potential disorder. 1D edge of a 2D topological insulator is predicted to have perfect conductance (2e2/h): right and left moving electrons carry opposite spins and potential disorder cannot flip spins and thus causes neither back-scattering nor the usual 1D localization.

What if there are localized spins coupled to the edge electrons? It turns out that the conductivity is still perfect provided that this coupling conserves the z-projection of the total spin of the impurities and electrons. Magnetic anisotropy violates this conservation and causes the backscattering even at T=0, i.e. an arbitrary small density of the spins with arbitrary weak anisotropy of the coupling leads to Anderson localization of the edge states in long enough samples [3]. The conclusion follows from the mapping of the electron-spin coupling to the well-studied problem [2] of disordered Luttinger liquid.

1. M.Z. Hasan and C.L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
2. T.Giamarchi and H.J.Schulz, Phys. Rev. B 37, 325 (1988).
3. B.L.Altshuler, I.L.Aleiner, V.I. Yudson Phys. Rev. Lett 111, 086401 (2013)

TT 91.2 Thu 11:00 TRE Ma

Multiple Exciton Generation in Si and Ge Nanoparticles with high pressure core structures — •Stefan Wippermann[1], Marton Vörös[2], Dario Rocca[3], Adam Gali[4], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Universite de Lorraine, Nancy — [4]Budapest University of Technology and Economics

Multiple exciton generation (MEG) in semiconductor nanoparticles (NPs) is a promising path towards surpassing the Shockley-Queisser limit in solar energy conversion efficiency. Recent studies demonstrate MEG to be more efficient in NPs than in the bulk, including Si. However, the increased efficiency is observed only on a relative energy scale in units of the gap: quantum confinement (QC) effects believed to be responsible for efficient MEG in NPs, also increase their optical gap, swiftly shifting the MEG threshold beyond the solar spectrum.

We present density functional and many body perturbation theory calculations of the electronic, optical, and impact ionization properties of Si and Ge nanoparticles (NPs) with core structures based on high-pressure bulk Si and Ge phases. Si and Ge particles with a BC8 or ST12 core structure exhibit significantly lower optical gaps and multiple exciton generation (MEG) thresholds, and an order of magnitude higher MEG rate than diamondlike ones of the same size (1).

(1) S. Wippermann et al., Phys. Rev. Lett. 110, 046804 (2013)

TT 91.3 Thu 11:15 TRE Ma

Advanced time-evolution method for optical absorption spectra calculations — •Tobias Sander and Georg Kresse — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The Green's function formalism from many-body perturbation theory gives access to electronic structure calculation within the quasiparticle picture, as well as provides for calculating optical absorption spectra. Within the traditional ansatz [1], a Bethe-Salpeter like equation for the polarizability is solved. This requires to diagonalize an in general non-hermitian and complex matrix (BSE matrix). Usually, the off-diagonal elements of the BSE matrix are neglected and this is referred to as Tamm-Dancoff approximation. The computational effort can be

reduced by using the time-evolution ansatz [2] which avoids the matrix diagonalization. We present a method based on the time-evolution algorithm, that finally avoids storing and diagonalizing the BSE matrix. This leads to a reduction of the scaling w.r.t the system size N from N^5 to N^3. Finally, we present first results for typical systems.

[1] S. Albrecht, L. Reining, R. Del Sole, G. Onida, PRL 80, 4510 (1998)
[2] W. G. Schmidt, S. Glutsch, P. H. Hahn, F. Bechstedt, PRB 67, 085307 (2003)

TT 91.4 Thu 11:30 TRE Ma

New starting point for the calculation of optical properties — •Igor Reshetnyak[1,2] and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF)

The Bethe-Salpeter Equation based on Hedin's GW approximation to the self-energy is a powerful approach for describing electron-hole interactions in optical properties and photo-absorption spectra. However, in its current formulation it is both computationally heavy and displays cancellation effects not accounted for analytically. We discuss the sources of these cancellations and the possibility of putting them forward explicitly. We furthermore assess alternative formulations and sets of approximations to the BSE. For each of them we examine its behavior on model systems as well as their computational applicability. Finally we suggest possible directions for further investigations.

TT 91.5 Thu 11:45 TRE Ma

Electron-Energy Loss and Inelastic X-ray Scattering of CuO from First Principles — •Claudia Rödl, Francesco Sottile, Matteo Gatti, and Lucia Reining — Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France and European Theoretical Spectroscopy Facility (ETSF)

Even though the strongly correlated transition-metal oxide CuO has many fields of application (potential absorber material in photovoltaic devices, pigment in glass and ceramics, building block of cuprate superconductors,...), surprisingly little is known about its electronic excitations from a theoretical point of view. The band gap and all electronic excitations in its vicinity are governed by the intricate interplay between itinerant O $2p$ and localized Cu $3d$ electrons. Complex many-body effects, that are still not well understood nowadays, determine the screening of the electron-electron interaction.

Electron-energy loss and inelastic x-ray scattering experiments yield direct access to the wave-vector- and frequency-dependent loss function $-\operatorname{Im}\varepsilon^{-1}_{\mathbf{GG'}}(\mathbf{q},\omega)$, and, hence, to the screened Coulomb interaction W. We use time-dependent density-functional theory (TDDFT) to calculate the loss spectrum of CuO and discuss the occurring d-d and plasmon excitations. This allows us, by comparing theory and experiment, to assess the quality of the screened Coulomb interaction which is a key quantity for many-body approaches, for instance, *GW* and Bethe-Salpeter calculations.

TT 91.6 Thu 12:00 TRE Ma

Optical Spectra from Molecules to Solids: Insight from Many-Body Perturbation Theory — •Caterina Cocchi and Claudia Draxl — Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

The spurious long-range behavior of time-dependent (TD) density functional theory (DFT) is a well known source of error in describing bound excitons in solids. Remarkably, TD-DFT is often able to capture the optical features of isolated systems, even with the most simple exchange-correlation kernels, like the TD local density approximation. With the example of molecular crystals, we aim at solving the puzzle when and why TD-DFT can be relied on. We answer this question by confronting TD-DFT with many-body perturbation theory (GW and Bethe-Salpeter equation), which is the most accurate methodology to describe optical excitations in solids. Our results are obtained with the all-electron code "exciting" (http://exciting-code.org), where all the quantities entering the two formalisms are treated on the same footing [1]. In-depth analysis allows us to identify the shortcomings of TD-DFT in predicting the excitonic spectra of extended systems and to understand when this methodology is capable of providing correct results.

[1] S. Sagmeister and C. Draxl, Phys. Chem. Chem. Phys. 11, 4451 (2009)

TT 91.7 Thu 12:15 TRE Ma

Relativistic Solar Cells — •Paolo Umari[1], Edoardo Mosconi[2], and Filippo De Angelis[2] — [1]Dipartimento di Fisica e Astronomia, Università di Padova, via Marzolo 8, I-35131 Padova, Italy — [2]Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM, Via Elce di Sotto 8, I-06123, Perugia, Italy

Hybrid AMX_3 perovskites (A=Cs, CH_3NH_3; M=Sn, Pb; X=halide) have revolutionized the scenario of emerging photovoltaic technologies. Indeed, a rapid evolution led, very recently, up to 15% efficient solar cells. $CH_3NH_3PbI_3$ has so far dominated the field, while the similar $CH_3NH_3SnI_3$ has not been explored for photovoltaic applications, despite the reduced band-gap. Replacement of Pb by the more environment-friendly Sn would facilitate the large uptake of perovskite-based photovoltaics. Despite the extremely fast progress, the materials electronic properties which are key to the photovoltaic performance are relatively little understood. Here we develop an effective GW method incorporating spin-orbit coupling which allows us to accurately model the electronic, optical and transport properties of $CH_3NH_3SnI_3$ and $CH_3NH_3PbI_3$, opening the way to new materials design. The different $CH_3NH_3SnI_3$ and $CH_3NH_3PbI_3$ properties are discussed in light of their exploitation for solar cells, and found to be entirely due to relativistic effects.

TT 91.8 Thu 12:30 TRE Ma

Solar nanocomposites with complementary charge extraction pathways for electrons and holes: Si embedded in ZnS — •Stefan Wippermann[1], Marton Vörös[2], Adam Gali[3], Francois Gygi[2], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Budapest University of Technology and Economics

We propose that embedding silicon nanoparticles (NP) into amorphous, non-stoichiometric ZnS leads to promising nanocomposites for solar energy conversion. Using ab initio molecular dynamics simulations we show that upon high temperature amorphization of the host chalcogenide, sulfur atoms are drawn to the NP surface. We found that the sulfur content may be engineered to form a type II heterojunction, with complementary charge transport channels for electrons and holes, and that sulfur capping is beneficial to lower the nanoparticle gap, with respect to that of NPs embedded in oxide matrices. Our analysis was conducted using density functional theory with local and hybrid functionals and many body perturbation theory at the GW level.

TT 91.9 Thu 12:45 TRE Ma

Ultraviolet photo-emission spectroscopies from Koopmans-compliant functionals — •Ngoc Linh Nguyen[1], Giovanni Borghi[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland. — [2]Centro S3, CNR-Istituto Nanoscienze, I-41125 Modena, Italy — [3]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, USA.

We study the photo-electron properties of organic photovoltaic molecules using Koopmans-compliant functionals [1] as well as the Perdew-Zunger self-interaction correction (PZ-SIC) [2] to density-functional theory. A simple method for simulating ultraviolet photoemission spectra (UPS) of molecules has been implemented. It is based on a plane-wave approximation for the final states to account for the spectra intensities. Our calculations show that Koopmans-compliant functionals provide ionization potentials and electron affinities closely comparable with those obtained by many-body perturbation theory (GW). In addition, we find that UPS spectra computed imposing the Koopmans' condition on the PZ-SIC functional are in remarkable agreement with experimental results.

Refs: [1] I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M. Cococcioni, Phys. Rev. B 82, 115121 (2010); [2] J. P. Perdew and A. Zunger, Phys. Rev. B 23, 5048 (1981).

TT 91.10 Thu 13:00 TRE Ma

Self-consistent dynamical embedding in real space — •Wael Chibani[1], Xinguo Ren[1,2], Patrick Rinke[1], and Matthias Scheffler[1] — [1]*Fritz Haber Institute of the Max Planck Society, Berlin, Germany* — [2]*Key Laboratory of Quantum Information, USTC, Hefei, China*

Density-functional theory with its local-density (LDA) and generalized gradient approximations (GGA) is known to fail for localized states.

To extend *ab initio* approaches to this domain, we have devised an embedding scheme that facilitates the treatment of the physically important part of a system with electronic structure methods, that are computationally too expensive for periodic systems, whereas the rest of the periodic system is treated with computationally less demanding approaches, i.e. LDA/GGA, in a self-consistent manner. Our scheme is based on the concept of dynamical mean-field theory (DMFT) [1]. However, in contrast to the original DMFT formulation for correlated model Hamiltonians, we consider here the unit cell as embedded cluster in an *ab initio* way, that includes all electronic degrees of freedom. The performance of our scheme is demonstrated by treating the embedded region with hybrid functionals for simple bulk systems, e.g. Si or NiO. The total energy and the density of states converge rapidly with respect to the computational parameters and approach their bulk limit with increasing cluster size. By treating the embedded region with *GW* we were able to improve the band gap using only a small cluster. The effect of self-consistency in *GW* for the embedded region will also be addressed. [1] A. Georges *et al.*, Rev. Mod. Phys. **68**,14 (2006)

TT 92: Superconductivity: Fe-based Superconductors - Theory II

Time: Thursday 15:00–16:15 Location: HSZ 201

TT 92.1 Thu 15:00 HSZ 201

Superconducting gap in LiFeAs from three-dimensional spin-fluctuation pairing calculations — •Yan Wang[1], Andreas Kreisel[1], Volodymyr B. Zabolotnyy[2,3], Sergey V. Borisenko[2], Bernd Büchner[2,4], Peter J. Hirschfeld[1], Thomas A. Maier[5], and Douglas J. Scalapino[6] — [1]Department of Physics, University of Florida, USA — [2]Leibniz-Institute for Solid State Research, IFW-Dresden, Germany — [3]Physikalisches Institut, EP IV, Universität Würzburg, Germany — [4]Institut für Festkörperphysik, Technische Universität Dresden, Germany — [5]Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, USA — [6]Department of Physics, University of California, Santa Barbara, USA

The lack of nesting of Fermi-surface sheets in the Fe-based superconductor LiFeAs, with a T_c of 18 K, has led to questions as to whether the origin of superconductivity in this material might be different from other Fe-based superconductors. Here we present calculations of the superconducting gap and pairing in the random-phase approximation using Fermi surfaces derived from ARPES. The gaps obtained are qualitatively different from previous 2D theoretical works and in good agreement with ARPES on the main Fermi-surface pockets. We analyze the contributions to the pairing vertex thus obtained and show that the scattering processes between electron and hole pockets still dominate the pairing as in other Fe-based superconductors despite the lack of nesting, leading to gaps with anisotropic $s_\pm$ structure.

TT 92.2 Thu 15:15 HSZ 201

Superconductivity from repulsion in LiFeAs: novel *s*-wave symmetry and potential time-reversal symmetry breaking — •Felix Ahn[1], Ilya Eremin[1], Johannes Knolle[2], Volodymyr Zabolotnyy[3], Sergey Borisenko[3], Bernd Büchner[3], and Andrey Chubukov[4] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, D-01171 Dresden,Germany — [4]Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

Using the ten orbital tight-binding model, derived from the ab-initio LDA calculations and fitted to the ARPES experiments, we analyze the structure of the superconducting gap in LiFeAs. We treat superconductivity as quasi-2D and decompose the pairing interaction for various k_z cuts into $s-$ and d-wave components. Analyzing the leading superconducting instabilities we find that in addition to the conventional s^{+-}-wave order parameter where the gap changes sign between electron and hole pockets LiFeAs possesses another instability where the superconducting gap also changes sign between two smaller inner hole pockets. This occurs due to relatively large repulsion between these two small pockets and also relatively weak interaction between outer and inner hole pockets. The sizes of the gaps on the inner hole pockets is larger than the average value of the superconducting gap on the outer hole pockets and electron pockets which agrees with experimental data.

TT 92.3 Thu 15:30 HSZ 201

$BaFe_2P_2$ and $LaFe_2P_2$: What makes the difference? — •Tobias Förster[1], Helge Rosner[2], Andrey Polyakov[1], Marek Bartkowiak[1], Andrea D. Bianchi[3], and Jochen Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Deutschland — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Deutschland — [3]Département de Physique and RQMP, Université de Montréal, Montréal H3C 3J7, Canada

The Fermi-surface topology of iron-pnictide superconductors stimulated many theories on the pairing mechanism in these materials. Especially the degree of nesting between quasi-two-dimensional hole and electron bands is regarded as a key ingredient. However, also more localized pictures and the duality of both itinerant and localized degrees of freedom of the Fe 3*d* electrons are considered.To challenge the different scenarios, a precise knowledge of the electronic structure is necessary. We, therefore, present a detailed DFT study on $LaFe_2P_2$ and $BaFe_2P_2$. Using the full potential local orbital (FPLO) code we work out the difference between both compounds and show in detail what changes when replacing Ba with La. As a surprise, we find that a rigid-band-like description is inappropriate, since the La 5*d* states provide sizable contributions to a part of the Fermi surface. Additionally we use our de Haas-van Alphen measurements of $LaFe_2P_2$ and literature data of $BaFe_2P_2$ to refine our calculations and estimate the renormalization strength acting on the electronic structure.

TT 92.4 Thu 15:45 HSZ 201

Is $LiFeO_2Fe_2Se_2$ a typical iron-based superconductor? — •Christoph Heil, Lilia Boeri, Markus Aichhorn, Heinrich Sormann, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, University of Technology Graz, Austria

We study the electronic and magnetic properties of the recently synthesised [Lu et al., arXiv 1309.3833 (2013)] new iron-based superconductor $LiFeO_2Fe_2Se_2$ from first principles using GGA, LDA+U and LDA+DMFT. This material is a very interesting new member of the class of iron superconductors as it features an intercalated $LiFeO_2$ layer with a Fe $3d^5$ configuration. We calculate different magnetic configurations with first-principle methods, and find that the $3d^5$ Fe in the $LiFeO_2$ layer has a very big magnetic moment of $\mu \approx 3.6$, which would block all spin fluctuations in the FeSe layer. Based on our LDA+U and LDA+DMFT results, we will compare $LiFeO_2Fe_2Se_2$ with other typical iron-based superconductors and also more "exotic" ones.

TT 92.5 Thu 16:00 HSZ 201

Spin fluctuations and superconductivity in $K_xFe_{2-y}Se_2$ — •Andreas Kreisel[1], Yan Wang[1], Thomas A. Maier[2], Peter J. Hirschfeld[1], and Douglas J. Scalapino[3] — [1]Department of Physics, University of Florida, USA — [2]Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, USA — [3]Department of Physics, University of California, USA

Superconductivity in alkali-intercalated iron selenide, with T_c's of 30 K and above, may have a different origin than that of the other Fe-based superconductors, since the Fermi surface seems not to have any sheets centered around the Γ point. Here we investigate the symmetry of the superconducting gap in the framework of spin-fluctuation pairing calculations using DFT bands downfolded onto a 3D, ten-orbital tight-binding model, treating the interactions in the random-phase approximation. We find a leading instability towards a state with *d*-wave symmetry, but show that the details of the gap function depend sensitively on electronic structure. The crystal symmetry requires quasi-nodes to occur, which are either horizontal, looplike or vertical depending on details. We investigate the possibility that spin-orbit coupling effects on the one-electron band structure, which lead to enhanced splitting of the two *M*-centered electron pockets in the 2-Fe zone, may stabilize the bonding-antibonding $s_\pm$-wave states. Finally, we discuss our results in the context of current phenomenological theories and experiments and address the question of the origin of the spin-resonance that has been observed in inelastic neutron scattering experiments.

TT 93: Superconductivity: (General) Theory

Time: Thursday 16:30–18:00 Location: HSZ 201

TT 93.1 Thu 16:30 HSZ 201

Symmetry-protected topological invariant and Majorana impurity states in time-reversal invariant superconductors — •Lukas Kimme[1], Timo Hyart[2], and Bernd Rosenow[1] — [1]Institut für Theoretische Physik, Universität Leipzig, D-04103 Leipzig, Germany — [2]Instituut-Lorentz, Universiteit Leiden, Post Office Box 9506, 2300 RA Leiden, The Netherlands

We address the question of whether individual nonmagnetic impurities can induce zero-energy states in time reversal invariant superconductors, and define a class of symmetries which guarantee the existence of such Majorana states for a specific value of the impurity strength [1]. These symmetries allow the definition of a position space topological $\mathbb{Z}_2$ invariant, which is related to the standard bulk topological $\mathbb{Z}_2$ invariant. Our general results are applied to the time reversal invariant p-wave phase of the doped Kitaev-Heisenberg model [2], where we also demonstrate how a lattice of impurities drives a topologically trivial system into the non-trivial phase and even causes gapless topological superconductivity. Finally, signatures of impurity states in the spin-susceptibility are described.

[1] L. Kimme, T. Hyart, and B. Rosenow, arXiv:1308.2496
[2] T. Hyart, A. R. Wright, G. Khaliullin, and B. Rosenow, Phys. Rev. B 85, 140510(R) (2012).

TT 93.2 Thu 16:45 HSZ 201

Flat bands at surfaces of nodal topological superconductors: Spin polarization and charge currents — •Carsten Timm[1], Philip M. R. Brydon[2,1], and Andreas P. Schnyder[3] — [1]Institute of Theoretical Physics, Technische Universität Dresden, Dresden, Germany — [2]Condensed Matter Theory Center, University of Maryland, College Park, USA — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Noncentrosymmetric superconductors with strong spin-orbit coupling generically show coexisting singlet and triplet pairing. If the superconducting gap has nodes on the Fermi surface, the system exhibits topologically protected flat surface bands. Employing exact diagonalization of lattice models and quasiclassical methods, we show that the flat-band states are strongly spin polarized. Since the spin polarization is odd in momentum, the surface states acquire a chiral dispersion if the superconductor is brought into contact with a ferromagnet. These chiral states carry a large charge current. We compare the results to a fully gapped topological superconductor.

TT 93.3 Thu 17:00 HSZ 201

Plasmons, gauge invariance and mass in non-centrosymmetric superconductors — •Nikolaj Bittner[1], Dietrich Einzel[2], Ludwig Klam[1], and Dirk Manske[1] — [1]Max–Planck–Institut für Festkörperforschung, Heisenbergstraße 1, D–70569 Stuttgart, Germany — [2]Walther–Meißner–Institut für Tieftemperaturforschung, Walther–Meißner–Straße 8, D–85748 Garching, Germany

We present for the first time a comprehensive, gauge–invariant description of the order parameter collective modes in the recently discovered non–centrosymmetric superconductors (NCS). The gauge mode (*Nambu–Goldstone Boson*, $\omega_{\rm G}$), common to all superconductors, and the new collective mode (*Leggett mode*, $\omega_{\rm L}$), which usually occurs in ordinary two–band superconductors, were specified by employing (Nambu–)matrix kinetic theory in the clean limit. Moreover, we investigate the dispersion and the general role of these collective excitations in NCS systems. In particular, the subtle interplay between the gauge mode and the Leggett mode is analyzed in view of the validity of the charge conservation law. The long–range Coulomb interaction is seen to introduce the condensate plasma frequency $\omega_{\rm P}$ into the description of NCS and to distinguish between the order parameter collective modes $\omega_{\rm G}$ and $\omega_{\rm L}$ with respect to their participation in the Anderson–Higgs mechanism [1,2]. In contrast to ordinary two–band superconductors, the possibility of a mass–less Leggett mode can be predicted to occur in NCS, which simulates the existence of a second gauge mode.

[1] P. W. Anderson, Phys. Rev. **130**, 439 (1963)
[2] P. Higgs, Phys. Rev. Lett. **13**, 508 (1964)

TT 93.4 Thu 17:15 HSZ 201

Phonon-mediated pairing in the new superconductor Ta_2PdS_5: A first principles study — •Rolf Heid and Klaus-Peter Bohnen — Institut für Festkörperphysik, Karlsruher Institut für Technologie

Recently, a new layered chalcogenide superconductor $Ta_2Pd_xS_5$, $x \approx 1$, with a T_c of 6 K was discovered and classified as a type-II s-wave superconductor [1]. The presence of the heavy $5d$ element Ta and the observation of a large upper critical field well above the estimated Pauli limit led to speculations of a strong influence of spin-orbit coupling on the superconducting state. A subsequent electronic-structure calculation classified this material as an anisotropic multiband metal [2]. From a comparison of the bandstructure density of states and the measured specific heat, a strong-coupling scenario with a coupling constant larger than 2 was inferred.

Here we address the question of a strong-coupling scenario for Ta_2PdS_5 within a first principles approach. We present results for the electronic bandstructure, phonon dispersion, and the phonon-mediated pairing interaction obtained via density-functional perturbation theory. We will also discuss the relevance of spin-orbit coupling for these quantities.

[1] Y. F. Lu et al., arXiv:1308.3766
[2] D. J. Singh, Phys. Rev. B 88, 174508 (2013)

TT 93.5 Thu 17:30 HSZ 201

Electron-phonon coupling of light-actinides: effect of spin-orbit coupling — Paola González-Castelazo[1], •Omar De la Peña-Seaman[1], Rolf Heid[2], and Klaus-Peter Bohnen[2] — [1]Benemérita Universidad Autónoma de Puebla (BUAP), Institute of Physics (IFUAP), México — [2]Karlsruher Institut für Technologie (KIT), Institut für Festkörperphysik (IFP), Germany

The physics of actinide metals is quite complex and rich due to the behavior of $5f$ electrons in the valence region: it goes from itinerant on the early stages of the actinide series to highly localized for the elements with a higher number of $5f$ electrons involved. In addition, in this systems should be mandatory the inclusion of spin-orbit coupling (SOC). However, only in few cases on electronic and lattice dynamical properties the SOC has been taking into account, while for the electron-phonon (e-ph) coupling such analysis has not been performed so far. Thus, as a first approach we have systematically studied the SOC influence on the full-phonon dispersion and the e-ph coupling for the simplest light-actinide metals: Ac and Th. These elements have been studied within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method. The full-phonon dispersion as well as the Eliashberg spectral function and the electron-phonon coupling parameter have been calculated with and without SOC. The observed effects of SOC in the full-phonon dispersion and Eliashberg function are discussed in detail, together with an analysis of the differences on the electronic properties due to the SOC inclusion in the calculations.

TT 93.6 Thu 17:45 HSZ 201

Electromagnetic response of strongly disordered superconductors — •Götz Seibold[1], Lara Benfatto[2], Claudio Castellani[2], and Jose Lorenzana[2] — [1]BTU Cottbus-Senftenberg, Germany — [2]University of Rome 'La Sapienza', Italy

By including fluctuations beyond the Bogoljubov-de Gennes approach we investigate the static and dynamical properties of current correlations in the attractive Hubbard model with strong on-site disorder. In the static limit we find a strong renormalization of the superfluid stiffness due to the occurence of quasi one-dimensional percolative current patterns which connect superconducting islands. Moreover we show that for strongly disordered superconductors phase modes acquire a dipole moment and appear as a subgap spectral feature in the optical conductivity.

TT 94: Low-Dimensional Systems: Oxide Hetero-Interfaces

Time: Thursday 15:00–17:45 Location: HSZ 204

TT 94.1 Thu 15:00 HSZ 204

Surface / interface interaction in $LaAlO_3/SrTiO_3$ heterostructures: an *in-situ* transport and photoemission study — •Philipp Scheiderer[1], Florian Pfaff[1], Judith Gabel[1], Mihaela Gorgoi[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems, Universität Würzburg, Germany — [2]Helmholtz Zentrum Berlin, Germany

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 has recently been 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* conductivity measurements and *in-situ* photoelectron spectroscopy (PES) on 6ML thick LAO/STO heterostructures exposed to a defined amount of water vapor. PES experiments indicate that water adsorbates induce additional charge carriers at titanium sites which are located at the interface. We correlate these spectroscopic findings with *in-situ* conductivity measurements.

[1] Ohtomo et al., Nature **427** (2004) 423
[2] Thiel et al., Science **313** (2006) 1942
[3] Xie et al., Nature Comm. **2** (2011) 494
[4] Bristowe et al., Phys. Rev. B **83** (2011) 205405

TT 94.2 Thu 15:15 HSZ 204

Direct k-space mapping of interface states in oxide-oxide heterostructures — •Florian Pfaff[1], Hidenori Fujiwara[2], Judith Gabel[1], Götz Berner[1], Atsushi Yamasaki[3], Akira Sekiyama[2], Yunzhong Chen[4], Nini Pryds[4], Shigemasa Suga[5,6], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg — [2]Graduate School of Engineering Science, Osaka University — [3]Department of Physics, Konan University — [4]Department of Energy Conversion and Storage, Technical University of Denmark, — [5]Institute of Scientific & Industrial Research, Osaka University — [6]Max-Planck-Institute for Microstructure Physics, Halle

The most prominent example of unexpected quantum phases that can form at oxide heterointerfaces is the 2D electron system (2DES) in $LaAlO_3/SrTiO_3$ (LAO/STO). Its origin has been related to electronic reconstruction due to the polar character of the LAO. The novel γ-Al_2O_3 (GAO)/STO also exhibits a 2DES with even higher mobility although GAO is regarded to be non-polar. Here, it is assumed that O vacancies at the STO side of the interface induce the 2DES. We have mapped the momentum-resolved electronic structure of the interface Ti 3d states by resonant soft x-ray photoemission for both types of heterostructures. While one can observe in both systems a dichotomy of mobile and trapped interface charges they also show remarkable differences regarding the proportion of mobile and trapped carriers as well as the electron dispersions and Fermi surfaces.

TT 94.3 Thu 15:30 HSZ 204

Correlated electron states in realistic oxide heterostructures — •Frank Lechermann[1], Lewin Boehnke[1], Christoph Piefke[1], and Daniel Grieger[2] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]SISSA, Via Bonomea 265, I-34136 Trieste

The interface physics that arises from merging different metal oxides is currently one of the most intensive condensed matter research areas. For instance, bringing bulk band- and/or Mott-insulating materials together most often leads to the formation of an intricate two-dimensional electron gas (2DEG) at the interface. This 2DEG may be susceptible to various orderings, e.g. ferromagnetism or superconductivity. Using the charge self-consistent combination of density functional theory (DFT) and dynamical mean-field theory (DMFT) with a continuous-time quantum Monte Carlo impurity solution to DMFT, the relevance of electron correlation in many of these novel designed materials will be elucidated. The methodology allows to treat many-body effects beyond static mean field on the realistic structural/chemical level of such challenging systems like $LaTiO_3/SrTiO_3$ superlattices [1].

[1] F. Lechermann, L. Boehnke, and D. Grieger, Phys. Rev. B 87, 241101(R) (2013)

TT 94.4 Thu 15:45 HSZ 204

Emerging magnetism and electronic phase separation at titanate interfaces — •Natalia Pavlenko[1], Thilo Kopp[1], and Jochen Mannhart[2] — [1]EKM und Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

The emergence of magnetism in otherwise nonmagnetic compounds and its underlying mechanisms have become the subject of intense research. Here we demonstrate that the nonmagnetic oxygen vacancies are responsible for an unconventional magnetic state common for titanate interfaces and surfaces. Using an effective multiorbital modelling, we find that the presence of localized vacancies leads to an interplay of ferromagnetic order in the itinerant t_{2g} band and complex magnetic oscillations in the orbitally-reconstructed e_g-band, which can be tuned by gate fields at oxide interfaces. The magnetic phase diagram includes highly fragmented regions of stable and phase-separated magnetic states forming beyond nonzero critical defect concentrations.

TT 94.5 Thu 16:00 HSZ 204

Interaction induced instabilities in $LaAlO_3/SrTiO_3$ interfaces — •Mathias Scheurer and Jörg Schmalian — Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

At the interface between insulating oxides, novel phases with peculiar electronic properties arise. In this talk, we focus on one specific example, the heterostructure formed by the perovskite oxides $LaAlO_3$ and $SrTiO_3$. Using the renormalization group approach, the effect of electron-electron interactions is studied. We consider all interaction terms consistent with the symmetries of the system and analyze the stability of the electron fluid towards the formation of symmetry broken phases.

15 min. break.

TT 94.6 Thu 16:30 HSZ 204

The Rashba spin-orbit coupling for superconductivity in oxide interfaces — •Stefan Beyl, Peter P. Orth, and Jörg Schmalian — Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

We investigate the role of the Rashba spin-orbit coupling on the superconducting order parameter and the phase stiffness at the interface of $LaAlO_3$ and $SrTiO_3$. In particular, we analyze the gate controlled crossover between BCS superconductivity and Bose-Einstein condensation of Cooper pairs, amplified by the Rashba coupling and the possibility of a phase fluctuation induced quantum critical point.

TT 94.7 Thu 16:45 HSZ 204

Spin-orbit coupling in 2DEGs at a polar/non-polar oxide interface — •Kourosh Rahmanizadeh, Gustav Bihlmayer, Daniel Wortmann, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The investigation of a two-dimensional electron gas (2DEG) at the polar / non-polar oxide interface (e.g. the discovery of highly mobile electrons at the $LaAlO_3$ / $SrTiO_3$ interface) is attractive for spintronic applications. Similar to the 2DEGs formed in semiconductor heterostructures, Rashba spin-orbit coupling (SOC) can have a big impact for the magnetotransport properties at these oxide interfaces [1]. Moreover, the combination of Rashba SOC and magnetic (or exchange) fields offer unique properties sought for in the hunt for Majorana fermions [2]. The $BiAlO_3$ (BAO) exhibits the same polar layers as $LaAlO_3$. The ferroelectricity of the material further allows to manipulate the carrier density at the interface. Using density functional theory, we investigated the 2DEG in BAO/$SrTiO_3$, BAO/$EuTiO_3$ and BAO/Sr_2NiWO_6 heterostructures. In the latter two structures, the proximity to ferroelectric insulators breaks the time-reversal symmetry in the 2DEG and leads, in combination with Rashba SOC to a single Fermi surface, analogous to the situation in topological insulators.

Financial support of the EU grant NMP3-LA-2010-246102 (IFOX) is gratefully acknowledged.
[1] A. D. Caviglia et al., Phys. Rev. Lett. **104**, 126803 (2010).
[2] J. D. Sau et al., Phys. Rev. Lett. **104**, 040502 (2010).

TT 94.8 Thu 17:00 HSZ 204

Confinement-driven electronic phases in $(LaAlO_3)_M/(LaNiO_3)_N(111)$ superlattices — •David Doennig and Rossitza Pentcheva — Ludwig-Maximilians University Munich

Complex oxide heterostructures exhibit a broad variability of functional properties and electronic states, not available in the bulk. Beyond the much studied (001)-oriented systems, here we highlight theoretical results on (111) perovskite superlattices (SLs) containing the correlated metal $LaNiO_3$ (LNO) and the band insulator $LaAlO_3$ (LAO). Density functional theory calculations with an on-site Coulomb repulsion term reveal a rich spectrum of electronic phases in $(LAO)_M/(LNO)_N(111)$ SLs as a function of the LNO and LAO thickness N and M in the superlattice. In the double perovskite 1/1 system, a Jahn-Teller distortion with d_{z^2} orbital polarization leads to a ferromagnetic Mott insulating phase, so far unanticipated for nickelates. For the LNO bilayer (N=2) with graphene topology, a Dirac-point Fermi surface is obtained, while symmetry breaking leads to band gap opening with two inequivalent interfaces. For $N \geq 3$ the confined LNO slab undergoes a metal-to-insulator transition to a half-semimetallic phase with conduction originating from the interfaces. Antiferromagnetic arrangements allow combining motifs of the bilayer and single trigonal layer band structures in engineered artificial mixed phases. We acknowledge funding by the DFG, SFB/TR80.

TT 94.9 Thu 17:15 HSZ 204

Enhanced ferromagnetism in $BiFeO_3$/$NgGaO_3$ thin film — •Chang-Yang Kuo[1], Zhiwei Hu[1], Jan-Chi Yang[2], Ying-Hao Chu[2], Stefano Agrestini[1], Tunwen Pi[3], Eric Pellegrin[4], and Liu Hao Tjeng[1] — [1]Max Planck Institut CPfS, Dresden, Germany — [2]National Chiao Tung University, Hsinchu, Taiwan — [3]National Synchrotron Radiation Research Center (NSRRC), Hsinchu, Taiwan — [4]CELLS-ALBA, Barcelona, Spain

Multiferroic material $BiFeO_3$ has attracted a tremendous interest from the fundamental research as well as application points of view because of its high ferroelectric Curie temperature of 820 °C and high Neel temperature of 370 °C. Recently, strain engineering has emerged as a powerful means for tuning the various properties of $BiFeO_3$ thin film remarkably, such as by modifying ferroelectric domain walls or direction in $BiFeO_3$, enhancing ferroelectricity. Also a weak ferromagnetic component, induced by spin canting, has been observed in strained thin films. Here we report a x-ray absorption magnetic circular dichroism (XMCD) and x-ray absorption magnetic linear dichroism (XMLD) study showing a strong enhancement of the ferromagnetic component and tetragonal distortion for $BiFeO_3$ thin film grown on $NdGaO_3$ substrate.

TT 94.10 Thu 17:30 HSZ 204

DFT+DMFT study of epitaxially strained $LaVO_3$ — •Gabriele Sclauzero, Krzysztof Dymkowski, and Claude Ederer — Materials Theory, ETH Zurich, Switzerland

$LaVO_3$ is a t_{2g} perovskite showing a rich phase diagram as a function of temperature, with a paramagnetic Mott-Hubbard insulating state at room temperature. Recently, it has become possible to produce and characterize strained lattices of $LaVO_3$ in thin films and superlattices of high structural quality. In such heterostructures both interface effects and epitaxial strain play an important role in the electronic reconstruction of the material, and it is often difficult to distinguish between these two effects in experiments. Moreover, the epitaxial strain can induce at least two different important modifications of the atomic geometry, namely: (i) a change in the amplitudes of the VO_6 octahedral rotations; (ii) a stretching or compression of V–O bonds.

In this work, we perform density functional theory plus dynamical mean field theory (DFT+DMFT) simulations to study how the correlated Mott-Hubbard phase of $LaVO_3$ is affected by epitaxial strain. We separate the effect of bond-length changes from that of octahedral rotations by comparing an idealized structure without rotations and a realistic one derived from the bulk orthorhombic phase. We interpret our findings through the strain-induced changes in the energies of the crystal-field t_{2g} levels of the local DFT Hamiltonian and in the occupation matrix obtained from DMFT. A comparison with the t_{2g} perovskite $LaTiO_3$, which shows an insulator-to-metal transition upon compressive strain, will also be presented.

TT 95: Focus Session: Theoretical Advances in Interacting Topological Phases (organized by TT)

Topological insulators have attracted considerable attention recently. Today, the theoretical and experimental understanding of such systems has become comparably well. The continued high interest in this topic is caused by exciting proposals and concepts for new exotic physics based on the interplay of the non-trivial band topology and strong electron-electron interactions. Fractional Chern insulators, topological Mott insulators, topological Kondo insulators, and spin liquids are just a few examples. Some of these phases have already been claimed to be found in experiments.

The aim of this focus session is to give an overview of the most recent advances in this exciting and rapidly evolving field presented by leading experts in the field.

Organizer: Stephan Rachel (TU Dresden)

Time: Thursday 15:00–18:25 Location: HSZ 03

Invited Talk TT 95.1 Thu 15:00 HSZ 03

Fractional Topological Insulators — •Andrei Bernevig — Princeton University

Topological insulators are remarkable materials whose insulating "boring" bulk nonetheless gives rise to perfectly metallic edge or surface states not disturbed by disorder. In this talk, I will relay new phenomena beyond the recently discovered topological insulators with time-reversal symmetry. I will show that topological insulators exist with any point group symmetry, and, upon adding interactions, can transform in much more interesting systems. I will show that fractionally filling a band of a one-body topological insulator and then subjecting its electrons to repulsive interaction can create new states of matter non-existent in the continuum, whose quasiparticles exhibit non-abelian braiding. I will then show that a new description of these states in terms of matrix product forms can greatly enhance our capability to calculate their many-body properties.

Invited Talk TT 95.2 Thu 15:30 HSZ 03

Non-Fermi Liquid, Quantum Critical, and Topological States in Iridates — •Leon Balents — Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA, USA

The combination of band topology and strong correlations is an intriguing and largely open area for theory and experiment. I will discuss a theory of a "parent state" for both topological and quantum critical descendants. This state is suggested to describe one of the prototypical materials families in this area: the pyrochlore iridates.

Parts of this work were done in collaboration with Yong-Baek Kim, Eun-Gook Moon, Lucile Savary, and Cenke Xu

Topical Talk TT 95.3 Thu 16:00 HSZ 03

Collective Spin-Orbit Physics in $j = 1/2$ Mott Insulators — •Simon Trebst — Universität zu Köln

The greatly enhanced spin-orbit coupling in 5d transition metal oxides can lead to a novel class of Mott insulators in which the local moment is a $j = 1/2$ spin-orbit entangled momentum. The rich physics arising in these novel Mott insulators has been extensively probed in the con-

text of the quasi two-dimensional compounds Sr_2IrO_4 (square lattice) with regard to superconducting instabilities and Na_2IrO_3 (honeycomb lattice) in context of possible spin liquid behavior. Here we report on our endeavor to understand the collective states of such spin-orbit entangled j=1/2 momenta when considering other lattice geometries, in particular the triangular lattice motivated by the recent synthesis of $Ba_3IrTi_2O_9$ and the three-dimensional hyperoctagon lattice in the context of β-Li_2IrO_3. For the triangular system we find that weak anisotropic Kitaev-like interactions stabilize a Z_2-vortex phase. For the hyperoctagon lattice (the premedial lattice of the hyperkagome lattice) we find that strong Kitaev-like couplings give rise to a gapless quantum spin liquid with a Majorana Fermi surface – a highly unusual spin liquid state, which is intimately connected to and protected by the lattice symmetries.

15 min. break.

Topical Talk TT 95.4 Thu 16:45 HSZ 03

Topological Kondo Insulators: An Example of Correlated Quantum Spin Hall States — •Fakher Assaad — Universität Würzburg

In the very same way as the heavy fermion paramagnetic state at $T = 0$ is adiabatically linked to a gas of free electrons, the topological Kondo insulator can be deformed to a quantum spin Hall insulator without going through a quantum phase transition. The interest however lies in the fact the quasi-particles forming this coherence state are dynamically created by correlation effects, and may be viewed as the Kondo screening clouds of the magnetic impurities. The minimal model to capture this piece of physics consists of odd parity localized f-states hybridizing with an even parity conduction band alongside strong spin-orbit coupling and time reversal symmetry. In this talk we will consider such a minimal model, and concentrate on the temperature dependence of various quantities from the mixed valence to local moment regimes [1-2] The quantities we consider include topological invariants as well as the single particle spectral function on slab topologies. We show that there is a single low energy scale, the coherence scale, below which one observes the emergence of the topological state.

This work has been carried out in collaboration with J. Werner.

[1] J. Werner and F. F. Assaad, Phys. Rev. B 88, 035113 (2013).
[2] J. Werner and F. F. Assaad, arXiv:1311.3668.

Topical Talk TT 95.5 Thu 17:15 HSZ 03

Fractional Chern Insulators in Strongly Correlated Multiorbital Systems — •Maria Daghofer, Stefanos Kourtis, Jörn W. F. Venderbos, and Jeroen van den Brink — IFW Dresden, Dresden, Germany

Interaction between itinerant carriers and localized spins on frustrated lattices can stabilize phases that are in many respects similar to a Landau level, with a non-coplanar spin background taking the role of the magnetic field. If the bands are nearly flat, longer-range Coulomb repulsion can then induce states that are like lattice-analogs of fractional Quantum-Hall (FQH) states, but do not require an external magnetic field. I will discuss a t_{2g}-orbital system on a triangular lattice that supports a spin-chiral magnetic ordering pattern with precisely the required topologically non-trivial and flat bands[1]. Exact-diagonalization methods reveal signatures of a FQH-like ground state. Moreover, we also find states that go beyond the physics of Landau levels: They show a combination of conventional (charge) and topological order and are related to the frustration of the underlying triangular lattice [2].

[1] J. W. F. Venderbos et al., PRL **108**, 126405 (2012)
[2] S. Kourtis and M. Daghofer, arXiv:1305.6948

TT 95.6 Thu 17:45 HSZ 03

Non-Abelian quasiparticles in strongly interacting helical liquids — •Thomas Schmidt, Christoph Orth, and Rakesh Tiwari — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

The interplay of strong Coulomb interactions with Rashba spin-orbit coupling can lead to the opening of a gap in the edge spectrum of a two-dimensional topological insulator, even if the system Hamiltonian is time-reversal invariant. We investigate the properties of such a strongly interacting helical system in proximity to an s-wave superconductor. We show that the interface between a region gapped out by the proximity effect and a region gapped out by strong interactions can host non-Abelian bound states, and determine their exchange statistics.

TT 95.7 Thu 18:05 HSZ 03

From fractionally charged solitons to Majorana bound states in a one-dimensional interacting model — •Frank Pollmann[1], Doru Sticlet[1,2], Luis Seabra[1,3], and Jerome Cayssol[1,2] — [1]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany — [2]CNRS and University Bordeaux, Talence, France — [3]Technion, Haifa, Israel

We investigate the one-dimensional Creutz model in the presence of induced superconductivity and Hubbard type interactions. We show that zero-energy Majorana edge modes develop in the presence of superconducting pairing for a certain range of parameters. Additionally, the system hosts regular electronic zero-energy modes in a trivial superconducting phase. We study the effect of interactions using a combination of density matrix renormalization group (DRMG) methods and mean field theory. It is shown how local repulsive interactions expand the parameter range for which a topological Majorana phase is stabilized. In contrast, we find that interactions remove the zero-energy modes found in the trivial superconducting phase.

TT 96: Correlated Electrons: Nonequilibrium Quantum Many-Body Systems II

Time: Thursday 15:00–17:00 Location: HSZ 304

TT 96.1 Thu 15:00 HSZ 304

Transient dynamics of open quantum systems — Oleksiy Kashuba[1] and •Herbert Schoeller[2] — [1]Institut fuer Theoretische Physik, TU Dresden — [2]Institut fuer Theorie der Statistischen Physik, RWTH Aachen

We present a renormalization group (RG) method which allows for an analytical study of the transient dynamics of open quantum systems on all time scales [1]. Whereas oscillation frequencies and decay rates of exponential time evolution follow from the fixed point positions, the long-time behavior of pre-exponential functions is related to the scaling behavior around the fixed points. We show that certain terms of the RG flow are only cut off by inverse time, which leads to a difference between infrared and ultraviolet scaling. An evaluation for the ohmic spin boson model at weak damping reveals significant deviations from previous predictions in the long-time regime. We propose that weak coupling problems for stationary quantities can in principle turn into strong coupling ones for the determination of the long-time behavior.

[1] O. Kashuba and H. Schoeller, Phys. Rev. B87, 201402(R) (2013)

TT 96.2 Thu 15:15 HSZ 304

Stationary properties of generic 2-level systems in nonequilibrium — •Stefan Goettel, Frank Reininghaus, and Herbert Schoeller — Institut für Theorie der Statistischen Physik, RWTH Aachen

We consider a generic quantum dot in nonequilibrium in the Coulomb blockade regime at fixed charge and zero temperature. In the weak coupling regime, we present a generic weak-coupling expansion of the stationary density matrix and the conductance based on a recent formulation of real-time renormalization group (RTRG) by using the Laplace variable as flow parameter, in analogy to the expansion presented in Ref.[3] where a Masubara-frequency cutoff has been used. We apply this expansion to a 2-level system and find generically that the effective Liouvillian contains terms linear or quadratic in the renormalized couplings which can not be described by perturbation theory with renormalized couplings from poor man scaling methods. At large bias voltage, we find that at vanishing and large magnetic fields renormalized perturbation theory works well whereas at intermediate magnetic fields of the same order as the typical renormalization, significant differences occur which can only be described from the full RTRG method. Furthermore, we present evidence that the same generic behaviour is expected for 3- and 4-level systems.

[1] M. Pletyukhov, H. Schoeller, Phys. Rev. Lett. 108, 260601 (2012)

[2] O. Kashuba and H. Schoeller, Phys. Rev. B87, 201402(R) (2013)
[3] H. Schoeller and F. Reininghaus, Phys. Rev. B80, 045117 (2009)

TT 96.3 Thu 15:30 HSZ 304

Quantum quenches and and statistics of projective quantum measurements — •Jonathan Lux and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln

Recently, it became possible to determine the position of ultracold atoms in a 2d optical lattice with single-site resolution[1]. This was used to perform time dependent projective quantum measurements in a many particle system.

Motivated by this development, we study a quench in the 2d XXZ Heisenberg model, where the initial state is a 1d chain of, for example, up-spins in a bath of down-spins. Here the zoology of quasiparticles and their reaction schemes are very rich. After a weak quench, the density of excitations induced by the quench is very low. This allows for a semiclassical approach: the creation and the scattering of the quasiparticles are quantum mechanical, while they propagate classically[2]. Using this method, we study the non-equilibrium statistics of projective quantum measurements, and find that many projective observables show algebraic long-time tails.

[1] T. Fukuhara, et al., Nature Phys. **9**, 235 (2013).
[2] S. Sachdev, and K. Damle, PRL **78**, 943 (1997).

TT 96.4 Thu 15:45 HSZ 304

Out of equilibrium quantum criticality and real-time dynamics — •Pedro Ribeiro[1,2,3], Farzaneh Zamani[1,2], and Stefan Kirchner[1,2] — [1]CFIF-IST, Universidade de Lisboa, Lisboa, Portugal. — [2]MPI-PKS, Dresden, Germany — [3]MPI-CPfS, Dresden, Germany,

A systematic understanding of the physical properties of correlated systems away from thermal equilibrium is currently actively pursued in a broad variety of contexts. This interest in the theoretical description of far-from-equilibrium dynamics is fueled by recent experimental achievements to probe non-thermal states in a controlled fashion. In this talk we report on recent progress in the understanding of real time evolution of certain impurity models near local critical quantum points away from thermal equilibrium. The reported results are based on a generalisation of the dynamic large-N approach to the Keldysh contour that can be used to efficiently obtain the full real-time dynamics. Particular attention is given to the approach to previously found steady-state solutions when the system is quenched near criticality.

TT 96.5 Thu 16:00 HSZ 304

Auxiliary master equation approach to nonequilibrium correlated impurities — •Antonius Dorda, Martin Nuss, Enrico Arrigoni, and Wolfgang von der Linden — Technische Universität Graz, Graz, Österreich

A theoretical scheme for the study of correlated quantum impurity problems out of equilibrium is presented, which is particularly suited to address steate steady properties within Dynamical Mean Field Theory. The approach, recently introduced in [1], is based upon a mapping of the original impurity problem to an auxiliary open quantum system consisting of the interacting impurity coupled to bath orbitals as well as to a Markovian environment. The dynamics of the auxiliary system are governed by a Lindblad master equation whose parameters are used to optimize the mapping. The accuracy of the method can be readily estimated and systematically improved by increasing the number of auxiliary bath orbitals. To solve for the Green's functions of the auxiliary impurity problem, a non-hermitian Lanczos diagonalization is used [2]. Results for the steady state current-voltage characteristics of the single impurity Anderson model are presented and compared against data from time evolving block decimation. Furthermore, the bias dependence of the single particle spectral function and the splitting of the Kondo resonance are discussed.

[1] E. Arrigoni et al., Phys. Rev. Lett. 110, 086403 (2013)
[2] A. Dorda et al., in preparation

TT 96.6 Thu 16:15 HSZ 304

Universal post-quench dynamics at quantum critical points — •Pia Gagel[1], Peter P. Orth[1], and Jörg Schmalian[1,2] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institute for Solid State Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

We consider a quench in a system initially located in the vicinity of a quantum critical point and that is suddenly moved to the critical point. In this regime one finds a universal exponent that is not related to the equilibrium exponents and that governs the post-quench short time dynamics. We calculate this exponent for an open quantum system and discuss the implications for the dynamics of the order parameter and response functions. The approach demonstrates that quantum-quenches can be efficient tools to manipulate and study quantum many body systems.

TT 96.7 Thu 16:30 HSZ 304

Many-body localization and entanglement in disordered quantum spin models — •Rajeev Singh, Jens Bardarson, and Frank Pollmann — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The presence of disorder in a non-interacting system can localize all the energy eigenstates, a phenomena dubbed Anderson localization. Many-body localization is a generalization of this phenomena to include *interactions*. The dynamics of disordered interacting quantum systems shows a logarithmic growth (associated with glassy systems) in the entanglement entropy after a global quench [1]. For finite systems, this growth saturates and the saturation value obeys a volume law. A volume law leads to a constant entanglement entropy per site which might be related to thermal entropy and imply partial thermalization of the system. In this work, we study further the dynamics of disordered quantum spin systems and parameter dependence of the long time saturation.

[1] J. H. Bardarson, F. Pollmann and J. E. Moore, Phys. Rev. Lett. 109, 107202 (2012)

TT 96.8 Thu 16:45 HSZ 304

Many body localization in a quantum Ising model: A numerical study — •Jonas Kjäll, Jens Bardarson, and Frank Pollmann — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

Closed correlated quantum systems with disorder can experience many-body localization. These systems do not thermalize and the properties of the individual finite energy eigenstates become important. Recently, Huse et. al. concluded that eigenstates with broken symmetry order the quantum system, even at energy densities where the corresponding thermal system is disordered. We perform a detailed exact diagonalization study of a random Ising chain with a short ranged interaction between the excitations. We find signatures of the three predicted localized phases. One is paramagnetic and the two others have a broken Z_2 symmetry with spin-glass order. These last two can further be distinguished by spectral properties.

TT 97: Spincaloric Transport I (organized by MA)

Time: Thursday 16:45–18:45 Location: HSZ 403

TT 97.1 Thu 16:45 HSZ 403

Spin Hall magnetoresistance in ferromagnetic insulator/normal metal hybrids — •M. Althammer[1], S. Meyer[1], S. Geprägs[1], M. Opel[1], R. Gross[1,2], and S. T. B. Goennenwein[1] — [1]Walther-Meißner-Institut, BAdW, Germany — [2]Physik-Department, Technische Universität München, Germany

Pure spin currents, i.e. the net flow of spin angular momentum without an accompanying charge current, represent a new paradigm for spin transport and spintronics. We have experimentally studied a new type of magnetoresistance effect, which arises from the interaction of charge and spin current flows in ferromagnetic insulator/normal metal hybrid structures. In more detail, we measured the resistance of yttrium iron garnet(YIG)/Pt, YIG/nonferromagnet/Pt, nickel ferrite/Pt, and magnetite/Pt hybrid structures as a function of the magnitude and the orientation of an external magnetic field. The resistance changes observed can be quantitatively traced back to the combined action of spin Hall and inverse spin Hall effect in the Pt metal layer, and are thus termed spin Hall magnetoresistance (SMR) [1, 2]. We show that the SMR is qualitatively different from the conventional anisotropic magnetoresistance effect arising in magnetic metals and is not due to a static proximity magnetization in Pt, as proposed by Huang et al. [3]. Financial support by the DFG via SPP 1538 (project no. GO 944/4) and the Nanoinitiative Munich (NIM) is gratefully acknowledged.

[1] Nakayama et al., PRL, **110**, 206601 (2013)
[2] Althammer et al., PRB, **87**, 224401 (2013)
[3] Huang et al., PRL, **109**, 107204 (2012)

TT 97.2 Thu 17:00 HSZ 403

Cooling nanodevices via spin-polarized currents — •Jochen Brüggemann[1], Stephan Weiss[2], Peter Nalbach[1], and Michael Thorwart[1] — [1]1. Institut für theoretische Physik, Universität Hamburg, Jungiusstrasse 9, 20355 Hamburg — [2]Theoretische Physik, Universität Duisburg-Essen & CENICE, 47048 Duisburg

We investigate a non-equilibrium cooling scheme for nanodevices utilizing spin-polarized currents inspired by the demagnetization cooling for macroscopic systems. A minimal model is employed including the following parts: First, a quantum dot coupled to ferromagnetic leads via electron tunneling, second, a localized magnetic moment on the dot interacting with the electron spins via exchange interaction and, finally, a single phonon mode coupled to both electric and spin degrees of freedom. By deriving and solving a quantum master equation for the reduced density matrix in the sequential tunneling limit, we are able to determine both spin and phonon dynamics. Due to the combination of spin-polarized currents and spin-phonon interaction we achieve an increase of the ground state population of the localized moment and thus, subsequently, of the phonon mode compared to its initial preparation.

TT 97.3 Thu 17:15 HSZ 403

Magneto-thermopower and Magnetoresistance of single Co-Ni alloy Nanowires — •Tim Böhnert[1], Victor Vega[2], Ann-Kathrin Michel[1], Victor M. Prida[2], and Kornelius Nielsch[1] — [1]Universität Hamburg, Hamburg, Germany — [2]Universidad de Oviedo, Oviedo, Spain

The magneto-thermopower is measured and correlated to the anisotropic magnetoresistance of Co-Ni alloyed nanowires with varying composition. The highest absolute and relative variation of the Seebeck coefficient in perpendicularly applied magnetic fields at room temperature are determined to be $1.5\,\mu\mathrm{VK}^{-1}$ for $Co_{0.24}Ni_{0.76}$ and 8.1 % for $Co_{0.39}Ni_{0.61}$ nanowires. Power factors of $3.7\,\mathrm{mW/mK}^2$ have been achieved, which is competitive with common thermoelectric materials like Bi_2Te_3. For Co-Ni nanowires containing up to 39 % Co a linear relationship between the magnetic field dependent change of the Seebeck coefficient and the electrical conductivity is found.

TT 97.4 Thu 17:30 HSZ 403

Magneto-thermopower on FeNi and FeCo thin films — •Sasmita Srichandan, Maximilian Schmid, Michael Vogel, Christoph Strunk, and Christian Back — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We present measurements on the magneto-thermoelectric effects of 20 nm thick ferromagnetic films of permalloy (Py) [1] and FeCo alloy. The Py has been deposited on bulk MgO and GaAs substrates as well as on 100 nm thick SiN membranes. The dominant contribution to these effects turns out to be planar Nernst effect (PNE). For bulk substrate samples, the out of the plane temperature gradient gives rise to the anomalous Nernst effect (ANE). No ANE or transverse spin Seebeck effect (TSSE) signals are detected for the membrane samples. The observed TSSE for Py on bulk substrates is at least two orders of magnitude smaller than in earlier experiments [2].

In addition we study thermoelectric effects for FeCo alloy of various compositions deposited on the membrane. The advantage with FeCo is that the Fermi energy can be tuned throughout the band structure [3]. The domain walls in our samples are clearly visible in the TEM images. We present preliminary results of the effect of the domains on the thermoelectric effects.

[1] M. Schmid, S. Srichandan et.al PRL **111**,187201(2013).
[2] K. Uchida et.al Nature **455**,778(2008).
[3] K. Schwarz et.al J. Phys. F **14**,2659(1984).

TT 97.5 Thu 17:45 HSZ 403

Magneto-Thermopower and Giant Magnetoresistance measurements on single multilayered Co-Ni/Cu nanowires — •Anna Niemann[1], Tim Böhnert[1], Ann-Katrin Michel[1], Svenja Bässler[1], Johannes Gooth[1], Katalin Neurohr[2], Bence Tóth[2], László Péter[2], Imre Bakonyi[2], and Kornelius Nielsch[1] — [1]Institute of Applied Physics, Universität Hamburg, Hamburg, Germany — [2]Wigner Institute, Budapest, Hungary

The magneto-thermopower (MTP) is linked to the giant magnetoresistance (GMR) of individual multilayered Co-Ni/Cu nanowires with varying Cu thickness. Both magneto effects are studied temperature dependent in perpendicular magnetic fields leading to cross plane GMR effects of up to 15 % at RT. This is a typical effect size for electrodeposited nanowires. A linear dependence between thermopower S and conductivity σ of the nanowires–with the magnetic field as an implicit variable–is found at a wide temperature range (50 K to 325 K). This observation is in agreement with the Mott formula with an additional thermopower offset, which allows the estimation of the absolute Seebeck coefficient of the contact material.

The linear behavior–S vs. σ–and the Mott formula are used to calculate the energy derivative of the resistivity, which can be further correlated to the transmission function serving as a starting point in theoretical models. Magneto-thermal conductance measurements are planned to complete the characterization of the spin-caloritronic properties, in particular to validate the Wiedemann-Franz law in cross-plane GMR structures.

TT 97.6 Thu 18:00 HSZ 403

The anomalous Nernst effect in the triplet superconductor Sr_2RuO_4 — •Martin Gradhand[1], Karol I. Wysokinski[2], and James F. Annett[1] — [1]H . H. Wills Physics Laboratory, University of Bristol, Tyndall Ave, BS8-1TL, UK — [2]Institute of Physics, M. Curie-Skłodowska University, Radziszewskiego 10, PL-20-031 Lublin, Poland

The existence of the time reversal symmetry breaking in the superconducting state of Sr_2RuO_4 is crucial for the understanding of the pairing mechanism in this material. It is believed to show triplet p-wave pairing with a finite orbital and spin momentum. The measured optical Kerr effect [1] in its superconducting state caused enormous theoretical effort with different possible explanations. [2]

Another way to proof or disproof the existence of the time reversal symmetry breaking would be highly desirable. Here we present, two routes strongly related to each other. On one hand we address the existence and magnitude of the orbital magnetic moment relying on the Berry curvature expression for periodic crystals. On the other hand we will discuss the possibility of a superconducting current induced by temperature gradients - the anomalous Nernst effect.

[1] J. Xia, et al. Phys. Rev. Lett. **97**, 167002 (2006)
[2] V. M. Yakovenko Phys. Rev. Lett.**98** 087003 (2007), V. P. Mineev Phys. Rev. B **76** 212501 (2007), E. Taylor C. Kallin Phys. Rev. Lett. **108** 157001 (2012), M. Gradhand et al. Phys. Rev. B **88**, 094504 (2013)

TT 97.7 Thu 18:15 HSZ 403

Magnetic field dependence of the thermal conductivity of LCMO — •Christoph Euler, Paulina Holuj, Tino Jäger, Christian Mix, and Gerhard Jakob — University of Mainz, Germany

We measured the low-temperature out-of-plane thermal conductivity of LCMO using the differential 3-omega technique and found substantial magnetic field dependence between 100 K and room temperature. The effect is observed to be largest in the vicinity of the metal-insulator transition, since the enhancement in thermal conductivity is caused by the colossal magnetoresistance effect increasing the electronic contribution to the thermal conductivity. Our measurements allow a discussion of the Wiedemann-Franz law in the framework of strong electron-lattice coupling.

TT 97.8 Thu 18:30 HSZ 403

Magnon Hall effect and topology in kagomé lattices: A theoretical investigation — •Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Ferromagnetic insulators with Dzyaloshinskii-Moriya interaction show the magnon Hall effect, i. e., a transverse heat current upon application of a temperature gradient [1,2]. In our theoretical investigation we establish a close connection of the magnon Hall effect in two-dimensional kagomé lattices with the topology of their magnon dispersion relation. From the topological phase diagram we predict systems which show a change of sign in the heat current in dependence of the temperature. Furthermore, we derive a high-temperature limit of the thermal Hall conductivity; this quantity provides a figure of merit for the strength of the magnon Hall effect. Eventually, we compare the temperature dependence of the magnon Hall conductivity of the three-dimensional pyrochlore $Lu_2V_2O_7$ with experiment.

[1] Y. Onose et al., Science **329**, 297 (2010).
[2] R. Matsumoto, S. Murakami, Phys. Rev. B **84**, 184406 (2011).

TT 98: Transport: Nanomechanics

Time: Thursday 15:00–18:00 Location: BEY 81

TT 98.1 Thu 15:00 BEY 81

Phonon lasing and non-linear phenomena with nitrogen-vacancy centers in diamond — •Kosmas Kepesidis — Institut of Atomic and Subatomic Physics, TU Wien, Wien, Austria

I this talk, I will describe a new approach for manipulating and detecting the state of single and multiple vibrational modes in nanoscale diamond structures by making use of the strain-induced coupling to a nitrogen-vacancy impurity. I will first show how this coupling can be used to either cool the resonator close to its vibrational ground state or drive it to a large-amplitude coherent state (phonon lasing). In the second part of the talk I will then describe the complex nonlinear phenomena that can arise in an array of coupled phonon-lasers under parity-time symmetric conditions, where phonon modes with alternating gain and loss of equal strength are coupled together.

TT 98.2 Thu 15:15 BEY 81

Nano-scale rotor driven by single-electron tunneling — •Alan Celestino[1], Alexander Croy[2], Marcus Werner Beims[3], and Alexander Eisfeld[1] — [1]MPIPKS, Dresden, Germany — [2]Chalmers University of Technology S-412 96, Göteborg, Sweden — [3]Federal University of Paraná, Curitiba, Brazil

We study theoretically the dynamics and the electronic transport in a nano-scale rotor. The rotor is driven by electron tunneling in the Coulomb-blockade regime. We show that a static bias can lead to self-excitation of intermittent oscillatory/rotatory or continuous rotational motion. We establish the connection between the dynamical regimes and the current through the device. The relevant device's parameters are identified and we study the dynamics' dependence on these parameters. Notably, in the intermittent 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. Finally, we show how to break the system's symmetry in order to recast it as a rectifier.
[1] A. Croy and A. Eisfeld, EPL 98, 68004

TT 98.3 Thu 15:30 BEY 81

Cooling a nanomechanical resonator using spin-dependent transport — •Pascal Stadler[1], Gianluca Rastelli[2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Zukunftskolleg, Fachbereich Physik, Universität Konstanz, 78457, Konstanz, Germany

We study spin-dependent transport in a quantum dot contacted to two ferromagnets and magnetically coupled to a nanomechanical oscillator in the quantum regime. Due to the magneto-vibrational coupling, the nanomechanical oscillator induces spin-flips of the electrons on the quantum dot. In such a spin-valve, owing to the sensitivity of the electron transport to the spin orientation, signatures of the nanomechanical motion appears in the I-V characteristic even for weak spin-vibrational coupling. Additionally, the feed-back action of the spin-polarized current on the state of the oscillator leads to an active cooling of the oscillator's eigenmode controlled by the applied voltage to the leads and by the parallel or antiparallel magnetization configuration.

TT 98.4 Thu 15:45 BEY 81

Optomechanical Metamaterials: Dirac polaritons, Gauge fields, and Instabilities — •Vittorio Peano, Michael Schmidt Schmidt, and Florian Marquardt — Friedrich Alexander Universität Erlangen

Freestanding photonic crystals can be used to trap both light and mechanical vibrations. These "optomechanical crystal" structures have already been experimentally demonstrated to yield strong coupling between a photon mode and a phonon mode, co-localized at a single defect site. Future devices may feature a regular superlattice of such defects, turning them into "optomechanical arrays". We predict that tailoring the optomechanical band structure of such arrays can be used to implement Dirac physics of photons and phonons, to create a photonic gauge field via mechanical vibrations, and to observe a novel optomechanical instability.

TT 98.5 Thu 16:00 BEY 81

Arbitrarily large steady-state bosonic squeezing via dissipation — •Andreas Kronwald[1], Florian Marquardt[1,2], and Aashish A. Clerk[3] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Max Planck Institute for the Science of Light, Günther-Scharowsky-Straße 1/Bau 24, D-91058 Erlangen, Germany — [3]Department of Physics, McGill University, Montreal, Quebec, Canada H3A 2T8

We discuss how large amounts of steady-state quantum squeezing (beyond 3 dB) of a mechanical resonator can be obtained by driving an optomechanical cavity with two control lasers with differing amplitudes. The scheme does not rely on any explicit measurement or feedback, nor does it simply involve a modulation of an optical spring constant. Instead, it uses a dissipative mechanism with the driven cavity acting as an engineered reservoir. It can equivalently be viewed as a coherent feedback process, related to the quantum non-demolition measurement of a single mechanical quadrature. We analyze how to optimize the scheme, how the squeezing scales with system parameters, and how it may be directly detected from the cavity output. Our scheme is extremely general, and could also be implemented with, e.g., superconducting circuits.

15 min. break.

Invited Talk TT 98.6 Thu 16:30 BEY 81

Real-Space Tailoring of the Electron-Phonon Coupling in Ultra-Clean Nanotube Mechanical Resonators — •Shahal Ilani[1], Avishai Benyamini[1], Assaf Hamo[1], Silvia Viola Kusminskiy[2], and Felix von Oppen[2] — [1]Dept. of Cond. Matt. Phys., Weizmann Institute — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin

The coupling between electrons and phonons is at the heart of many fundamental phenomena in physics. In nature, this coupling is generally predetermined for both, molecules and solids. Although tremendous advances have been made in controlling electrons and phonons in engineered nanosystems, to date the control over the coupling between

these degrees of freedom is still widely lacking. Here we demonstrate the ability to fully tailor electron-phonon interactions in a new class of suspended carbon nanotube devices, in which we can form highly-tunable single and double quantum dots at arbitrary locations along a nanotube mechanical resonator. We find that electron-phonon coupling can be turned on and off by controlling the position of a quantum dot along the resonator. Using more elaborate double quantum dots we structure the interactions in real space to couple specific electronic and phononic modes. Exploiting this tailored coupling we measure the parity of phonons in real space and directly image their mode shapes. Interestingly, we demonstrate tailored coupling of phonons to internal electrons in an isolated system, decoupled from the random environment of the electronic leads, a crucial step towards fully-engineered quantum coherent electron-phonon systems.

TT 98.7 Thu 17:00 BEY 81

Microwave Cavity Readout of Graphene NEMS — •Peter Weber, Johannes Guettinger, Ioannis Tsioutsios, and Adrian Bachtold — ICFO-Institut de Ciencies Fotoniques, 08660 Castelldefels (Barcelona), Spain

Graphene is an interesting material for the realization of nano-electromechanical systems (NEMS), because of its high mechanical strength and its ultra low mass density. In optomechanical sideband cooling experiments [1] the low mass offers the advantage that graphene has a comparatively large motional amplitude in the quantum mechanical ground state. Additionally, mechanical nonlinearities of graphene could still remain significant in the quantum regime. We developed a new method to detect the mechanical vibrations of a graphene resonator by coupling it capacitively to a superconducting microwave cavity. The cavity resonance frequency is modulated by the graphene motion and leads to sideband peaks in the cavity spectrum [2]. In particular, we present fabrication, microwave readout and characterisation of few-layer graphene NEMS at millikelvin temperatures. The fabrication is based on a graphene transfere process on predefined gate structures being part of the superconducting cavity. Our measurements demonstrate, that microwave readout of graphene NEMS is a promising technique enabling the possibility to detect thermal vibrations as well as making cooling experiments feasible with graphene.

[1] J. D. Teufel et al., Nature 475, 359 (2011)
[2] X. Song et al., Nano Letters 12, 198 (2012)

TT 98.8 Thu 17:15 BEY 81

Coupled Graphene Mechanical Resonators — •Ioannis Tsioutsios[1,2], Joel Moser[1,2], José Antonio Plaza[3], and Adrian Bachtold[1,2] — [1]ICFO, Av. Carl Friedrich Gauss, 08860 Castelldefels, Barcelona, Spain — [2]ICN, CIN2-CSIC, Campus UAB, 08193 Barcelona, Spain — [3]IMB-CNM (CSIC), E-08193 Bellaterra, Barcelona, Spain

Coupled mechanical resonators show reach variety of non-linear dynamics such as synchronization and chaos. Moreover, they offer new strategies to improve the quality factor and detect charge and mass with high sensitivity. Such devices have been mainly fabricated form metallic and silicon-based materials using top-down micromachining.

Single mechanical resonators based on alternative materials like carbon nanotubes and graphene sheets have been demonstrated and show a wide variety of useful properties like very high resonant frequency, extremely high mass and force sensitivity, and strong mechanical nonlinearities. However, so far it has not been possible to use them as building blocks to create coupled resonator devices.

In this work, we demonstrate a multi-element resonant structure consisting of two graphene sheets linked by a carbon nanotube beam. The mechanical vibrations are actuated and detected electrically using the mixing technique. Two mechanical eigenmodes are measured, each corresponding to vibrations localized in a different graphene sheet. Coupling between the eigenmodes is observed and is evaluated by measuring the shift of the resonance frequency of one graphene sheet as a function of the vibration amplitude of the other.

TT 98.9 Thu 17:30 BEY 81

Intrinsic mode-coupling and thermalization in nanomechanical graphene drums — •Daniel Midtvedt[1], Zenan Qi[2], Alexander Croy[1], Harold S. Park[2], and Andreas Isacsson[1] — [1]Chalmers University of Technology, Sweden — [2]Boston University, Boston, MA, United States

Nanomechanical graphene resonators display strong nonlinear behavior, which leads to coupling between normal modes. This coupling allows for intermodal energy-transfer, which facilitates the redistribution of energy initially localized in a single mode. Further, the mode-coupling intrinsically limits the quality factor of the device. We study the mode-coupling in a circular graphene resonator using molecular dynamics and continuum mechanics. Mimicking a ring-down setup, the fundamental mode is excited with a given energy, and the time-evolution of this energy is computed. At $T > 0$, we find a relaxation rate independent of system size and proportional to $T^*/\epsilon_{\text{pre}}^2$, where T^* is the effective temperature and ϵ_{pre} is the pre-strain of the system [Midtvedt et al, arXiv:1309.1622]. At low temperatures, the system enters a metastable state where only very few low-frequency modes are excited, the life-time of which increases exponentially with decreasing excitation energy. This is similar to what is seen in the much studied Fermi-Pasta-Ulam (FPU) problem. We make a detailed comparison between the dynamics of a graphene drum and the FPU system, and propose to use graphene drums as test beds for FPU physics.

TT 98.10 Thu 17:45 BEY 81

Dissipation-induced entanglement and excitation transport in quantum nanomechanical systems — Aurora Voje, Andreas Isacsson, and •Alexander Croy — Department of Applied Physics, Chalmers University of Technology, Göteborg, Sweden

Nanoelectromechanical (NEM) resonators are important systems for the study of quantum phenomena in macroscopic, mechanical man-made objects. Only recently, cooling of NEM resonators to the ground state was experimentally demonstrated. We investigate possibilities to generate non-classical states in carbon-based resonators, which are highly promising for the study of nonlinear mechanical systems in the quantum regime. Our proposals are based on the presence of nonlinear (two-phonon) dissipation found in those systems. We show that the latter facilitates the emergence of non-classical states for a single oscillator [1] and leads to generation of entanglement of two oscillators, which are individually subject to two-phonon dissipation [2]. Finally, the implications and prospects for arrays of such NEM resonators are discussed.

[1] A. Voje, A. Croy, and A. Isacsson, NJP **15**, 053041 (2013).
[2] A. Voje, A. Isacsson, and A. Croy, PRA **88**, 022309 (2013).

TT 99: Graphene: Spintronics, Transistors, and Sensors (organized by HL)

Time: Thursday 15:00–18:00 Location: POT 081

TT 99.1 Thu 15:00 POT 081

Graphene's RF Potential: How harmful is the Zero Bandgap? — Kyle D. Holland[1], Navid Paydavosi[1], Neophytos Neophytou[2], •Diego Kienle[3], and Mani Vaidyanathan[1] — [1]Department of Electical and Computer Engineering, University of Alberta — [2]Institute for Microelectronics, Technical University of Vienna — [3]Institute of Theoretical Physics I, University of Bayreuth

With the aid of self-consistent quantum-mechanical simulations and simple expressions for the radio-frequency (RF) metrics, we examine the impact of a lack of a bandgap on limiting the RF potential of graphene transistors. Considering various RF figures of merit, we show that the lack of a bandgap leads to all RF metrics being optimal when the bias point is chosen such that the drain Fermi level aligns with the Dirac point at the midpoint of the channel. We further quantify the precise extent to which the lack of a bandgap limits the transistor's cutoff frequencies, an issue that has been flagged as requiring crucial attention to make graphene transistors competitive. For an 18-nm channel length, we show that the extrinsic unity-current-gain frequency could be improved by 300 GHz and the unity-power-gain frequency could be doubled if a bandgap could be introduced to reduce the output conductance to zero. [1] K. D. Holland, N. Paydavosi, N. Neophytou, D. Kienle, and M. Vaidyanathan, IEEE Trans. Nanotechnol. 12, 566 (2013).

TT 99.2 Thu 15:15 POT 081

Atomic layer deposited aluminum oxide on epitaxial graphene without surface activation — •Peter Wehrfritz[1], Florian Speck[2], Felix Fromm[1], Stefan Malzer[3], and Thomas Seyller[1] — [1]TU Chemnitz, Institut für Physik, Chemnitz, Deutschland — [2]FAU Erlangen-Nürnberg, Department Physik, Erlangen, Deutschland — [3]FAU Erlangen-Nürnberg, Angewandte Physik, Erlangen, Deutschland

Graphene with its high charge carrier mobility is a promising material for analog RF field effect transistors. The preparation of the required insulating layer is still challenging. Atomic layer deposition (ALD) has been extensively studied in the context of alternative dielectrics for silicon-based field effect transistors owing to its capabilities to produce high-quality, homogeneous oxide layers. However, nucleation of ALD growth is strongly suppressed on inert graphene surfaces.

In this contribution we present an approach to obtain conformal aluminum oxide (Al_2O_3) on epitaxial monolayer graphene on silicon carbide (SiC). We demonstrate that closed layers of Al_2O_3 can be deposited on the so called buffer layer. This buffer layer covered by ALD-Al_2O_3 can then be decoupled from the SiC substrate by means of hydrogen intercalation yielding quasi-freestanding monolayer graphene with an insulating dielectric on top. We investigated the quality of the graphene layer and ALD-Al_2O_3 using X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, AFM, and Hall effect measurements.

TT 99.3 Thu 15:30 POT 081

Spin-dependent negative differential resistance in composite graphene superlattices — •Christopher Gaul[1,2], Javier Munárriz[2], Andrey V Malyshev[2], Pedro A Orellana[3], Cord A Müller[4], and Francisco Domínguez-Adame[2] — [1]Max-Planck-Institut für Physik Komplexer Systeme, Dresden — [2]Universidad Complutense de Madrid, Spain — [3]Universidad Técnica Federico Santa María, Casilla 110 V, Valparaíso, Chile — [4]Fachbereich Physik, Universität Konstanz

We propose and study a compound system of a graphene nanoribbon and a set of ferromagnetic insulator strips deposited on top of it. The periodic array of ferromagnetic strips induces a proximity exchange splitting of the electronic states in graphene, resulting in the appearance of a superlattice with a spin-dependent energy spectrum. We find clear signatures of spin-dependent negative differential resistance. The electric current through the device can be highly polarized and both the current and its polarization manifest non-monotonic dependence on the bias voltage. The device operates therefore as an Esaki spin diode, which opens possibilities to design new spintronic circuits.

Phys. Rev. B 88, 155423 (2013)

TT 99.4 Thu 15:45 POT 081

Exchange coupling between localized defect states in graphene nanoflakes — •Matthias Droth and Guido Burkard — University of Konstanz, Germany

Graphene nanoflakes are interesting because electrons are naturally confined in these quasi zero-dimensional structures, thus eluding the need for a bandgap. Defects inside the graphene lattice lead to localized states and the spins of two such localized states may be used for spintronics. We perform a tight-binding description on the entire system and, by virtue of a Schrieffer-Wolff-transformation on the bonding and antibonding states, we extract the coupling strength between the localized states. The coupling strength allows us to estimate the exchange coupling, which governs the dynamics of singlet-triplet spintronics.

TT 99.5 Thu 16:00 POT 081

Novel fabrication method of lateral spin valve devices based on graphene on hexagonal boron nitride — Marc Drögeler[1], Frank Volmer[1], •Maik Wolter[1], Bernat Terrés[1], Kenji Watanabe[3], Takashi Taniguchi[3], Gernot Güntherodt[1], Christoph Stampfer[1,2], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany, EU — [2]Peter Grünberg Institute (PGI-8/9), Forschungszentrum Jülich, 52425 Jülich, Germany, EU — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Despite tremendous efforts in improving graphene-based spin transport devices the measured spin lifetimes are still orders of magnitude less than theoretically predicted. Contact-induced spin dephasing has recently been identified as the bottleneck for spin transport through Co/MgO spin injection and detection electrodes. It can, however, significantly be suppressed for devices with large contact resistance area products [1]. Simultaneously, a strong reduction of the charge carrier mobility is usually observed. We present a new method to fabricate graphene-based non-local spin valves on hexagonal boron nitride yielding spin lifetimes above 3 ns, spin diffusion length above 10 μm and large charge carrier mobilities above 30.000 cm^2/Vs.

[1] F. Volmer *et al.*, Phys. Rev. B **88**, 161405(R) (2013).

This work has been supported by DFG through FOR 912 and by EU through Graphene Flagship.

TT 99.6 Thu 16:15 POT 081

Suppression of contact-induced spin dephasing in graphene/Co/MgO_x spin-valve devices by successive oxygen treatments — Frank Volmer, •Christopher Franzen, Marc Drögeler, Eva Maynicke, Nils von den Driesch, Maren Laura Boschen, Gernot Güntherodt, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

By successive oxygen treatments of graphene non-local spin-valve devices we achieve a gradual increase of the contact resistance area products R_cA of the Co/MgO_x spin injection and detection electrodes and a transition from linear to non-linear characteristics in the corresponding dV/dI-curves. With this manipulation of the contacts both spin lifetime and amplitude of the spin signal can significantly be increased by a factor of seven in the same device. This demonstrates that contact-induced spin dephasing is the bottleneck for spin transport in graphene devices with small R_cA values [1]. With increasing R_cA we furthermore observe the appearance of a second charge neutrality point (CNP) in gate dependent resistance measurements. Simultaneously we observe a decrease of the gate voltage separation between the two CNPs. The strong enhancement of the spin transport properties as well as the charge transport will be explained by the same gradual suppression of a Co/graphene interaction by improving the oxide barrier.

Work was supported by DFG/FOR 912 and EU/Graphene Flagship.

[1] F. Volmer *et al.* Phys. Rev. B **88**, 161405 (2013).

Coffee break (15 min.)

TT 99.7 Thu 16:45 POT 081

Development of an amperometric H2O2 sensor based on graphene — •Masoumeh Sisakhti[1], Alexander Zöpfl[2], Jonathan Eroms[1], Thomas Hirsch[2], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik,Universität Regensburg —

[2]Institut für analytische Chemie,Universität Regensburg

The precise detection of Hydrogen peroxide (H2O2) has been a widely researched topic and the focus of a vast amount of attention, owing to its vital role in biological systems, as well as its utility in food, pharmaceutical and biochemical industries.

The objective of this work is to investigate a novel nonenzymatic, amperometric sensor for reliable determination of H2O2 based on graphene.

We produced graphene sensors based on three types of graphene: exfoliated graphene, CVD grown graphene and reduced graphene oxide and carried out cyclic voltammetry and amperometric experiments using a CH Instrument electrochemical analyzer. We demonstrate that all three graphene materials show excellent sensitivity to the catalytic reduction of H2O2 and are able to detect H2O2 concentrations down to 0.1 mM. rGO as well as graphene prepared by CVD are promising candidates for sensor applications since they are able to detect hydrogen peroxide with high sensitivity at moderate electrode potentials. Both materials are superior in the signal-to-noise ratio compared to exfoliated graphene. A further conjugation of enzymes to the defects within the carbon nano material as well as the assembly of 2D-layered composite materials will be perspective to biosensor applications.

TT 99.8 Thu 17:00 POT 081

Controlled chemical modification of graphene for applications in biosensing — •Marco R. Bobinger, Max Seifert, Anna Cattani-Scholz, and Jose A. Garrido — Walter Schottky Institut, Technische Universität München, Germany

Given its exceptional chemical and mechanical stability as well as its unique electronic properties, graphene is an extremely promising platform for biosensors. In order to use graphene in the biological environment and to improve sensing specificity and device performance, chemical functionalization schemes are needed to allow stable grafting of organic and bioorganic molecules onto graphene. In particular for applications in bioelectronics, the influence of the chemical functionalization of graphene on the generation of defects, strain, and doping has to be balanced with the desired modulation of the electronic properties of the produced graphene-organic hybrid material. In this work the effect of the controlled chemical modification of large area CVD-grown graphene via ozone treatment is investigated. This process creates sp3-like defects, related to covalently bound surface groups, e.g. OH-. Such ozone-treated surfaces are characterized by Raman- and X-ray photoelectron spectroscopy in order to investigate the degree of surface modification and the chemical composition of the surface terminations. The generated anchor groups are further used as binding sites for the modification of graphene with organic molecules.

TT 99.9 Thu 17:15 POT 081

Functionalization of Graphene for Bioelectronic Applications — •Alina Lyuleeva[1], Lucas Hess[1], Frank Deubel[2], and Jose Antonio Garrido[1] — [1]Walter Schottky Institut, TU München, 85748 Garching — [2]Wacker Chemie AG, 81379 München, Germany

With its fascinating structural, chemical and electronic properties, graphene outperforms many materials and is expected to pare the way for a vast range of applications such as transparent electrodes, energy storage devices, high-frequency electronics, or biosensors. The performance of the devices for these various applications can be enhanced with the help of surface functionalization, allowing a versatile modification of the properties of this material. Here, we report on the covalent and thus robust functionalization of CVD graphene with enzymes for the development of novel devices for bioelectronic applications. Graphene solution-gated field-effect transistors (SGFETs) are functionalized using a controlled grafting of polymethacrylate (PMA) brushes. We will show how this material platform can be used for further functionalization with the enzyme acetylcholinesterase (AChE). The enzymes' activity can be monitored with the modified-graphene transistor allowing both the measurement of the concentration of the neurotransmitter acetylcholine as well as the inhibition of the enzyme by neurotoxins such as nerve agents or pesticides. Our study demonstrates the potential of graphene-based functionalized transistors for biosensing and bioelectronic application.

TT 99.10 Thu 17:30 POT 081

Coupling of electrogenic cells to graphene devices — Michael Sejer Wismer, Felix Rolf, Damia Viana, •Martin Lottner, Lucas Hess, and Jose A. Garrido — Walter Schottky Institut - Technische Universität München, Am Coulombwall 4, 85748 Garching

In this contribution, we will demonstrate the electrical coupling between electrogenic cells and graphene-based solution-gated field effect transistors (SGFETs). To this end, HEK293 and HL1 cells were cultured on 8x8 arrays of graphene SGFETs with feature sizes of 10 mu x 20 mu. Graphene was grown by chemical vapour deposition (CVD) on copper foil and transferred to sapphire substrates, on which field effect transistors were fabricated using standard semiconductor technology. The devices show a typical maximum transconductance of >100 muS at 0.1 V drain-source voltage. This value is stable over months of storage. HEK293 cells were used to analyse the electrical coupling between cells and transistors. A model considering the distribution of ions within the cell transistor cleft and ion sensitivity of the graphene SGFETs fits the measured signals very well. Additionally, nano-transistors were defined by e-beam lithography, which allowed feature sizes down to 50 nm. With these nanoscale devices a signal-to-noise ratio of 2.5 could be obtained within single recordings of HL1 activity. Analysis of the measured ionic currents allowed to draw conclusions about local inhomogeneities of ion channel concentration within the membrane. Further, experiments for the stimulation of PC12 cells using arrays of graphene SGFET and graphene-based microelectrode arrays (MEAs) are under preparation.

TT 99.11 Thu 17:45 POT 081

Graphene solution-gated field effect transistors on flexible substrates — •Andrea Bonaccini Calia, Benno M. Blaschke, Lucas H. Hess, Max Seifert, and Jose A. Garrido — Walter Schottky Institut, Technische Universität München, Germany

Graphene based solution-gated field effect transistors (SGFETs) hold great promise for biosensors and bioelectronic applications. Due to its unique combination of electronic, mechanical, and chemical properties, such as high charge carrier mobility, flexibility and good biocompatibility, graphene has been shown to be an excellent material for sensing in electrolyte environments. Sensors based on graphene SGFETs have already been realized on rigid substrates for various analytes, as well as for the detection of cell signals. However, this technology hold some severe problems for biomedical and in vivo applications. One of the major problems is the rigidity of the substrate itself, which does not allow a proper mechanical matching to the biological tissue, resulting in the formation of scar tissue. Therefore, flexible devices are currently considered as a major step towards the development of more biocompatible implants. In this work, an array of graphene SGFETs is fabricated on a flexible polymer substrate. We present a detailed electrical characterization of the flexible graphene SGFETs in electrolyte and compare their performance to graphene SGFETs on rigid substrates. In addition, we analyze the effect of changes in the electrolyte's pH and ionic strength on the transistor performance and present a model to explain the obtained results. Furthermore, the low-frequency noise performance of graphene devices on flexible substrates is discussed.

TT 100: Graphene: Adsorption, Intercalation, Doping (organized by O)

Time: Thursday 16:00–18:45 Location: WIL C107

TT 100.1 Thu 16:00 WIL C107

Covalent binding of single iron phtalocyanine molecules to graphene on Ir(111) — •Simon J. Altenburg[1], Shiri R. Burema[2], Bin Wang[3], Richard Berndt[1], and Marie-Laure Bocquet[2,4] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Université de Lyon, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, CNRS, F69007 Lyon, France — [3]Department of Physics & Astronomy, Vanderbilt University, Nashville, TN 37235 — [4]Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

Single iron phtalocyanine (FePc) molecules on graphene on Ir(111) are studied by low temperature scanning tunneling microscopy. The molecules are either unperturbed and weakly coupled to the substrate or bound to graphene by a lobe in a specific region of the moiré unit cell. Concomittant density functional calculations reveal that the binding between the FePc lobe and graphene is the result of a new kind of cyclization reaction. This reaction is activated in certain regions of the moiré unit cell by the presence of the iridium substrate.

TT 100.2 Thu 16:15 WIL C107

Adsorption of Pentacene on Epitaxial Graphene and BN — •Alexei Nefedov[1], Wenua Zhang[1,2], Hikmet Sezen[1], Alexandr Fedorov[3], Nikolay Verbitskiy[4], Alexander Grüneis[3,4], and Christof Woell[1] — [1]Institute of Funcional Interfaces, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]NSRL, Hefei, China — [3]IFW, Dresden, Germany — [4]University of Vienna, Vienna, Austria

Smooth interfaces are a prerequisite for future high-performance and low-cost organic electronic devices based on small conjugated molecules. Since all important charge transport processes are confined to the first several monolayers, the quality of the first layer plays a key role on device performance. Pentacene stands out as a model molecule among organic semiconductors due to its ability to form well-ordered films showing a high field effect mobility. Moreover, the morphology of the first layer of a thin Pn film is known to be strongly influenced by the substrate termination, which further decisively affects the interfacial charge transport properties. Thus, information on the molecular orientation of pentacene in a case of (sub)monolayer coverages can provide a key information on improvement of device performance. In this study the adsorption of pentacene on a single layer of graphene or boron nitride (BN) has been investigated by means of XPS and NEXAFS spectroscopy. The experiments were performed on the HE-SGM beamline at BESSY II in Berlin. It was found that pentacene molecules demonstrate a dependence of their orientation and electronic structure on the coverage.

TT 100.3 Thu 16:30 WIL C107

Wetting properties of parahexaphenyl on exfoliated graphene — •Markus Kratzer[1], Stefan Klima[1], Borislav Vasić[1], Aleksandar Matković[2], Marijana Milićević[2], Rados Gajić[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben,Franz Josef Straße 18, 8700 Leoben, Austria — [2]Institute of Physics, University of Belgrade, Pregrevica 118 P.O. Box 68, 11080 Belgrade, Serbia

Graphene (Gr) bears potential to serve as transparent and flexible electrode material in organic electronics. Therefore, understanding of the growth of organic thin films on it is essential. Here, we investigated the growth morphology of films formed by the rodlike para-hexaphenyl (6P) molecule on Gr as a model system. As substrates exfoliated graphene transferred onto a silicon oxide support were used. Submonolayer amounts of 6P were deposited by means of hot-wall epitaxy between 333 K and 393K. The evolving film morphologies, investigated by atomic-force microscopy (AFM), exhibited a strong dependence on temperature and number of supporting Gr layers. At 333 K, needle like structures - which are known to be composed of flat lying molecules [1]- and islands composed of upright standing molecules coexist on the Gr. For the higher temperatures solely needles, forming networks, are found. The needles forming at 363 K exhibit an increasing dewetting with increasing number of Gr layers which is attributed to Gr layer dependent changes in surface energy, diffusion properties and preferential adsorption sites.

[1] C. Teichert et al. Appl. Phys. A 82 (2006) 665.

TT 100.4 Thu 16:45 WIL C107

H-adsorption and H_2-splitting on graphene/SiC(0001) — •Gabriele Sclauzero and Alfredo Pasquarello — École Polytechnique Fédérale de Lausanne (EPFL), Lausanne (Switzerland)

High-quality graphene grown epitaxially on SiC(0001) can be regarded as a convenient template for the realization of graphene-based electronics. However, the presence of a carbon "buffer" layer buried at the interface between the SiC surface and the epitaxial graphene is detrimental to the electronic transport properties of graphene. Hydrogen intercalation at high temperatures can be used to convert the buffer layer into a quasi-free standing graphene lying directly above a H-saturated SiC(0001) surface, which provides a much more effective decoupling from the substrate.

Here, the processes of H-adsorption and H_2-splitting at the graphene/SiC(0001) interface is addressed through first-principles atomistic simulations based on realistic interface models, including the experimentally observed $6\sqrt{(3)}\times 6\sqrt{(3)}R30°$ reconstruction. Our main finding is a great enhancement of the chemical reactivity of the carbon buffer layer with respect to pristine graphene, as a result of the partial sp^2 to sp^3 rehybridization of the C atoms in the buffer. H-binding energies on threefold-coordinated C atoms of the buffer are three-to-four times larger than on graphene and H_2-splitting becomes an exothermic process, with activation barriers that can be up to four times smaller than on graphene. On favorable sites, energy barriers can become as low as 1 eV and are in agreement with the observation of atomic-H intercalation also when H_2 is used as hydrogen source.

TT 100.5 Thu 17:00 WIL C107

Deuterium adsorption on (and desorption from) SiC(0001)-(3x3), (R3xR3)R30°, (6R3x6R3)R30° and quasi-free-standing graphene obtained by hydrogen intercalation — •Bocquet F.C.[1], Bisson R.[2], Themlin J.-M.[3], Layet J.-M.[2], and Angot T.[2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich - 52425 Jülich, Germany — [2]Aix-Marseille Université, PIIM, CNRS, UMR 7345, 13013 Marseille, France — [3]Aix-Marseille Université, IM2NP, 13397, Marseille, France and CNRS, UMR 7334, 13397, Marseille - Toulon, France

I present a comparative High-Resolution Electron Energy-Loss Spectroscopy (HREELS) study on the interaction of atomic hydrogen and deuterium with various reconstructions of SiC(0001). We show that deuterium passivation of the (3x3) is only reversible when exposed to atomic deuterium at a surface temperature of 700 K since tri- and dideuterides, necessary precursors for silicon etching, are not stable at this temperature. On the other hand, we show that the deuteration of the (R3xR3)R30° is always reversible because precursors to silicon etching are scarce on the surface [1]. Further, the comparison of the deuterium binding in the intercalation layer of quasi-free-standing graphene with the deuterated (R3xR3)R30° surface provides some indication on the bonding structure at the substrate intercalation layer [1,2].

[1] F.C. Bocquet et al. J. Phys. D: Appl. Phys. (2014) in press
[2] F.C. Bocquet et al. Phys. Rev. B. 85 (2012) 201401

TT 100.6 Thu 17:15 WIL C107

Charge doping induced phase transitions in hydrogenated and fluorinated graphene — •Tim Wehling[1,2], Bernhard Grundkötter-Stock[2], Bálint Aradi[2], Thomas Niehaus[3], and Thomas Frauenheim[2] — [1]Institute for Theoretical Physics, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Material Science, Universität Bremen, Am Fallturm 1, 28359 Bremen, Germany — [3]Department of Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We show that charge doping can induce transitions between three distinct adsorbate phases in hydrogenated and fluorinated graphene. By combining ab initio, approximate density functional theory and tight binding calculations we identify a transition from islands of C_8H_2 and C_8F_2 to random adsorbate distributions around a doping level of ± 0.05 e/C-atom. Furthermore, in situations with random adsorbate coverage, charge doping is shown to trigger an ordering transition

where the sublattice symmetry is spontaneously broken when the doping level exceeds the adsorbate concentration. Rehybridization and lattice distortion energies make graphene which is covalently functionalized from one side only most susceptible to these two kinds of phase transitions. The energy gains associated with the clustering and ordering transitions exceed room temperature thermal energies.

TT 100.7 Thu 17:30 WIL C107

Graphene Oxide Formation by Adsorption and Photolysis of NO_2 and SO_2 on Graphene/Ir(111) — •Stefan Böttcher, Hendrik Vita, and Karsten Horn — Fritz-Haber Institute of the Max-Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Graphene oxide is a widely discussed precursor for the technological application of graphene-based systems; for example, its controlled reduction into graphene may lead to a tunable band gap. We report on the formation of oxidized graphene layers on Ir(111) by adsorption and photodissociation of NO_2 and SO_2 at low temperatures. Both adsorbates induce atomic oxygen on the surface when irradiated with intense UV light, leading to an oxidation of the graphene layer. The method presented here is expected to be less intrusive compared for example to oxygen bombardment methods. We also believe the photon induced oxidation to be more selective compared to other physical or wet chemical methods. A band gap opening at room temperature is observed, showing that the graphene oxide phase is also stable above 100 K. High quality graphene can be recovered after annealing, judged by the reappearance of its core and valence level spectral features. Apart from the selective formation of the epoxidic phase, the reaction can also be driven towards a metastable oxide phase from NO_2 using low photon flux. SO_2 on the other hand produces fragments upon dissociation, which have a strong influence on the hybridization state of the graphene backbone.

TT 100.8 Thu 17:45 WIL C107

Tuning the van der Waals Interaction of Graphene with Molecules by Doping — •Felix Huttmann[1], Antonio Javier Martinez-Galera[1], Nicolae Atodiresei[2], Vasile Caciuc[2], Stefan Blügel[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [2]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

Strong n-doping of graphene on its epitaxial substrate can be introduced via intercalation of highly electropositive elements such as Cs and Eu, and has recently been shown to lead to reduced binding energy for electropositive, ionic adsorbates [1].

Here, we explore tuning of graphene's van der Waals (vdW) interaction with adsorbates via doping. Employing an all in-situ surface science approach, we find by scanning tunneling microscopy and thermal desorption spectroscopy a significantly higher binding energy on n-doped as opposed to undoped graphene for the vdW-bonded molecules benzene and naphthalene. This is just opposite to the case of electropositive, ionic adsorbates. Based on the model character of these simple pi-conjugated molecules [2], we propose that the strength of the van der Waals interaction is modified by doping. The experimental results are compared to density functional calculations, including van der Waals interactions.

References:
[1] S. Schumacher et al., Nano Lett. 13, 5013 (2013)
[2] S. D. Chakarova-Käck et al., Phys. Rev. Lett. 96, 146107 (2006)

TT 100.9 Thu 18:00 WIL C107

Li intercalation at the graphene/Cu interface: An electronic structure view of synchrotron-based spectroscopy — •Liang Zhang[1,2], Jinghua Guo[2], and Junfa Zhu[1] — [1]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, 230029, China — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA

The synthesis of graphene on metal surfaces (such as Ni, Pd, Ru or Cu) by chemical vapor deposition (CVD) is one of the most promising, inexpensive and readily accessible methods to prepare single-layer graphene, which is a prerequisite for the fabrication of graphene-based electronic devices. In particular, graphene grown on Cu foils over large areas has allowed access to high quality of this material.

In this presentation, we report our recent studies on the electronic structure of graphene/Cu and Li-intercalated graphene/Cu by synchrotron-based spectroscopy. The results indicate a high degree of alignment and a slight corrugation/rippling of the graphene layer on Cu. The deposition of Li atoms on graphene surface under ultrahigh vacuum condition at room temperature results in a charge transfer from the adsorbed Li atoms to graphene. After annealing the as-deposited Li/graphene/Cu sample at 300 °C for 10 min, the Li atoms intercalate into the interface of graphene/Cu. These interfacial Li atoms show a strong passivation from oxidation environment due to the protection of graphene layer.

TT 100.10 Thu 18:15 WIL C107

Progressive nitrogen-doping of graphene on SiC(0001) — •Mykola Telychko, Pingo Mutombo, Martin Ondráček, Prokop Hapala, Jan Berger, Pavel Jelinek, and Martin Švec — Institute of Physics ASCR, Cukrovarnická 10, Praha, Czech republic

Doping of epitaxial graphene on SiC substrates was achieved by direct nitrogen ion implantation and stabilization at temperatures above 1300K. Scanning tunneling microscopy reveals very well-defined single substitutional defects on single and bilayer graphene. Repeated nitrogen implantation and stabilization leads to formation of double defects, which comprise of two nitrogen defects in a second-nearest-neighbour (meta) configuration. DFT calculations and scanning tunneling microscopy simulations are used to evaluate the electronic properties and to explain varying contrast of these defects in the atomically-resolved images, depending on the probe type. A mechanism of defect formation is proposed.

TT 100.11 Thu 18:30 WIL C107

Electronic and magnetic properties of cobalt interaction with graphene on Ir(111) — Hendrik Vita, Stefan Böttcher, and •Karsten Horn — Fritz-Haber-Institut of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany

The interaction of graphene with transition metal surfaces has attracted much interest because these are ideal templates for the growth of high quality films. Ferromagnetic substrates such as Ni(111) and Co(0001) are interesting since graphene grown on these surfaces can act as a spin filter. We have earlier found that the proximity of graphene to the ferromagnetic Ni(111) substrate induces a sizeable magnetic moment in the carbon π -states as determined from carbon K edge XMCD. Here we study the influence of thin layers of ferromagnetic Co sandwiched between Ir(111) and graphene with consequences for the magnetic properties expected. We find that the cobalt films show ferromagnetic behavior even for very low thicknesses. In order to study the behavior of magnetic heterostructures utilizing graphene as an interlayer we examine sandwich systems consisting of a thin layer of cobalt on top graphene/Ni(111). Using element-specific XMCD and hysteresis measurements it is possible to gain insight into the magnetic coupling across this magnetic heterostructure.

TT 101: Transport - Poster Session

Time: Thursday 15:00–19:00 Location: P2

TT 101.1 Thu 15:00 P2

Non-equilibrium transport through a QD using Keldysh-fRG — •Dennis Schimmel[1,2], Florian Bauer[1,2], Jan Heyder[1,2], and Jan von Delft[1,2] — [1]Arnold Sommerfeld Center München — [2]LMU München, Germany

The functional renormalization group (fRG) is a powerful resummation technique which recasts the computation of diagrams into a diffential equation. We apply the non-equilibrium (Keldysh) version of it to a single impurity Anderson model and analyze various choices of the flow parameter. We focus on the weakly interacting region to establish the quality of the fRG-scheme. From previous studies, it is known that the truncation involved in fRG schemes inevitably leads to a violation of the particle-conservation law. As a consequence of this, physical quantities need to be computed without resorting to derivations using the particle-conservation law, unless the quantitative violation is negligible. The scheme used here can readily be generalized to quantum chain models, e.g. to treat nonequilibrium transport through (weakly) interacting quantum wires.

TT 101.2 Thu 15:00 P2

Nonequilibrium BCS-Anderson model- ISPI approach — •Stephan Weiss and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

Using the scheme of iterative summation of real-time path integrals (ISPI) [1-2], we compute the $I(V)$ characteristics of a single spin-degenerate quantum dot tunnel coupled to superconducting (BCS) leads. By means of a Hubbard-Stratonovich transformation, the path integral is mapped to a finite spin sum inheriting nonlocal-in-time correlations among the spins. Anomalous Green's functions components are truncated according to the established rules [1-2] on the same footing as the normal Keldysh components. The remaining spin-path summation is capable for the ISPI scheme. Since we treat tunneling exactly to all orders, we are able to resolve the subgap structure in terms of multiple Andreev reflections (MAR). We present results of the $I(V)$ for the non-perturbative regime ($U/\Gamma, T/\Gamma, eV/\Gamma \gg 1$), whereas in the noninteracting limit we compare our results to previous analytical results [3]. For $U/\Gamma \ll 1$ we compare to a perturbative calculation [4] as well as to a real-time diagrammatic approach for $\Gamma_S \ll 1$ [5].

[1] S. Weiss, et al., Phys. Rev B, **77**, 195316, (2008).
[2] S. Weiss, et al., Phys. Status Solidi B **250**, 2298 (2013).
[3] A. Levy-Yeyati, et al., Phys. Rev. B **55**, 6137(R) (1996).
[4] L. Dell Anna, et al., Phys. Rev. B **77**, 104525 (2008).
[5] M. Governale, et al., Phys. Rev. B **77**, 134513 (2008).

TT 101.3 Thu 15:00 P2

Exact solutions of collective heat transport — •Gabriel Topp, Tobias Brandes, and Gernot Schaller — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

In the last decades a lot of different tools to describe transport processes in open quantum systems have been developed. Prominent examples include e.g. master equations or Green's functions. The model of a single impurity coupled to two reservoirs is therefore a well-known problem [1].

We show that several collective transport setups can be mapped to the single impurity model. Using exact solutions of the Heisenberg equations of motion we calculate stationary transport properties, both in fermionic and bosonic systems. With our proper solutions we investigate the validity of simple markovian master equations.

[1] G. Schaller, P. Zedler, and T. Brandes, Phys. Rev. A 79, 032110 (2009)

TT 101.4 Thu 15:00 P2

Electronic current switching at finite temperature by magnetic focusing in a soft-wall quantum dot — •Christian Morfonios and Peter Schmelcher — Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

We demonstrate a mechanism enabling efficient switching of the finite-temperature magnetoconductance in an electronic quantum dot with designed soft-wall confinement. The mechanism relies on the effective increase of the available area of motion within the dot with increasing energy, so that the magnetically deflected electron density retains invariant spatial characteristics at an optimal low field strength. Heavily suppressed background transmission can then be achieved along the entire ground propagation channel of the incoming electrons, while resonant states couple very weakly to the attached leads, even for a large number of dot levels. The presence of soft walls in an elliptically shaped quantum dot simultaneously aids collimated electron transport and high transmission for zero field, leading to efficient finite-temperature magnetoconductance switching at linear response. The effect is investigated in terms of the influence of the width of the soft wall and its profile at given temperatures, as well as for arrays of connected dots.

TT 101.5 Thu 15:00 P2

Spin-thermoelectric effects in metals — •Sebastian Tölle[1], Cosimo Gorini[2], and Ulrich Eckern[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Service de Physique de l'Etat Condensé, CEA-Saclay, 91191 Gif sur Yvette, France

Via spin-orbit coupling, and even in the absence of magnetic fields, a temperature gradient applied to a two-dimensional electron gas can generate both spin currents and spin polarizations. These phenomena are the thermal counterpart of well-known ones such as the spin Hall effect and the voltage-induced spin polarization, and belong to the fast growing field of spin caloritronics. We study them by means of a generalized Boltzmann equation which takes into account spin-orbit coupling of both intrinsic and extrinsic origin within an $SU(2)$ formulation. We show, in particular, that a thermal gradient induces an in-plane spin polarization and a spin current transverse to the field and polarized out-of-plane (spin Nernst effect). We find that the interplay between intrinsic and extrinsic mechanisms is critical, and that the relation between spin currents and spin polarizations – well understood in the presence of simple electric drivings – is nontrivially affected by the thermal driving.

TT 101.6 Thu 15:00 P2

Magnetotransport in ferromagnetic Mn_5Ge_3 and $Mn_5Ge_3C_{0.8}$ thin films — •Christoph Sürgers[1], Patrick Winkel[1], Gerda Fischer[1], Inga A. Fischer[2], and Li-Te Chang[3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76049 Karlsruhe — [2]Institut für Halbleitertechnik, Universität Stuttgart, 70569 Stuttgart — [3]Device Research Lab., Dept. of Electrical Engineering., University of California, Los Angeles, CA 90095, USA

Ferromagnetic Mn_5Ge_3 and $Mn_5Ge_3C_{0.8}$ compounds with Curie temperatures of $\approx$ 300 K and 450 K, respectively, are potential electrode-materials for spin injection into Si and Ge due to their high resistivity and compatibility with CMOS technology [1]. We investigate the temperature dependence of the anisotropic magnetoresistance (AMR) and the anomalous Hall effect of sputtered thin films. The AMR changes sign from negative to positive with increasing temperature with a concomitant increase and sign change of the ordinary Hall coefficient R_0 while the anomalous Hall coefficient is independent of temperature. The correlation between the temperature dependence of R_0 and of the AMR ratio is discussed by considering a change of the different contributions arising from the electron-like minority-spin band and the hole-like majority-spin band to the conductance with increasing temperature. Magnetoresistance measurements in the Hanle geometry on $Mn_5Ge_3C_{0.8}$ electrodes deposited on highly doped n-Ge reveal that spin injection and spin extraction occur, however, at temperatures below 15 K.

[1] I. A. Fischer et al., Semicond. Sci. Technol. **28**, 125002 (2013)

TT 101.7 Thu 15:00 P2

Conductance Quantization in Rare-Earth-Metal Nanocontacts — •Oliver Berg[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76049 Karlsruhe — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe

We present conductance measurements of Gd, Dy, and Ce obtained on mechanically controlled break-junctions (MBCJ) made from polycrystalline wires at l-He temperatures. The contact formation and switching between metallic and tunneling conductance G is investigated in dependence of the electrode distance Δx. From a number of measurements of $G(\Delta x)$, exhibiting conductance plateaus, we ob-

tain conductance histograms. We focus on the conductance G^* of the last plateau before with increasing Δx, G enters the tunneling regime. While for Gd and Dy the last "plateau" occurs at $G^* \approx 0.6\,G_0$ and $0.9\,G_0$ ($G_0 = 2e^2/h$), respectively, $G^* \simeq 1.7\,G_0$ is observed for Ce. For Gd and Dy the $4f$ state is far below the Fermi level and does not contribute to the electronic transport. A possible explanation for the large G^* value of Ce is the additional contribution from the $4f$ state being shifted toward the Fermi level, when cooling the sample through the $\gamma - \alpha$ phase transition.

TT 101.8 Thu 15:00 P2

Renormalization of subband anticrossings in interacting quantum wires with spin-orbit interactions — •Tobias Meng[1], Jelena Klinovaja[1,2], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

We discuss how electron-electron interactions renormalize the anticrossings between different subbands in quantum wires with spin-orbit interactions. Depending on the wire's parameters, interactions may either increase or decrease the width of the anticrossings. When the anticrossings are closed using a special combination of Rashba and Dresselhaus spin-orbit interactions, their width tends to zero as an interaction dependent power law of the spin-orbit couplings, which is a consequence of Luttinger liquid physics. Monitoring the closing of the anticrossings would allow to directly measure the related renormalization group (RG) scaling dimensions in an experiment.

TT 101.9 Thu 15:00 P2

Quantum transport and response to electric fields in non-Abelian systems with spin-orbit coupling and magnetic fields — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Electronic transport in spin-polarized systems with impurity and electron-electron interactions as well as spin-dependent meanfields is discussed. The appropriate quantum kinetic equation for SU(2) are derived with special consideration of spin-orbit coupling and magnetic fields. Linearizing, the spin and density dynamical responses to electric fields (polarized light) are calculated and several effects are described: spin-Hall, anomalous Hall and optical Hall effect, spin-heat coupling, extended quasiparticle picture and polarization effect from correlated density. Clarifying the relative importance of meanfield and scattering correlations, new modes due to magnetic fields and spin-orbit coupling are found.

[1] EPL 104 (2013) 2700

TT 101.10 Thu 15:00 P2

Orbital dependent absorbing boundary conditions for nanoscale spin transport — •Sebastian Frank and David Jacob — MPI of Microstructure Physics, Weinberg 2, 06120 Halle/Saale, Germany

Atomic and molecular junctions containing magnetic atoms are an intriguing field of research that may give rise to the development of nanoscale spintronic devices [1]. This type of system is particularly challenging: it is infinite, but non-periodic in the transport direction. In order to model the effect of the leads, we implement a novel methodology making use of absorbing boundary conditions (ABC) [2,3] within the ab initio quantum transport method for nanoscale devices based on DFT [4]. Our method allows us to determine orbital dependent ABC. This is crucial for the correct description of transition metal leads which have s-, p- and d-orbital channels. The orbital-dependence is included via a non-empirical criterion. The two free parameters are chosen by comparision with exact results for infinite chains and prove to be universal, i.e. have to be chosen only once and can then be applied to all types of systems. We apply our method to transition metal nanocontacts and find smooth density of states and transmission functions in agreement with experimental data.

[1] A. R. Rocha, Nature Mater. 4 (2005) 335
[2] A. Goldberg et al., J. Phys. B 11 (1978) 3339
[3] F. Evers et al., CFN Lectures on Functional Nanostructures 2 (2011) 27
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TT 101.11 Thu 15:00 P2

Electronic Properties of Spirobifluorene Molecules — •Amin Karimi[1], Michal Valasek[2], Fabian Pauly[1], Maya Lukas[2], Marcel Mayor[2], and Elke Scheer[1] — [1]University of Konstanz — [2]Karlsruhe Institute of Technology

The knowledge about the fundamental correlations between a molecule's functional chemical groups, its contacts, and surroundings and the resulting electronic properties is imperative for the design of future molecular electronic building blocks [1,2]. The electronic properties of multipodal molecules have been studied in recent years mainly by inserting them into mechanically controlled break junctions (MCBJ) [3] or by scanning tunneling microscopy (STM) [4]. We present charge transport measurements through single spirobifluorene tripodal molecules, performed with the help of the low-temperature MCBJ technique. Inelastic electron tunneling spectra are measured to study the influence of vibronic coupling on the conductance of molecular junctions and to obtain in this way knowledge about the contact geometry and electrode-molecule coupling.

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TT 101.12 Thu 15:00 P2

Transport measurements of diarylethene molecules with long conjugated linkers in solution — •Katharina Luka-Guth[1], Daniel Schmid[1], Jannic Wolf[2], Thomas Huhn[2], and Elke Scheer[1] — [1]Universität Konstanz, FB Physik — [2]Universität Konstanz, FB Chemie

We measure the conductance of several different diarylethene molecules via the mechanically controllable break junction (MCBJ) technique at room temperature. Diarylethenes are photochromic molecules that undergo a ring-opening ring-closure reaction upon irradiation with light with suitable wavelength. This reaction changes the conjugation of the pi-system of the molecules that are therefore discussed as optically driven molecular switches. To measure their transport properties, a solution of molecules is directly applied to the gold electrodes in a glass pipette sealed by a PDMS gasket. While opening and closing the MCBJ, molecules get into contact with the electrodes and bridge the gap between two electrodes. Simultaneously the conductance of the molecules is measured, from which conductance histograms are calculated. We compare our results to previous findings. The information is completed by current-voltage characteristics that enable us to determine the position of the current-dominating molecular orbital. We compare our findings with those from previous studies on diarylethenes with shorter linkers [1,2]. Furthermore, we discuss the role of the solvent.

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TT 101.13 Thu 15:00 P2

Switching the Conductance of a Molecular Junction using a Proton Transfer Reaction — •Chriszandro Hofmeister[1], Pedro B. Coto[1], Óscar Rubio-Pons[1], Andrzej L. Sobolewski[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland

The possibility of using single molecules as components in electronic circuits has motivated intensive experimental and theoretical research on the conductance characteristics of these systems. In this contribution, we present theoretical results suggesting that a molecular junction can work as a nano switch [1] using a mechanism that based on a ground state proton transfer reaction [2]. Employing density functional theory and the Landauer transport theory we show that the keto and enol forms of our selected molecule have different conductance characteristics which can be explained in terms of the different conjugation patterns exhibited by both tautomers. We also provide a proof of principle showing that both forms can be reversibly interconverted using an external electrostatic field. The dynamics of the process is investigated using a quantum master equation approach.

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TT 101.14 Thu 15:00 P2

Effects of electronic correlations and magnetic field on a molecular ring out of equilibrium — •Martin Nuss, Enrico Arrigoni, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, Graz University of Technology

We study effects of electron-electron interactions on the steady-state characteristics of a hexagonal molecular ring in a magnetic field, as a model for a benzene molecular junction. The system is driven out of equilibrium by applying a bias voltage across two metallic leads. We employ a model Hamiltonian approach to evaluate the effects of on-site as well as nearest-neighbor density-density type interactions in a physically relevant parameter regime. Results for the steady-state current, charge density and magnetization in three different junction setups (para, meta and ortho) are presented. Our findings indicate that interactions beyond the mean-field level renormalize voltage thresholds as well as current plateaus. Electron-electron interactions lead to substantial charge redistribution as compared to the mean-field results. It is shown that electron-electron interactions do not qualitatively change the current-voltage characteristics in magnetic fields as compared to the noninteracting case in a charge-neutral setup. We identify a strong response of the circular current on the electronic structure of the metallic leads. Our results are obtained by steady-state Cluster Perturbation Theory, a systematically improvable approximation to study interacting molecular junctions out of equilibrium, even in magnetic fields. The method is flexible and fast and can straight-forwardly be applied to effective models as obtained from ab-initio calculations.

TT 101.15 Thu 15:00 P2

Intramolecular interference in an extended benzenelike molecule, due to a three-path analogy — Tim Ludwig and •Carsten Timm — TU Dresden, Dresden, Germany

In the last few years so-called intramolecular interference gained attention. It is the effect of interference in electronic transport through single molecules, leading to proposals for devices in molecular electronics and spintronics. Previous works have investigated spatially symmetric molecules or structures with two degenerate many-body states, analogous to a semiclassical two-path setup. We report on electronic-transport calculations within the quantum master-equation-formalism, investigating an extended Hubbard model of a six-sided ring with an additional central site, inspired by, e.g., benzene-vanadium. One can archieve a threefold-degenerate groundstate by tuning the parameters of the central site corresponding to a semiclassical three path setup.

TT 101.16 Thu 15:00 P2

Electrical Characterization of a Switchable Molecular Wire via Mechanically Controllable Break Junctions — •Torsten Sendler[1], Matthias Wieser[1], Jannic Wolf[2], Thomas Huhn[2], Elke Scheer[2], Francesca Moresco[3], Jochen Grebing[1], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]University of Konstanz, Germany — [3]Max Bergmann Center of Biomaterials, Dresden, Germany

Molecular electronics has been a field of big interest for the last years. Using the technique of mechanically controllable break junctions we characterize the Switchable Molecular Wire Oligo(phenylene ethynylene)-embedded Difurylperfluorocyclopentenes (SMW) in liquid environment. Via light irradiation the SMW can be switched between two well-defined conductance states.

Conductance and hysteresis measurements allow us to identify the two states providing the basis for a comprehensive study of the in situ switching process. Based on the analysis with the transport model assuming transport through a single molecular level, we confirm that a reliable contact of the molecules to the gold contacts is formed and extract the energy of the molecular levels and the coupling constants between molecule and electrodes.

TT 101.17 Thu 15:00 P2

Electronic structure of photosensitive molecular switches: A first-principle investigation — •Lokamani L[1], Daijiro Nozaki[1], Arezoo Dianat[1], Tahereh Ghane[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Sciences and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, Germany — [3]Center for Advancing Electronics Dresden, TU Dresden, Germany

The investigation of networks of nano-particles interconnected with functional molecular components is an active research field. Some potential applications include the realization of elementary computing units, able to act as memory nano-devices. However, to achieve this goal a detailed understanding of the electronic, structural, and electrical transport properties of potentially relevant molecular building blocks is mandatory. Here, we study such properties at the level of single molecules, for merocyanine derivatives, a photosensitive organic complex. In particular, we analyse the interplay between molecular conformation and corresponding modifications in the electrical response. First steps towards the inclusion of structural fluctuations via molecular dynamics simulations and its impact on the charge transport are also discussed.

TT 101.18 Thu 15:00 P2

Dynamics of a nano-electromechanical rotor driven by single-electron tunneling — •Alan Celestino[1], Alexander Croy[2], Marcus Werner Beims[3], and Alexander Eisfeld[1] — [1]MPIPKS, Dresden, Germany — [2]Chalmers University of Technology S-412 96, Göteborg, Sweden — [3]Federal University of Paraná, Curitiba, Brazil

We discuss a nano-electromechanical rotor driven by single-electron tunneling. A possible realization could be a nanotube with quantum dots attached on its extremities, which can freely rotate about a double-walled nanotube axis. The system is driven using a bias voltage between source and drain contacts. Using a few relevant parameters one can set the rotor's dynamics to either intermittent oscillations/rotations or continuous rotational motion. The connection between the dynamical regimes and the current through the device is established. The effect of tuning initial conditions is also addressed, showing a bistable behaviour in the system's phase space. Among the possible applications of such device stand out the signal amplification, current rectification and viscosity measurements.

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TT 101.19 Thu 15:00 P2

Hierarchical Quantum Master Equation Approach to Vibrationally Coupled Electron Transport in Single-Molecule Junctions — •Christian Schinabeck[1], Rainer Härtle[2], and Michael Thoss[1] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

In this contribution we investigate vibrationally coupled transport in single-molecule junctions using the hierarchical quantum master equation approach [1,2]. This method allows a systematic convergence of the reduced dynamics of open quantum systems beyond the traditional Markovian rate equations. We consider a model consisting of a molecular level coupled to fermionic leads as well as a vibrational mode. For this system the numerically accurate results of the hierarchical quantum master equation approach are compared with Markovian rate equation calculations in different parameter regimes. The performance of the method with respect to numerical efficiency and convergence is analyzed in detail.

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TT 101.20 Thu 15:00 P2

Model study of nonadiabatic electronic-vibrational interactions in single-molecule junctions — •André Erpenbeck and Michael Thoss — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen- Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany

The interaction between electronic and vibrational degrees of freedom in single-molecule junctions results from a dependence of the electronic energies on the nuclear displacement, but also from the dependence of the electronic states of the molecular bridge on the nuclear coordinates. The latter mechanism leads to a direct coupling between different electronic states and is referred to as nonadiabatic electronic-vibrational coupling. Employing a perturbative non-equilibrium Green's function approach, we study the influence of nonadiabatic electronic-vibrational coupling on the transport properties of model molecular junctions. In particular, we investigate the validity of the adiabatic approximation and show that nonadiabatic electronic-vibrational interaction gives rise to new transport channels. Furthermore, we explore the properties of nonadiabatic vibrational effects and their manifestation in observables such as the current-voltage characteristics.

TT 101.21 Thu 15:00 P2

Ab-initio phonon transport through single-molecule junctions — •Jan Klöckner[1], Robert Gossman[1], Thomas Hellmuth[2], Marius Bürkle[3], and Fabian Pauly[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Germany — [3]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan

We study the phononic contribution to thermal transport in single-molecule junctions. For this purpose we determine contact geometries and force constants on the level of density functional theory. The phonon transport is computed in the harmonic approximation by use of Green's function techniques. We study the following two basic problems: (i) Length-dependent transport and (ii) quantum interference effects. For (i) we study Au-alkane-Au junctions of varying molecular length. In (ii) we consider para- and meta-coupled Au-benzene-Au contacts to search for the phononic analogon of destructive electronic interference.

TT 101.22 Thu 15:00 P2

Real-time Dynamics in the Anderson-Holstein Model with phonon dependent hybridization — •Andre Jovchev and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

We study the real-time dynamics after a quench in the one-lead Anderson-Holstein model with a modified hybridization term using the time-dependent numerical renormalization group (TD-NRG). In molecular devices hysteresis effects and negative differential conductions have been reported. Experiments give hints, that these physics are due to the electron-phonon interactions inside the molecule. In our model we show that the short time dynamics of an electronic level in contact with a electronic bath is strongly dependent on the coupling with a phononic mode. The expectation value of the occupancy of the electronic level oscillates with the frequency of the phonon. For long times we show that we reach the equilibrium expectation values.

TT 101.23 Thu 15:00 P2

Magnetostriction in Nanomechanical Beams — •Rasmus Hollaender[1], M. Pernpeintner[1], M. J. Seitner[2,3], J. P. Kotthaus[2], E. M. Weig[2,3], S. T. B. Goennenwein[1], R. Gross[1], and H. Huebl[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Center for NanoScience (CeNS) and Fakultät für Physik, LMU, München, Germany — [3]Fachbereich Physik, Universität Konstanz, Germany

Nanomechanical sensors have demonstrated excellent force sensitivity [1], allowing for the detection of individual spins on surfaces [2]. Here, we apply this sensor concept to the detection of magnetostriction in nanometer thick ferromagnetic cobalt films. To this end we experimentally investigate the eigenfrequency of a 25 μm long and 300 nm wide highly stressed silicon nitride beam covered by a 10 nm thin film of cobalt at room temperature as function of the direction and magnitude of the applied magnetic field in the plane of the film using optical interferometry. For magnetic fields applied in the direction perpendicular to the beam, we find a decrease in the resonance frequency by 7.6 kHz compared to fields applied along the beam direction. We explain this 10^{-4} change in the resonance frequency quantitatively by modeling the impact of the magnetization orientation dependent magnetostriction. This opens the path for further magneto-mechanical experiments in nanostructures. Financial support via the Nanosystems Initiative Munich is gratefully acknowledged.

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TT 101.24 Thu 15:00 P2

Exploring mechanical material parameters from spectroscopy of nano-electromechanical systems — •Anh Tu Bohn[1], F. Hocke[1], M. Pernpeintner[1], X. Zhou[3,5], A. Schliesser[4], T. J. Kippenberg[3,5], R. Gross[1,2], and H. Huebl[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Germany — [2]Physik-Department, TU München, Germany — [3]École Polytechnique Fédérale de Lausanne, Switzerland — [4]Niels Bohr Institute, University of Copenhagen, Denmark — [5]Max-Planck-Institut für Quantenoptik, Germany

The field of nano-electromechanics combines nanomechanical resonators with electrical circuits. In our nano-electromechanics experiments, we investigate a double layer nanomechanical beam consisting of Si_3N_4 and Niobium coupled to a superconducting microwave resonator. Using microwave noise spectroscopy, we determine the electromechanical coupling. Furthermore, the investigation of the nonlinear Duffing regime gives access to the Young's modulus of the nano-beam. We compare our results with finite element modelling corroborating our experimental data. Additionally, we show that our experimental results can be well modelled by standard beam theory. Our technique provides a new way to explore the mechanical parameters of nanomechanical beams and could be extended to other hybrid structures. Financial support via the Nanosystems Initiative Munich is gratefully acknowledged.

TT 101.25 Thu 15:00 P2

Spin relaxation of phosporus donors in silicon at millikelvin temperatures — •Christoph W. Zollitsch[1,2], 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

In the field of quantum information processing spin ensembles are promising candidates for quantum memories. To allow for the transfer of quantum information to the memory, the spin ensembles used are typically coupled to a microwave resonator, acting as a quantum bus. Regarding practical realizations, phosphorus dopants in silicon are very attractive due to their long spin coherence times [1,2]. Here, we investigate the coupling between an ensemble of phosphorus donors in silicon and a superconducting coplanar waveguide microwave resonator (CPWR) at temperatures below 1.4 K and study the electron spin resonance (ESR) saturation behavior to extract the relaxation time of the spin system. We find the expected linear dependence of the relaxation time on temperature between 1.4 K and 200 mK [3]. Additionally, we present initial pulsed ESR experiments allowing to access the full dynamics of the system.

Financial support by the DFG via SFB 631 and the Excellence Initiative via NIM is gratefully acknowledged.

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TT 101.26 Thu 15:00 P2

Entangled photon pairs from three coupled optomechanical cells — •Zhi Jiao Deng[1,2], Steven Habraken[1], and Florian Marquardt[1] — [1]Institute for Theoretical Physics, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen,Germany — [2]Department of Physics, College of Science, National University of Defense Technology,Changsha,China

Optomechanics, which couples light to the mechanical motion of an object, is a very important research field both for fundamental studies of quantum physics and for potential applications. To show features different or superior to the classical counterparts, one major goal in the field of optomechanics is to generate nonclassical states such as squeezed states, entangled states, or states with negative Wigner functions for either or both the optical and mechanical degrees of freedom. In this work, we will discuss on how to generate entangled photon pairs from three coupled optomechanical cells, where each cell consists of a standard optomechanical system and different cells are coupled by photon tunneling. Due to the symmetry of the setup and with the help of mechanical motion, the photons in the driven optical normal mode will be scattered into the other two optical normal modes, where the entangled photon pairs correlated by frequency can be collected. We have investigated the squeezing and entanglement properties of the output light beams, and how these properties would be changed under the influence of the mechanical thermal noise and intrinsic optical losses. Moreover, we find that a suitable choice of parameters can lead to large steady-state entanglement in this proposed setup.

TT 101.27 Thu 15:00 P2

Quasiparticle induced qubit dephasing — •Sebastian Zanker, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Karlsruhe, Germany

We investigate dephasing in superconducting qubits due to quasiparticle tunneling. Contrary to qubit relaxation dephasing cannot be treated with golden rule calculations. Nonetheless one can define a dephasing rate which has to be obtained self-consistently. However, we show that qubit dephasing doesn't obey a simple exponential decay

but has a more complex time dependence.

TT 101.28 Thu 15:00 P2

Fluctuations in the susceptibility of spin systems — •Pablo Schad[1], Boris Narozhny[1], Alexander Shnirman[1,2], and Gerd Schön[2,3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [3]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Motivated by experiments in the context of 1/f flux noise in SQUIDs and Josephson qubits [1], which is widely attributed to magnetic impurities on the device surfaces [e.g. 2,3,4], we consider fluctuations in the susceptibility of spin systems. We use the Majorana fermion representation for spins [5] and take advantage of generalized relations between spin and Majorana correlators [6]. A path integral formulation allows us to study the role of slow modes and their influence on higher-order correlators, e.g. fluctuations of the spin susceptibility.

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TT 101.29 Thu 15:00 P2

Non-Markovian noninvasive measurements in coupled quantum systems — •Johannes Buelte and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457, Germany

The standard textbook introduction of quantum measurement uses the projection postulate implying a instantaneous collapse of the systems wave function in the measurement process. In many real systems a less invasive measurement is performed by coupling a detector to the measured system for a finite time and with a weak interaction. We investigate the generalized measurement scheme by positive operator-valued measures (POVM) in the weak coupling limit with a focus on a non-Markovian interaction [1]. Such a scheme with memory allows to directly measure nonsymmetrized correlations and is hence related to absorption and emission noise. We calculate the memory function which couples the detector to the system in general and for a harmonic oscillator as detector and discuss the resulting quasiprobabilities, in particular the possible violation of weak positivity [2] by second-order correlation functions.

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TT 101.30 Thu 15:00 P2

Resonance-assisted tunneling of Cooper pairs — •Pierre-Luc Dallaire-Demers and Frank Wilhelm-Mauch — Universität des Saarlandes, Saarbrücken, Deutschland

Superconducting tunnel junctions can be designed to have femtofarad capacitance with their charging energy larger than their Josephson energy E_J. When biased with a constant voltage V below the superconducting gap, the supercurrent starts to oscillate at a frequency $\omega = \frac{2eV}{\hbar}$. If the junction is capacitively coupled to an external electromagnetic environment, a net current appears through the junction as Cooper pairs tunnel and emit photons in the external modes, allowing for the spectroscopy of the environment. We investigate the situation where Cooper pair tunneling is coupled to a perfect LC mode, high order processes such as sequential coherent tunnel events involving many photons and pairs can contribute to the net current, departing significantly from the traditional picture of incoherent tunneling given by $P(E)$ theory. At low temperature, different regimes can be observed varying with the ratio of the mode frequency and the tunneling rate. We present the main diagrams contributing to each of those regimes and compute the asymptotic current in each case. Finally, the full perturbative series in E_J is cast in terms of a $P(E)$ framework in order to extend the method to more general environmental impedances.

TT 101.31 Thu 15:00 P2

Ab-initio calculation of local current-flow in functionalized graphene armchair nano-ribbons — •Jan Wilhelm, Michael Walz, and Ferdinand Evers — Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76133 Karlsruhe, Germany and Institut für Theorie der Kondensierten Materie, D-76128 Karlsruhe, Germany

We calculate the local current density in graphene armchair nanoribbons employing AITRANSS, our DFT-based transport simulation tool. [1,2] The simulations for pristine ribbons indicate that the current flows along streamlines. Neighboring streamlines are separated by stripes of almost vanishing flow. These streamlines form a strongly textured current pattern with gradients that exceed an order of magnitude on the scale of the lattice constant.

Due to the pronounced texture of current flows, the ribbon exhibits a very strong sensitivity to the placing of adsorbates. Backscattering off the adsorbates is strong, if they are located within a streamline and weak, otherwise. We observe that a single adsorbant, e.g., H or OH, when properly placed on the ribbon (width, e.g., 11 carbon atoms) can suppress the current by more than two orders of magnitude.

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TT 101.32 Thu 15:00 P2

Effects of disorder and contacts on transport through graphene nanoribbons — •Andreas Pieper[1], Gerald Schubert[2], Gerhard Wellein[3], and Holger Fehske[1] — [1]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17487 Greifswald, Germany — [2]Philips Healthcare, Äyritie 4, 01510 Vantaa, Finland — [3]Regionales Rechenzentrum Erlangen, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We study the transport of charge carriers through finite graphene structures. The use of numerical exact kernel polynomial and Green function techniques allows us to treat actual sized samples beyond the Dirac-cone approximation. Particularly we investigate disordered nanoribbons, normal-conductor/graphene interfaces, and normal-conductor/graphene/normal-conductor junctions with a focus on the behavior of the local density of states, single-particle spectral function, optical conductivity, and conductance. We demonstrate that the contacts and bulk disorder will have a major impact on the electronic properties of graphene-based devices.

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TT 101.33 Thu 15:00 P2

Electron dynamics in graphene with gate-defined quantum dots — •Rafael Leslie Heinisch, Andreas Pieper, and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald

We study transport through circular graphene quantum dots. We use numerically exact Chebyshev expansion and kernel polynomial methods in the framework of a tight-binding honeycomb lattice model [1]. Thereby, we confirm the scattering resonances and bound states for small dots found in the Dirac approximation. Our focus lies on the regime where individual modes of the electrostatically defined dot dominate the charge carrier dynamics. In particular, we discuss the scattering of an injected Dirac electron wave packet for a single quantum dot, electron confinement in the dot, the optical excitation of dot-bound modes, and the propagation of an electronic excitation along a linear array of dots.

[1] A. Pieper, R. L. Heinisch, and H. Fehske arXiv:1311.6271

TT 101.34 Thu 15:00 P2

Dynamics of Dirac Electrons in a Photon Cavity — •Lisa Hesse, Viktor Krückl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We consider low energy excitations of monolayer graphene embedded in an optical cavity and exposed to a perpendicular constant magnetic field. The influence of an additional radiation field can yield resonant cyclotron transitions of the Dirac fermions of graphene which can be studied using techniques known from cavity quantum electrodynamics. The coupling of cavity photons with condensed matter has been realized in the context of electron gases[1] and very recently also proposed for graphene[2, 3] and therefore opens a new subfield of research in graphene. By considering the interaction of cavity photon modes with Landau quantized states in graphene numerically based on a realistic tight-binding model we aim at clarifying the recent contradicting issue[2, 3] concerning the existance of a superradiant ground state in such systems.

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TT 101.35 Thu 15:00 P2

Phonon-drag thermopower in monolayer and bilayer graphene - significance of flexural phonons — •Eugen Wolf and Dietmar Lehmann — Institut für Theoretische Physik, TU Dresden, 01062 Dresden, Germany

Recent realizations of suspended monolayer graphene (MLG) and bilayer graphene (BLG) samples have enabled a direct probe of their intrinsic properties. It turns out that MLG and its bilayer possess high magnitudes of electron mobility and thermopower, thus promising attractive applications. A detailed study of the (intrinsic) scattering mechanisms, like electron-phonon-interaction, is therefore of large interest. A quite sensitive tool for investigating the coupling of electrons to acoustic phonons is the phonon-drag thermopower S^{g}. In freestanding graphene, electrons couple noticeably not only to in-plane longitudinal and transversal phonons, but also to out-of-plane (flexural) phonons. In our study, we indicate the contribution of flexural acoustic phonons to S^{g} in graphene for the first time. We have calculated S^{g} in doped, suspended MLG and BLG as function of temperature for different carrier densities by using a generalized Cantrell-Butcher formalism up to 2-phonon processes. Electron-phonon coupling by a screened deformation potential (proportional to the local contraction or dilatation of the lattice) as well as by an effective gauge field (induced by changes in bond length and bond angle between the carbon atoms) are included. We find that for reasonable coupling constants the electron scattering by out-of-plane phonons below 10 K cannot be neglected, especially for MLG.

TT 101.36 Thu 15:00 P2

Magnetic impurities at the edge of a two-dimensional topological insulator — •Johanna Kleinen, Markus Garst, and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, Germany

We investigate the effect of a magnetic impurity in a helical Luttinger liquid representing the edge states of a two-dimensional topological insulator. Analyzing the renormalization group flow in the presence of Kondo- as well as Rashba-interactions, we find that the magnetic impurity always couples strongly to the spin-polarized electrons. Moreover, we identify, in principle, two strong-coupling fixed-points with completely different transport characteristics. The magnetic impurity might either be Kondo-screened and only forward-scattering the electrons or it could develop into a strong backscatterer effectively inhibiting transport along the edge.

TT 101.37 Thu 15:00 P2

Electronic correlations in bulk Bi-chalcogenide topological insulators and elemental bismuth — •Luis Craco[1] and Stefano Leoni[2] — [1]Instituto de Fisica, Universidade Federal de Mato Grosso, 78060-900, Cuiaba, MT, Brazil — [2]School of Chemistry, Cardiff University, Cardiff, CF10 3AT, UK

In recent years three-dimensional (3D) topological insulators (TIs) have attracted great fundamental interest as systems that can lead to new phases of quantum matter. Theoretical and experimental work have revealed that intrinsic spin-orbit (SO) coupling can drive qualitative new effects on the electronic structure of Bi-chalcogenide p-band systems in general. In this poster, we present our recent work on electronic structure and transport properties of bulk Bi_2Se_3 [1] and Bi_2Te_2Se [2] TIs. We will also revisit the long-standing issues of transport and magnetoresistance responses in elemental bismuth [3]. Basing ourselves on LDA+DMFT calculations we show that the interplay between SO and multi-orbital Coulomb interactions has quantitative new effects in their semimetal electronic structure. We show, for example, why the intricate interplay between local Coulomb and SO interaction promotes a spin-orbit Kondo state in elemental bismuth. Taken together our work represents a realization of complex dynamical correlation effects in p-band semimetals and in bulk Bi-chalcogenide TIs.
[1] L. Craco and S. Leoni, Phys. Rev. B 85, 075114 (2012)
[2] L. Craco and S. Leoni, Phys. Rev. B 85, 195124 (2012)
[3] L. Craco and S. Leoni, in preparation

TT 101.38 Thu 15:00 P2

Transition between n-type and p-type transport in MBE-grown topological insulator $(Bi_{1-x}Sb_x)_2Te_3$ thin films — Tobias Merzenich[1], •Melissa Schall[1], Christian Weyrich[1], Igor E. Batov[1,2], Gregor Mussler[1], Jörn Kampmeier[1], Yulieth Arango[1], Jürgen Schubert[1], Thomas Schäpers[1,3], and Detlev Grützmacher[1] — [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 transition between n-type and p-type conduction in the ternary compound $(Bi_{1-x}Sb_x)_2Te_3$ $(0 < x < 1)$ films grown by molecular beam epitaxy. They were grown on silicon on insulator (SOI) substrates with Si(111)-top layer harbouring. A top-gate was used to deplete the intrinsic n-doped bulk. By performing Hall measurements on several samples with varying x, we obtain a change of sign of the Hall resistivity at $x = 0.43$. This is attributed to compensation effects. For samples with $x < 0.43$ we obtain a n-type conduction, i.e. an electron transport, whereas samples with $x > 0.43$ show a p-type conduction, i.e. a hole transport. This transition is an evidence that the Fermi energy is initially located above the conduction band edge and is shifted into the valence band for higher Sb concentration.

TT 101.39 Thu 15:00 P2

Transport simulations of nanowires hosting Majorana Bound States — •Felix Weiner and Peter Schmitteckert — Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany

Semiconductor nanowires with proximity-induced s-wave superconductivity and spin-orbit coupling have been shown theoretically to host Majorana Bound States (MBS) on the boundaries of topological segments. The unambiguous identification of these states in experiments is still an ongoing challenge. Several groups have reported the observation of a zero-bias peak in the differential conductance of tunneling experiments, which hints at the existence of a MBS at the end of the wire. We investigate numerically the transport properties of inhomogenous nanowires by means of wavepacket evolution. The aim is to address open questions regarding the I-V characteristic such as the signature of the excitation gap, which is expected to close when passing through the topological phase transition.

TT 101.40 Thu 15:00 P2

Real time dynamics of Majorana bound states — •Michael Sekania[1], Felix Weiner[2], Ronny Thomale[1], and Peter Schmitteckert[2] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilian University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany

Majorana fermions have been attracting substantial interest during recent years. Considerable attention is devoted to the robust and unambiguous probing of Majorana bound states and the error-tolerant manipulations of them, particularly in the view of possible applications in topological quantum computing. Here we present the investigation of the real-time dynamics of the Majorana bound states in different lattice geometries and discuss application of the real-time simulations in a context of braiding of Majorana fermions.

TT 101.41 Thu 15:00 P2

Majorana Fermions: Anholonomy of Bound States — •Sourin Das[1] and Indu Satija[2] — [1]MPIPKS, Dresden, Germany & University of Delhi, India — [2]Department of Physics and Astronomy, George Mason University, USA

Majorana modes in p-wave superconducting quantum wires are shown to result in exotic quantum holonomy of both the eigenvalue and the eigenstates. Induced by a degeneracy hidden in complex Bloch vector space, Majorana bound states are characterized by Kohn branch point (also known as exceptional points) singularities leading to Mobius strip-like structure of the eigenspace. This may provide yet another elegant framework to characterize topological aspect of Majorana detection in p-wave superocndcutor. This topological characterization is shown to be valid also for the periodically driven superconducting wires that supports two species of Majorana.

TT 101.42 Thu 15:00 P2

Majorana fermions at the quantum spin Hall edge —

Shuo Mi[1], Dimitry Pikulin[1], •Michael Wimmer[1,2], and Carlo Beenakker[1] — [1]Universiteit Leiden, The Netherlands — [2]TU Delft, The Netherlands

One of the earliest proposals for Majorana fermions in condensed matter systems involves quantum spin Hall (QSH) insulators [1]. In fact, Majorana fermions appear naturally if QSH insulators are coupled to superconductors, and are in this setting also inherently more stable than for example the now very popular proposal of obtaining Majorana fermions in semiconducting nanowires.

Yet, the proposals for Majorana fermions in QSH always involved elements (magnetic insulators, or very strong magnetic fields) that pose experimental problems. Here, we present a much simpler setup involving only gates and a weak magnetic field that will allow for an unambiguous signature of Majorana fermions in this system. In addition, we explain how to prove the non-Abelian statistics in a QSH setup [2].

[1] L. Fu & C. Kane. Phys. Rev. B **79**, 161408(R) (2009)
[2] S. Mi *et al.* Phys. Rev. B **87**, 241405(R) (2013)

TT 101.43 Thu 15:00 P2

Stability of Majorana metals — •Kevin O'Brien and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

The topological nature of exotic quantum states with non-Abelian vortices, such as $p_x + ip_y$ superconductors, the Moore-Read quantum Hall state or certain heterostructures of topological insulators and s-wave superconductors, can be discussed in terms of Majorana fermion zero modes. If the non-Abelian vortices hosting these zero modes form a regular triangular lattice – a natural situation for an Abrikosov lattice in a superconductor or a Wigner crystal in the context of quantum Hall liquids – the corresponding model of Majorana fermions hopping on a triangular lattice becomes particularly tractable. In terms of symmetry classification, such a Majorana model is in class D and allows for three types of ground states – a trivial insulator, a Chern insulator and a thermal metal state. While the Chern insulator is found for uniform hopping [1], sufficiently strong sign-disorder in the hopping amplitudes will drive the system into the thermal metal state [2].

Here we investigate the stability of this thermal metal state when introducing an additional level of disorder – random bond or site depletion of the underlying triangular lattice. In particular, we are interested in addressing whether the thermal metal state is stable up to the respective percolation threshold of site/bond disorder.

First results will be discussed on this poster.

[1] E. Grosfeld and A. Stern, Phys. Rev. B **73**, 201303(R) (2006).
[2] C. R. Laumann *et al.*, Phys. Rev. B **85**, 161301(R) (2012).

TT 101.44 Thu 15:00 P2

Absorption and transport properties of quantum aggregates with heavy-tailed disorder — •Sebastiaan Vlaming[1], Sebastian Möbius[1], Victor 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, The Netherlands

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 contribution to the energy fluctuations.

Recent developments in generating and trapping highly excited Rydberg atoms, allow for quantum simulations of molecular aggregates. We show that by controlling the environment, e.g. a polar background gas, non-Gaussian static disorder can be studied. We analyze how the environment generates disorder distributions with heavy tails, so called Lévy-stable distributions, and discuss novel effects in Lévy disordered systems such as broadening of the absorption bandwidth [1] as well as a subdiffusive exciton transfer.[2]

[1] A. Eisfeld, S.M. Vlaming, V.A. Malyshev, J. Knoester, PRL 105, 137402 (2010)
[2] S.M. Vlaming, V.A. Malyshev, A. Eisfeld, J. Knoester, JCP 138, 214316 (2013)

TT 101.45 Thu 15:00 P2

Full counting statistics of energy dissipated by a driven two level system — •Philip Wollfarth[1] and Alexander Shnirman[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

Within the last decades fluctuation relations[1-4] have been established. Recent experiments have shown the validity of such fluctuation relations for entropy production in the microscopic regime[5]. However the extension of fluctuation relations of heat and work to the quantum regime is still under discussion, since non-ambiguous definitions for heat and work have not yet been established. In this context we consider the statistics of energy emitted by a driven two level system into a bosonic bath using the full counting statistics technique.

[1] G. N. Bochkov, Yu. E. Kuzovlev, Sov. Phys. JETP, Vol. **45**, 125 (1977)
[2] C. Jarzynski, Phys. Rev. Lett. **78**, 2690 (1997)
[3] G. E. Crooks, Phys. Rev. E, **60**, 2721 (1999)
[4] M. Campisi, P. Hänggi, P. Talkner, Rev. Mod. Phys, **83**, 771, (2011)
[5] J. V. Koski, *et al.*, Nature Physics **9**, 644 (2013)

TT 102: Cold Atomic Gases - Poster Session

Time: Thursday 15:00–19:00 Location: P2

TT 102.1 Thu 15:00 P2

Second order self-energy of fermions with dipolar interaction — Jan Krieg[1], •Philipp Lange[1,2], and Peter Kopietz[1,2] — [1]Institut für Theoretische Physik, Universität Frankfurt, Frankfurt am Main, Germany — [2]Department of Physics, University of Florida, Gainesville, Florida, USA

We calculate the self-energy, the quasiparticle residue and the effective mass of a two- and three-dimensional system of dipolar fermions, which are aligned by an external field, up to second order perturbation theory. The influence of the anisotropy of the dipolar interaction on these quantities is investigated as a function of the interaction strength and, for two-dimensional systems, the tilting angle between the external field and the normal of the plane of dipoles.

TT 102.2 Thu 15:00 P2

Quantum quench dynamics in the Bose-Bose resonance model — •Florian Dorfner and Fabian Heidrich-Meisner — Ludwig-Maximilian-University Munich

We study quantum quenches between the three phases of the Bose-Bose resonance model, a one-dimensional model of bosonic atoms and diatomic molecules interacting via resonant Feshbach-type interactions. The three phases are: (i) Mott insulator (MI), (ii) molecular condensate (MC) and (iii) atomic and molecular condensate (AC+MC) [1]. We are interested in the temporal evolution of optimal modes that are the eigenstates of the one-site reduced density matrix. We also investigate the distribution of weights by computing the associated von-Neumann entropy. The optimal mode spectra and weights are calculated using exact diagonalization. We find that for quenches from the AC+MC to the MC phase the optimal mode weights and spectra stay almost constant in time. For this quench, the number of particles of the two species is studied and found to be oscillating in time. This is understood by decomposing the starting state into the eigenstates of the quenched system showing that there is significant overlap with only two eigenstates. In other cases the optimal mode spectra and weights change more significantly.

Support from the DFG through FOR1807 is gratefully acknowledged.

[1] S. Ejima, M. J. Bhaseen, M. Hohenadler, F. H. L. Essler, H. Fehske and B. D. Simons, PRL 106, 015303 (2011)

TT 102.3 Thu 15:00 P2

Relaxation and thermalization dynamics in the one-dimensional Bose-Hubbard-Model — •Stefan Sorg, Lode

Pollet, and Fabian Heidrich-Meisner — Ludwig-Maximilians-Universität München

Motivated by experiments recently carried out with ultracold atomic gases [1], we study the relaxation and thermalization dynamics of several observables in the one-dimensional Bose-Hubbard-Model with integer filling after a global interaction quantum quench. Using exact diagonalization, we analyze the distribution of the diagonal matrix elements of several observables and the energy distribution of quench initial states in the framework of the eigenstate thermalization hypothesis, discussing its applicability in different regimes of U/J.

We acknowledge financial support through DFG FOR 801 and 1807.
[1] Ronzheimer et al., Phys. Rev. Lett. **110**, 205301 (2013)

TT 102.4 Thu 15:00 P2

Numerical calculation of spectral functions of the Bose-Hubbard model using B-DMFT — •Jaromir Panas[1,3], Anna Kauch[2], Jan Kunes[2], Dieter Vollhardt[3], and Krzysztof Byczuk[1] — [1]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Hoza 69, 00-681 Warszawa, Poland — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Praha, Czech Republic — [3]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Spectral functions of the Bose-Hubbard model are computed within the bosonic dynamical mean field theory (B-DMFT) [1] using a continuous-time quantum Monte Carlo (CT-QMC) solver together with maximum entropy method for analytic continuation. Results are obtained for different interaction strengths and chemical potentials and are compared with approximate results from a strong coupling solution of the B-DMFT equations [2].
[1] K. Byczuk and D. Vollhardt, Phys. Rev. B 77, 235106 (2008)
[2] A. Kauch, K. Byczuk, D. Vollhardt, Phys. Rev. B 85, 205115 (2012)

TT 102.5 Thu 15:00 P2

Ferromagnetism in a two-component Bose-Hubbard model with synthetic spin-orbit coupling — Jize Zhao[1,2], •Shijie Hu[3], Jun Chang[4], Ping Zhang[1,2], and Xiaoqun Wang[5] — [1]LCP, Institute of Applied Physics and Computational Mathematics, Beijing 100088, China — [2]Beijing Computational Science Research Center, Beijing 100084, China — [3]Max-Plank Institute fuer Physik Komplexer Systeme, Dresden 01187, Germany — [4]Institute of Theoretical Physics and Kavli Institute for Theoretical Physics, CAS, Beijing 10080, China — [5]Department of Physics, Renmin University of China, Beijing 100872, China

We study the effect of the synthetic spin-orbit coupling in a two-component Bose-Hubbard model in one dimension by employing the density-matrix renormalization group method. A ferromagnetic long range order emerges in both Mott insulator and superfluid phases resulting from the spontaneous breaking of the Z_2 symmetry, when the spin-orbit coupling term becomes comparable to the hopping kinetic energy and the inter-component interaction is smaller than the intra-one. In the symmetry-broken phase, the system behaves effectively as a one-component model. The novel effects are expected to be detectable with the present realization of the synthetic spin-orbit coupling in experiments.

TT 102.6 Thu 15:00 P2

Dimensional crossover of topological insulators and cold-atom realization of gapless Mott insulators — •Peter P. Orth[1], Mathias Scheurer[1], and Stephan Rachel[2] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), , 76131 Karlsruhe, Germany — [2]Institute for Theoretical Physics, TU Dresden, 01062 Dresden, Germany

We propose a realistic cold-atom setup which allows for a dimensional crossover from a two-dimensional quantum spin Hall insulating phase to a three-dimensional strong topological insulator phase by simply tuning the hopping between the layers. We further employ cluster slave-rotor mean-field theory to study the effect of additional Hubbard onsite interactions that give rise to various spin liquid-like phases such as gapless and semi-metallic Mott insulating states.

TT 103: Symposium One-Dimensional Metals: Reality or Fiction (organized by DS; with HL, O, TT)

Time: Friday 9:30–12:30 Location: HSZ 02

Invited Talk TT 103.1 Fri 9:30 HSZ 02

Atomic-scale dopant wires for quantum computer architectures — •Michelle Y Simmons — Centre of Excellence for Quantum Computation and Communication Technology, University of New South Wales, Sydney, NSW 2052, Australia

Down-scaling has been the leading paradigm of the semiconductor industry since the invention of the first transistor in 1947. As silicon electronics approaches the atomic scale, interconnects and circuitry become comparable in size to the active device components. Maintaining low electrical resistivity at this scale is challenging because of the presence of confining surfaces and interfaces. We report on the fabrication of wires in silicon-only one atom tall and four atoms wide-with exceptionally low resistivity ˜ 0.3 milliohm-centimeters. By embedding phosphorus atoms within a silicon crystal with an average spacing of less than 1 nanometer we achieved a diameter-independent resistivity [1]. Atomistic tight-binding calculations confirm the low resistivity of these atomic-scale wires [2], which pave the way for single-atom device architectures for both classical and quantum information processing. I will demonstrate how we have incorporated these wires into single atom transistors [3] and performed single-shot spin read-out of precisely-positioned P donor electron spins as potential qubits in Si [4].

[1] B. Weber et al., Science 335, 6064 (2012). [2] H. Ryu et al., Nanoscale 5, 8666 (2013). [3] M. Fuechsle et al., Nature Nanotechnology 7, 242 (2012). [4] H. Buch et al., Nature Communications 4, 2017 (2011).

Invited Talk TT 103.2 Fri 10:10 HSZ 02

$1+\delta$: Tuning the Dimensionality of Organic Conductors — •Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

Organic charge-transfer salts are prime candidates for tuning the dimension by applying pressure. Strictly one-dimensional systems, such as the Fabre salts $(TMTTF)_2X$, are Mott insulators that undergo a deconfinement transition towards a Luttinger liquid and eventually a two-dimensional Fermi liquid if the interchain interaction increases with pressure. The deconfinement transition can be identified when the transverse hopping integral $2t_\perp = \Delta_\rho$, the Mott gap. Ab-initio density functional theory allows us to study the influence of temperature and pressure on the electronic band structure.

Quasi-one-dimensional organic conductors, like the Bechgaard salts $(TMTSF)_2X$, exhibit a cross-over from a Luttinger liquid to a Fermi liquid behavior upon cooling and application of external pressure. Frequency and temperature dependent transport measurement yield a change in power-laws and Luttinger exponent.

Often the metallic phase is not stable in reduced dimensions: at low temperatures the electronic charges and spins tend to arrange themselves in an orderly fashion due to relatively strong correlations. There are a growing number of molecular materials where electronic degrees of freedom and electronic interactions are directly responsible for electric polarization and ferroelectric transition, termed electronic ferroelectricity. Recently, it was discovered that charge order not only produces ferroelectricity but also breaks the symmetry of the magnetic degree of freedom in organic quantum spin chains.

Coffee break (20 min)

Invited Talk TT 103.3 Fri 11:10 HSZ 02

Spectral and transport properties of one-dimensional correlated electrons — •Volker Meden — Institut für Theorie der Statistischen Physik, RWTH Aachen University

Two-particle interactions strongly alter the low-energy physics of electrons confined to one spatial dimension. Excitations cannot be described by fermionic quasi-particles. Metallic systems of this type fall into the Luttinger liquid universality class and are characterized

by power-law decay of correlation functions. I will give an overview over the one-particle spectral and transport properties of such systems including a discussion of the model dependent low-energy scale beyond which Luttinger liquid power laws are observable. Leaving the framework of equilibrium physics I will report on recent progress in understanding the non-equilibrium steady state as well as relaxation dynamics of isolated and contacted quantum wires.

Invited Talk TT 103.4 Fri 11:50 HSZ 02

Atomic nanowires on surfaces: Spectroscopic reality versus theoretical fiction — •Ralph Claessen — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Solids with electrons confined to only one spatial dimension are predicted to behave quite different from conventional metals. Many-body theory finds that electronic interactions may lead to Peierls-type instabilities or even a breakdown of Landau's quasiparticle picture, which works so well in higher dimensions. Atomic nanowires formed by self-organized growth of metal atoms on suitable semiconductor surfaces can be viewed as closest approach to perfect 1D electron confinement, and therefore serve well as model systems for experimental tests of the expected 1D physics. In my presentation I will discuss current experiments on atomic nanowires, using photoelectron spectroscopy and scanning tunneling microscopy as experimental probes, and compare the results to corresponding theoretical predictions. Examples include the observation of Tomonaga-Luttinger behavior as well as the possible detection of (quasi-)1D antiferromagnetic order.

TT 104: Topological Insulators (organized by MA)

Time: Friday 9:30–12:00 Location: HSZ 04

TT 104.1 Fri 9:30 HSZ 04

Experimental characterization and simulation of quasiparticle-interference in the Bi-bilayer topological insulator — •Matteo Michiardi[1], Andreas Eich[2], Gustav Bihlmayer[3], Alex A. Khajetoorians[2], Jens Wiebe[2], Jianli Mi[4], Bo B. Iversen[4], Philip Hofmann[1], and Roland Wiesendanger[2] — [1]Department of physics and astronomy, Aarhus University, Denmark — [2]Institute of Applied Physics, University of Hamburg, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [4]Center for Materials Crystallography, Aarhus University, Denmark

Topological insulators (TI) are a new class of materials that host gapless surface states with spin helicity. While several 3D TIs have been discovered, the interest in 2D TI systems that can host topological edge state is rising. A single bilayer of bismuth is predicted to be such a 2D TI. Here we present an experimental and theoretical study of a Bi-bilayer grown on 3D TI Bi_2Se_3. The use of Bi_2Se_3 as substrate allows the epitaxial growth of the bilayer in the rhombohedral structure, as shown by Scanning Tunnelling Microscopy. We calculate the band structure of the Bi-bilayer/Bi_2Se_3 system by Density Function Theory (DFT) and experimentally study the quasi particle interference (QPI) on the bilayer. In order to clarify the scattering channels responsible for the QPI, we perform simulations based on the Joint Density of States method starting from our DFT calculations. The comparison with the experimental results reveals a good match for a wide range of binding energies for both occupied and unoccupied states.

TT 104.2 Fri 9:45 HSZ 04

Quasiparticle self-consistent *GW* study of bismuth under strain — •Irene Aguilera, Christoph Friedrich, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

It has been recently claimed on the basis of ARPES measurements that bulk bismuth is a topological semimetal. The discrepancies between this result and previous *ab-initio* calculations were attributed to the failure of density functional theory (DFT) in the prediction of band gaps, because the topological or trivial character of Bi depends only on the "sign" of the very small direct band gap at the L point. We show that bulk Bi is indeed predicted by DFT in the local-density approximation (LDA) to be a trivial semimetal, with a surprisingly overestimated gap at L. We have performed quasiparticle self-consistent *GW* (QS*GW*) calculations for bulk bismuth that support its trivial character. The QS*GW* gap at L as well as the energy overlap between the electron and hole pockets are in much better agreement with experiments than the LDA ones. Thus, the QS*GW* approach appears as the right tool to study the trivial-to-topological transition that Bi experiences under stress, as a result of a change of sign of the gap at L. We have analyzed the effect of strain on the topological properties of bulk Bi. Whereas LDA predicts that an impractical stress is needed for such a transition, QS*GW* shows that bulk Bi becomes a topological semimetal already under very small stress. This work is supported by the Helmholtz Virtual Institute for Topological Insulators (VITI).

TT 104.3 Fri 10:00 HSZ 04

Combined STM/STS- and ARPES-investigation of the quaternary Topological Insulator $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ — •Thomas Bathon[1], Felix Reis[1], Christoph Seibel[2], Hendrik Bentmann[2], Paolo Sessi[1], Friedrich Reinert[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We present a combined scanning tunneling microscopy/spectroscopy (STM/STS) and angular-resolved photoemission spectroscopy (ARPES) characterization of the electronic properties of the quaternary compound $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$. ARPES-data evidence that this compound is still a Topological Insulator (TI) with a single Dirac cone, which is characteristic for the Bi_2X_3-class. The topological properties of the surface state, i.e. forbidden backscattering, have been confirmed by Fourier-transformed differential conductance (dI/dU) maps. Measurements performed both above and below the Fermi level allow us to determine the energy dispersion relation, the carrier velocity, and—by extrapolation to zero momentum—the position of the Dirac point. The observed scattering vectors are not as well-defined as those observed in binary compounds, probably due to substitutional disorder which results in a spatial fluctuation of the chemical potential. Our investigations illustrate how the properties of the well-known TI Bi_2Te_3 can be changed by chemical substitution.

TT 104.4 Fri 10:15 HSZ 04

Surface and bulk contributions to the electronic structure of the topological insulator Sb_2Te_3(0001) — •Christoph Seibel[1,2], Hendrik Bentmann[1,2], Henriette Maass[1,2], Jürgen Braun[3], Jan Minár[3], Kenya Shimada[4], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe — [3]Department Chemie, Physikalische Chemie, Universität München, Butenandtstraße 5-13, D-81377 München — [4]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Photon energy dependent angle-resolved photoemission measurements were performed to disentangle surface and bulk contributions to the electronic structure of the 3D topological insulator (TI) Sb_2Te_3. We discover a penetration of the topological surface state (TSS) into the bulk valence band regime where it coexists with bulk states without considerable hybridization. Our results indicate an emerging $k_\perp$-dispersion of the TSS at higher binding energies, which we attribute to an increasing bulk character. These observations deviate from previous findings for the isostructural TIs Bi_2Se_3 and Bi_2Te_3. Our results are supported by fully relativistic one-step photoemission calculations. [1] Seibel *et al.* PRB 86, 161105(R) (2012)

15 min. break

TT 104.5 Fri 10:45 HSZ 04

Spin-dependent unoccupied electronic structure of the topological insulator Sb_2Te_3 — •Anna Zumbülte[1], Anke B. Schmidt[1], Markus Donath[1], Peter Krüger[2], Gregor Mussler[3], and Detlev Grützmacher[3] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Festkörpertheo-

rie, Westfälische Wilhelms-Universität Münster, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

Studies on three-dimensional topological insulators focus mainly on the well-known systems of Bi_2Se_3 and Bi_2Te_3 and the related ternary compounds. Theoretical predictions of chalcogenides as topological insulators with a single Dirac cone [1] include an additional compound, Sb_2Te_3. There, due to p-type doping of the available samples, the Dirac point lies above the Fermi level, making it inaccessible to photoemission experiments unless the surface is modified with an adsorbate [2]. Consequently, the electronic structure of this system has been left almost unstudied.

We present spin- and angle-resolved inverse-photoemission measurements of the unoccupied electronic states of Sb_2Te_3. In addition to the Dirac state, further spin-dependent features have been obtained which show a distinct Rashba splitting. The experimental data will be discussed along with bandstructure calculations.

[1] H. Zhang *et al.*, Nat. Phys. **5**, 438 (2009)
[2] C. Seibel *et al.*, Phys. Rev. B **86**, 161105 (2012)

TT 104.6 Fri 11:00 HSZ 04

Comparitive study of the ternary topological insulators Bi_2Se_2Te and Bi_2Te_2Se — •Felix Reis[1], Thomas Bathon[1], Christoph Seibel[2], Hendrik Bentmann[2], Paolo Sessi[1], Friedrich Reinert[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The 3D topological insulators Bi_2Se_2Te and Bi_2Te_2Se have been investigated by combining the complementary experimental techniques scanning tunneling microscopy (STM/STS) and angular-resolved photoemission spectroscopy (ARPES). With low temperature STM/STS technique we investigate the structural and electronic properties of both systems. Fourier-transformed quasi-particle interference (QPI) maps give access to the scattering events within the topological surface state. Taking QPI maps for several energies allows us to obtain information on the position of the Dirac point and the carrier velocity by fitting the linear energy dispersion relation of the Dirac fermions. These results will be compared with the band structure as obtained by ARPES measurements.

TT 104.7 Fri 11:15 HSZ 04

A large-energy-gap oxide topological insulator based on the superconductor BaBiO3 — •Binghai Yan[1,2,3], Martin Jansen[1], and Claudia Felser[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden — [3]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg University of Mainz, 55099 Mainz

Topological insulators are a new class of quantum materials that are characterized by robust topological surface states (TSSs) inside the bulk-insulating gap, which hold great potential for applications in quantum information and spintronics as well as thermoelectrics. One major obstacle is the relatively small size of the bulk bandgap, which is typically around 0.3eV for the known topological insulator materials. Here we demonstrate through ab initio calculations that a known superconductor BaBiO3 (BBO) with a Tc of nearly 30 K emerges as a topological insulator in the electron-doped region. BBO exhibits a large topological energy gap of 0.7 eV, inside which a Dirac type of TSSs exists. As the first oxide topological insulator, BBO is naturally stable against surface oxidization and degradation, distinct from chalcogenide topological insulators. An extra advantage of BBO lies in its ability to serve as an interface between TSSs and superconductors to realize Majorana fermions for future applications in quantum computation.

Reference: B. Yan, M. Jansen, C. Feler, Nature Physics 9, 709*711 (2013) (arXiv:1308.2303).

TT 104.8 Fri 11:30 HSZ 04

Topological surface states of HgTe and Heulser compounds — •Shu-Chun Wu[1], Binghai Yan[1,2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany. — [2]Max Planck Institute for Physics of Complex Systems, Dresden, Germany.

We studied the topological electronic structures of HgTe and half Heusler compounds (e.g.: XYZ, X = rare earth elements, Y = trasition metal and Z = main group elements) by both *ab initio* calculations. The topological surface structures were investigated by the Wannier function based tight-binding method. The effects of external strains induced from the substrate and surface terminations are taken into account by the atomic positions. Our results agree well with recent photoemission experiments.

TT 104.9 Fri 11:45 HSZ 04

Sputter Deposition of Half-Heusler Topological Insulators — •Benedikt Ernst, Daniel Ebke, Stanislav Chadov, Gerhard Fecher, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Heusler compounds have exhibited manifold physical properties in the recent years and attracted a lot of interest in the field of spintronic applications due to their half-metallic properties. Recently, a topological insulating state has been predicted by theory for some of these compounds.

In this work, we have prepared Heusler materials such as LaPdBi and LaPtBi for which a topological insulating behavior was predicted. Co-deposition by DC- and RF magnetron sputtering was used to prepare corresponding thin films. To realize an epitaxial film growth in the crystallographic $C1_b$ structure on MgO-substrates, a buffer layer was applied and optimized. Initial transport properties will be discussed with regard to the film composition and the crystallographic properties.

TT 105: Graphene: Bi- and Multi-Layers (organized by HL)

Time: Friday 9:30–11:00 Location: POT 081

TT 105.1 Fri 9:30 POT 081

Atomistic simulations of dislocations in bilayer graphene — •Konstantin Weber[1], Christian Dolle[2], Florian Niekiel[2], Benjamin Butz[2], Erdmann Spieker[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — [2]Center for Nanoanalysis and Electron Microscopy, FAU Erlangen-Nürnberg

The atomic structure and the properties of basal-plane dislocations in bilayer graphene, the thinnest imaginable crystal that can host such 1D defects, has been investigated by atomistic simulations based on the registry-dependent potential of Kolmogorov and Crespi [1] and the classical AIREBO potential.

Our calculations show that the dislocations lead to a pronounced buckling of the graphene bilayers in order to release strain energy, leading to a complete delocalization of the residual compressive/tensile strain in the two graphene sheets [2]. Furthermore, the absence of a stacking-fault energy, a unique peculiarity of bilayer graphene, gives rise to a splitting of the dislocations into equidistant partials with alternating Burgers vectors [2]. Thus, dislocations in bilayer graphene show a distinctly different behavior than corresponding dislocations in graphite or other 3D crystals.

[1] A. Kolmogorov, V. Crespi, *Phys. Rev. B* **71**, 235415 (2005).
[2] B.Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spieker, *Nature*, (2013) (accepted for publication).

TT 105.2 Fri 9:45 POT 081

Study of the magnetoresistance of biased graphene bilayers — •Dmitri Smirnov[1], Galina Y. Vasileva[1,2], Yurij B. Vasilyev[2], Pavel S. Alekseev[2], Yurij L. Ivanov[2], Hennrik Schmidt[1], Alexander W. Heine[1], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Ioffe Physical Technical Institute, Russian Academy of Sciences, St. Petersburg

We demonstrate magnetotransport behaviour of bilayer graphene. In contrast to monolayer graphene, bilayer has a parabolic band structure with a zero band gap, which can be opened by applying an electrical field perpendicular to the samples [1]. One of the consequences of such

a band structure is the coexistence of two different types of charge carriers with the Fermi energy placed near the charge neutrality point.

Several bilayer graphene samples with different electrical properties (charge neutrality point, mobility) have been investigated. A positive and negative magnetoresistance is observed for electrons and holes. We can show that that the positive magnetotransport can be described well with a two carrier Drude model which allows us a new approach to probe parameters of electrons and holes separately.

[1] McCann, E., and V. Fal'ko Phys. Rev. Lett. 96, 086805 (2006)

TT 105.3 Fri 10:00 POT 081

Transport in Dual Gated Encapsulated Bilayer Graphene — •Jonas Hesselmann[1], Stephan Engels[1,2], Bernat Terrés[1,2], Kenji Watanabe[3], Takashi Taniguchi[3], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Bilayer graphene (BLG) is a promising material which combines superior electronic properties like high charge carrier mobilities with the possibility of opening a band gap. The band gap can be induced by applying a perpendicular electric field resulting in a gap in the order of a few 10 meV. This makes BLG a possible candidate for future nanoelectronic applications. Here, we present the fabrication and low temperature (T=2K) transport measurements of dual gated BLG which is encapsulated in hexagonal boron nitride serving as an atomically flat gate dielectric. We show that the investigated devices exhibit mobilities of up to 80.000 cm^2/Vs. Quantum Hall effect measurements show a distinct sequence of Hall plateaus together with a full symmetry breaking of the eightfold degenerate zero Landau level. By temperature dependent measurements we investigate the energy gap opening as function of a perpendicular electric field. We find that the transport via localized states at low temperatures exhibits a strong asymmetric behavior with respect to the sign of the applied electric field while the temperature activated transport is fully symmetric.

TT 105.4 Fri 10:15 POT 081

An emergent momentum scale and low energy theory for the graphene twist bilayer. — •Sam Shallcross, Nicolas Ray, Dominik Weckbecker, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

We identify an angle dependent *momentum scale* as the fundamental property of a bilayer composed of mutually rotated graphene layers [1]. This leads to (i) a numerical method that increases, for the twist bilayer, the efficiency of the standard tight-binding method by a factor of $\approx 10^3$, at no loss of accuracy, and (ii) a low energy theory that can be deployed, without distinction, for both the low angle regime and the large angle regime. In the low angle regime this leads to a theory that is close to that of Bistritzer *et al.* [2], but differs in the choice of momentum scale. In the large angle this approach yields electronic versions of the Hamiltonians first derived on symmetry grounds by Mele [3]. We use these low energy approaches to give an overview of the $T = 0$ electronic properties of the twist bilayer system, with a particular focus on the localization of electrons, mixing of single layer graphene states by the interaction, and low energy density of states features.

[1] S. Shallcross, S. Sharma, and O. Pankratov, *Phys. Rev. B* **87**, 245403, 2012.
[2] R. Bistritzer and A. H. MacDonald. *Proc. Natl Acad. Sci.*, **108:12233**, 2010.
[3] E. J. Mele. *Journal of Physics D Applied Physics*, **45:154004**, 2012.

TT 105.5 Fri 10:30 POT 081

RKKY interaction in the AB stacked graphene bilayer: interstitial impurities and a diverging propagator. — •Nicolas Klier, Sam Shallcross, and Oleg Pankratov — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

The interaction between spin polarised impurities in graphene displays a number of novel features that arise both from the valley degree of freedom that graphene possesses, as well as the linearly vanishing density of states at the Dirac point [1,2]. Multilayer graphene systems offer both the possibility of realistic interstitial (i.e., interlayer) impurities, as well as novel electronic features. In particular, the Bernal stacked (AB) bilayer exhibits low energy (chiral) bands as well as high energy bonding and anti-bonding bands. We demonstrate that at the bonding to anti-bonding *gap edge* there is an logarithmic divergence $\log(E - E_g)$ in the propagator on one sublattice, with E the energy and E_g the energy of the bonding to anti-bonding gap (0.38 eV). This leads to a number of dramatic consequences for the RKKY interaction, most notably: (i) a $R^{-5/2}$ impurity interaction at the gap edge, and, (ii) for interstitial impurities a discontinuous change in the Fermi surface spanning vector that drives the RKKY at the gap edge. We further derive the finite temperature behaviour of this system on the basis of finite temperature perturbation theory.

[1] M.Sherafati, and S.Satpathy, Phys. Rev. B 84, 125416, 2011.
[2] F.Parhizgar, and M.Sherafati, and R.Asgari, and S.Satpathy, Phys. Rev. B 87, 165429, 2013.

TT 105.6 Fri 10:45 POT 081

Conductivity of two-dimensional charge carriers with non-parabolic dispersion — Bretislav Sopik[1], Janik Kailasvuori[2,3], and •Maxim Trushin[4] — [1]Central European Institute of Technology, Masaryk University, Kamenice 735, 62500 Brno, Czech Republic — [2]International Institute of Physics, Universidade Federal do Rio Grande do Norte, 59078-400 Natal-RN, Brazil — [3]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [4]University of Konstanz, Fachbereich Physik, M703 D-78457 Konstanz

We investigate the conductivity of two-dimensional charge carriers with the non-parabolic dispersion k^N with N being an arbitrary natural number assuming the delta-shaped scattering potential as a major source of disorder. We employ the exact solution of the Lippmann-Schwinger equation to derive an analytical Boltzmann conductivity formula valid for an arbitrary scattering potential strength. We proceed further with a numerical study based on the finite size Kubo formula which assesses the applicability range of our analytical model. We find that for any $N > 1$, the conductivity demonstrates a linear dependence on the carrier concentration in the limit of a strong scattering potential strength. This finding agrees with the conductivity measurements performed recently on chirally stacked multilayer graphene [1] where the lowest two bands are non-parabolic and the adsorbed hydrocarbons might act as strong short-range scatterers.

[1] L. Zhang, Y. Zhang, J. Camacho, M. Khodas I. Zaliznyak, Nature Physics **7**, 953-957 (2011).

TT 106: Graphene: Interaction with the Substrate (organized by HL)

Time: Friday 11:15–13:00 Location: POT 081

TT 106.1 Fri 11:15 POT 081

Phonons of graphene on metallic and semiconductor surfaces, an ab-inito approach — •Alejandro Molina-Sanchez and Ludger Wirtz — Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg

The interaction of graphene with substrates can alter its electronic and vibrational properties and is relevant for the practical use of graphene. In this work, we describe the graphene-substrate interaction through the theoretical study of the vibrational properties. We focus on three paradigmatic cases where the interaction strength changes gradually: graphene@BN, graphene@Ir(111), and graphene@SiC (i.e., the buffer layer). We use ab-initio methods to obtain the phonon modes, the density of states, and the strength of the electron-phonon coupling. When we deal with large supercells, we use an unfolding scheme to visualize the phonon bands in the primitive unit cell. Thus, we can distinguish clearly the changes in the phonon dispersion of perturbed-graphene with respect to the one of pristine graphene. Graphene on boron nitride exhibits a weak interaction but a non-negligible shift of the 2D Raman band. We explain this observation as due to a weakening of the electron-phonon interaction via screening of electron-electron correlation by the dielectric substrate. Graphene on iridium, also displays weak interaction but the underlying material is a metal. This leads to an even more pronounced screening of the electron-electron interaction in graphene. In the last case, we study the buffer layer of graphene on silicon carbide. The hybridization of graphene with silicon carbide changes the electronic structure of graphene and the phonon bands.

TT 106.2 Fri 11:30 POT 081

The (3×3)-SiC($\bar{1}\bar{1}\bar{1}$) reconstruction: Surface phase equilibria near the graphene formation regime on 3C-SiC($\bar{1}\bar{1}\bar{1}$) — •Lydia Nemec[1], Florian Lazarevic[2], Patrick Rinke[1], Volker Blum[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]AQcomputare GmbH, Chemnitz — [3]MEMS Department, Duke University, Durham, NC, USA

To refine the growth quality of epitaxial graphene on the C-side of SiC and improve the resulting electronic character of these films, it is important to understand the atomic- and electronic-structure of the interface. A phase mixture of different surface phases is observed just when surface graphitization first sets in. However, the atomic structure of some of the competing surface phases, as well as of the SiC-graphene interface, is unknown.

We performed a density functional theory study on the C-side of the polar SiC($\bar{1}\bar{1}\bar{1}$) surface using the all-electron, numeric, atom-centered basis function code FHI-aims. The formation energy of different reconstructions and model systems for the interface is presented within the thermodynamically allowed range.

The surface energies of the known (2×2) phase is compared with several structural models of the (3×3) phase proposed in the literature. In comparison all the previously suggested (3×3) models are higher in energy than the known (2×2) phase. We present a new model for the (3×3) reconstruction. Its formation energy crosses that of the (2×2) phase just at the carbon rich limit of the chemical potential, which could explain the observed phase mixture.

TT 106.3 Fri 11:45 POT 081

Reststrahl band assisted photocurrents in epitaxial graphene layers — •P. Olbrich[1], C. Drexler[1], L.E. Golub[2], S.N. Danilov[1], V.A. Shalygin[3], V.A. Shalygin[3], R. Yakimova[4], S. Lara-Avila[5], S. Kubatkin[5], B. Redlich[6], R. Huber[1], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]State Polytechnic University, St. Petersburg, Russia — [4]Linköping University, Linköping, Sweden — [5]Chalmers University of Technology, Göteborg, Sweden — [6]FOM Institute for Plasma Physics, Nieuwegein, The Netherlands

We report on the observation of reststrahl band assisted photocurrents in epitaxial graphene on SiC. The samples were excited by the infrared radiation from the tunable free electron laser "FELIX" and a CO_2 gas laser [1]. We show that the photoresponse due to linearly (circularly) polarized mid-infrared light is strongly enhanced (suppressed) in the vicinity of the reststrahl band of SiC. Our data, in particular a complex spectral behavior, are well described by the developed theory taking into account photon drag and photogalvanic effects affected by an enhanced light-matter interaction in the range of substrate's negative dielectric function in its reststrahl band. Moreover, our work demonstrates that substrate phonons strongly influence the transport properties of the carriers in graphene.

[1] P. Olbrich *et al.*, arXiv:1308.0123

TT 106.4 Fri 12:00 POT 081

Towards superlattices: Lateral bipolar multibarriers in graphene — •Martin Drienovsky[1], Franz-Xaver Schrettenbrunner[1], Andreas Sandner[1], Ming-Hao Liu[2], Fedor Tkatschenko[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik Universität Regensburg — [2]Institut für Theoretische Physik Universität Regensburg

We report on transport properties of monolayer-graphene (MLG) with a laterally modulated charge carrier density profile. For that we employed a planar back gate and striped top gate electrodes of 25 nm width and a spacing of 100 nm up to 200 nm, separated from the MLG by an Al_2O_3 dielectric. Tuning of top and back gate voltages gives rise to multiple potential barriers and wells, enabling the investigation of resistance either in the unipolar or the bipolar transport regime. In the latter pronounced single- and multibarrier Fabry-Pérot (FP) resonances are observed. The experimental data of different devices with alternating numbers of top gate stripes and pitch, taken at different temperatures, is consistent with a ballistic transport calculation, employing a realistic potential profile, extracted from classical electrostatic simulation combined with the quantum capacitance model. The origin of resistance oscillations in our multibarrier graphene system can be explained in the FP-picture, without resorting to an artificial band structure.

TT 106.5 Fri 12:15 POT 081

Scanning Tunnelling Spectroscopy of Moiré Patterns on Graphene/Rh(111) — •Anne Holtsch, Tobias Euwens, Hussein Schanak, and Uwe Hartmann — Institut für Experimentalphysik, Universität des Saarlandes, Saarbrücken

The lattices of graphene and Rh(111) provide a difference of approximately 9% between the two lattice constants. This mismatch results in the formation of a Moiré pattern with a lattice constant of 2.9 nm. Each unit cell of the pattern exhibits four regions where the graphene lattice is aligned differently with respect to the Rh(111) atoms. Scanning tunnelling microscopy and spectroscopy are used to investigate changes in the electronic properties at the four regions of the Moiré unit cell. Density functional theory (DFT) calculations show that a decreasing C-Rh distance at different symmetry points coincides with an increasing interaction strength between graphene and Rh(111) [1]. The locations of the minima in the dI/dV curves are identical for the different symmetry regions. Beyond the minimum, the symmetry points show differences in the dI/dV curves according to the C-Rh interaction strength.

[1] M. Iannuzzi and J. Hutter, Surf. Sci. 605, 1360 (2011).

TT 106.6 Fri 12:30 POT 081

Varied Moiré patterns of graphene/Rh(111) measured by scanning tunnelling microscopy — •Tobias Euwens, Anne Holtsch, Hussein Schanak, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Scanning tunnelling microscopy measurements on graphene deposited on a Rh(111) surface are conducted to investigate the superstructures that originate from the different lattice parameters of the graphene and the substrate. Different kinds of superstructures, also called Moiré patterns, can be seen in the resulting images. Their origin lies in either the surface inhomogenities of the Rh(111) substrate or in the form of folds and steps in the graphene itself. Knowing the properties of the growth of graphene on the rhodium surface is important for the construction of more complex graphene-based electronics. Understanding the specific structure of the Moiré patterns can help in that regard as it relays information about the angle between the carbon and the rhodium lattice and potential reasons for the twisting between the two lattices.

TT 106.7 Fri 12:45 POT 081

Impact of the substrate on the electronic properties of graphene — •Hussein Shanak, Anne Holtsch, Tobias Euwens, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Electronic properties of graphene grown on different substrates such as Rh, Cu and SiO2 were investigated using scanning tunnelling microscopy and spectroscopy. The different kinds of substrates result in different types of superstructures due to the mismatch between graphene and substrate. Comparison of the electronic properties obtained for graphene on the different substrates leads to a better understanding of the graphene doping behaviour. Additionally, the existence of different superstructures leads to different growing properties of the materials on top of graphene itself.

TT 107: Quantum Information Systems II (organized by HL)

Time: Friday 9:30–10:45 Location: POT 151

TT 107.1 Fri 9:30 POT 151

Coherent pulse re-shaping in a semiconductor optical amplifier — •Mitra Pasche, Mirco Kolarczik, Yücel Kaptan, Nina Owschimikow, and Ulrike Woggon — Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany

Recently it was demonstrated that Rabi oscillations in Quantum Dots (QDS) induce a laser pulse re-shaping in a semiconductor optical amplifier (SOA) at room temperature[1]. Here we present the results of a systematic investigation of the dependence of the pulse re-shaping on pulse power, detuning and the electrical injection level. The measurements are performed using frequency resolved optical short-pulse characterization by heterodyning (FROSCH)[1]. The method allows to observe simultaneously the amplitude and phase of the light field of the laser pulse relative to a reference pulse. In numerical simulations, we vary the parameters of the probe pulse and quantify their influence on the shape of the cross-correlation of the probe and reference pulse. We can thus assign characteristic phase jumps observed in the experiment to a coherent exchange of energy in the light-matter system.

[1] M.Kolarczik, N.Owschimikow, J.Korn, B.Lingnau, Y.Kaptan, D.Bimberg, E.Schöll, K.Lüdge, U.Woggon, *Nat. Commun.*, accepted (2013).

TT 107.2 Fri 9:45 POT 151

Ambient Temperature Spin Pumping of Silicon Carbide Quantum Defects — •Hannes Kraus[1], Franziska Fuchs[1], Daniel Riedel[1], Victor Soltamov[2], Dmitrij Simin[1], Stefan Väth[1], Andreas Sperlich[1], Pavel Baranov[2], Georgy Astakhov[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, Germany — [2]Ioffe Physical-Technical Institute, St. Petersburg, Russia

Silicon carbide is best known as a high performance power electronics semiconductor, although intrinsic defects in this material, particularly silicon vacancies, are very promising for quantum information processing, photonics and magnetometry [1]. This is due to the defects' intriguing quantum properties: The SiC defect spin states can be initialized and subsequently read using optically detected magnetic resonance (ODMR), and the high-spin ground state of these defects can be selectively populated by optical pumping. Similar to a lasing system, this leads to a population inversion and, consequently, to a stimulated radio emission [2]. We show this effect also works at room temperature, which opens an interesting perspective to construct low noise, low cost and low maintenance solid state radio amplifiers. Another opportunity is the defect ODMR's dependence on magnetic field orientation and temperature, suggesting SiC applications in quantum sensing.

[1] D. Riedel et al., Phys. Rev. Lett. 109, 226402 (2012)
[2] H. Kraus et al., Nature Physics (2013), doi:10.1038/NPHYS2826

TT 107.3 Fri 10:00 POT 151

Silicon Vacancies in Silicon Carbide as a Vector Magnetometer — •Dmitrij Simin[1], Franziska Fuchs[1], Hannes Kraus[1], Victor Soltamov[2], Andreas Sperlich[1], Pavel Baranov[2], Georgy Astakhov[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany — [2]Ioffe Physical-Technical Institute, 194021 St. Petersburg, Russia

The determination of both the magnitude and orientation of ambient magnetic fields has become a crucial convenience and safety factor in smartphones, spacecrafts, and satellites. Due to severe requirements for these devices, including compactness, temperature stability, and inexpensive fabrication, there are few devices that meet them all. In this study, we present a new approach, utilizing the spin properties of the silicon vacancies in silicon carbide [1]. Using room temperature optically detected magnetic resonance [2], we measure the change in optical emission due to vacancy specific electronic transitions that are dependent on the magnitude as well as on the direction of the external magnetic field. Using these relationships, we show how silicon carbide can be used as a compact and cost-effective solution for vector magnetometry applications with a good accuracy.

[1]Riedel et al.: Phys. Rev. Lett. 109, 226402 (2012)
[2]Kraus et al.: Nat. Phys., DOI 10.1038/nphys2826 (2013)

TT 107.4 Fri 10:15 POT 151

Spin defect engineering in silicon carbide using neutron irradiation — •Franziska Fuchs[1], Michael Trupke[2], Georgy Astakhov[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, A-1020 Wien

Atom-like defects in semiconductors are promising systems for spin-based quantum information applications. With its advanced growth and device technologies, Silicon carbide (SiC) is an eligible host for such defects, e.g. silicon vacancies (V_{Si}). This spin-$\frac{3}{2}$ system can be addressed and manipulated [1] and could serve as a room temperature source for single photons [2] or a room temperature maser amplifier [3]. With these applications in mind, one main challenge is to thoroughly create, isolate, and control the defects. Here, we report defect engineering of V_{Si} defects in SiC by means of neutron irradiation. Our photoluminescence measurements show that the defect density is well controllable via the irradiation dose. The irradiation flux has been varied over 10 orders of magnitude, from 10^8 to 10^{18} neutrons/cm^2. Two specific cases are of interest. The generation of the maximum V_{Si} concentration possible without destroying the crystal structure is required for the implementation of maser amplifiers. On the other hand, the creation of very few, isolated defects is crucial for the realization of single photon sources. [1] Riedel et al.: Phys. Rev. Lett. 109, 226402 (2012), [2] Castelletto et al.: Nat Mat 12 (2013), DOI 10.1038/namt3806 [3] Kraus et al.: Nat Phys (2013), DOI 10.1038/nphys2826

TT 107.5 Fri 10:30 POT 151

Mapping the D1-transition of Caesium by dressed-state resonance fluorescence from a single (In,Ga)As quantum dot — •Sven M. Ulrich[1], Markus Oster[1], Michael Jetter[1], Alban Urvoy[2], Robert Löw[2], Tilmann Pfau[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]5. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Hybrid quantum systems combining semiconductor quantum dots (QDs) and atomic vapors promise interesting applications in quantum information technology. Recent research in this field has explored the resonant coupling between single GaAs QDs and Rubidium gas to generate e.g. frequency-stabilized non-classical emission ($\sim$ 780 nm) as well as slow light for qubit storage/retrieval operations.

As an alternative hybrid approach we use a cw laser-driven single (In,Ga)As QD (4 K) in the "dressed state" resonance fluorescence (RF) regime to address the D_1 transitions of atomic Caesium (Cs) vapor (300 K). QD-atom resonance is achieved by tuning the frequency of the dressing laser close to the QD ground state $\nu_0 \approx 335.116$ THz (894.592 nm) and shifting the narrow-band center and side channels of the QD Mollow triplet. Using this laser frequency controlled QD probe light for absorption measurements allows to precisely identify all four Cs hyperfine-split transitions. Therefore, narrow-band (In,Ga)As QD RF is demonstrated as suitable to optically address individual channels of the D_1 quadruplet without magnetic field or electric field tuning.

TT 108: Graphene (joint session with TT, MA, HL, DY, O)

Time: Friday 11:30–13:15 Location: CHE 89

TT 108.1 Fri 11:30 CHE 89

Plasma-enhanced chemical vapor deposition of graphene on copper substrates — •Nicolas Wöhrl, Oliver Ochedowski, Steven Gottlieb, and Volker Buck — Universität Duisburg-Essen und CENIDE, 47057 Duisburg, Germany

In this work we present the synthesis of graphene on copper by microwave Plasma-enhanced Chemical Vapor Deposition (PE-CVD) process. The special construction of the plasma source allows the deposition at a wide range of different process parameters giving a fast and inexpensive method to synthesize graphene. Additional advantages of the plasma deposition of graphene are lower substrate temperatures compared with thermal CVD processes. The PE-CVD process uses hydrogen and methane as reaction gases exactly like thermal CVD process does. The gaseous precursors are decomposed in the plasma and the catalytic influence of copper and the minor solubility of carbon in copper lead to the growth of one monolayer of graphene. Plasma parameters are varied to investigate the influence on the graphene properties. Raman spectroscopy and AFM measurements are used as nondestructive tools for the characterization of the synthesized graphene films. Especially Raman spectroscopy is used as an efficient tool to determine the number of graphene layers, the disorder and the defect density. We present a possible way to produce large area of monolayer graphene on a copper based substrate. This technology can help to make graphene available for industrial applications.

TT 108.2 Fri 11:45 CHE 89

Continuous wafer-scale graphene on cubic-SiC(001) — •Victor Aristov[1,2], Olga Molodtsova[2], Alexei Zakharov[3], Dmitry Marchenko[4], Jaime Sánchez-Barriga[4], Andrei Varykhalov[4], Marc Portail[5], Marcin Zielinski[6], Igor Shvets[7], and Alexander Chaika[1,7] — [1]ISSP RAS, Chernogolovka, Moscow dist. 142432, Russia — [2]HASYLAB at DESY, D-22607 Hamburg, Germany — [3]MAX-lab, Lund University, Box 118, 22100 Lund, Sweden — [4]HZB für Materialien und Energie, D-12489 Berlin, Germany — [5]CNRS-CRHEA, 06560 Valbonne, France — [6]NOVASiC, BP267-F73375 Le Bourget du Lac Cedex, France — [7]CRANN, School of Physics, Trinity College, Dublin 2, Ireland

The atomic and electronic structure of graphene synthesized on commercially available cubic SiC(001)/Si(001) wafers have been studied. LEED, LEEM, PEEM, STM and ARPES data prove the wafer-scale continuity and uniform thickness of the graphene overlayer and reveal that the graphene overlayer consists of only a few monolayers with physical properties of quasi-freestanding graphene: atomic-scale rippling, asymmetric distributions of carbon-carbon bond lengths etc. In addition, graphene overlayer consists of rotated nanometer-sized ribbons with four different lattice orientations connected through the grain boundaries. Thus, this graphene could be adapted for graphene-based electronic technologies and directly patterned using Si-electronic lithographic process. Supported by RFBR grant 14-02-00949, by Marie Curie IIF grant (7th ECFP) and by SPP 1459 of DPG.

TT 108.3 Fri 12:00 CHE 89

Characterization of single and few layer of molybdenum disulfide with spectroscopic imaging ellipsometry — •P. H. Thiesen[1], B. Miller[2], C. Röling[1], E. Parzinger[2], A. W. Holleitner[2], and U. Wurstbauer[2] — [1]Accurion GmbH, Göttingen, Germany — [2]Technische Universität München, Walter Schottky Institut, 85748 Garching, Germany

Molybdenum disulfide is a layered transition metal dichalcogenide. From the point of current research, 2D-materials based on MoS2 are very promising because of the special semiconducting properties. The bulk material has an indirect 1.2 eV electronic bandgap, but single layer MoS2 has a direct 1.8 eV bandgap. The monolayer can be used in prospective electronic devices like transistors or photo detectors. Like in the initial period of graphene research, the issue is to identify and characterize MoS2 crystallites of microscopic scale. Imaging ellipsometry is a nondestructive optical method in thin film metrology with a lateral resolution down to 1 micro meter. Imaging ellipsometry has been applied to characterize graphene flakes of few micrometer size [1],[2] and also to identify single layer steps in multilayer graphene/graphite stacks [3]. Delta and Psi Spectra of MoS2 monolayers as well as maps of the ellipsometric angles will be presented. The practical aspect of single layer identification will be addressed and the capability of ellipsometric contrast micrographs as a fast tool for single layer identification will be demonstrated. [1] Wurstbauer et al., Appl. Phys. Lett. 97, 231901 (2010) [2] Matkovic et al. J. Appl. Phys. 112, 123523 (2012) [3] Albrektsen et al. J. Appl. Phys. 111, 064305 (2012)

TT 108.4 Fri 12:15 CHE 89

Charge and Spin Transport in Turbostratic Graphene and Graphene Nanoribbons — •Nils Richter[1], Sebastian Schweizer[2], Ajit Kumar Patra[2], Yenny Hernandez[3], Akimitsu Narita[3], Xinliang Feng[3], Petr Ostrizek[1], Klaus Müllen[3], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]FB Physik, Universität Konstanz, 78457 Konstanz, Germany — [3]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

We present two specially selected allotropes of graphene: Turbostratic graphene (TG) and graphene nanoribbons (GNRs).

TG discs are graphitic microstructures where the twisting of adjacent layers leads to an electronic decoupling. Electrical transport measurements reveal quantum effects such as weak localization and huge charge carrier mobilities (100,000 cm^2/Vs) in protected bulk layers [1]. In non-local spin valves we find efficient spin injection over micrometer distances showing large spin diffusion lengths.

Using electromigrated nanojunctions we are able to investigate electrical and spin transport in chemically synthesized GNRs. As they are dispersed in a solvent [2] they can be drop cast on such junctions. With GNRs of different widths and edge geometries we will probe the exciting unconventional properties that have been predicted for these nanostructures [3].

[1] Y. Hernandez et al., arXiv:1301.6087 (under review 2013). [2] A. Narita et al., Nature Chem., in press, DOI: 10.1038/NCHEM.1819. [3] O. Yazyev, Rep. Prog. Phys. 73, 056501 (2010).

TT 108.5 Fri 12:30 CHE 89

Graphene functionalisation with N and O: reversible or permanent modification of the electronic properties? — •Peter Brommer[1,2], Alex Marsden[1], Neil Wilson[1], Gavin Bell[1], and David Quigley[1,2] — [1]Department of Physics, University of Warwick, Coventry, UK — [2]Centre for Scientific Computing, University of Warwick, Coventry, UK

For many applications it is essential to modify the electronic properties of graphene in a controlled fashion. This can be achieved via oxygen and nitrogen functionalisation in ultra-high vacuum, leading to a system in which electronic and structural properties can be systematically studied. Low dose oxygen functionalisation (< 5 atomic percent) can be reversed completely by annealing at 200 °C, while nitrogen permanently integrates itself into the material. Here we present insights from DFT calculations on this system, such as the low-energy configurations and simulated transmission electron microscopy (TEM) images, binding energies and effective band structures of the N and O decorated graphene sheets. We directly compare our results with experiments on CVD grown graphene. Angle-resolved photoemission spectroscopy (ARPES) resolves the band structure changes on functionalization, whilst X-ray photoelectron spectroscopy (XPS) provides information about the chemical environment of the defect atoms. Combined, the computational and experimental data can offer insights into the structural changes induced by the functionalisation process and their consequences on the electronic properties of the material.

TT 108.6 Fri 12:45 CHE 89

Revealing the ultrafast process behind the photoreduction of graphene oxide — •Daniel S. Badali[1], Regis Y.N. Gengler[1], Dongfang Zhang[1], Kostantinos Dimos[2], Kostantinos Spyrou[2], Dimitrios Gournis[2], and R.J. Dwayne Miller[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg Center for Ultrafast Imaging, University of Hamburg, Hamburg, Germany — [2]Department of Material Science and Engineering, University of Ioannina, Ioannina, Greece

Because of its unique electronic and structural properties, graphene has brought two-dimensional materials to the foreground of material science and nanoelectronic research. As such, reliable methods for producing graphene are in demand and have significant impact on the field

of thin films. In recent years it has been found that irradiating dispersions of graphene oxide in water with ultraviolet light has led to the production of graphene. Although this has been observed in a variety of experimental conditionals, the exact mechanism of the reduction has remained elusive until now. To this end, we have performed careful optical pump-probe measurements which have revealed the chemistry of this process: rather than direct photoreduction, the reduction is mediated by solvated electrons which have been liberated from water molecules by the ultraviolet light. We show that this occurs on an ultrafast timescale in the tens of picoseconds range. Characterization of the final product confirms the removal of oxygen containing groups and the restoration of the honeycomb carbon network of graphene.

TT 108.7 Fri 13:00 CHE 89

Tuning of structural, electronic and optical properties in twisted bilayer MoS_2 — •Jens Kunstmann[1], Arend M. van der Zande[1], Alexey Chernikov[1], Daniel A. Chenet[1], YuMeng You[1], XiaoXiao Zhang[1], Timothy C. Berkelbach[1], Pinshane Y. Huang[2], Lei Wang[1], Fan Zhang[1], Mark Hybertsen[1,3], David A. Muller[2], David R. Reichman[1], Tony F. Heinz[1], and James C. Hone[1] — [1]Columbia University, New York, New York, 10027, USA — [2]Cornell University, Ithaca, New York, 14853, USA — [3]Brookhaven National Laboratory, Upton, New York 11973, USA

With the rise of graphene, atomically thin 2D materials have become the focus of many researchers worldwide. Among them, group 6 transition metal dichalcogenides, such as MoS_2 are new 2D direct gap semiconductors, have been used as field effect transistors and are promising for applications in valleytronics. However, little is understood about the interlayer interactions between 2D materials. We measured dozens of MoS_2 bilayers with well-defined twist angle by stacking single crystal monolayers using ultraclean transfer techniques. We observe that continuous changes in the interlayer twist angle lead to strong, continuous tuning in the indirect optical transitions, the Raman modes, the second harmonic generation, and the reflection spectra. We use electronic structure calculations to show that the tuning in the indirect band transitions arise from an increase of the bilayer separation caused by the van der Waals repulsion of sulfur atoms. These results indicate the possibility of producing new 2D materials with desired properties by tailoring the interlayer alignment in 2D heterostructures.