Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(Lecture halls H2, H4, H7, H22, H23, H48, and Theater; Poster D)

Tutorial "Next generation of SI-Units (joint session VA/TT/TUT)"

VA 1.1	Sun	16:00–16:35	H2	**A Quantum-Based Pressure Standard for a New SI Realization of the Pascal** — •Jay Hendricks
VA 1.2	Sun	16:35–17:10	H2	**Redefinition of the Kelvin - With what accuracy can temperatures be measured?** — •Steffen Rudtsch
VA 1.3	Sun	17:10–17:45	H2	**The new kilogram - Now approachable for extraterrestrials and nonhumans** — •Frank Härting
VA 1.4	Sun	17:45–18:20	H2	**Counting electrons for the new ampere** — •Frank Hohls

Plenary Talks

PLV I	Mon	8:30– 9:15	H1	**Linking the International System of Units to Fundamental Constants** — •Joachim Ullrich
PLV V	Tue	17:15–18:00	H1	**The Dark Energy of Quantum Materials** — •Laura H Greene
PLV IX	Wed	14:00–14:45	H2	**Vestigial order in quantum materials** — •Jörg Schmalian
PLV XII	Thu	14:00–14:45	H1	**Quantum computing - progress towards applications** — •Heike Riel

Invited talks of the joint Symposium SKM Dissertation-Prize 2019

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:50	H2	**Synchronization and Waves in Confined Complex Active Media** — •Jan Frederik Totz
SYSD 1.2	Mon	9:50–10:10	H2	**Spin scattering of topologically protected electrons at defects** — •Philipp Rüssmann
SYSD 1.3	Mon	10:10–10:30	H2	**Beyond the molecular movie: Revealing the microscopic processes behind photo-induced phase transitions** — •Chris W. Nicholson
SYSD 1.4	Mon	10:30–10:50	H2	**Thermodynamic bounds on current fluctuations** — •Patrick Pietzonka
SYSD 1.5	Mon	10:50–11:10	H2	**Lightwave-driven quasiparticle acceleration** — •Fabian Langer
SYSD 1.6	Mon	11:10–11:30	H2	**Ultrafast plasmon-driven point-projection electron microscopy** — •Jan Vogelsang
SYSD 1.7	Mon	11:30–11:50	H2	**Helimagnets, sand patterns and fingerprints linked by topology** — •Peggy Schönherr

Invited talks of the joint Symposium Geometry, Topology, and Condensed Matter

See SYGT for the full program of the symposium.

SYGT 1.1	Tue	9:30–10:00	H1	**Thermal Properties of Vortices on Curved Surfaces** — •José Lorenzana
SYGT 1.2	Tue	10:00–10:30	H1	**Curvature–induced effects in manomagnets** — •Denis Sheka
SYGT 1.3	Tue	10:30–11:00	H1	**Magnetization configurations and reversal of individual ferromagnetic nanotubes** — •Martino Poggio

SYGT 1.4	Tue	11:15–11:45	H1	**An experimental perspective on topology and nanoelectronics in graphene and related 2D materials.** — •Ivan J. Vera-Marun
SYGT 1.5	Tue	11:45–12:15	H1	**Roles of the curvature in two-dimensional nematic films** — •Gaetano Napoli

Invited talks of the joint Symposium Hydrodynamic Electronics: Transport in ultra-pure Quantum Systems

See SYHE for the full program of the symposium.

SYHE 1.1	Wed	9:30–10:00	H1	**Hydrodynamic theory of dissipative magnetophonons** — •Sean Hartnoll
SYHE 1.2	Wed	10:00–10:30	H1	**Unconventional transport in mesostructures of ultra-pure delafossite metals** — •Andrew Mackenzie
SYHE 1.3	Wed	10:30–11:00	H1	**Topological Materials with liquid electrons** — •Claudia Felser
SYHE 1.4	Wed	11:15–11:45	H1	**Hydrodynamic approach to electronic transport** — •Boris Narozhny
SYHE 1.5	Wed	11:45–12:15	H1	**Electron hydrodynamics in graphene: introduction and status** — •Denis Bandurin

Invited talks of the joint Symposium Czech Republic as Guest of Honor

See SYCZ for the full program of the symposium.

SYCZ 1.1	Thu	9:30–10:00	H4	**Crystal symmetries and transport phenomena in antiferromagnets** — •Tomas Jungwirth
SYCZ 1.2	Thu	10:00–10:30	H4	**Terahertz subcycle charge and spin control** — •Rupert Huber
SYCZ 1.3	Thu	10:30–11:00	H4	**1D molecular system on surfaces** — •Pavel Jelinek
SYCZ 1.4	Thu	11:15–11:45	H4	**Tunneling microscopy on insulators provides access to out-of-equilibrium charge states** — •Jascha Repp
SYCZ 1.5	Thu	11:45–12:15	H4	**Occam's razor and complex networks from brain to climate** — •Jaroslav Hlinka
SYCZ 1.6	Thu	12:15–12:45	H4	**Long range temporal correlations in complex systems** — •Holger Kantz

Invited talks of the joint Symposium Interactions and Spin in 2D Heterostructures

See SYIS for the full program of the symposium.

SYIS 1.1	Thu	15:00–15:30	H1	**Magic Angle Graphene: a New Platform for Strongly Correlated Physics** — •Pablo Jarillo-Herrero
SYIS 1.2	Thu	15:30–16:00	H1	**Bilayer Graphene Quantum Devices** — •Klaus Ensslin
SYIS 1.3	Thu	16:00–16:30	H1	**Light-Matter interaction in van der Waals heterostructures** — •Tobias Korn
SYIS 1.4	Thu	16:45–17:15	H1	**Spin transport in Van der Waals materials and heterostructures** — •Bart Van Wees
SYIS 1.5	Thu	17:15–17:45	H1	**Flipping the valley in graphene quantum dots** — •Markus Morgenstern

Invited talks of the joint Symposium Identifying Optimal Physical Implementations for beyond von Neumann Computing Concepts

See SYCC for the full program of the symposium.

SYCC 1.1	Fri	9:30–10:00	H1	**On the Link Between Energy and Information for the Design of Neuromorphic Systems** — •Narayan Srinivasa
SYCC 1.2	Fri	10:00–10:30	H1	**Encoding neural and synaptic functionalities in electron spin: A pathway to efficient neuromorphic computing** — •Kaushik Roy
SYCC 1.3	Fri	10:30–11:00	H1	**Neuromorphic computing with spintronic nano-oscillators** — •Philippe Talatchian
SYCC 1.4	Fri	11:15–11:45	H1	**Artifcial Intelligence and beyond von Neumann architectures, a mutual opportunity** — •Mirko Prezioso
SYCC 1.5	Fri	11:45–12:15	H1	**Brain-inspired approaches in ultrafast magnetism** — •Johan H. Mentink

Focus Session "New Bright Sources of Quantum Microwaves"

TT 10.1	Mon	15:00–15:30	H2	**Quantum dynamics of a microwave resonator strongly coupled to a tunnel junction** — •Jérôme Esteve
TT 10.2	Mon	15:30–16:00	H2	**Quantum optics with artificial atoms in an open space** — •Oleg Astafiev
TT 10.3	Mon	16:00–16:30	H2	**Quantum microwaves with a DC-biased Josephson junction** — •Fabien Portier
TT 10.4	Mon	16:45–17:15	H2	**Photodetectors and metamaterials for on-chip microwave photonics** — •Frank K. Wilhelm-Mauch
TT 10.5	Mon	17:15–17:45	H2	**Correlated Cooper pair transport and microwave photon emission in the Coulomb blockade** — •Juha Leppäkangas

Focus Session "Quantum Dynamics of Kinetically Constrained Many-Body Systems"

TT 21.1	Tue	9:30–10:00	H2	**Quantum dynamics, scars, and integrability in constrained Rydberg systems** — •Vedika Khemani
TT 21.2	Tue	10:00–10:30	H2	**DMRG investigation of constrained models: from quantum dimer and quantum loop ladders to hard-boson and Fibonacci anyon chains** — •Natalia Chepiga
TT 21.3	Tue	10:30–11:00	H2	**Localization in Fractonic Random Circuits** — •Michael Pretko
TT 21.4	Tue	11:15–11:45	H2	**Many-body localization dynamics from gauge invariance** — •Markus Heyl
TT 21.5	Tue	11:45–12:15	H2	**Slow dynamics due to kinetic constraints, from classical to quantum** — •Juan Garrahan

Focus Session "Topology in 3D Reciprocal Space: Beyond Dirac and Weyl Quasiparticles"

TT 43.1	Wed	15:00–15:30	H2	**Novel optical and electrical responses in topological semimetals** — •Joel Moore
TT 43.2	Wed	15:30–16:00	H2	**Beyond the elementary particles and the 10-fold classification of non-interacting topological phases** — •Alexey Soluyanov
TT 43.3	Wed	16:00–16:30	H2	**Direct optical detection of Weyl fermion chirality in a topological semimetal** — •Nuh Gedik
TT 43.4	Wed	16:45–17:15	H2	**Evidence for an axionic charge density wave in the Weyl semimetal $(TaSe_4)_2I$** — •Johannes Gooth
TT 43.5	Wed	17:15–17:45	H2	**Investigations of Dirac/Weyl semimetals under external stimuli** — •Ece Uykur

Focus Session "Broken Time Reversal Symmetry in Multiband Superconductors"

TT 51.1	Thu	9:30–10:00	H2	**Evaluation of chiral superconductivity in Sr_2RuO_4** — •Clifford Hicks
TT 51.2	Thu	10:00–10:30	H2	**Magnetic excitations and their possible role in the superconducting pairing in Sr_2RuO_4** — •Markus Braden
TT 51.3	Thu	10:30–11:00	H2	**Topologically protected Bogoliubov Fermi surfaces** — •Daniel Agterberg
TT 51.4	Thu	11:15–11:45	H2	**Time-reversal symmetry breaking in Fe-based superconductors** — •Andrey Chubukov
TT 51.5	Thu	11:45–12:15	H2	**Emerging superconductivity with broken time reversal symmetry inside a superconducting s-wave state** — •Vadim Grinenko

Invited Talks not included in Focus Sessions

TT 11.4	Mon	15:45–16:15	H4	**Majorana states in carbon nanotubes** — •Magdalena Marganska
TT 14.8	Mon	17:00–17:30	H22	**Gate-defined quantum point contacts and quantum dots in bilayer graphene** — •Christoph Stampfer
TT 15.10	Mon	17:30–18:00	H23	**Theory of superconducting pairing in iron-based superconductors** — •Andreas Kreisel
TT 22.10	Tue	12:00–12:30	H7	**Superconducting films and interfaces: Novel features from spin imbalance and Rashba spin-orbit coupling** — •Gertrud Zwicknagl
TT 29.1	Tue	14:00–14:30	H2	**Mesoscopic quantum electrodynamics with carbon nanotubes** — •Takis Kontos

TT 29.2	Tue	14:30–15:00	H2	**Nanomechanical characterization of the Kondo charge dynamics in a carbon nanotube** — •Andreas K. Hüttel
TT 38.1	Wed	9:30–10:00	H23	**A new heavy-fermion superconductor $CeRh_2As_2$ with Rashba and quadrupolar interactions** — •Seunghyun Khim
TT 66.1	Fri	9:30–10:00	H2	**Non-equilibrium superconductivity: from post-quench dynamics to controlling competing orders** — •Peter P. Orth

Sessions

TT 1.1–1.4	Sun	16:00–18:20	H2	**Next generation of SI-Units (joint session VA/TT/TUT)**
TT 2.1–2.13	Mon	9:30–13:00	H7	**Correlated Electrons: Electronic Structure Calculations and Other Theoretical Topics**
TT 3.1–3.13	Mon	9:30–13:00	Theater	**Topological Insulators (joint session TT/MA)**
TT 4.1–4.12	Mon	9:30–12:45	H22	**Nonequilibrium Quantum Many-Body Systems 1 (joint session TT/DY)**
TT 5.1–5.13	Mon	9:30–13:00	H23	**Superconductivity: Fe-based Superconductors - FeSe and 122**
TT 6.1–6.14	Mon	9:30–13:15	H53	**Surface magnetism and magnetic coupling phenomena (joint session MA/O/TT)**
TT 7.1–7.11	Mon	10:00–13:00	H19	**Dynamics in many-body systems: Equilibration and localization I (joint session DY/TT)**
TT 8.1–8.9	Mon	10:30–13:00	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge I (joint session O/TT/CPP/DS)**
TT 9.1–9.9	Mon	10:30–13:00	H24	**Graphene I: Structure and Growth (joint session O/TT)**
TT 10.1–10.9	Mon	15:00–18:45	H2	**Focus Session: New Bright Sources of Quantum Microwaves**
TT 11.1–11.13	Mon	15:00–18:45	H4	**Majorana Physics**
TT 12.1–12.10	Mon	15:00–17:30	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge II (joint session O/TT/DS/CPP)**
TT 13.1–13.14	Mon	15:00–18:45	Theater	**Frustrated Magnets - Spin Liquids (joint session TT/MA)**
TT 14.1–14.14	Mon	15:00–19:00	H22	**Graphene**
TT 15.1–15.14	Mon	15:00–19:00	H23	**Superconductivity: Fe-based Superconductors - Other Materials and Theory**
TT 16.1–16.12	Mon	15:00–18:00	H24	**Graphene II: Excitations and Nanoribbons (joint session O/TT)**
TT 17.1–17.49	Mon	15:00–18:30	Poster D	**Poster Session: Correlated Electrons 1**
TT 18.1–18.13	Mon	15:00–18:30	Poster D	**Poster Session: Topological Topics (joint session TT/MA)**
TT 19.1–19.3	Mon	15:00–18:30	Poster D	**Poster Session: Disordered Quantum Systems**
TT 20.1–20.9	Mon	15:30–18:00	H19	**Dynamics in many-body systems: Equilibration and localization II (joint session DY/TT)**
TT 21.1–21.8	Tue	9:30–13:00	H2	**Focus Session: Quantum Dynamics of Kinetically Constrained Many-Body Systems (joint session TT/DY)**
TT 22.1–22.10	Tue	9:30–12:30	H7	**Superconductivity: Theory**
TT 23.1–23.13	Tue	9:30–13:00	Theater	**Frustrated Magnets - General 1 (joint session TT/MA)**
TT 24.1–24.10	Tue	9:30–12:15	H22	**Molecular Electronics and Photonics**
TT 25.1–25.6	Tue	9:30–11:00	H23	**Disordered Quantum Systems**
TT 26.1–26.9	Tue	10:30–13:00	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge III (joint session O/CPP/DS/TT)**
TT 27.1–27.7	Tue	10:30–12:45	H15	**Focus Session: Designer Quantum Systems I (joint session O/TT)**
TT 28.1–28.6	Tue	11:15–12:45	H23	**Cryotechnique: Refrigeration and Thermometry**
TT 29.1–29.6	Tue	14:00–16:00	H2	**Nanotubes and Nanoribbons**
TT 30.1–30.7	Tue	14:00–15:45	H4	**Correlated Electrons: 1D Theory**
TT 31.1–31.10	Tue	14:00–16:45	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge IV (joint session O/CPP/DS/TT)**
TT 32.1–32.5	Tue	14:00–15:45	H15	**Focus Session: Designer Quantum Systems II (joint session O/TT)**
TT 33.1–33.8	Tue	14:00–16:00	Theater	**Frustrated Magnets - General 2 (joint session TT/MA)**
TT 34.1–34.8	Tue	14:00–16:00	H22	**Nonequilibrium Quantum Many-Body Systems 2**
TT 35.1–35.8	Tue	14:00–16:00	H23	**Spintronics (joint session TT/MA/DY)**
TT 36.1–36.4	Wed	9:30–10:30	H7	**Fluctuations, Noise and Quantum Coherence**
TT 37.1–37.11	Wed	9:30–12:30	H22	**Topological Semimetals - Theory (joint session TT/MA)**

TT 38.1–38.11	Wed	9:30–12:45	H23	**f-Electron Systems and Heavy Fermions**
TT 39.1–39.9	Wed	9:30–12:30	H32	**Focus Session: Direct-Write Nanofabrication and Applications I (Electron Beam Induced Processing) (joint session DS/TT)**
TT 40.1–40.13	Wed	9:30–13:00	H48	**Superconductivity: Qubits 1**
TT 41.1–41.9	Wed	10:30–13:15	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge V (joint session O/CPP/DS/TT)**
TT 42.1–42.7	Wed	10:45–12:30	H7	**Nano- and Optomechanics**
TT 43.1–43.7	Wed	15:00–18:15	H2	**Focus Session: Topology in 3D Reciprocal Space: Beyond Dirac and Weyl Quasiparticles (joint session TT/MA)**
TT 44.1–44.15	Wed	15:00–19:00	H7	**Correlated Electrons: Method Development**
TT 45.1–45.11	Wed	15:00–17:45	H9	**Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge VI (joint session O/DS/CPP/TT)**
TT 46.1–46.13	Wed	15:00–18:30	H22	**Quantum Dots, Quantum Wires, Point Contacts**
TT 47.1–47.14	Wed	15:00–18:45	H23	**Quantum Magnets, Molecular Magnets and Skyrmions**
TT 48.1–48.9	Wed	15:00–18:00	H32	**Focus Session: Direct-Write Nanofabrication and Applications II (Electron Beam Induced Processing) (joint session DS/TT)**
TT 49.1–49.50	Wed	15:00–18:30	Poster D	**Poster Session: Superconductivity**
TT 50.1–50.26	Wed	15:00–18:30	Poster D	**Poster Session: Correlated Electrons 2**
TT 51.1–51.8	Thu	9:30–13:00	H2	**Focus Session: Broken Time Reversal Symmetry in Multiband Superconductors**
TT 52.1–52.12	Thu	9:30–12:45	H7	**Quantum Impurities and Kondo Physics**
TT 53.1–53.13	Thu	9:30–13:00	Theater	**Frustrated Magnets - Strong Spin-Orbit Coupling (joint session TT/MA)**
TT 54.1–54.13	Thu	9:30–13:00	H22	**Correlated Electrons: Complex Oxides and Other Materials**
TT 55.1–55.13	Thu	9:30–13:00	H23	**Superconductivity: Tunneling and Josephson Junctions**
TT 56.1–56.10	Thu	15:00–17:45	H2	**Topological Semimetals - Experiment (joint session TT/MA)**
TT 57.1–57.11	Thu	15:00–18:00	H7	**Superconductivity: Properties and Electronic Structure**
TT 58.1–58.13	Thu	15:00–18:30	Theater	**Superconductivity: Qubits 2**
TT 59.1–59.11	Thu	15:00–18:00	H22	**Complex Oxides Interfaces and Charge Order**
TT 60.1–60.11	Thu	15:00–18:00	H23	**Quantum-Critical Phenomena (joint session TT/DY)**
TT 61.1–61.9	Thu	15:00–17:45	H24	**Topology and Symmetry-Protected Materials (joint session O/MA/TT)**
TT 62.1–62.8	Thu	15:00–17:45	H32	**Direct-Write Nanofabrication and Applications III (Electron Beam Induced Processing) (joint session DS/TT)**
TT 63.1–63.13	Thu	15:00–18:30	Poster D	**Poster Session: Cryogenic Particle Detectors and Cryotechnique**
TT 64.1–64.17	Thu	15:00–18:30	Poster D	**Poster Session: Transport**
TT 65	Thu	18:30–20:00	H7	**Annual General Meeting of the Low Temperature Physics Division**
TT 66.1–66.11	Fri	9:30–12:45	H2	**Ultrafast Dynamics of Light-Driven Systems**
TT 67.1–67.10	Fri	9:30–12:00	H4	**Cryogenic Particle Detectors and Other Superconducting Electronics**
TT 68.1–68.10	Fri	9:30–12:15	H22	**Topology: Other Topics**
TT 69.1–69.8	Fri	9:30–11:30	H23	**Cold Atomic Gases and Superfluids**

Annual General Meeting of the Low Temperature Physics Division

Thursday 18:30–20:00 H7

- Bericht
- Verschiedenes

TT 1: Next generation of SI-Units (joint session VA/TT/TUT)

Time: Sunday 16:00–18:20 Location: H2

Tutorial TT 1.1 Sun 16:00 H2

A Quantum-Based Pressure Standard for a New SI Realization of the Pascal — •Jay Hendricks — NIST Thermodynamic Metrology Group, Gaithersburg, MD, US

Moving forward, the next generation of pressure standards will provide a new route of SI traceability for the pascal. By taking advantage of both the properties of light interacting with a gas and that the pressure dependent refractive index of helium can be precisely predicted from fundamental, first-principles quantum-chemistry calculations, a new route of realizing the pascal has been demonstrated. This lecture will briefly cover the classical methods of realizing pressure that have served the metrology community well for the past 375 years. And then will take a deeper dive into the next generation of light-based pressure standards that will enable the elimination of mercury manometers, replacing them with a smaller, lighter, faster, and higher precision standards. From a metrology stand point, the new quantum-based SI pascal will move us from the classical force/area definition, to an energy density (joules per unit volume) definition. Should the technique be further miniaturized, it will lead to a revolution in pressure metrology, enabling a photonics based device that serves both a gas pressure sensor and a portable gas pressure standard all in one.

Tutorial TT 1.2 Sun 16:35 H2

Redefinition of the Kelvin - With what accuracy can temperatures be measured? — •Steffen Rudtsch — Physikalisch-Technische Bundesanstalt (PTB), Abbstraße 2-12, 10587 Berlin

On 20 May 2019, World Metrology Day, the revised International System of Units (SI) will enter into force. From this day on, all units will be traced back to natural constants. The redefinition of the Kelvin via the Boltzmann constant opens up new possibilities in the field of high-precision temperature measurements and metrological traceability. The lecture gives an overview of the currently used precision measurement methods in contact thermometry, in the range from 1 mK to 2000 °C, and shows which changes result from the new definitions.

Tutorial TT 1.3 Sun 17:10 H2

The new kilogram - Now approachable for extraterrestrials and nonhumans — •Frank Härting — Physikalisch-Technische Bundesanstalt (PTB), Abbstraße 2-12, 10587 Berlin

The presentation gives an overview of the work that have been done and which is still in progress in order to realize the new kilogram after the redefinition of the SI on Mach 20, 2019. Beside some historical information, the presentations will focus on the actual and future scientific challenges that have to be solved in mass metrology.

Tutorial TT 1.4 Sun 17:45 H2

Counting electrons for the new ampere — •Frank Hohls — Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany

On November 16th 2018 the General Conference for Weights and Measures, CGPM, adopted the resolution on the biggest revision of the International System of Units (SI) in its history: From May 20th on the SI system is completely determined by fixing the values of 7 constants of nature. One of these constants is the elementary charge which will have the exact value e = 1.602 176 634 * 10-19 As. For the unit of electrical current, the Ampere, this has the nice consequence, that the physics of electrical current and the definition of the ampere are rejoined: Counting or controlling the number of electrons passing a conductor in each second will be the natural realization of the ampere. This could be achieved by a single-electron transport (SET) pump that transfers exactly n electrons in each of its operation cycles, generating a quantized current I = nef when operated at a frequency f. The present state of the art of the SET based current standard with emphasis on the most advanced candidate will be reviewed, a SET pump based on dynamic semiconductor quantum dots with electrically tunable energy barriers.

TT 2: Correlated Electrons: Electronic Structure Calculations and Other Theoretical Topics

Time: Monday 9:30–13:00 Location: H7

TT 2.1 Mon 9:30 H7

Pressure-induced spin-state ordering in Sr_2CoO_3F — •Juan Fernandez Afonso, Andrii Sotnikov, Atsushi Hariki, and Jan Kunes — Institute of Solid State Physics, TU Wien, Wien, Austria

Sr_2CoO_3F is a recently-synthesized compound that has an antiferromagnetic high-spin (HS) order at ambient pressure with a Néel temperature of 323 K. Under pressure, the HS nature of the ground-state transforms into a low-spin (LS). In this talk, we provide a theoretical analysis combining LDA+DMFT and strong-coupling effective model consistent with the experimental studies [1] that, in addition to the observed paramagnetic and antiferromagnetic regimes, points to the existence of a spin-state ordered (SSO) phase in between. This order is characterized by a checkerboard arrangement of HS and LS + IS (mixture of low- and intermediate-spin states).
[1] Y. Tsujimoto et al., Sci. Rep. 6, 36253 (2016)

TT 2.2 Mon 9:45 H7

Modeling the X-ray absorption spectra and magnetism in UGa_2 using LDA+U and LDA+DMFT — •Banhi Chatterjee and Jindrich Kolorenc — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

We study the electronic structure and magnetic properties of the uranium inter-metallic compound UGa_2. We focus on theoretical modeling of the M-edge X-ray absorption spectra (XAS), and investigate the magnetic moments formed at the uranium atoms. Correlations between the uranium 5f electrons are considered using the static orbital-dependent LDA+U functional and the dynamical mean-field theory (LDA+DMFT). We show that the LDA+DMFT reproduces the XAS spectra more accurately than LDA or LDA+U. Distinctive spectral features are identified with atomic multiplets, which favors the localized picture of the 5f electrons in this compound. It turns out that LDA substantially underestimates the size of the magnetic moments at the uranium atoms and even LDA+U does not reach the experimental moments with reasonable values of Coulomb U. We investigate whether LDA+DMFT improves the description of the magnetic moments.

TT 2.3 Mon 10:00 H7

Efficient LDA+DMFT response functions for correlated systems — •Julian Musshoff[1,2] and Eva Pavarini[1,3] — [1]Forschungszentrum Juelich GmbH, Institute for Advanced Simulation, Juelich, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]JARA-HPC, RWTH Aachen University, Aachen, Germany

Linear-response functions are essential for comparing theory to experiments, and yet for strongly correlated systems their calculation is very challenging. The state-of-the-art technique to calculate susceptibilities for real materials is based on the dynamical mean-field (DMFT) approach and the local-vertex approximation and its extensions. The bottleneck of this method is the calculation of 3-frequencies local susceptibilities. For this we employ an efficient scheme based on the massively-parallel general implementation of the continuous-time quantum Monte Carlo impurity solver of Ref. [1]. We explore different possible polynomial bases. To calculate lattice susceptibilities, we solve the multi-orbital and multi-site Bethe-Salpeter equation. We present results for representative orbitally ordered systems [2].
[1] A. Flesch, E. Gorelov, E. Koch, E. Pavarini, Phys. Rev. B **87**, (2013) 195141
[2] J. Musshoff and E. Pavarini, in preparation

TT 2.4 Mon 10:15 H7

Lattice Dynamics of Palladium in the Presence of Electronic Correlations — •Wilhelm Appelt[1,3], Andreas Östlin[2], Ivan Leonov[4,5], Michael Sekania[2,6], Liviu Chioncel[2,3], and Dieter Vollhardt[2] — [1]Theoretical Physics II, Institute of Physics, University of Augsburg, Germany — [2]Theoretical Physics III, Cen-

ter for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [3]Augsburg Center for Innovative Technologies, University of Augsburg, Germany — [4]Institute of Metal Physics, Yekaterinburg, Russia — [5]Materials Modeling and Development Laboratory, NUST "MISiS", Moscow, Russia — [6]Andronikashvili Institute of Physics, Tbilisi, Georgia

We compute the phonon dispersion, density of states, and the Grüneisen parameters of bulk palladium in the combined Density Functional Theory (DFT) and Dynamical Mean-Field Theory. When electronic correlations are taken into account we find a good agreement with the measured phonon spectra, and ground state properties (equilibrium lattice parameter and bulk modulus). In particular, the ground state properties are improved in comparison with DFT results. At the same time we demonstrate that the previously predicted softening of the phonon mode along the [110] direction is absent in the presence of electronic correlations.

TT 2.5 Mon 10:30 H7

Correlated electronic structure with uncorrelated disorder — •Andreas Östlin[1], Levente Vitos[2,3,4], and Liviu Chioncel[5,1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [2]KTH Royal Institute of Technology, Stockholm, Sweden — [3]Uppsala University, Sweden — [4]Wigner Research Center for Physics, Budapest, Hungary — [5]Augsburg Center for Innovative Technologies, University of Augsburg, Germany

We introduce a computational scheme for calculating the electronic structure of random alloys that includes electronic correlations within the framework of the combined density functional and dynamical mean-field theory. By making use of the particularly simple parameterization of the electron Green's function within the linearized muffin-tin orbitals method, we show that it is possible to greatly simplify the embedding of the self-energy. This in turn facilitates the implementation of the coherent potential approximation, which is used to model the substitutional disorder. The computational technique is tested on the Cu-Pd binary alloy system, and for disordered Mn-Ni interchange in the half-metallic NiMnSb.

TT 2.6 Mon 10:45 H7

Charge Reconstruction in Magnetic Heterostructures — •Andreas Weh[1], Liviu Chioncel[1], Ulrich Eckern[1], and Junya Otsuki[2] — [1]Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Department of Physics, Tohoku University, Sendai, Japan

We present a self-consistent method for using real-space dynamical mean-field theory (r-DMFT) to address local and intersite Coulomb interactions in heterostructures. The local in-plane many-body problem is solved using the continuous-time quantum Monte Carlo approach for the Hubbard model in hybridization expansion (CT-Hyb). The mean-field interlayer Coulomb potential generates a classical electrostatic problem which is solved by employing the Poisson equation for the multilayered geometry. Using this method we study half-metallic heterostructures consisting of coupled layers of single-band Hubbard models.

15 min. break.

TT 2.7 Mon 11:15 H7

The smothered phase separation - Microscopic Fermi liquid theory of the Mott transition — •Friedrich Krien[1], Erik Gerardus Cornelis Petrus van Loon[2], Mikhail Katsnelson[2], Alexander Lichtenstein[3], and Massimo Capone[1] — [1]Sissa, Trieste, Italien — [2]Radboud University, Nijmegen, The Netherlands — [3]University of Hamburg, Germany

The compressibility of the Mott insulating phase is vanishingly small, the doped Mott insulator however often exhibits a phase separation (divergence of the compressibility), which is a Pomeranchuk instability of the Fermi liquid in the charge sector. In order to better understand the counter-intuitive proximity of the two phases we calculate the two-particle Fermi liquid parameters in the DMFT approximation. Our analysis shows that the vanishing compressibility of the Mott insulator in fact requires the divergence of the charge forward scattering vertex at the Mott transition, which for finite quasi-particle weight would lead to a divergence of the compressibility. The proximity of the Mott phase is therefore connected to a tendency towards phase separation.

TT 2.8 Mon 11:30 H7

Thermodynamics of the metal-insulator transition in the extended Hubbard model — •Malte Schüler[1,2], Erik van Loon[1,2], Mikhail Katsnelson[3], and Tim Wehling[1,2] — [1]Institut for Theoretical Physics, Universtity of Bremen — [2]Bremen Center for Computational Materials Science, Universtity of Bremen — [3]Institute for Molecules and Materials, Radboud University, Nijmegen

Due to ineffective screening, low-dimensional materials often comprise strong local and non-local Coulomb interaction at the same time. In the corresponding extended Hubbard model, nonlocal interactions can raise the order of the metal-insulator transition and under certain circumstances lead to a discontinuous first-order transition. Here, we investigate the square lattice at half filling and find a first-order transition which is far from any charge-density instability. We discuss the thermodynamics of this transition and elucidate its experimental observability based on the corresponding jump on entropy. We use the Peierls-Feynman variational principle to approximate the extended Hubbard model by an effective Hubbard model. This requires the calculation of non-local charge correlation functions for various parameters of the effective Hubbard model, which we obtain by the determinant quantum Monte Carlo method.

TT 2.9 Mon 11:45 H7

Extended Hubbard Model with nearest neighbor exchange interaction — •Edin Kapetanovic[1,2], Malte Schüler[1,2], Gerd Czycholl[1], and Tim Wehling[1,2] — [1]Institute for Theoretical Physics, Universtity of Bremen — [2]Bremen Center for Computational Materials Science, Universtity of Bremen

We study an extended Hubbard model (EHM) taking into account nearest neighbor direct Coulomb and exchange interactions. Whereas the simple EHM (without exchange interaction) can be mapped on a simple Hubbard model with renormalized on-site interaction $\tilde{U}$, the EHM with ferromagnetic exchange (i.e. the extended Hubbard-Heisenberg model) at half filling, allows for both, ferro- and antiferromagnetic phases, which is not captured by a simple Hubbard model. For the case of intermediate coupling strengths, which cannot be addressed by perturbation theory or similar approaches, we apply a variational scheme by mapping the EHM with exchange on an effective Hubbard model within an effective magnetic field. In the aforementioned parameter regime we find a partly magnetized phase where the kinetic energy is still significant. In contrast to the known limiting cases, a first order magnetic transition to the fully magnetized state occurs. Further study of these phenomena may provide insight on exotic magnetic phases within correlated materials. For performing the variation we rely on exact numerical solutions of the effective Hubbard model on finite clusters using determinant quantum Monte Carlo.

TT 2.10 Mon 12:00 H7

Lefschetz thimbles approach for the sign problem in Hubbard model away of half-filling — •Maksim Ulybyshev[1], Christopher Winterowd[2], and Savvas Zafeiropoulos[3] — [1]Institut für Theoretische Physik, Julius-Maximilians-Universität, 97074 Würzburg, Germany — [2]University of Kent, School of Physical Sciences, Canterbury CT2 7NH, UK — [3]Institute for Theoretical Physics, Universität Heidelberg, Philosophenweg 12, D-69120 Germany

Quantum Monte Carlo simulation of the Hubbard model away of half filling suffer from the sign problem which makes the method almost inapplicable in this case. We applied the Lefschetz thimble approach to the Hubbard model on hexagonal lattice with chemical chemical at van Hove singularity. In this method the integration contour for continuous auxiliary fields is shifted into complex space. There are optimal manifolds ("Lefschetz thimbles"), where fluctuations of the phase of the Monte Carlo weight are substantially suppressed. Thus the sign problem is also suppressed and can be dealt with using conventional reweighting technique. Thimbles are attached to saddle points of the action in complex space. Thus the algorithm includes the search for these saddle points and also the special methods for sampling over curved surfaces in complex space. We made the practical implementation of the above mentioned algorithms, suitable for the Hubbard model, and estimated the complexity of the residual sign problem. We also show that it is possible to manipulate the saddle points of the action using different versions of the Hubbard-Stratonovich transformation, thus also changing the complexity of the sign problem.

TT 2.11 Mon 12:15 H7

From gapped Goldstone to Higgs modes in excitonic magnets — •Jan Kuneš[1], Dominique Geffroy[1,2], Josef Kaufmann[1], At-

sushi Hariki[1], Andreas Hausoel[3], and Patrik Gunacker[1] — [1]TU Wien, Austria — [2]Masaryk University, Brno, Czechia — [3]Univesity of Würzburg, Germany

We present a dynamical mean-field study of dynamical susceptibility in two-orbital Hubbard model across the exciton condensation transition. We observe appearance of Goldstone modes consistent with the broken symmetries. Reducing continuously the symmetry of the Hamiltonian we open gaps in the Goldstone modes. Upon increasing the amplitude of the symmetry breaking terms the character of the gapped modes smoothly changes from gapped Goldstone modes to Higgs amplitude fluctuations. Another notable observation is a qualitative change of the dynamical spin structure factor upon exciton condensation, which may be used as an experimentally accessible probe of the spin-triplet exciton condensate.

[1] Geffroy et al., arXiv:1808.08046

TT 2.12 Mon 12:30 H7

A Fractionalized Metal in a Falicov-Kimball Model — •Martin Hohenadler and Fakher Assaad — Universität Würzburg

Quantum Monte Carlo simulations are used to reveal two different metallic regimes in a 2D spinful Falicov-Kimball model with a three-body interaction. For weak to intermediate coupling, gapless single-particle excitations are consistent with a Fermi liquid. In contrast, for strong coupling, metallic behavior is observed despite the absence of quasiparticles. This regime can be understood using the concepts of orthogonal metals and fractionalization. Interesting connections to lattice-gauge and slave-spin theories are highlighted.

TT 2.13 Mon 12:45 H7

Fluctuation effects at the onset of the $2k_F$ density wave order in two-dimensional metals — •Jachym Sykora[1], Tobias Holder[2], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel 76100

We analyze quantum fluctuation effects at the onset of charge or spin density wave order in two-dimensional metals with an incommensurate $2k_F$ wave vector. We distinguish two cases where the ordering vector connects either a single pair of hot spots on the Fermi surface or two pairs of hot spots. For both cases we evaluate the self-energy to leading order in fluctuation expansion (one loop). For the case of single pair of hot spots we find anomalous frequency scaling and a divergent renormalization of Fermi velocity. However this one loop result is found to not be self-consistent casting doubt on the existence of such a quantum critical point. The case of two pairs of hot spots also exhibits non-Fermi liquid behavior, however of a weaker kind and is the subject of current investigation.

TT 3: Topological Insulators (joint session TT/MA)

Time: Monday 9:30–13:00 Location: Theater

TT 3.1 Mon 9:30 Theater

Coexistence of trivial and topological edge states in two-dimensional topological insulators — T. L. van den Berg[1,2], M. R. Calvo[3,4], and •D. Bercioux[1,4] — [1]Donostia International Physics Center, Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [2]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU,E-20018 Donostia-San Sebastián, Spain — [3]CIC nanoGUNE, 20018 Donostia – San Sebastián, Spain — [4]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain

In this work, we show how the coexistence of trivial and topological edge states for the case of two-dimensional topological insulators (2DTIs) can occur in two different scenarios. In one case, we consider a space modulation of the gap parameter from topological to trivial. This scenario results in the so-called Volkov-Pankratov states (VPSs) [1]. In a second case, we consider the modulation of the chemical potential in an inverted gap 2DTI, similar to the traditional band pinning of semiconductors [2]. Also within this method, we obtain trivial edge states similar to the VPSs. In both cases, the trivial states lead to an enhancement of the edge conductance over the nominal maximum values of $2e^2/h$ expected in the presence of topological edge states. We propose several experiments that could demonstrate the presence of such trivial states in 2DTIs.

[1] B.A. Volkov & O.A. Pankratov, JETP Lett. **42**, 178 (1985).
[2] R. T. Tung, Appl. Phys. Rev. **1**, 011304 (2014).

TT 3.2 Mon 9:45 Theater

An anomalous higher-order topological insulator — •Selma Franca — Institute for Theoretical Solid State Physics, IFW Dresden, 01171 Dresden, Germany

Topological multipole insulators are a class of higher order topological insulators (HOTI) in which robust fractional corner charges appear due to a quantized electric multipole moment of the bulk. This bulk-corner correspondence has been expressed in terms of a topological invariant computed using the eigenstates of the Wilson loop operator, a so called "nested Wilson loop" procedure. We show that, similar to the unitary Floquet operator describing periodically driven systems, the unitary Wilson loop operator can realize "anomalous" phases, that are topologically non-trivial despite having a trivial topological invariant. We introduce a concrete example of an anomalous HOTI, which has a quantized bulk quadrupole moment and fractional corner charges, but a vanishing nested Wilson loop index. A new invariant able to capture the topology of this phase is then constructed. Our work shows that anomalous topological phases, previously thought to be unique to periodically driven systems, can occur and be used to understand purely time-independent HOTIs.

TT 3.3 Mon 10:00 Theater

Quantum Phase Transitions between $\mathbb{Z}_n \times \mathbb{Z}_n$ Symmetry Protected Topological Phases — •Julian Bibo[1], Ruben Verresen[1,2], and Frank Pollmann[1] — [1]Technische Universität München — [2]Max-Planck-Institut für komplexe Systeme, Dresden

Symmetry protected topological (SPT) phases are phases of matter without local order parameters. Instead, they are characterized by how a global symmetry G acts projectively on the edges. The projective transformations at the boundaries are in turn classified by the second cohomology group $H^2(G, U(1))$. Given this classification scheme, we can construct so called „fixed-point" models describing the universal features of these phases. For $G = \mathbb{Z}_n \times \mathbb{Z}_n$, there are $n-1$ non-trivial SPT phases and hence $n-1$ „fixed-point" models. For $n \leq 4$, it has been proven that the corresponding „fixed-point" models have direct transitions between adjacent phases. For $n \geq 5$, however, the expectation was that there are intermediate gapless phases instead of direct transitions. Contrary to this expectation, we use local symmetries to construct a path, proving that there are indeed direct transitions in cases, where n is divisible by 2, 3 or 4. We numerically confirm these arguments and show that these transitions are not fine-tuned.

TT 3.4 Mon 10:15 Theater

Quasiparticle interference and spin momentum locking of topological insulator surface states — •Henry Legg[1], Wouter Jolie[2], Timo Knispel[2], Nick Borgwardt[2], Zhiwei Wang[2], Markus Grüninger[2], Yoichi Ando[2], Thomas Michely[2], and Carsten Busse[2] — [1]Institut für Theoretische Physik, Universität zu Köln, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany

In a normal Schrödinger material, with quadratic dispersion, the Fourier-transform of an STM quasi-particle interference (QPI) image is strongly enhanced close to momenta corresponding to $2k_F$ back-scattering. In constrast, the surface states of 3D topological insulators are protected from back-scattering due to spin-momentum locking and this protection suppresses the otherwise divergent QPI signal at $2k_F$.

Performing a self-consistent T-matrix calculation for several different scattering potentials, we demonstrate that spin-momentum locking leads to only a smooth dependence of QPI intensity as function of momentum, in particular no sharp features occur close to $2k_F$.

Our theory will be quantatively compared to measurements on compensated $BiSbTeSe_2$ allowing us to perform a detailed and precise characterisation of the topological insulator surface by extracting the full dispersion, scattering rates, and screening length of charged impurities. Intriguingly the experimental QPI intensity close to $2k_F$ shows a slight deviation from that expected due to perfect protection from

backscattering, we will discuss the potential scattering mechanism that results in this effect.

TT 3.5 Mon 10:30 Theater

Topological insulator - ferrimagnet interface: Bi_2Te_3 on Fe_3O_4 — •Vanda M. Pereira[1], Chi-Nan Wu[1,2], Cariad Knight[1,3], Simone G. Altendorf[1], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Physics, National Tsing Hua University, Hsinchu, Taiwan — [3]University of British Columbia, Vancouver, Canada

Breaking the time reversal symmetry (TRS) of a topological insulator (TI) can lead to exotic phenomena such as the quantum anomalous Hall effect. In order to break the TRS, one can dope the system with transition metal elements. An alternative way to introduce magnetic order is to interface the TI with a magnetic layer, for instance a ferrimagnetic insulator (FI), making use of the proximity effect. This approach can be more advantageous, since it avoids the non-uniformity and disorder of the doping process. Here we present the study on the growth of TI/FI heterostructures, namely Bi_2Te_3/Fe_3O_4, making use of our expertise in growing high quality thin films of these materials [1,2]. The preparation of the films by molecular beam epitaxy and their *in-situ* structural and spectroscopic characterization will be discussed. We were able to achieve a good quality interface, indicated by the minimal chemical reaction observed by X-ray photoelectron spectroscopy. Furthermore, angle-resolved photoemission spectroscopy indicates the presence of a sharp Dirac cone and the consequent preservation of the top topological surface states of the TI layer.

[1] K. Hoefer *et al.* PNAS, **111(42)**, 14979 (2014)
[2] X.H. Liu *et al.*, Phys. Rev. B **90**, 125142 (2014)

TT 3.6 Mon 10:45 Theater

Transport properties of MBE grown Bi_2Te_3 on Fe_3O_4 thin film heterostructure — •Chi-Nan Wu[1,2], Vanda M. Pereira[1], Cariad Knight[1,3], Simone G. Altendorf[1], Minghwei Hong[4], Jueinai Kwo[2], and Liu Hao Tjeng[1] — [1]MPI CPfS, Dresden, Germany — [2]Dept. of Phys., NTHU, Hsinchu, Taiwan — [3]UBC, Vancouver, Canada — [4]Dept. of Phys., NTU, Taipei, Taiwan

Quantum anomalous Hall effect (QAHE) is expected to be observed when magnetic ordering is introduced in a topological insulator (TI) system. This effect is due to time reversal symmetry breaking and can be experimentally achieved by doping transition metals into the TI or by using the magnetic proximity effect (MPE) in TI/ferromagnetic insulator (FI) heterostructures to magnetize the topological surface state (TSS) at the interface. The MPE in TI/FIs has the advantage of less defects in the TI, and it might have a higher T_c to exhibit the QAHE. However, the QAHE has not yet been experimentally observed for TI/FI heterostructures. We have successfully grown heterostructures of Bi_2Te_3/Fe_3O_4 thin films by molecular beam epitaxy with minimum chemical reaction at the interface which is crucial for the short ranged MPE. In order to study the MPE induced gap opening of the TSSs, we conducted electrical transport measurements. The temperature dependent resistance shows a sharp Verwey transition of Fe_3O_4 at 122K indicating very good quality of the FI layer. From magnetoresistance measurement at low temperature, we observed the suppression of the weak antilocalization in the TI layer, indicating a TSS gap opening by the MPE.

TT 3.7 Mon 11:00 Theater

Towards Topological Quasi-Freestanding Stanene via Substrate Engineering — •Philipp Eck[1], Domenico Di Sante[1], Maximilian Bauernfeind[2], Marius Will[2], Ronny Thomale[1], Jörg Schäfer[2], Ralph Claessen[2], and Giorgio Sangiovanni[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg — [2]Physikalisches Institut and Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg

Although two-dimensional (2D) Kane-Mele-type group-IV (C-, Si-, Ge-, Sn-) honeycomb lattices have been successfully grown on a vast number of substrates, strain, deformation and/or hybridization often destroy their topological properties. Utilizing heavy atoms (Sn, Pb) increases the SOC strength and stabilizes the non-trivial phase but comes at the prize of low-buckled structurally unstable monolayers. Here we present a systematic density functional study of stanene (Sn) on group-III and -V adatom buffered SiC(0001) and shed light on the buffer-stanene interaction physics by investigating the impact of covalent and Van-der-Waals-type bonding on the topological phase of stanene and its structural stability. We find for some buffer layers weakly interacting configurations which preserve the freestanding stanene geometry and its non-trivial phase while rendering the low-buckled structure stable. The theoretical study is supported by experimental data on an Al buffer.

[1)] D. Di Sante et al., arXiv:1807.09006

15 min. break.

TT 3.8 Mon 11:30 Theater

VLS-Growth and characterization of bulk-insulating topological insulator nanowires — •Felix Münning[1], Oliver Breunig[1], Zhiwei Wang[1], Mengmeng Bai[1], Stefan Roitsch[2], Klaus Meerholz[2], Thomas Fischer[3], Sanjay Mathur[3], and Yoichi Ando[1] — [1]Physics Institute II, University of Cologne — [2]Institute of Physical Chemistry, University of Cologne — [3]Institute of Inorganic Chemistry, University of Cologne, Germany

We report on the growth of $Bi_2Te_xSe_{3-x}$ and $Bi_xSb_{2-x}Te_3$ nanowires and their characterization in terms of morphology, material composition and electronic transport at low temperatures. Growth is performed using the vapour-liquid-solid (VLS) method on Si/SiO_2 substrates decorated with 20-nm Au nanoparticles. Growth parameters such as temperature distribution, mass and ratio of source materials, inert gas flow, pressure and growth time are optimized and the results are examined using scanning and transmission electron microscopy (SEM, TEM) and electron dispersive X-ray spectroscopy (EDX). Devices featuring ohmic contacts to the nanowires are fabricated using electron-beam lithography. Subsequently, the electronic transport properties of the nanowires are measured for their dependencies on temperature, magnetic field and electrostatic gating at temperatures down to 1.7 K.

TT 3.9 Mon 11:45 Theater

Crossed Andreev reflection in Superconductor-TI nanowire junctions — •Michael Barth, Jacob Fuchs, Cosimo Gorini, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

Topological Insulators (TIs) are materials with an ordinary bulk band gap and metallic surface/edge states. The latter are helical, meaning that we have spin-momentum-locking, and they are topologically protected by time-reversal symmetry [1]. Topologically non-trivial superconducting states can be obtained by putting a TI in close proximity to a normal superconductor. This kind of system is characterized by modifications of phenomena such as crossed Andreev reflection [2], which for example can be fully suppressed in 2-dimensional TIs [3]. We consider instead a hybrid 3-dimensional TI - superconductor T-junction, where crossed Andreev reflection is in principle tunable via external magnetic fields. This is confirmed by our 3D numerical simulations for T-junctions, showing clear signatures of tunable crossed-Andreev reflection.

[1] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011)
[2] G. Falci, D. Feinberg, and F. W. J. Hekking, EPL 54, 255 (2001)
[3] P. Adroguer et al., Phys. Rev. B 82, 081303 (2010)

TT 3.10 Mon 12:00 Theater

Coulomb Blockade in Topological Insulator Quantum Dots — Klaus Richter, Cosimo Gorini, Raphael Kozlovsky, •Ansgar Graf, and Andreas Hackl — Universität Regensburg, Institut für Theoretische Physik, 93053 Regensburg

Three-dimensional topological insulator (3DTI) nanowires host topologically non-trivial surface states wrapped around an insulating bulk. We model these states by two-dimensional effective Dirac Hamiltonians. A coaxial magnetic field is known to produce Aharonov-Bohm (AB) type oscillations in the conductance. The corresponding AB phase and a Berry phase originating from spin-momentum locking affect the angular momentum wave number. We investigate 3DTI nanowires where additionally the longitudinal wave number gets quantized by size confinement, such that a '3DTI quantum dot' exhibiting a fully discrete energy spectrum is obtained. Such confinement is not possible by electrostatic means (Klein tunneling) but can be achieved via the interplay between non-trivial geometry (shaped nanowire) and a homogeneous coaxial magnetic field. We are looking for signatures of Berry phase and Dirac states in the single-electron transport regime (in particular in the Coulomb diamonds) of such a 3DTI quantum dot.

TT 3.11 Mon 12:15 Theater

On-demand thermoelectric generation of equal-spin Cooper

pairs — •Felix Keidel[1], Pablo Burset[2], Sun-Yong Hwang[3], Björn Sothmann[3], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany — [2]Department of Applied Physics, Aalto University, 00076 Aalto, Finland — [3]Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany

A central goal for the application of superconductors in spintronics is the on-demand generation of spin-polarized supercurrents or, analogously, of equal-spin Cooper pairs. Most proposals rely on a careful manipulation of magnetic materials to electrically generate equal-spin Cooper pairs in ferromagnet (F)-superconductor (S) hybrid junctions.

Here, we propose a quantum heat engine that utilizes the helicity of the edge states of a quantum spin Hall insulator instead, where nonlocal transport necessarily takes place through equal-spin channels. We demonstrate that a temperature bias applied to an S-F-S junction can drive a nonlocal polarized supercurrent, while the normal contribution from electron tunneling is suppressed. Remarkably, the relative phase between the superconductors serves as a switch to turn the thermoelectric current on and off, allowing for the creation of equal-spin Cooper pairs on demand.

TT 3.12 Mon 12:30 Theater

Edge plasmons in topological 2D materials — •Luca Vannucci[1], Nicola Marzari[2], and Kristian S. Thygesen[1] — [1]CAMD, Technical University of Denmark, 2800 Kongens Lyngby, Denmark — [2]THEOS, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

We discuss topologically-protected collective excitations in 1D systems formed at the edge of novel 2D materials, combining both theoretical models and first-principles simulations. With the help of newly-developed computational 2D materials databases [1, 2], containing thousands of 2D materials and forming the ideal starting point for the investigation of unexplored topological materials, we focus both on known quantum spin Hall systems and new interesting candidates [3]. We then explore the electronic and plasmonic band structures in different nanoribbon geometries, highlighting the emergence of plasmonic excitations from the inspection of the dielectric function and discussing the influence of topological protection on their properties. This topological plasmonics [4] may lead to several important applications in the context of opto-electronics, where the coupling of electromagnetic fields to collective edge excitations of topological 2D materials could pave the way to new and innovative recipes for transmitting information in a robust, protected way.

[1] N. Mounet et al., Nat Nanotechnol. 13, 246 (2018)
[2] S. Haastrup et al., 2D Mater. 5, 042002 (2018)
[3] A. Marrazzo et al., Phys. Rev. Lett. 120, 117701 (2018)
[4] D. Jin et al., Phys. Rev. Lett. 118, 245301 (2017)

TT 3.13 Mon 12:45 Theater

Topological Devil's staircase in atomic two-leg ladders — Simone Barbarino[1,2], Davide Rossini[3], •Matteo Rizzi[4], Rosario Fazio[5,6], Giuseppe E. Santoro[1,5,7], and Marcello Dalmonte[1,5] — [1]SISSA, Trieste, Italy — [2]Technische Universität Dresden, Germany — [3]Università di Pisa and INFN, Italy — [4]Johannes Gutenberg-Universität, Mainz, Germany — [5]ICTP, Trieste, Italy — [6]NEST, SNS & Istituto Nanoscienze-CNR, Pisa, Italy — [7]CNR-IOM Democritos, Trieste, Italy

We show that a hierarchy of symmetry-protected topological (SPT) phases in 1D –a topological Devil's staircase – can emerge at fractional filling fractions in interacting systems, whose single-particle band structure describes a (crystalline) topological insulator. Focusing on a specific example in the BDI class, we present a field-theoretical argument based on bosonization that indicates how the system phase diagram, as a function of the filling fraction, hosts a series of density waves. Subsequently, based on a numerical investigation of spectral properties, Wilczek-Zee phases, and entanglement spectra, we show that these phases can support SPT order. In sharp contrast to the non-interacting limit, these topological density waves do not follow the boundary-edge correspondence, as their edge modes are gapped. We then discuss how these results are immediately applicable to models in the AIII class, and to crystalline topological insulators protected by inversion symmetry. Our findings are immediately relevant to cold atom experiments with alkaline-earth atoms in optical lattices, where the band structure properties we exploit have been recently realized.

TT 4: Nonequilibrium Quantum Many-Body Systems 1 (joint session TT/DY)

Time: Monday 9:30–12:45 Location: H22

TT 4.1 Mon 9:30 H22

Quantum Loschmidt echo in quenched Hubbard model — •Nikodem Szpak[1] and Ralf Schützhold[2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Institut für Theoretische Physik, Technische Universität Dresden

A quantum Loschmidt echo (also referred to as quantum time mirror) corresponds to an effective time inversion after which the quantum wave function reverses its previous time evolution and eventually reaches its initial distribution again. We consider a Hubbard model describing free dispersion in a lattice and impose a sudden pulse-like perturbation (pi-pulse) which reverses the sign of all quasi-momenta simultaneously. After equal period of time, we observe the rebuild of the initial state. We generalize previous results obtained in this field and propose a comparably simple protocol for ultra-cold atoms in optical lattices which should be easier to realize experimentally than previous proposals.

TT 4.2 Mon 9:45 H22

Ion Impact induced Doublon Creation in Strongly Correlated Finite Hubbard Systems — •Maximilian Rodriguez Rasmussen, Karsten Balzer, Niclas Schlünzen, Jan-Philip Joost, and Michael Bonitz — CAU Kiel, Germany

Under certain conditions strongly correlated fermions in lattice systems are known to form doublons - quasi-particles consisting of two electrons on the same site. Due to the interesting resulting electronic properties doublon formation processes have been the subject of various studies. Here a new mechanism of doublon production due the impact of energetic ions is presented. The processes leading to doublon creation are described and verified by numerical results [1, 2] obtained by exact diagonalization for small systems and non-equilibrium Green functions approach [3] for larger systems.

[1] K. Balzer, M.R. Rasmussen, N. Schlünzen, J.-P. Joost, M. Bonitz, submitted to Phys. Rev. Lett., arXiv:1801.05267
[2] M. Bonitz, K. Balzer, N. Schlünzen, M.R. Rasmussen, J.-P. Joost, Phys. Stat. Sol. (b) (2018), arXiv:1808.07868
[3] K. Balzer and M. Bonitz, "Nonequilibrium Green's Functions Approach to Inhomogeneous Systems", Springer 2013

TT 4.3 Mon 10:00 H22

Hidden phases in the photodoped two-band Hubbard model — •Jiajun Li and Martin Eckstein — University of Erlangen-Nuremberg, Erlangen, Germany

Recent years have witnessed intense interest in controlling materials through non-equilibrium protocols. In particular, a strong electric pulse can drastically disturb a Mott insulator, giving rise to a transient photo-doped state featuring charge excitations across the insulating gap. This protocol of photo-doping can yield non-trivial physical consequences, such as non-thermal melting of symmetry-breaking phases and the formation of hidden states with entangled spin-orbital ordering which are inaccessible in equilibrium. We demonstrate the scenarios in a two-band Hubbard model using non-equilibirum Dynamical Mean-Field Theory. Furthermore, controlled studies of the photo-doped state are often prone to the limited time range that is numerically accessible. Thus, we adopt a non-equilibrium steady-state formulation of Dynamical Mean-Field Theory to describe a longlived photo-doped system, which is constantly perturbed to maintain a stationary state containing charge excitations across the gap. The perturbation can be adjusted to control the excitation density continuously. Using this method, we study a photo-doped two-band Hubbard model. We find the photo-doping drives the system to a hidden phase, which exhibits non-thermal ordering essentially distinct from an equilibrium or Floquet engineered system.

TT 4.4 Mon 10:15 H22

Non-equilibrium optical conductivity for the antiferromagnetic single-band Hubbard model: Time-dependent Gutzwiller analysis — •Christian Martens[1], Jörg Bünemann[2], and Götz Seibold[1] — [1]Institut für Physik, BTU Cottbus-Senftenberg, Postfach 101344, 03013 Cottbus, Germany — [2]Fakultät Physik, TU Dortmund, 44227 Dortmund, Germany

Based on the time-dependent Gutzwiller approximation (TDGA) for the Hubbard model we analyze the optical conductivity $\sigma(\omega)$ in an out-of equilibrium situation for underlying antiferromagnetic ground states. The equilibrium state is perturbed by an instant quench of the local Coulomb interaction parameter U or by an electric field $E(t)$. We analyze various shapes for the applied electric field and discuss our results with regard to the optical conductivity determination from pump-probe experiments. In the linear response regime, RPA corrections to the TDGA vanish, so that the optical response is determined by the bare current-current correlation function. In contrast, far from the linear response regime the out-of equilibrium case shows a more interesting behavior and in particular mixes double occupancy fluctuations to the current response.

TT 4.5 Mon 10:30 H22

Time-dependent wave functions with multiple correlators for the Hubbard model in nonequilibrium — •Patricia Mayer[1], Masud Haque[2], and Marcus Kollar[1] — [1]Theoretische Physik III, Universität Augsburg — [2]Department of Theoretical Physics, Maynooth University, Ireland

For the solvable $1/r$-Hubbard chain [1], the double occupation relaxes to nonthermal values after an interaction quench [2]. We apply time-dependent variational wave functions to this problem to assess their descriptive capabilities. We find that the Gutzwiller wave function, which acts on the Fermi sea with the exponentiated double occupation as correlator, can describe the time evolution accurately only for short times and then keeps oscillating with a single frequency, similar to the infinite-dimensional case [3]. On the other hand, in the Gutzwiller-Baeriswyl wave function the exponentiated kinetic energy is applied in turn to the Gutzwiller wave function [4], which leads to accurate expectation values up to longer times followed by a more complicated oscillating pattern. We conclude that multiple variational correlators substantially improve the description of Hubbard models in nonequilibrium.

[1] F. Gebhard and A.E. Ruckenstein, Phys. Rev. Lett. **68**, 244 (1992)
[2] M. Kollar and M. Eckstein, Phys. Rev. A **78**, 013626 (2008)
[3] M. Schiró and M. Fabrizio, Phys. Rev. Lett. **105**, 076401 (2010)
[4] M. Dzierzawa et al., Phys. Rev. B **51**, 1993 (1995)

TT 4.6 Mon 10:45 H22

Dynamics of densities and currents in spin ladders — •Jonas Richter[1], Fengping Jin[2], Lars Knipschild[1], Jacek Herbrych[3], Hans De Raedt[4], Kristel Michielsen[2], Jochen Gemmer[1], and Robin Steinigeweg[1] — [1]University of Osnabrück, Germany — [2]Forschungszentrum Jülich, Germany — [3]The University of Tennessee, USA — [4]University of Groningen, The Netherlands

The impact of integrability or nonintegrability on the dynamics of isolated quantum systems is a longstanding issue. For integrable models, a macroscopic set of (quasi)local conservation laws can lead to partially conserved currents and ballistic transport. In generic situations, however, integrability is lifted due to various perturbations and currents are expected to decay. Still, since the dynamics of interacting quantum many-body systems poses a formidable challenge to theory and numerics, it remains open whether nonintegrability as such already implies the emergence of diffusion. In this context, we study the dynamics of spin and energy in the two-leg spin-1/2 ladder with up to 40 lattice sites, using an efficient pure-state approach based on the concept of typicality. We discuss correlation functions in real and momentum space, and in the time and frequency domain, providing a comprehensive picture of high-temperature dynamics in this archetypal nonintegrable quantum model. Particularly, we unveil the occurence of diffusion for both spin and energy.

[1] J. Richter *et al.*, Phys. Rev. B **97**, 174430 (2018)
[2] J. Richter *et al.*, arXiv:1811.02806

15 min. break.

TT 4.7 Mon 11:15 H22

Inhomogeneous quench on the Bethe lattice — •Marc Alexander and Marcus Kollar — Theoretische Physik III, Universität Augsburg

An abrupt change of the on-site energy for a single site in a one-dimensional non-interacting tight-binding model generates dynamical Friedel oscillations of the disturbed Fermi sea [1]. In order to study this phenomenon in higher dimensions we obtain exact time evolution for such an inhomogeneous quench for a Bethe lattice with arbitrary coordination number. We use the exact eigenstates of finite Cayley trees without [2,3] or with an impurity at the central site. For the Bethe lattice with infinite coordination number we observe dynamical Friedel oscillations with two qualitative different long-time limits depending on the strength of the impurity potential.

[1] J. M. Zhang and Y. Liu, Phys. Rev. B. **97**, 075151 (2018)
[2] M. van den Berg et al., J. Stat. Phys. **69**, 307 (1992)
[3] G. D. Mahan, Phys. Rev. B **63**, 155110 (2001)

TT 4.8 Mon 11:30 H22

Steady-state charge transport through Falicov-Kimball system connected to metallic leads — Martin Žonda and •Michael Thoss — Institute of Physics, Albert-Ludwig University of Freiburg, Hermann-Herder-Strasse 3, 791 04 Freiburg, Germany

We study steady-state nonequilibrium charge transport in a model heterostructure, where a two-dimensional spin-less Falicov-Kimball system is coupled to two noninteracting leads, using a combination of a sign-problem-free Monte Carlo approach and nonequilibrium Green's function techniques. We show that the transport characteristic depends sensitively on the electrostatic potential in the system and exhibits different properties for different phases of the Falicov-Kimball model. In particular, pronounced step-like changes of the current and transmission are observed at the phase boundaries, evident even on a logarithmic scale. Analyzing finite size effects, we find that with the method used a relatively small system can be utilized to address specific thermodynamic limits.

TT 4.9 Mon 11:45 H22

Heating Dynamics in a Periodically Driven SYK-Model — •Clemens Kuhlenkamp, Simon Weidinger, and Michael Knap — Technische Universität München

Periodically driven quantum matter can realize exotic dynamical phases that do not even exist in equilibrium. In order to understand how ubiquitous and robust these phases are, it is important to understand the heating dynamics of generic interacting quantum systems. We study the thermalization and heating dynamics in a generalized SYK-model subjected to a periodic drive, which realize a Fermi-Liquid (FL) to Non-FL crossover at a certain energy scale. Using an exact field theoretic approach we determine two regimes in the heating dynamics. Only at energies above this crossover scale the system is efficiently thermalizing and heats up exponentially. The crossover in the heating dynamics may be experimentally studied by measuring the absorption of THz laser light that impinges on an irregularly shaped graphene flake in a strong magnetic field, which has been proposed to realize exotic SYK physics.

TT 4.10 Mon 12:00 H22

Periodically Driven Manybody System: a Density Matrix Renormalization Group Study — Shaon Sahoo, •Imke Schneider, and Sebastian Eggert — Department of Physics and Research Center OPTIMAS, Technical University of Kaiserslautern

Driving a quantum system periodically in time can profoundly alter its long-time dynamics and trigger exotic quantum states of matter. We propose a new DMRG method which directly deals with the Fourier components of the eigenstates of a periodically driven system using Floquet theory. With this new method we can go beyond effective Hamiltonians and take into account higher Floquet modes. Numerical results are presented for the isotropic Heisenberg antiferromagnetic spin-1/2 chain under both local (edge) and global driving for energies, spin-spin correlation and temporal fluctuations. As the frequency is lowered, the spin system enters into a Floquet regime with coherent excitations of a large number of Floquet modes, which shows characteristic quantum correlations that cannot be described by any effective static model.

TT 4.11 Mon 12:15 H22

Matrix Product Operator Algorithm for Quantum Hydrodynamics — •Tibor Rakovszky[1], Curt von Keyserlingk[2], Ehud Altman[3], and Frank Pollmann[1] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748

Garching, Germany — [2]University of Birmingham, School of Physics & Astronomy, B15 2TT, UK — [3]Department of Physics, University of California, Berkeley, California 94720, USA

Motivated by recent understanding of the Heisenberg picture evolution of operators in many-body systems, and the growth of quantum entanglement in systems subject to weak measurements, we propose a novel numerical algorithm for extracting the long-time hydrodynamic transport properties of strongly interacting spin chains. Our algorithm is based on time evolving local operators corresponding to conserved densities, making use of the so-called matrix product operator representation, and adding an artificial dissipative term that reduces the weight of large, un-physical operators that do not contribute to the physically relevant few-point correlations. The dissipation leads to a significant reduction in the number of parameters needed to represent the operator and allows us to compute the aforementioned correlation functions up to much longer times then would otherwise be possible. Using this we extract the diffusion constants of several model Hamiltonians and benchmark them against existing results in the literature.

TT 4.12 Mon 12:30 H22

Diffusion and operator spreading in matrix product operators — •Johannes Hauschild and Frank Pollmann — Department of Physics, Technische Universität München, Garching, Germany

Matrix product states (MPS) became one of the standard tools for the simulation of real time dynamics in quantum many-body systems in one dimensional systems. The fast growth of entanglement during a real time evolution usually restricts the evolution of pure MPS to short to intermediate times. In certain cases, the operator entanglement entropy of a single-site operator evolved in the Heisenberg picture grows much slower. We discuss advantages and disadvantages of the different methods in the context of extracting diffusion constants and the study of operator spreading in disordered systems. Starting from a model which displays diffusion already after short times, we study the transition to a many-body localized phase and perform a careful convergence analysis in the bond dimension.

TT 5: Superconductivity: Fe-based Superconductors - FeSe and 122

Time: Monday 9:30–13:00 Location: H23

TT 5.1 Mon 9:30 H23

Elastoresistance and resistivity anisotropy in FeSe under uniaxial strain — •Alexander Steppke[1], Jack Bartlett[1,2], Suguru Hosoi[3], Takasada Shibauchi[3], Andrew Mackenzie[1,2], and Clifford Hicks[1] — [1]Max-Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, Dresden, 01187, Germany — [2]University of St Andrews, School of Physics and Astronomy, St Andrews KY16 9SS, United Kingdom — [3]University of Tokyo, Department of Advanced Materials Science, Kashiwa, Chiba 277-8561, Japan

The phase diagram of iron-based superconductors features breaking of rotational symmetry, the electronic nematic order. Its microscopic origin and consequences for the transport and magnetic properties are under intense debate. We set out to tune the crystal structure of FeSe using uniaxial strain. Without magnetic order at ambient pressure this material undergoes a tetragonal-to-orthorombic transition around 90 K. Whereas this transition only leads to small changes in the lattice constants, the electrical transport, i.e., the resistivity can exhibit anisotropies of several percent. With the development of a sample-on-platform technique we were able to apply uniaxial strains up to 0.6% in a wide temperature range for this very ductile material. This enables continuous tuning of FeSe from the twinned to fully detwinned state and beyond. We report on the non-monotonic elastoresistance, the resistance anisotropy and characterize the contribution of domains to the resistivity within the nematic phase.

TT 5.2 Mon 9:45 H23

Thermal expansion study on $Fe_{1+y}Te_{1-x}Se_x$ — •Liran Wang[1,2], Anna Böhmer[2], Frédéric Hardy[2], Thomas Wolf[2], Peter Adelmann[2], Michael Merz[2], Mahmoud Abdel-Hafiez[3], Rüdiger Klingeler[1], and Christoph Meingast[2] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany — [3]Physikalisches Institute Goethe-Universität,Germany

The $Fe_{1+y}Te_{1-x}Se_x$ series presents one of the main families of high T_C Fe-based superconductors. To provide further insight into these materials, we present detailed thermal expansion study on high quality single-crystalline $Fe_{1+y}Te_{1-x}Se_x$ ($0 \leq x \leq 0.4$) by means of high-precision capacitance dilatometry. Clear anomalies in the thermal expansivity are observed at both the magneto/structural and superconducting transitions. Further, the electronic component of the thermal expansion is quite large and can be extracted from the data. We discuss these data in light of strong electronic correlations and possible quantum criticality.

TT 5.3 Mon 10:00 H23

Electronic structure of iron-based superconductors: BKFA and FeSe — •Volodymyr Bezguba[1,3] and Alexander Kordyuk[1,2] — [1]Kyiv Academic University, 36 Vernadsky blvd., Kyiv 03142, Ukraine — [2]G. V. Kurdyumov Institute for Metal Physics, 36 Vernadsky blvd., Kyiv 03142, Ukraine — [3]IFW Dresden, Helmholtz-Straße 20, D-01069 Dresden, Germany

The nature of high-temperature superconductivity (HTSC) remains unclear. There are many different theoretical models, which describe some of HTSC aspects and peculiarities, but none of them is neither fully predictive nor coherent enough. Because of the extremely complicated electronic structure, the iron-based superconductors (IBS) are one of the most interesting classes of HTSC to study. In particular, the effect of three-dimensionality of electronic structure on electronic properties of IBS is not clear at all.

Using angle-resolved photoemission spectroscopy (ARPES) we have measured and studied the kz-dependence of electronic structure in BKFA. We focus on peak positions of unoccupied bands in different points of Brillouin zone, Fermi surface and renormalization dependencies. A number of unexpected effects have been observed such as the swap of known excitation energy values for Γ and Z points and renormalization dependence from kz in BKFA.

In addition, temperature dependence of FeSe was carefully studied and leads to new explanation of dxy-band shift in the center of Brillouin's zone.

TT 5.4 Mon 10:15 H23

Impact of magnetic disorder and van der Waals interaction on structure parameters of FeSe and FeTe superconductors by density functional theory calculations — •Felix Lochner[1,2], Ilya Eremin[2], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany

Density functional theory (DFT) calculations for iron base superconductors often show deviations in the lattice constants compared to experiment. Therefore, we have studied the impact of the magnetic phase on the lattice parameters of FeSe and FeTe. We focus on the competition between stripe-type anti ferromagnetism (AFM) and paramagnetic disorder (PM). The PM state is implemented by using the spin-space average approach [1]. We find for both magnetic states an unphysical behavior of the structural ground state. The reason is the lack of Van der Waals (vdW) interaction in the employed PBE-GGA functional. Therefore, we have applied several approaches to include vdW. Our results show, that the additional vdW forces have a large impact on the out-of-plane lattice constant. Using the PM spin configuration together with the Van der Waals corrections we obtain lattice constants that are in excellent agreement with those obtained from experiment [2].

[1] F. Körmann, A. Dick, B. Grabowski, T. Hickel, and J. Neugebauer, Phys. Rev. B **85**, 125104 (2012)
[2] F. Ricci and G. Profetta, Phys. Rev. B **87**, 184105 (2013)

TT 5.5 Mon 10:30 H23

Magnetic fluctuations in FeSe: effect of orbital selectivity — •Andreas Kreisel[1], Johannes H. J. Martiny[2], Brian M. Andersen[3], and Peter J. Hirschfeld[4] — [1]Universität Leipzig, Germany — [2]Center for Nanostructured Graphene, Technical University of Denmark, Denmark — [3]Niels Bohr Institute, University of

Copenhagen, Denmark — [4]University of Florida, USA

Recent STM experiments and theoretical considerations have highlighted the role of interaction-driven orbital selectivity in FeSe, and its role in generating the extremely anisotropic superconducting gap structure in this material. We study the magnetic excitation spectrum resulting from the coherent quasiparticles within the same renormalized random phase approximation approach used to explain the STM experiments, and show that it agrees well with the low-energy momentum and energy dependent response measured by inelastic neutron scattering experiments. We find a correlation-induced suppression of (π, π) scattering due to a small quasiparticle weight of states of d_{xy} character [1]. We compare predictions for twinned and untwinned crystals, and predict in particular a strongly $(\pi, 0)$-dominated susceptibility at low energies in untwinned systems. Since the system is known to be close to a magnetic phase transition, it is possible that impurities can pin local magnetic order in this system. Within a mean field approach in real space, we deduce the structure of such local magnetic order and predict implications of this as been visible in a STM experiment even if a non-spinpolarized technique is used [2].

[1] A. Kreisel et al., arXiv:1807.09482
[2] J. Martiny et al., arXiv:1811.01788

TT 5.6 Mon 10:45 H23

Non-local Correlations in FeSe within the Two-Particle Self-Consistent approach — •Karim Zantout[1], Steffen Backes[2], and Roser Valentí[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany — [2]CPHT, Ecole Polytechnique, 91128 Palaiseau cedex, France

In this talk we will present results on non-local correlations in FeSe obtained with the non-perturbative Two-Particle Self-Consistent approach that provides a frequency- and momentum-dependent Self energy. We will compare our calculations to results obtained by local approximation techniques as DMFT and discuss their relevance to experimental observations such as ARPES experiments.

TT 5.7 Mon 11:00 H23

Band engineering in the iron pnictides: Search for topological surface states — •Lars Lauke[1], Rolf Heid[1], Michael Merz[1], Amir-Abbas Haghighirad[1], and Jörg Schmalian[1,2] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie (KIT), 76344 Eggenstein-Leopoldshafen, Deutschland — [2]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe, Deutschland

By band engineering the iron pnictide Fe(SeTe) via ab-initio calculations, we search for topological surface states and realizations of Majorana bound states. Proposed topological states are expected to occur for non-stoichiometric compositions on a surface Dirac cone where issues like disorder scattering and charge transfer between the relevant electronic states have to be addressed. However, this surface Dirac cone is well above the Fermi-level. The goal is to make the surface Dirac cone experimentally accessible by modifying the bulk material without disturbing the surface. Going beyond conventional density functional theory (DFT), we apply the coherent potential approximation (BEB-CPA) in a mixed basis pseudopotential framework to scan the substitutional phase-space of co-substitutions on the Fe- and Se-sites. We find that substitution on the transition-metal-site is not a viable option but a number of viable candidates at the Se-site achiev the desired effect of bringing the Dirac cone into vicinity of the Fermi-level. We further seek to experimentally realize these predicted compounds.

15 min. break.

TT 5.8 Mon 11:30 H23

Temperature dependence of quasiparticle states in superconducting monolayer FeSe on STO: a theoretical study — •Fabian Schrodi, Alex Aperis, and Peter Oppeneer — Department of Physics and Astronomy, Uppsala University, Sweden

We study the temperature evolution of the quasiparticle bands of the FeSe monolayer on the $SrTiO_3$ (STO) substrate from 10 to 300 K by applying the anisotropic, multiband and full-bandwidth Eliashberg theory. To achieve this, we extend this theory by self-consistently coupling the chemical potential to the full set of Eliashberg equations. In this way, regardless of the temperature, the electron filling can be kept at a constant level with high accuracy. Solving the coupled equations self-consistently, and with focus on the interfacial electron-phonon coupling, we predict a non-trivial evolution of the global chemical potential. Focusing on the ARPES spectra, we suggest a new route to determine the energy scale of the interfacial phonon mode by measuring the energy position of second-order replica bands. Finally, our results reveal potential implications for the determination of the momentum anisotropy of the superconducting gap in ARPES measurements [1].

[1] F. Schrodi, A. Aperis, P. M. Oppeneer, Phys. Rev. **98**, 094509 (2018)

TT 5.9 Mon 11:45 H23

Cavity-enhanced electron-phonon coupling in monolayer FeSe/STO — •Michael Sentef[1], Michael Ruggenthaler[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010

Laser control of solids was so far mainly discussed in the context of strong classical nonlinear light-matter coupling in a pump-probe framework. Here we propose a quantum-electrodynamical setting to address the coupling of a low-dimensional quantum material to quantized electromagnetic fields in quantum cavities [1]. Using a protoypical model system describing $FeSe/SrTiO_3$ with electron-phonon long-range forward scattering, we study how the formation of phonon polaritons at the 2D interface of the material modifies effective couplings and superconducting properties in a Migdal-Eliashberg simulation. We find that through highly polarizable dipolar phonons, large cavity-enhanced electron-phonon couplings are possible but superconductivity is not enhanced for the forward-scattering pairing mechanism due to the interplay between coupling enhancement and mode softening. Our results demonstrate that quantum cavities enable the engineering of fundamental couplings in solids paving the way to unprecedented control of material properties.

[1] M. A. Sentef, M. Ruggenthaler, A. Rubio, Science Advances 4, eaau6969 (2018).

TT 5.10 Mon 12:00 H23

Interplay of lattice, electronic, and spin degrees of freedom in detwinned $BaFe_2As_2$: A Raman scattering study — •Andreas Baum[1,2], Ying Li[3], Milan Tomić[3], Nenad Lazarević[4], Daniel Jost[1,2], Florian Löffler[1,2], Bernhard Muschler[1], Thomas Böhm[1,2], Jiun-Haw Chu[5,6,7], Ian R. Fisher[5,6], Roser Valentí[3], Igor I. Mazin[8], and Rudi Hackl[1] — [1]Walther-Meissner-Institut, 85748 Garching, Germany — [2]Fakultät für Physik E23, Technische Universität München, 85748 Garching, Germany — [3]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [4]Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia — [5]SIMES, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — [6]GLAM and Department of Applied Physics, Stanford University, Stanford, CA 94305, USA — [7]Department of Physics, University of Washington, Seattle WA 98195, USA — [8]Code 6393, Naval Research Laboratory, Washington, DC 20375, USA

The magneto-structural phase transition of $BaFe_2As_2$ is studied by Raman spectroscopy with a focus on lattice dynamics. Using uniaxial pressure to detwin the sample allows us to resolve anisotropic features. The As A_{1g} phonon shows a resonance at 3.1 eV with distinct differences between the antiferromagnetically and the ferromagnetically ordered direction. The E_g phonon at 130 cm^{-1} splits into two modes having B_{2g} and B_{3g} symmetry which differ by 10 cm^{-1}. Both effects can be attributed to the emergence of magnetic order, rather than the structural transition, by DFT calculations.

TT 5.11 Mon 12:15 H23

Unusual thermoelectric properties of $BaFe_2As_2$ in high magnetic fields — •Martina Meinero[1,2], Federico Caglieris[3], Gianrico Lamura[2], Ilaria Pallecchi[2], Andreas Jost[4], Uli Zeitler[4], Shigeyuki Ishida[5], Hiroshi Eisaki[5], and Marina Putti[1,2] — [1]Dipartimento di Fisica, Università di Genova, Via Dodecaneso 33, 16146 Genova, Italy — [2]CNR-SPIN, Corso Perrone 24, 16152 Genova, Italy — [3]IFW Dresden, Helmholtz Strasse 33, Dresden, Germany — [4]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Toernooiveld 7, 6525ED Nijmegen, The Netherlands — [5]National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8568, Japan

Electric and thermoelectric transport properties are mutually intertangled in diffusive transport equations. In particular, in high mobility multiband systems an anomalous behavior may occur, which can be

tracked down to the properties of the individual bands. Here, we present magneto-electric and magneto-thermoelectric transport properties of a $BaFe_2As_2$ high-quality single crystal, for different magnetic field directions up to 30 T. We detect a giant Nernst effect and an anomalous field dependence of the Seebeck coefficient. The extraction of the Peltier tensor coefficients α_{xx}, α_{xy} and α_{xz} allows us to disentangle the main transport mechanisms in play. The large α_{xy} and α_{xz} values and their field dependence provide evidence of the presence of a high mobility band, compatible with a Dirac dispersion band, crossing the Fermi level, and suggest a possible three-dimensional nature of the Dirac fermions.

TT 5.12 Mon 12:30 H23

Charge density wave instability in $Ba(Ni_{1-x}Fe_x)_2As_2$ probed by time-resolved optical spectroscopy. — •V. Yu. Grigorev[1,2], A. Mejas[3], T. Dong[1], Th. Wolf[4], A. A. Haghighirad[4], C. Meingast[4], M. Le Tacon[4], M. Merz[4], and J. Demsar[1] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, Mainz, Germany — [2]Graduate School of Excellence, Materials Science in Mainz (MAINZ), Mainz, Germany — [3]Institute for solid state physics, TU Wien, Vienna, Austria — [4]Institute for Solid State Physics, KIT, Karlsruhe, Germany

In Fe-based superconductor $BaFe_2As_2$, which displays the spin-density wave order, superconductivity is induced by chemical doping, reaching the maximum T_c of 24 K [1]. In its structural homologue $BaNi_2As_2$, however, superconductivity is observed even in undoped samples, yet the maximal T_c in Co-doped samples does not exceed 3 K [2,3]. Recent diffraction studies [4] suggest that superconductivity in $BaNi_2As_2$ is competing with the unidirectional charge-density-wave (CDW) order. Here we report on optical femtosecond time-resolved spectroscopy on weakly doped $BaNi_{1.93}Fe_{0.07}As_2$, aiming at investigating the CDW collective modes - see e.g. [4]. We present a clear evidence for a commensurate-to-incommensurate CDW lock-in phase transition at 45 K, and the low temperature amplitude mode at 1 THz in the commensurate CDW phase.

[1] J. Paglione and R. L. Greene, Nat. Phys. 6, 645 (2010)
[2] Z. G. Chen et al., Phys. Rev. B 80, 094506 (2009)
[3] S. Lee et al., arXiv:1801.04874
[4] H. Schäfer et al., Phys. Rev. B. 89, 045106 (2014)

TT 5.13 Mon 12:45 H23

Nematic susceptibility in heavily hole-doped iron-based superconductors — •Xiaochen Hong[1], Saicharan Aswartham[1], Igor Morozov[1,2], Steffen Sykora[1], Federico Caglieris[1], Silvia Seiro[1], Bernd Büchner[1,3,4], and Christian Hess[1,4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden (IFW-Dresden), Dresden, Germany — [2]Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia — [3]Institute of Solid State Physics, TU Dresden, Dresden, Germany — [4]Center for Transport and Device, TU Dresden, Dresden, Germany

Unconventional superconductivity typically is closely related to the suppression of ordered states which possibly compete or coexist with superconductivity in the underdoped region. The overdoped systems are usually assumed to stay in a rather conventional Fermi liquid state. However, for iron-based superconductors, experiments indicate that the heavily hole-doped end-member KFe_2As_2, together with its sister compounds, are more complicated including the possibility of emerging electronic nematic order.

We present elasto-resistivity measurements of KFe_2As_2, revealing a divergent nematic susceptibility. The evolution of nematic susceptibility is also tracked with isovalent doping and electron doping on the K site. Our results point to unexpected nematic critical point(s) in those overdoped superconductors.

TT 6: Surface magnetism and magnetic coupling phenomena (joint session MA/O/TT)

Time: Monday 9:30–13:15 Location: H53

TT 6.1 Mon 9:30 H53

Magneto-Seebeck Tunneling on the Atomic Scale — Cody Friesen, •Hermann Osterhage, Johannes Friedlein, Anika Schlenhoff, Roland Wiesendanger, and Stefan Krause — Department of Physics, University of Hamburg, Germany

The tunneling of spin-polarized electrons in a magnetic tunnel junction driven by a temperature gradient is a fundamental process for the thermal control of electron spin transport. As we have shown recently, scanning Seebeck tunneling microscopy is a technique that enables spin-averaged thermopower measurements in a metal-vacuum-metal tunnel junction with atomic-scale lateral resolution [1]. Using a magnetic tip and sample allows for the experimental investigation of the details of the magneto-Seebeck tunneling, with vacuum serving as the tunneling barrier. Heating the tip with a laser and measuring the thermopower of the junction while scanning across the spin texture of the sample leads to spin-resolved Seebeck coefficients that can be determined and mapped with atomic-scale lateral resolution [2].

The experiments on Fe/W(110) and Fe/Ir(111) will be presented and discussed in terms of spin-averaged, magneto-Seebeck and anisotropic magneto-Seebeck thermopower in an ideal single atom tunnel junction. Based on the experimental findings we propose a spin detector for spintronics applications that is solely driven by waste heat, utilizing magneto-Seebeck tunneling to convert spin information into a voltage that can be used for further data processing.

[1] C. Friesen *et al.*, J. Phys. D: Appl. Phys. **51**, 324001 (2018).
[2] C. Friesen *et al.*, Science (accepted).

TT 6.2 Mon 9:45 H53

Tunable spin-superconductor coupling of spin 1/2 molecules — •Luigi Malavolti[1,2,3], Matteo Briganti[4], Max Hänze[1,2,3], Giulia Serrano[4], Irene Cimatti[4], Gregory McMurtie[1,2,3], Edwige Otero[5], Philippe Ohresser[5], Federico Totti[4], Matteo Mannini[4], Roberta Sessoli[4], and Sebastian Loth[1,2,3] — [1]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany — [4]Università degli Studi di Firenze, Sesto Fiorentino (Firenze), Italy — [5]Synchrotron SOLEIL, Gif-sur-Yvette, France

Assemblies of magnetic molecules with long coherence time are being investigated as quantum bits that may be embedded in superconducting resonators [1]. Bringing the spin center into contact with the superconducting surface maximizes coupling to the resonator but may also reduce the spin's coherence time by increased scattering of quasiparticles. Here we report the capability to tune the exchange coupling of spin 1/2 vanadyl phthalocyanine molecules (VOPc) with a Pb superconducting surface. This system offers a fully tunable spin superconductor coupling from uncoupled spin to strongly coupled, screened spin [2]. These findings highlight the possibility to scale superconducting resonator experiments down to single molecule sensitivity.

[1] M. D. Jenkins, et al., Dalt. Trans. 2016, 45, 16682.
[2] L. Malavolti, et al., Nano Letters DOI: 10.1021/acs.nanolett.8b03921

TT 6.3 Mon 10:00 H53

Reduced magnetic moment in polycrystalline Co thin films — •Sabine Pütter[1], Amir Syed Mohd[1], Artur Glavic[2], Stefan Mattauch[1], and Thomas Brückel[3] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ, Garching, Germany — [2]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Villigen PSI, Switzerland — [3]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) and Peter Grünberg Institute (PGI): JCNS-2, PGI-4: Quantum Materials and Collective Phenomena, Jülich, Germany

The variation of the magnetic moment with dimensionality of magnetic materials, i. e. from atoms to bulk, is a longtime studied issue. For thin films, a constant magnetic moment is often assumed in modelling, however, intermixing and surface roughness may also have an impact.

With the help of polarised neutron reflectometry (PNR) we study the magnetic moment of polycrystalline Co/20 nm Pt/MgO(001). The samples were grown by molecular beam epitaxy and subsequently measured with PNR at room temperature and in saturation in UHV.

Our results reveal the vertical depth profile of the magnetic moment of the Co films. In fact, the magnetisation is not constant but smeared out at the edges, due to roughness. Measurements at different film thicknesses reveal the evolution of the magnetic moment which is sep-

arated in a bulk and a surface contribution and discussed with respect to published results.

This project has received funding from the EU's H2020 research and innovation programme under grant agreement n. 654360.

TT 6.4 Mon 10:15 H53

Investigation of the structural and magnetic properties of self-organized MnO_2 chains on Pt(001) — •Chong-Heeon Park, Martin Schmitt, Matthias Vogt, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, Würzburg, Germany

Recently, the self organized growth of 3d transition metal oxide (TMO) chains on Ir(001) and Pt(001) was investigated by STM, LEED, and DFT calculations [1,2]. Along with the structural (3×1) phase of the MnO_2 chains, antiferromagnetic (AFM) coupling on Ir(001) was predicted along and between adjacent chains. In this study, we investigate the structural and magnetic properties of self-organized MnO_2 chains, grown on Pt(001), with low temperature spin-polarized scanning tunneling microscopy (SP-STM). Similar to Ir(001), we observe a perfectly ordered (3×1) structural phase with an inter-chain periodicity of $3a_{\mathrm{Pt}}$. When these chains are scanned with either an in-plane or out-of-plane polarized tip (Cr-coated W tip), we observe a spin structure that can be modeled by a (15×2) magnetic unit cell. It is formed by AFM coupling along the MnO_2 chains and 72° spin spiraling across the chains.

[1] P. Ferstl, *et. al.*, Phys. Rev. B. **96**, 085407 (2017)
[2] P. Ferstl, *et. al.*, Phys. Rev. Lett. **120**, 089901 (2018)

TT 6.5 Mon 10:30 H53

Coexistence of RW-AFM and 3Q state in the Mn/Re(0001) monolayer investigated with SP-STM — •Jonas Spethmann, Jonas Sassmannshausen, André Kubetzka, Roland Wiesendanger, and Kirsten von Bergmann — Institut für Nanostruktur- und Festkörperphysik, Hamburg

Exciting new physics is predicted to arise at the interface of non-collinear magnetic and superconducting materials. In order to study this subject, promising model systems need to be found. Therefore, we investigated the growth and the magnetism of a monolayer of Mn on Re(0001) using spin-polarized scanning tunneling microscopy.

Re becomes superconducting below a critical temperature of 1.69 K, which is a temperature well accessible with modern cryogenics. Mn typically prefers an antiferromagnetic order. If it is forced into a hexagonal atomic lattice, like the (0001) surface of Re, complex magnetic structures might arise due to geometric frustration. Furthermore, it is known that differently stacked monolayers of the same material can show different magnetic ground states. By adding Co to the Re surface prior to the Mn deposition, we managed to grow the Mn in two different stackings. We show that the fcc stacking exhibits a row-wise antiferromagnetic state with three symmetry-equivalent rotational domains. The hcp-stacked area shows a magnetic texture that is compatible with a so-called 3Q state [1], which is a non-collinear state with four spins in the unit cell that have an angle of 109.4° between each other.

[1] Ph. Kurz, G. Bihlmayer, K. Hirai, and S. Blügel. Phys. Rev. Lett., 86:1106-1109, Feb 2001.

TT 6.6 Mon 10:45 H53

Zero field sub-10 nm skyrmions and antiskyrmions in ultrathin Co films — •Sebastian Meyer[1], Stephan von Malottki[1], Marco Perini[2], André Kubetzka[2], Roland Wiesendanger[2], Kirsten von Bergmann[2], and Stefan Heinze[1] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel — [2]Department of Physics, University of Hamburg

Non-collinear spin structures such as skyrmions are being intensively studied due to their promise for spintronic devices [1]. For applications it is envisioned to use isolated skyrmions with diameters below 10 nm that are stable at zero magnetic field [2]. Here, we use density functional theory and atomistic spin dynamics simulations [3] to show how we can stabilize magnetic skyrmions and antiskyrmions in ultrathin Co films in zero external magnetic field. In contrast to Co being a ferromagnetic material with a strong exchange stiffness we obtain very large frustration effects in the magnetic interactions of ultrathin Co films which imperatively requires an atomistic spin model. We find that the frustration enhances the energy barriers for skyrmions and antiskyrmions against collapse into the ferromagnetic ground state.

[1] A. Fert, V. Cros, and J. Sampaio, Nat. Nanotech. **8**, 152 (2013)
[2] A. Fert, N. Reyren, and V. Cros, Nat. Rev. Mater. **2**, 17031 (2017)
[3] S. Haldar, *et al.*, Phys. Rev. B **98**, 060413 (2018)

TT 6.7 Mon 11:00 H53

Scanning Seebeck Tunneling Microscopy — Cody Friesen, Hermann Osterhage, Johannes Friedlein, Anika Schlenhoff, Roland Wiesendanger, and •Stefan Krause — Department of Physics, University of Hamburg, Germany

The field of spin caloritronics is specifically concerned with effects that arise in the presence of a temperature gradient, and their effect on spin-dependent electronic transport. The advent of increasingly detailed techniques for nano-scale fabrication, measurement, and manipulation have led to an improved understanding of spin caloritronic effects, and their potential uses in engineering sensors and devices at all size scales, e.g. waste-heat recycling and efficient computing.

Within this field, the thermally induced Seebeck tunneling of electrons is a fundamental effect. In our experiments, it is studied in a metal-vacuum-metal junction using scanning tunneling microscopy (STM). Selective heating of the tip with a laser generates a well-defined temperature difference at the tunnel junction. The thermovoltage between the tip and the sample is measured with atomic-scale lateral resolution and related to the band structure of the junction, as revealed by local tunneling spectroscopy. Tunnel current rectification experiments in compensated conditions allow for a direct measurement of the Seebeck coefficient without the need for tip heating, thereby realizing Seebeck mapping on the atomic scale. The STM studies will be presented and discussed in terms of thermally induced tunneling across a single-atom ideal vacuum barrier.

C. Friesen *et al.*, J. Phys. D: Appl. Phys. **51**, 324001 (2018).

15 min. break

TT 6.8 Mon 11:30 H53

***Ab initio* simulations of 2D-materials interacting with magnetic clusters and surfaces** — •Nicolae Atodiresei, Vasile Caciuc, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich, Germany

Using density functional theory calculations we elucidate how the subtle interplay between the electrostatic, the weak van der Waals and the strong chemical interactions determines the geometric, electronic and magnetic structure of hybrid systems formed by magnetic substrates and atomic clusters with 2D materials as transition metal dichalcogenites (TMDs) monolayers and graphene (Gr). More precisely, the interaction between 2D and magnetic materials (i.e. surfaces, atomic clusters) shapes the (i) spin-polarization, (ii) magnetic exchange couplings, (iii) magnetic moments and (iv) their orientation of the hybrid systems. This work has been supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project number 277146847 - CRC 1238 (C01).

[1] R. Brede *et al.*, Nature Nanotech. **9**, 1018 (2014).
[2] F. Huttmann *et al.*, Phys. Rev. Lett. **115**, 236101 (2015).
[3] F. Huttmann *et al.*, Phys. Rev. B **95**, 075427 (2017).
[4] V. Caciuc *et al.*, Phys. Rev. Mat. **2**, 084001 (2018).

TT 6.9 Mon 11:45 H53

Electronic and magnetic structure of monolayer and double layer GdFe/W(100) surface alloy — •Vikas Kashid, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The rare earth-transition metal alloy films are attractive materials for high density mageto-optic storage due to their magnetic recording and magneto-optical anisotropy. We investigate by virtue of spin density functional theory (DFT) as realized in the FLEUR code [1], the structural and magnetic properties of the monolayer and double layer film of GdFe on the W(100) substrate in $c(2 \times 2)$ unit cell, where highly localized Gd-4f orbitals are treated within GGA+U method. Gd buckles outward by 0.96 Å and 0.88 Å with respect to Fe atoms in the monolayer and double layer surfaces, respectively. The calculated monolayer and double layer GdFe/W(100) exhibits a checkerboard antiferromagnetic ground state configurations between Fe and Gd atoms. The Fe atoms in the double layer GdFe/W(100) exhibit large magnetic moment of 2.30 μ_{B}, larger than that of 1.45 μ_{B} in the monolayer film. The easy axes for the spin quantization arising from spin-orbit coupling in both the surfaces lie in the surface plane and along the diagonal of $c(2 \times 2)$ cell with the magneto-crystalline anisotropy energy larger for

the double layer than for the monolayer.
We acknowledge discussions with Prof. Alexander Ako Khajetoorians.
[1] www.flapw.de

TT 6.10 Mon 12:00 H53

Nonlocal electron correlations in an itinerant ferromagnet — •Christian Tusche[1,2], Martin Ellguth[3], Vitaliy Feyer[1], Alexander Krasyuk[3], Carsten Wiemann[1], Jürgen Henk[4], Claus M. Schneider[1,2], and Jürgen Kirschner[3,4] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-6), Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [3]Max-Planck-Institut für Mikrostrukturphysik, Halle — [4]Martin-Luther-Universität Halle-Wittenberg, Halle

A fundamental concept in solid state physics describes the electrons in a solid by the relation of the energy E vs. the crystal momentum $\boldsymbol{k}$ in a band structure of independent quasi particles. However, even for the most simple elemental ferromagnets, electron correlations are prevalent, requiring descriptions of their electronic structure beyond this simple single-electron picture. Our comprehensive measurements of the spectral-function by spin-resolved momentum microscopy show that in itinerant ferromagnets like cobalt these electron correlations are of nonlocal origin. This manifests in a complex self-energy $\Sigma_\sigma(E, \boldsymbol{k})$ that disperses as function of spin σ, energy E, and momentum $\boldsymbol{k}$. Combining the experiments with one-step photoemission calculations, we quantify the dispersion of the self-energy over the whole Brillouin zone [1]. The observation of nonlocal electron correlations in cobalt substantially affects our understanding of electron interactions, and makes itinerant ferromagnets a paradigmatic test case for the interplay between band structure, magnetism, and correlations.

[1] C. Tusche et al., Nat. Commun. 9, 3727 (2018)

TT 6.11 Mon 12:15 H53

Magnetic coupling of ferromagnetic $SrRuO_3$ epitaxial layers separated by ultrathin spacers with large spin-orbit coupling — •Lena Wysocki[1], Michael Ziese[2], Lin Yang[1], Jörg Schöpf[1], Rolf Versteeg[1], András Kovács[3], Lei Jin[3], Felix Gunkel[4], Regina Dittmann[4], Paul H.M. van Loosdrecht[1], and Ionela Lindfors-Vrejoiu[1] — [1]University of Cologne, Institute of Physics II, Germany — [2]Felix Bloch Institute for Solid State Physics, University of Leipzig, Germany — [3]Forschungszentrum Jülich, PGI-5, Germany — [4]Forschungszentrum Jülich, PGI-7, Germany

$SrRuO_3$, a 4d ferromagnet exhibiting several Weyl nodes in proximity of the Fermi level, offers a rich playground to tailor its physical properties in epitaxial heterostructures and superlattices. Interfacing $SrRuO_3$ with large spin-orbit coupling perovskite oxides, as $SrIrO_3$, results in intriguing physical phenomena like pronounced anomalies in the Hall resistivity, attributed either to the existence of Néel type skyrmions or to modifications of the Berry curvature of electronic bands with non-trivial topology. The nature of the coupling between the magnetic layers in such superlattices is an important component influencing the global multilayer properties. We present the investigation of the magnetic coupling between ferromagnetic $SrRuO_3$ layers separated by ultrathin spacers of perovskite oxides exhibiting strong spin-orbit coupling[1]. The type and strength of the magnetic interlayer coupling was determined by major and minor magnetization measurements for various spacer geometries.

[1] L. Wysocki et al., Appl. Phys. Lett. **113**, 192402 (2018)

TT 6.12 Mon 12:30 H53

Charge-transfer driven ferromagnetism in a disordered three-dimensional $3d$-$5d$ spin system — •Philipp Komissinskiy[1], Supratik Dasgupta[1], Ilya Radulov[1], Andrei Rogalev[2], Fabrice Wilhelm[2], Marton Major[1], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany — [2]European Synchrotron Radiation Facility, 71 Avenue des Martyrs, 38000 Grenoble, France

A three-dimensional disordered spin system consisting of the $3d$ transitional metal ion Mn^{4+} with strong electronic correlations and the heavy $5d$ transition metal ion Ir^{4+} with large spin-orbit coupling has been investigated in form of a perovskite thin film. The studied compound of the composition $SrMn_{0.5}Ir_{0.5}O_3$ does not exist as bulk or single crystal, but can be stabilized by epitaxy as fully disordered double perovskite thin film onto $SrTiO_3$ single-crystal substrate using pulsed laser deposition. As measured by X-ray circular dichroism, the ground state of this material is ferromagnetic with both, Mn and Ir, spins aligned in parallel. This unusual ground state can be qualitatively explained by charge-transfer driven magnetic exchange involving the effective $J = 1/2$ state of Ir. Due to the coexistence of competing magnetic interactions and randomness in the system, spin-glass features are observed at low temperatures.

TT 6.13 Mon 12:45 H53

Thickness independent magnetism of the magnetic MAX phase films $(Cr_{0.5}Mn_{0.5})_2GaC$ — •Iuliia P. Novoselova[1], Andrejs Petruhins[2], Ulf Wiedwald[1], Johanna Rosen[2], Michael Farle[1], and Ruslan Salikhov[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [2]Department of Physics, Linköping University, Linköping, Sweden

Atomically laminated magnetic MAX phases $M_{n+1}AX_n$ (n = 1, 2, 3) have attracted interest as novel materials exhibiting both ceramic and metallic properties. Here 12.5 to 156 nm thick films $(Cr_{0.5}Mn_{0.5})_2GaC$ were investigated by ferromagnetic resonance, electron scanning microscopy and magnetometry. The X-ray diffraction reveals a high crystalline quality and phase purity. Magnetocrystalline anisotropy energy density of 140 mT as well as magnetization of 240 kA/m are found to not depend on thickness. All films are environmentally stable without a change of magnetic properties for more than one year at ambient conditions and without any protection layer. Such independence on thickness combined with the chemical stability makes the $(Cr_{0.5}Mn_{0.5})_2GaC$ films attractive for various applications such as spintronic devices or corrosion resistant magnetic sensors. This work is supported by DFG, Grant SA 3095/2-1 and DAAD Doctoral Programmes in Germany,57214224. [1] M. W. Barsoum, Prog. Solid State Chem. 28, 201 (2000).[2] A. Petruhins, et al. Journal of Mat. Sci. 50-13, 4495 (2015).[3] R. Salikhov, et al. Mat. Res, Lett. 3-3, 156-160 (2015).[4] I. P. Novoselova, Sci. Reports 8, 2637 (2018).

TT 6.14 Mon 13:00 H53

The polar distortion and its relation to magnetic order in multiferroic HoMnO3 — •Nazaret Ortiz[1], Yoav William Windsor[2], Jose Renato Linares Mardegan[1], Christof Schneider[1], Gareth Nisbet[3], and Urs Staub[1] — [1]Paul Scherrer Institute, Swiss Light Source, Switzerland — [2]Fritz Haber Institut der Max Planck Gesellschaft, Germany, — [3]Diamond Light Source, United Kingdom

The orthorhombic (Pbnm) HoMnO3 is of particular interest due to its high magnetically-induced polarization values (P) and magnetoelectric coupling strength. The mechanism behind this involves high magnetic frustration, which results in a magnetic order that creates a distortion in the crystal lattice. This distortion breaks inversion symmetry and creates a macroscopic electric polarization P along the a-axis.

We investigated the atomic distortion to identify the broken symmetry of Pbnm in thin films of HoMnO3 at low temperature and the relation between the magnetic order of Ho and the structural distortion. Forbidden reflections for Pbnm has been observed, showing that the distortion does not exclusively affect to the atomic position along the polar axis, it also moves atoms along other directions. Moreover, studying reflections with component along the polar axis we observe the polar distortion directly, visualized by the difference diffraction intensity from opposite domains.

TT 7: Dynamics in many-body systems: Equilibration and localization I (joint session DY/TT)

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

TT 7.1 Mon 10:00 H19

Modern Principles of Equilibration in Closed Quantum Systems do Not Rule Out Strange Relaxation Dynamics — Lars Knipschild and •Jochen Gemmer — Universität Osnabrück, Germany

The quest for equilibration and thermalization in closed quantum systems has stimulated vast scientific effort, especially in the last decades. Various principles and approaches have been put forth, such as the eigenstate thermalization hypothesis, quantum chaos, typicality, the non-resonance principle, the unfeasibility of fine-tuned initial states, etc. While these approaches are well suited to explain that observables will assume specific "equilibrium" values for most points in time in between some initial time and a very distant future, they do not address the concrete dynamics towards these values. Furthermore they do not rule out substantial observable revivals on relevant timescales . We demonstrate that indeed very unexpected dynamics may result for systems and observables complying with all the above principles. This occurs for a very large set of non-fine tuned initial states.

TT 7.2 Mon 10:15 H19

Entanglement-ergodic quantum systems equilibrate exponentially well — Henrik Wilming[1], •Marcel Goihl[2], Ingo Roth[2], and Jens Eisert[2] — [1]Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland — [2]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

One of the outstanding problems in non-equilibrium physics is to precisely understand when and how physically relevant observables in many-body systems equilibrate under unitary time evolution. General equilibration results have been proven that show that equilibration is generic provided that the initial state has overlap with sufficiently many energy levels and the energy spectrum is sufficiently generic. At the same time results showing that natural initial states fulfill this condition are lacking. We present stringent results for equilibration of lattice systems in which the amount of entanglement in energy eigenstates with finite energy density is extensive for some subset of the lattice. Concretely, we carefully formalize a notion of "entanglement-ergodicity" in terms of Rényi entropies and derive that systems fulfilling this condition equilibrate exponentially well. Our proof uses insights about Rényi entropies and combines them with recent results about the probability distribution of energy in local lattice systems with initial states that are weakly correlated.

TT 7.3 Mon 10:30 H19

Out-Of-Time-Ordered Correlators in critical systems - Instability and the onset of chaos — •Dominik Hahn, Benjamin Geiger, Quirin Hummel, and Klaus Richter — Universität Regensburg

It is known from mean field theory that a system of bosons with attractive contact interaction in one dimension exhibits a quantum phase transition at a certain critical coupling. This transition has its manifestation in the formation of a local instability in the integrable mean-field dynamics. By adding an external potential, we investigate the transition from integrability to chaos in this system. A characteristic feature of chaotic motion, the exponential sensitivity to initial conditions, can be also detected in the corresponding quantum mechanical system using Out-Of-Time-Ordered Correlators (OTOCs). It can be shown, that a local instability is sufficient to generate an exponential growth of certain OTOCs. After breaking the integrability, we find evidence, that the OTOC growth is affected by an additional exponent, which can be related to the largest Lyapunov exponent of the system.

TT 7.4 Mon 10:45 H19

Thermalization and eigenstate thermalization hypothesis in the Holstein polaron model — David Jansen[1], •Jan Stolpp[2], Lev Vidmar[3], and Fabian Heidrich-Meisner[2] — [1]Arnold-Sommerfeld-Center for Theoretical Physics, LMU Munich — [2]Institute for Theoretical Physics, University of Göttingen — [3]Jozef Stefan Institute, Ljubljana

The 1d Holstein model is a paradigmatic system to study polaron physics and the nonequilibrium dynamics of charge carriers coupled to phonons. While the electronic relaxation dynamics of a single charge carrier is a much studied topic (see, e.g. [1]), here, we systematically investigate whether the 1d Holstein model in the single-polaron limit is ergodic by checking the criteria of the eigenstate thermalization hypothesis and by testing for established quantum chaos indicators. Using exact diagonalization techniques we find that the level spacing distribution is Wigner-Dyson, which is characteristic for a quantum chaotic system. Remarkably, both the diagonal and offdiagonal matrix elements of typical observables obey properties predicted by the eigenstate thermalization hypothesis. Thus, we found an example in which the coupling term between the electronic and phononic subspaces leads to ergodic behavior, even though the phonon system itself consists of uncoupled, local harmonic oscillators.

[1] Phys. Rev. B 91, 104302 (2015)

TT 7.5 Mon 11:00 H19

Bounds on equilibration time scales — •Robin Heveling, Lars Knipschild, and Jochen Gemmer — University of Osnabrueck, Osnabrueck, Germany

We consider closed quantum systems consisting of a single system-spin and a spin-bath. Starting from a product state of a microcanonical bath at some energy and a fully aligned system-spin, equilibration time scales of the magnetization are calculated for various coupling strengths. The paper PRX 7, 031027 (2017) conjectures a relation between short time behaviour and long equilibration time scales. We probe this conjecture. For small couplings, we find exponential relaxation to an equilibrium value. The exponential nature of the decay may break down at some point when decreasing the coupling strength.

TT 7.6 Mon 11:15 H19

Decoherence Entails Exponential Forgetting in Systems Complying with the Eigenstate Thermalization Hypothesis — •Lars Knipschild and Jochen Gemmer — University of Osnabrück, D-49069 Osnabrück, Germany

According to the eigenstate thermalization ansatz, matrices representing generic few-body observables exhibit a specific form when displayed regarding the eigenbasis of the Hamiltonian. We examine the effect of environmental induced decoherence on the expectation value dynamics of observables confirming with said eigenstate thermalization ansatz. We find that this influence is equivalent to an exponential damping of the memory-kernel appearing in an equation of motion for the expectation value. The statement is formulated as a rigorous theorem.

15 min. break

TT 7.7 Mon 11:45 H19

Many body localized system weakly coupled to thermal environment — •Ling-Na Wu, Alexander Schnell, Giuseppe De Tomasi, Markus Heyl, and André Eckardt — Max Planck Institute for the Physics of Complex Systems

Many body localization (MBL), which describes the failing of an interacting system under disorder to reach thermalization, has attracted widespread attentions. In recent years, the imperfect experimental environment has excited an intense interest in the effect of dissipations on MBL. We formulate an efficient method for the description of MBL systems in weak contact with thermal environments at temperature T. As an example, we study the transport property of a fermion Hubbard chain coupled to a thermal bath and recover a conductivity following Mott's law for variable range hopping. Weak attractive (repulsive) interactions are found to enhance (decrease) the transport, which is attributed to an interaction-induced modification of the density of states due to spatio-energetic correlations. We also study the effect of dissipations on disorder-free localized system and compare it with the conventional disorder-induced localized system.

TT 7.8 Mon 12:00 H19

Many-body localization and delocalization in large quantum chains — •Elmer V. H. Doggen[1], Frank Schindler[2], Konstantin S. Tikhonov[1,3], Alexander D. Mirlin[1,3,4,5], Titus Neupert[2], Dmitry G. Polyakov[1], and Igor V. Gornyi[1,3,4,6] — [1]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Department of Physics, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland — [3]L. D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia

— [4]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [5]Petersburg Nuclear Physics Institute, 188300 St. Petersburg, Russia — [6]A. F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia

We theoretically study the quench dynamics for an isolated Heisenberg spin chain with a random on-site magnetic field, which is one of the paradigmatic models of a many-body localization transition. We use the time-dependent variational principle as applied to matrix product states, which allows us to controllably study chains of a length up to L=100 spins. We find that the consideration of the larger system sizes substantially increases the estimate for the critical disorder that separates the ergodic and many-body localized regimes, compared to the values in the literature. From a technical perspective, we develop an adaptation of the "learning by confusion" machine-learning approach that can determine the critical disorder.

TT 7.9 Mon 12:15 H19

Detection and characterization of many-body localization in central spin models — •Daniel Hetterich[1,4], Norman Yao[2], Maksym Serbyn[3], Frank Pollmann[4], and Björn Trauzettel[1] — [1]Institute for theoretical Physics, University of Würzburg — [2]Department of Physics, University of California, Berkeley — [3]Insitute of Science and Technology, Wien — [4]Department of Physics, Technical University Munich

We analyze a disordered central spin model, where a central spin interacts equally with each spin in a periodic one-dimensional (1D) random-field Heisenberg chain. If the Heisenberg chain is initially in the many-body localized (MBL) phase, we find that the coupling to the central spin suffices to delocalize the chain for a substantial range of coupling strengths. We calculate the phase diagram of the model and identify the phase boundary between the MBL and ergodic phase. Within the localized phase, the central spin significantly enhances the rate of the logarithmic entanglement growth and its saturation value. We attribute the increase in entanglement entropy to a nonextensive enhancement of magnetization fluctuations induced by the central spin. Finally, we demonstrate that correlation functions of the central spin can be utilized to distinguish between MBL and ergodic phases of the 1D chain. Hence, we propose the use of a central spin as a possible experimental probe to identify the MBL phase.

TT 7.10 Mon 12:30 H19

Magnetization and Entanglement after a geometric quench in the XXZ chain — •Matthias Gruber and Viktor Eisler — TU Graz, Graz, Österreich

We consider the XXZ spin chain in the gapless regime and study magnetization and entropy profiles after a geometric quench. This quench is realized by preparing the ground states with zero and maximum magnetizations on the two halves of a chain and letting it evolve subsequently. The magnetization profiles during time evolution are studied numerically by tDMRG and compared to the predictions obtained from generalized hydrodynamics (GHD). We find that the GHD description of the dynamics provides a very good agreement with the numerical data. Furthermore, entanglement entropy profiles are also studied, finding a closed form expression in the non-interacting XX case. For the general interacting case, the propagation velocities of the entropy fronts are studied both before and after the reflection from the boundaries. Finally, we also study the relationship between magnetization fluctuations and entanglement entropy.

TT 7.11 Mon 12:45 H19

Equilibration of expectation values for statically and dynamically generated initial conditions — •Christian Bartsch — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, D-49069 Osnabrück

We investigate dynamical equilibration of expectation values in closed quantum systems for realistic non-equilibrium initial states. For statically generated initial states we find that the long time expectation values depend on the initial expectation values if eigenstate thermalization is violated. An analytical expression for the deviation from the expected ensemble value is derived for small displacements from equilibrium based on linear response theory. Analogous derivations show that this deviation vanishes for dynamically generated initial states, at least within the linear response regime. Additional numerics for magnetization and energy equilibration in an asymmetric anisotropic spin-1/2-ladder illustrate the behavior beyond linear response for both cases.

TT 8: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge I (joint session O/TT/CPP/DS)

First-principles electronic structure calculations have become an indispensable tool in many research areas where materials surfaces or interfaces play a central role. Corresponding calculations provide insight into catalytic mechanisms, interfacial ionic and charge transport in batteries or solar cells, materials degradation through corrosion or wear, and many other highly relevant application areas. Despite this prolific use, corresponding calculations face multiple issues. While the invited lectures will have a focus on this interface challenge, the symposium will also cover the general field of computational materials science and electronic-structure theory.

Organizers: Jens Nørskov (Technical University of Denmark), Karsten Reuter (Technical University Munich), and Matthias Scheffler (Fritz Haber Institute of the Max Planck Society, Berlin)

Time: Monday 10:30–13:00 Location: H9

Topical Talk TT 8.1 Mon 10:30 H9

Scaling relations and beyond for kinetic Monte Carlo models in heterogeneous catalysis — •Mie Andersen — Theoretical Chemistry, Technische Universität München, Germany

Heterogeneous catalysis typically operates at the interface between a gas or liquid and a solid catalytic material. In my talk, I will discuss mean-field and kinetic Monte Carlo models for the operating catalyst. These often rely on input data calculated using either first principles or more approximate methods, e.g. scaling relations, which use only selected adsorption energies as descriptors for the catalyst function [1,2]. I will also discuss recent work [3] where we used compressed sensing methods to identify new low-cost and accurate descriptors that allow to predict adsorption energies for a wide range of adsorbates, multimetallic transition metal surfaces and facets. The descriptors are expressed as non-linear functions of intrinsic properties of the clean catalyst surface, e.g. coordination numbers and *d*-band moments. From a single DFT calculation of these properties, we predict adsorption energies at all potential surface sites, and thereby also the most stable geometry. Compared to previous approaches such as scaling relations, we find our approach to be both more general and more accurate for the prediction of adsorption energies on alloys with mixed-metal surfaces, already when based on training data including only pure metals.

[1] M. Andersen *et al.*, Ang. Chem. Int. Ed. **55**, 5210 (2016)
[2] M. Andersen *et al.*, J. Chem. Phys. **147**, 152705 (2017)
[3] M. Andersen *et al.*, submitted

TT 8.2 Mon 11:00 H9

The Teacher and the Student: Exchange-Correlation Energy Densities from Quantum Chemistry and Machine-Learning — •Johannes T. Margraf, Christian Kunkel, and Karsten Reuter — Chair for Theoretical Chemistry, Technische Universität München, Germany

(Semi-)local density functional approximations (DFAs) are the workhorse electronic structure methods in condensed matter theory and surface science. Central to defining such DFAs is the exchange-correlation energy density ϵ_{xc}, a spatial function that yields the

exchange-correlation energy E_{xc} upon integration.

Unlike E_{xc}, ϵ_{xc} is not uniquely defined. Indeed, there are infinitely many functions that integrate to the correct E_{xc} for a given electron density ρ. The challenge for constructing a useful DFA is to find a systematic connection between ρ and ϵ_{xc}. While several empirical and rigorous approaches to this problem are known, there has been little innovation with respect to the fundamental functional forms of DFAs in recent years.

Herein, we discuss two less explored routes to constructing DFAs. Specifically, a recipe for deriving ϵ_{xc} directly from many-body wavefunctions is compared to a machine learning (ML) approach that infers the optimal ϵ_{xc} for a given functional form. We find that local DFAs based on the many-body ϵ_{xc} are not transferrable between systems because the underlying energy densities are inherently non-local. In contrast, the ML ϵ_{xc} is by construction as local as possible. The extension of both approaches to non-local DFAs will be discussed.

TT 8.3 Mon 11:15 H9

Self-Interaction Corrected SCAN for Molecules and Solids: All-Electron Implementation with Numerical Atom-Centered Basis Functions — •Sheng Bi, Igor Ying Zhang, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Electronic self-interaction is the most severe cause of inaccuracies in all semilocal density-functional approximations (DFAs), including the promising meta-GGA "strongly constrained and appropriately normed" (SCAN) functional [1]. This error can be alleviated via localized orbital scaling corrections [2] or via self-interaction corrections (SIC) based on Fermi-orbitals [3]. In this contribution, we follow the latter concept which involves solving a set of SIC constraints. Here, we present an all-electron implementation of the self-consistent SIC for semilocal DFAs, including SCAN. We first validate our implementation by inspecting certain properties (HOMO and dissociation energies) for a molecular test set, showing that SIC improves SCAN calculations. Furthermore, we compare the performance of SCAN-SIC and SCANα, i.e., SCAN with a fraction of exact exchange, in predicting the broken symmetry in pentacene – note that standard semilocal DFAs always favor symmetric solutions. Eventually, we discuss the extension of our SIC approach to periodic solids.

[1] J. Sun *et al.*, *Phys. Rev. Lett.* **115**, 036402 (2015).
[2] N. Q. Su *et al.*, *Proc. Natl. Acad. Sci.* **115**, 9678 (2018).
[3] Z. Yan *et al.*, *Phys. Rev. A* **95**, 052505 (2017).

TT 8.4 Mon 11:30 H9

Progress in Fermi-Löwdin orbital self-interaction correction to DFT — •Torsten Hahn, Sebastian Schwalbe, and Jens Kortus — Institute for Theoretical Physics, Freiberg, Germany

The accuracy of density functional theory (DFT) calculations is limited by the so called self-interaction error [1]. The recently proposed Fermi-Löwdin orbital based method [2,3,4] for self-interaction correction (FLO-SIC) is a unitary invariant and size extensive approach to overcome this error. We present the current state of the method and discuss selected applications. In addition we discuss strategies to improve the thermochemical and numerical performance of the FLO-SIC approach in combination with state-of-the-art exchange-correlation functionals.

[1] J. P. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)
[2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[3] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)
[4] S. Schwalbe et al., J. Comp. Chem., vol. 39, 2463 (2018).

TT 8.5 Mon 11:45 H9

Time evolution of the natural occupation numbers — •Carlos Benavides-Riveros and Miguel A. L. Marques — Martin-Luther Universität Halle Wittenberg

Reduced density matrix functional theory (RDMFT) is based on the Gilbert theorem, which asserts that the ground-state wave function can be written as a functional of the one-body reduced density matrix. Since RDMFT accounts for fractional natural occupation numbers, it captures quite well static (strong) electron correlation (unlike DFT, RDMFT correctly predicts the insulating behavior of Mott-type insulators). Yet the time-dependent extension of RDMFT suffers from various shortcomings. Chief among them, the current status of the theory does not allow the fermionic occupation numbers to evolve in time. It is known that this deficiency is connected to the failure of RDMFT to account for relative phases at the level of the two-body reduced density matrix. Based on recent results on fermionic exchange symmetry, we propose a new equation for the time evolution of the fermionic occupation numbers.

TT 8.6 Mon 12:00 H9

Nonempricial hybrid functionals constructed through adjustable potential probes for band gap predictions of extended systems — •Thomas Bischoff, Igor Reshetnyak, and Alfredo Pasquarello — Chaire de Simulation a l'Echelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

We describe a nonempirical procedure for achieving accurate band gaps of extended systems through the insertion of suitably defined potential probes. By enforcing Koopmans' condition on the resulting localized electronic states, we determine the optimal fraction of Fock exchange to be used in the adopted hybrid functional. As potential probes, we consider native defects, the extrinsic hydrogen impurity, and various adjustable potentials that allow us to vary the energy level of the localized state in the band gap and its degree of localization. By monitoring the delocalized screening charge, we achieve a measure of the hybridization with the band states, which can be used to improve the band gap estimate. Application of this methodology to AlP, C and MgO yields band gaps differing by less than 0.2 eV from experiment.

TT 8.7 Mon 12:15 H9

Quantum-mechanical relation between atomic dipole polarizability and van der Waals radius — •Dmitry Fedorov, Mainak Sadhukhan, Martin Stöhr, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

The atomic dipole polarizability α and the van der Waals (vdW) radius R_{vdW} are two key quantities to describe the ubiquitous vdW forces important for the structure and dynamics of molecules and materials [1]. The commonly assumed relation between them, $R_{\mathrm{vdW}} \propto \alpha^{1/3}$, is based on a classical picture of hard-sphere atoms. Employing the quantum Drude oscillator model [2], we reveal [3] the quantum-mechanical relation $R_{\mathrm{vdW}} = const. \times \alpha^{1/7}$ which is markedly different from its classical counterpart. Based on the accessible accurate reference data for α and R_{vdW}, we demonstrate that the obtained formula can be used as a unified definition of the vdW radius solely in terms of the atomic polarizability for all chemical elements. Moreover, for vdW-bonded heteronuclear dimers consisting of atoms A and B, the simple combination rule $\alpha = (\alpha_A + \alpha_B)/2$ provides a remarkably accurate way to calculate their equilibrium interatomic distance. These findings unveil a fundamental relationship between the geometric and electronic properties of atoms. From a practical point of view, they allow us to reduce the empiricism and improve the efficiency of computational models for vdW interactions.

[1] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[2] Jones *et al.*, Phys. Rev. B **87**, 144103 (2013)
[3] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)

TT 8.8 Mon 12:30 H9

impact of continuum electronic states on van der Waals dispersion interactions — •Mohammad Reza Karimpour, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

The ubiquitous van der Waals (vdW) forces play an important role for structure, stability, and dynamics of molecules and materials. Their description on atomistic level is important for molecular physics, crystal chemistry, surface science, structural biology, and pharmacy. To this end, the development of simple yet efficient models is of high importance. Normally, such models focus only on fluctuations to bound electron states, described via quantum harmonic oscillator potentials. However, the polarizability of real atomic and molecular systems has important contributions also from fluctuations to continuum states. To study their influence on the vdW dispersion interactions from a general point of view, here we consider models based on the Dirac delta-function potentials. In one-dimensional case, such a potential provides just one bound state whereas all excited states belong to the continuum electron spectrum. We apply both the atomistic method and the scattering picture representing the van der Waals and Casimir approaches for dispersion interactions, respectively. In the atomistic framework we compare our results to the ones of the quantum oscillator models. Within the other picture, we discuss an obtained new scaling law in comparison to the results known for excited atomic systems.

[1] Woods *et al.*, Rev. Mod. Phys. **88**, 045003 (2016)
[2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)

TT 8.9 Mon 12:45 H9

Relation between the van der Waals radius and higher-order atomic polarizabilities — •Ornella Vaccarelli, Dmitry Fedorov, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

The atomic polarizabilities and van der Waals (vdW) radii describe the electronic and geometric aspects of the ubiquitous vdW interactions [1, 2], respectively. Normally, these quantities are assumed to be independent. Therefore, they are determined separately from each other. Based on the quantum Drude oscillator model [3], recently we revealed [4] a remarkable direct relationship between the vdW radius and the dipole polarizability. This provides a unified determination of the vdW radius for all chemical elements solely in terms of their dipole polarizabilities. In addition, further relations between the vdW radius R_{vdW} and higher-order atomic polarizabilities α_n $(n = 1, 2, ...)$ were found empirically. Here, we present a physical background for these results. The derivation of the corresponding scaling laws is performed by going beyond the dipole approximation for the Coulomb interaction to obtain higher-order contributions to attractive and repulsive forces acting on atoms in a vdW-bonded homonuclear dimer. We focus on the derivation of the proportionality constants C_n in the general relation $R_{\mathrm{vdW}}(\alpha_n) = C_n\ \alpha_n^{2/7(n+1)}$ unveiling their quantum nature.

[1] Woods *et al.*, Rev. Mod. Phys. **88**, 045003 (2016)
[2] Hermann *et al.*, Chem. Rev. **117**, 4714 (2017)
[3] Jones *et al.*, Phys. Rev. B **87**, 144103 (2013)
[4] Fedorov *et al.*, Phys. Rev. Lett. **121**, 183401 (2018)

TT 9: Graphene I: Structure and Growth (joint session O/TT)

Time: Monday 10:30–13:00 Location: H24

Invited Talk TT 9.1 Mon 10:30 H24

Real-time imaging of adatom-promoted graphene growth on nickel — •Laerte L. Patera — Department of Physics, University of Trieste, 34127 Trieste, Italy — IOM-CNR - TASC Laboratory, Basovizza, 34149 Trieste, Italy — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Single adatoms are expected to participate in many processes and chemical reactions occurring at solid surfaces. We demonstrate, both experimentally and theoretically, the catalytic role played by single metal adatoms during the graphene growth on Ni(111). The catalytic action of individual Ni atoms at the edges of a growing graphene flake was directly captured by scanning tunneling microscopy imaging at video-rate, allowing the precise determination of the atomic structure of reaction intermediates in the ms time-scale. Force field molecular dynamics and density functional theory calculations rationalize the experimental observations. Our results unveil the mechanism governing the activity of a single-atom catalyst at work [1].

[1] L. L. Patera et al., Science 359, 1243-1246 (2018)

TT 9.2 Mon 11:00 H24

Adsorption Heights and Coupling Strength at Graphene/Ni(111) and h-BN/Ni(111) interfaces — •Christina Schott[1], Johannes Seidel[1], Markus Franke[2], Anja Haags[2], You-Ron Lin[2], Martin Aeschlimann[1], Christian Kumpf[2], and Benjamin Stadtmüller[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Peter Grünberg Institut, Functional Nanostructures at Surfaces, 52425 Jülich, Germany

From a technological point of view, 2D material stacks consisting of light elements grown on ferromagnetic surfaces are highly promising for spintronic applications due to their low spin-orbit coupling and the large charge and spin carrier velocity. However, utilizing the exotic properties requires a minimization of the chemical interaction between the 2D layers and the ferromagnet. Therefore, we have investigated the interlayer interaction strength and coupling mechanisms in bilayer films of prototypical 2D materials on the ferromagnetic surface Ni(111) by using the NIXSW technique. The small vertical bonding distance between graphene or the nano-graphene molecule coronene and the Ni(111) surface suggests a strong chemical interaction across the interface. To achieve a decoupling of coronene from Ni, we used one layer of h-BN as a buffer layer between one the coronene layer and the Ni substrate. Here, we will discuss the modifications of the vertical adsorption height of gr and coronene upon the passivation of the Ni surface and correlate our findings to the chemical interaction and the vertical distortions of these 2D layers.

TT 9.3 Mon 11:15 H24

Thermodynamically Stable Small-Angle Twisted Domains in Graphene on Iridium (111) — •Karim M. Omambac[1], Christian Brand[1], Hichem Hattab[1], Laurenz Kremeyer[1], Giriraj Jnawali[1], Alpha T. N'Diaye[2], Johann Coraux[2], Raoul van Gastel[3], Bene Poelsema[3], Thomas Michely[2], Frank-Jörg Meyer zu Heringdorf[1], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen, Germany — [2]Universität zu Köln, Germany — [3]University of Twente, The Netherlands

Lattice rotations or twists is one to the characteristics in the catalytic growth of monolayer graphene on a hot metallic surface. In particular, these small-angle twists have not yet been found experimentally but have been predicted partly through density functional theory calculations [1]. In this low energy electron diffraction study we evaluated the distribution of twisted domains of the epitaxially grown graphene on Ir(111) through spot profile analysis of the moiré spots. We find a new class of small-angle twisted domains with clear and distinct twist angles of 1.7°, 1.1° and 0.6° at growth temperatures of 1255 K, 1350 K, and 1460 K, respectively. To further analyze, we performed a simple two-dimensional in-plane coincidence site lattice analysis taking only into account the thermal expansion coefficients between the substrate and the epitaxially grown graphene. The results show a very good agreement with the experimental findings suggesting the origin of these small-angle twisted domains is strongly dependent on the variation of the lattice mismatch between graphene and Ir(111) substrate during growth. [1] J. Phys.: Condens. Matter **24**, 314214 (2012)

TT 9.4 Mon 11:30 H24

Buckling of graphene on Ir(111) by the intercalation of cobalt — •David A Duncan[1], Nicolae Atodiresei[2], Simone Lisi[3], Phil J Blowey[1,4], Vasile Caciuc[2], James Lawrence[4], Tien-Lin Lee[1], Maria Grazia Betti[5], Pardeep Thakur Kumar[1], Ada Della Pia[5], Giovanni Costantini[4], and D. Phil Woodruff[4] — [1]Diamond Light Source, Didcot, UK — [2]Forschungzentrum Jülich, Jülich, Germany — [3]Institut Néel, Grenoble, France — [4]University of Warwick, Coventry, UK — [5]University Sapienza of Rome, Rome, Italy

The intercalation of Co between graphene and Ir(111) results in a corrugated network of strongly and weakly bound carbon [1]. Utilising the X-ray standing wave method to monitor the chemical-state resolved C 1s photoemission components [2], we determine that the strongly bound C atoms adsorb with a mean adsorption height, above the Co layer, of 2.06(3) Å, almost 0.75 Å lower than that of the weakly bound C atoms (2.76(5) Å). DFT calculations using DFT-D2 and vdW-DF corrections predict a subtle difference corrugation structure, with DFT-D2 predicting a local maximum where the vdW-DF predicts a global minimum. The DFT-D2 calculations result in a structural model that more closely matches the experimental results, with the vdW-DF calculations predicting mean adsorption heights for the strongly and weakly bound C atoms that are 0.10 Å and 0.37 Å closer to the Co intercalant, respectively, than measured experimentally. Despite this difference, both functionals predict a covalent like interaction between the Co and the C, resulting in a weak nearest-neighbour C-C buckling.

[1] PRB 87 (2013), 041403; [2] PRB, 90 (2014), 195446

TT 9.5 Mon 11:45 H24

Understanding the first steps of graphene growth: a study of small carbon clusters on Cu surfaces — •Juan Santiago Cingolani, Mie Andersen, and Karsten Reuter — Chair of Theoretical Chemistry, Technical University of Munich, Germany

It has been shown that high quality single layer graphene can be obtained through chemical vapor deposition on liquid Cu [1]. The role of the liquid surface in carbon nucleation as well as in defect healing is not yet well understood. While a comprehensive description of the growth mechanism would require molecular dynamics (MD) simulations, a first step is to study the precursors for graphene growth and

the influence of the surface on them.

We performed a series of density-functional theory (DFT) calculations of carbon clusters of different sizes adsorbed to different Cu facets aiming to shed some light on the effects of the surface on relative stabilities, as well as on experimentally accessible properties such as vibrational frequencies. We also take advantage of the data generated to fit the parameters of density-functional tight binding, a semi-empirical method, which in turn allows us to carry out MD simulations for longer timescales and in larger systems than otherwise accessible through *ab initio* methods. We then simulate graphene flakes on liquid Cu at different levels of theory to get a clearer picture of what the Cu surface might look like under growth conditions.

[1] L. Tan, M. Zeng, T. Zhang, L. Fu, Nanoscale 7, 9105 (2015).

TT 9.6 Mon 12:00 H24

Aperiodically ordered nano-graphene — •Mahalingam Maniraj[1], Lu Lyu[1], Sebastian Becker[1,2], Dominik Jungkenn[1], Sebastian Emmerich[1], Sina Mousavion[1], D L Schlagel[3], T A Lograsso[3], Sudipta Roy Barman[4], Stefan Mathias[5], Benjamin Stadtmuller[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany — [2]Department of Chemistry, TU Kaiserslautern, Germany — [3]Division of Materials Sciences and Engineering, Ames Laboratory, USA — [4]UGC-DAE Consortium for Scientific Research, Indore (M.P.), India — [5]I. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

We demonstrate that the quasiperiodic order of surfaces can be transferred to 2D adsorbate systems by investigating the self-assembly of the nano graphene molecule coronene on the icosahedral(i)-Al-Pd-Mn quasicrystalline surfaces using multiple surface sensitive techniques. We find a quasiperiodic ordering of coronene on the i-Al-Pd-Mn surface which can be explained qualitatively by the P1 Penrose tilling. Using angle resolved photoemission spectroscopy, we observe a 5-fold symmetric modulation of the photoemission intensity distribution in the kx-ky-plane with a clear band dispersion along the high symmetry axis in momentum space. The latter suggests a direct correlation between the energy and momenta of the electrons in the quasicrystal and the rotational symmetry of the system. Moreover, the pseudogap of the bare Al-Pd-Mn persists even after the adsorption of the aperiodically ordered coronene confirming the quasiperiodic nature of the interface.

TT 9.7 Mon 12:15 H24

The role of the curvature of graphitic materials in the oxygen adoption reaction — Jakob Hauns, Julian Wüst, Jürgen Weippert, Regina Fischer, Frank Hennrich, Dmitry Strelnikov, •Artur Böttcher, and Manfred M. Kappes — Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

The capability of graphitic materials to bind atomic oxygen has been studied under ultrahigh vacuum conditions by monitoring the oxygen-induced evolution of the XPS-*O1s*, -*C1s* and the valence band states, UPS-VB. Three groups of solid films were investigated: HOPG (planar graphene sheet), felts of metallicity-sorted single walled carbon nanotubes S-, M-SWCNTs and solid C_{60} films. The monodispersed materials chosen here differ by the curvature $\boldsymbol{C}$ of the graphene layers. In order to quantify the role of strained C-C-C bonds in the oxidation pathway exactly the same oxidation procedure has been applied to all graphitic materials. The VB-DOS profiles measured for oxidized films differ clearly by their oxygen-derived bands and the work functions. The evolution of the XPS-*O1s* and -*C1s* states indicate that whereas the oxidation of planar graphene sheets proceeds via epoxy species [1], ether functionalities dominate the oxidative scenario of the curved surfaces of SWCNT and $C_{\mathbf{60}}$. The yield for the initial oxygen-adoption reaction for all curved surfaces is significantly higher than that measured for planar graphene sheets. This finding stresses the unique role of the strained -C-C-C- bonds which facilitate the formation of ether functionalities. [1] A. Barinov, et al. J. Phys. Chem. C 2009, 113, 9009.

TT 9.8 Mon 12:30 H24

Thermal reduction of graphene oxide studied by electron spectroscopy — •Gianluca Di Filippo[1], Andrea Liscio[2], and Alessandro Ruocco[1] — [1]Dipartimento di Scienze, Università degli Studi Roma Tre, Rome, Italy — [2]Consiglio Nazionale delle Ricerche, Istituto per la Microelettronica e Microsistemi, Rome, Italy

Graphene oxide (GO) is a purely 2D material composed of a conductive filter given by sp^2 domains and an insulating matrix containing sp3-carbons, defects, holes and oxygen functional groups. The latter make GO an insulator, but its electronic, optical and structural properties can be tailored via controlled removal of the oxygen groups. This enables reduced graphene oxide (rGO) to be used in many fields such as sensors development and energy storage applications.
In this work, we investigated the thermal reduction of GO in ultra-high-vacuum by combining several electron spectroscopies. Photoemission spectroscopy (XPS and UPS) was used to investigate variations in the chemical and electronic structure of GO reduced in the 150 °C - 750 °C temperature range. The optical properties of rGO were investigated using electron energy loss spectroscopy (EELS). The build-up of the $\pi-$plasmon excitation was observed upon reduction at 300 °C, this revealing the formation of ordered graphene-like areas with dimensions around 5 nm. The vibrational spectrum revealed the presence of CH groups on the surface. Most of the hydrogen atoms are bound to sp^3-carbon and are probably located in oxidized regions in the basal plane of rGO. The sp^3-CH impurities can be removed upon annealing at 750 °C where only sp^2 CH defects are observed.

TT 9.9 Mon 12:45 H24

Intercalation dynamics of sulfur underneath graphene on Ru(0001) — •Lars Buss[1], Jens Falta[1,2], and Jan Ingo Flege[3] — [1]Institute for Solid State Physics, University of Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Germany — [3]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany

It is known that the binding of epitaxially grown graphene to the substrate has a detrimental effect on its electronic properties. This is especially true for the strong binding to various transition metals and particularly ruthenium. However, via intercalation the interlayer coupling can be lifted and its unique electronic properties can be restored. Therefore, we have investigated the interaction of sulfur with single-layer graphene grown on Ru(0001) via surface segregation and CVD of ethylene under UHV conditions with in situ low-energy electron microscopy (LEEM) and micro-diffraction (μLEED). At elevated temperature and under dimethyl disulfide background pressure, we observe that sulfur intercalates through the open edges of the graphene islands. Prolonged exposure to sulfur induces wrinkling of the graphene islands, consistent with substantial relief of tensile strain after successful sulfur insertion underneath the graphene. It can be seen that the intercalation dynamics are both dependent on the temperature during intercalation and the preparation method of the graphene sheets. Furthermore, darkfield imaging and μLEED of the intercalated graphene reveal a graphene induced improved ordering of sulfur underneath.

TT 10: Focus Session: New Bright Sources of Quantum Microwaves

Quantum microwaves are an important building block of future quantum technologies. The Focus Session brings together groups that are currently pioneering the use of conventional quantum microwave sources to demonstrate the first proof of principle experiments in quantum communication and sensing, with groups that have recently realized new bright sources of quantum microwaves operating based on completely novel and simple schemes. The goal is to provide a bridge of shared expertise between two parts of the community aiming from different angles at novel quantum technologies using microwaves.

Organized by: Joachim Ankerhold, Björn Kubala, Ciprian Padurariu (Ulm University)

Time: Monday 15:00–18:45 Location: H2

Invited Talk TT 10.1 Mon 15:00 H2

Quantum dynamics of a microwave resonator strongly coupled to a tunnel junction — •Jérôme Esteve — Laboratoire de Physique des Solides, CNRS, Université Paris-Sud, Université Paris-Saclay, Orsay, France

The coupling of a quantum system, such as an atom or a resonator, to a bath can be modeled under certain hypotheses by a quantum master equation in the Lindblad form. In this description, two effects arise from the coupling to the bath: the first is a shift of the energy levels, called Lamb shift, and the second is an irreversible energy exchange with the bath in the form of quantum jumps.

A tunnel junction galvanically coupled to a resonator realizes a bath for the resonator mode. In the strong coupling regime, where the characteristic impedance Z_c of the resonator is on the order of the quantum of resistance $R_K = h/e^2$, we will show that both the Lamb shift and the jump operators strongly depend on the resonator state. Different Fock states experience different Lamb shifts, which introduces a nonlinearity, and quantum jumps from a specific Fock state to another can be forbidden by tuning the coupling parameter $\sqrt{\pi Z_c/R_K}$ to specific values.

We will discuss the dynamics of the resonator mode resulting from this engineered bath and consider possible applications including quantum Zeno dynamics and the realization of a qubit without Josephson effect.

Invited Talk TT 10.2 Mon 15:30 H2

Quantum optics with artificial atoms in an open space — •Oleg Astafiev — Royal Holloway University of London, Egham, UK

Superconducting quantum systems in open space allow one to reproduce textbook phenomena of quantum optics on a new basis of fully controllable artificial quantum systems (artificial atoms). Such systems, differently from natural atoms, can be easily coupled to their environment and other circuit elements and therefore new quantum-optical phenomena can be demonstrated with the single quantum systems. Particularly, a regime of strong coupling to an open 1D transmission line, when the atom relaxes with high probability of the photon emission into the line, has been experimentally achieved. With the strong coupling we were able to experimentally realise a series of effects, useful for applications and also interesting from the fundamental point of view, using the artificial atom as a quantum source and a sensor of specific properties of electromagnetic waves. The following phenomena have been demonstrated: a tuneable on-demand single-photon source, an absolute power sensor, a quantum wave mixer, etc. All these effects are difficult to demonstrate with natural atoms.

Invited Talk TT 10.3 Mon 16:00 H2

Quantum microwaves with a DC-biased Josephson junction — •Fabien Portier[1], Ambroise Peugeot[1], Chloé Rolland[1], Marc Westig[1], Gerbold Ménard[1], Yuri Mukharsky[1], Hélène le Sueur[1], Patrice Roche[1], Philippe Joyez[1], Carles Altimiras[1], Patrice Bertet[1], Daniel Esteve[1], Denis Vion[1], Max Hofheinz[1], Pérola Milman[2], Bjoern Kubala[3], Simon Dambach[3], and Joachim Ankerhold[3] — [1]SPEC (UMR 3680 CEA-CNRS), CEA Paris-Saclay, 91191 Gif-sur-Yvette, France — [2]LMPQ, Université Paris Diderot, CNRS UMR 7162, 75013, Paris, France — [3]ICQS and IQST, University of Ulm, 89069 Ulm, Germany

Tunneling of a Cooper pair through a dc-biased Josephson junction is possible only if collective excitations (photons) are produced in the rest of the circuit to conserve the energy. The probability of tunneling and photon creation, well described by the theory of dynamical Coulomb blockade, increases with the coupling strength between the tunneling charge and the circuit mode, which scales as the mode impedance. Using very simple circuits with only one or two high impedance series resonators, we first show the equality between Cooper pair tunneling rate and photon production rate. Then we demonstrate a blockade regime for which the presence of a single photon blocks the next tunneling event and the creation of a second photon. Finally, using two resonator with different frequencies, we demonstrate photon pair production, two-mode squeezing, and entanglement between the two modes leaking out of the resonators.

15 min. break.

Invited Talk TT 10.4 Mon 16:45 H2

Photodetectors and metamaterials for on-chip microwave photonics — •Frank K. Wilhelm-Mauch — Theoretical Physics, Saarland University, Campus E2.6, 66123 Saarbrücken, Germany

Superconducting quantum nanodevices are a unique platform for on-chip microwave photonics. They allow engineered sources, strong quantum nonlinearities, and excellent amplification. In this presentation, I will describe two additional toolsets for this platform: For one, the Josephson-Photomultiplier (JPM) allows photodetection of microwaves that is insensitive to the phase. This. on the one hand, can be used to taylor measurement backaction to, e.g., selectively detect only the parity of a quantum register but to not resolve fixed-parity states, and to use create nonclassical microwave states by measurement and displacement only. On the other hand, the JPM is an attractive platform for qubit measurement due to its low technological overhead. I will present new results on the possibility of generalizing this concept to reaching number resolution. On the other hand, superconducting metamaterials can be used to taylor the spectrum of propagating photons. Left-handed transmission lines create a large density of states that can be enhanced even further by using left-handed superlattices. This allows to study a wealth of unconventional dissipative phase-transitions with long-range order.

Invited Talk TT 10.5 Mon 17:15 H2

Correlated Cooper pair transport and microwave photon emission in the Coulomb blockade — •Juha Leppäkangas[1,2], Michael Marthaler[1], Mikael Fogelström[2], and Göran Johansson[2] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Microtechnology and Nanoscience, MC2, Chalmers University of Technology, Göteborg, Sweden

We study theoretically electromagnetic radiation emitted by inelastic Cooper-pair tunneling. We consider a dc-voltage-biased superconducting transmission line terminated by a Josephson junction. The leading-order expansion in the tunneling coupling, similar to the "P(E)-theory", can be used to investigate the photon emission statistics in the limit of sequential (independent) Cooper-pair tunneling. By explicitly evaluating the system characteristics up to the fourth-order in the tunneling coupling, we account for dynamics between consecutively tunneling Cooper pairs. Within this approach we investigate how temporal correlations in the charge transport can be seen in the second-order coherence of the emitted microwave radiation. In particular, we find that a Coulomb blockade provided by a high zero-frequency impedance can be used to create antibunched microwave photons at a very high rate.

TT 10.6 Mon 17:45 H2

Nonlinear quantum dynamics and hidden cats states in a cavity conductor hybrid — •Andrew Armour[1], Bjoern Kubala[2], and Joachim Ankerhold[2] — [1]School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, UK — [2]Institute

for Complex Quantum Systems and IQST, Ulm University, Albert Einstein-Allee 11, 89069 Ulm, Germany

Coupling a mesoscopic conductor to a microwave cavity can lead to fascinating feedback effects which generate strong correlations between the dynamics of photons and charges. We explore the connection between cavity dynamics and charge transport in a model system consisting of a voltage-biased Josephson junction embedded in a high-Q cavity. We find that strong nonlinearities which occur in the cavity dynamics are associated with the emergence of novel regimes of charge and photonic transport. We also show that when the state of the cavity is conditioned on measurements of the number of photons emitted one can reveal fragile features, such as cat states, which are lost within the usual unconditioned dynamics.

TT 10.7 Mon 18:00 H2

Generating Pairs of Entangled Microwave Photons by Josephson-Photonics Devices — •Simon Dambach[1], Ambroise Peugeot[2], Juha Leppäkangas[3], Björn Kubala[1], Marc Westig[2], Yuri Mukharsky[2], Carles Altimiras[2], Denis Vion[2], Daniel Esteve[2], Fabien Portier[2], and Joachim Ankerhold[1] — [1]Institut für komplexe Quantensysteme, Universität Ulm, Germany — [2]SPEC (UMR 3680 CEA-CNRS), CEA Paris-Saclay, France — [3]Physikalisches Institut, Karlsruher Institut für Technologie, Germany

The realization of bright and efficient sources for entangled microwave photons is considered of paramount importance for many future applications of quantum technology. Josephson-photonics devices are very promising candidates for this task since they allow one to create a broad range of different entangled states in a surprisingly simple way [1]. In these devices, Cooper-pair tunneling across a dc-voltage–biased Josephson junction simultaneously creates photons in several series-connected microwave cavities. Steady states with multifaceted entanglement properties are reached naturally due to the interplay of these multiphoton creation processes and subsequent individual photon leakage from the cavities. Sophisticated pulse shaping as required in conventional circuit-QED architectures is thus not necessary here. In this talk, we present a theoretical study of the bipartite entanglement in both the cavity modes and the output transmission lines. Analytical results for weak driving, complemented by numerical calculations for the full nonlinear case, show good agreement with experimental data.
[1] S. Dambach et al., New J. Phys. **19**, 023027 (2017).

TT 10.8 Mon 18:15 H2

Full photon counting statistics at non-degenerate Josephson parametric resonance — •Lisa Arndt and Fabian Hassler — JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

Due to parametric down conversion, a dc-biased Josephson junction coupled to two microwave resonators emits photon pairs when the Josephson frequency matches the sum of the two resonance frequencies. Recent experiments have shown that such a setup permits analyzing the correlation of the radiation [1]. Motivated by these results, we study theoretically the full counting statistics (FCS) of a non-degenerate parametric oscillator below the instability threshold. We focus on the limit of long measurement times and derive the FCS for arbitrary detuning between the driving frequency and the sum of the resonance frequencies. Additionally, we study the impact of asymmetry in the linewidth of the modes—a distinctive property of the non-degenerate resonance effect. In particular, we find that the frequency of the photons emitted by the mode with the larger linewidth is shifted by the total detuning, while the other mode emits photons at the resonance frequency.
[1] M. Westig, B. Kubala, O. Parlavecchio, Y. Mukharsky, C. Altimiras, P. Joyez, D. Vion, P. Roche, D. Esteve, M. Hofheinz, M. Trif, P. Simon, J. Ankerhold, and F. Portier, Phys. Rev. Lett. **119**, 137001 (2017)

TT 10.9 Mon 18:30 H2

Steady-state generation of Wigner-negative states in 1D resonance fluorescence — •Fernando Quijandria, Ingrid Strandberg, and Göran Johansson — Microtechnology and Nanoscience, MC2, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

In this work, we generate nonclassical states of the electromagnetic field by utilizing the strong coupling between an artificial two-level atom and a one-dimensional waveguide. We use the negativity of the Wigner function as an indicator of nonclassicality. States characterized by a negative Wigner function are a necessary element for protocols promising to overcome classical computational power. We study the steady-state emission from a continuously driven atom using the method of quantum trajectories. We simulate the conditioned evolution of an atom being subjected to quadrature meassurement. In turn, from the measurement statistics we are able to reconstruct the state of the emitted field. We show that using this setup it is possible to generate coherent superpositions of Fock states beyond vacuum and single-photons.
[1] F. Quijandría, I. Strandberg and G. Johansson. arXiv:1806.01355 (2018), accepted in Phys. Rev. Lett. (in press).

TT 11: Majorana Physics

Time: Monday 15:00–18:45 Location: H4

TT 11.1 Mon 15:00 H4

Kitaev spin liquid at quantum criticality and beyond — •Dirk Wulferding[1,2], Youngsu Choi[3], Yann Gallais[4], Peter Lemmens[1,2], Seunghwan Do[5], and Kwang-Yong Choi[3] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]Chung-Ang Univ., Seoul, Korea — [4]Univ. Paris-Diderot, Paris, France — [5]MPK / POSTECH, Pohang, Korea

The honeycomb lattice α-$RuCl_3$ is among the most promising candidates to realize a Kitaev spin liquid [1] that hosts Majorana fermions. In applied magnetic fields, the low temperature zig-zag antiferromagnetic order is suppressed, and α-$RuCl_3$ approaches quantum criticality at $H_c = 6.5$ T [2,3]. Our Raman study reveals distinct changes in low energy magnetic excitations as a function of applied fields. Based on a detailed temperature analysis [4,5] we comment on the fate of Majorana fermionic excitations and multiparticle quasiparticles at and beyond the quantum critical point.

Work supported by QUANOMET NL-4 and DFG LE967/16-1.

[1] Sandilands et al., PRL 114, 147201 (2014)
[2] Wang et al., PRL 119, 227202 (2017)
[3] Wolter et al., PRB 96, 041405(R) (2017)
[4] Glamazda et al., PRB 95, 174429 (2017)
[5] Glamazda et al., Nat. Commun. 7, 12286 (2016)

TT 11.2 Mon 15:15 H4

Probing Majorana bound states with an optical quantum dot — •Lena Bittermann[1], Daniel Frombach[1], Christophe De Beule[1], and Patrik Recher[1,2] — [1]Institut für Mathematische Physik, TU Braunschweig — [2]Laboratory for Emerging Nanometrology Braunschweig

Majorana bound states (MBSs) arise at the ends of a semiconducting nanowire in proximity to a superconductor when a sufficiently strong magnetic field is applied. Ever since signatures of MBSs were discovered, there has been a lot of research exploring their properties. Nevertheless, their spin structure [1] has only recently gotten attention. By coupling a quantum dot to one of the ends of the wire [2], the spin and non-local properties can be investigated [3].

Here, we propose a setup where we use an optical quantum dot as a spectroscopic tool. At first we solve the low-energy model for the wire coupled to the quantum dot and calculate the corresponding transition rates for creation of photons via optical recombination. Furthermore, we use a master equation formalism to obtain the steady-state occupation probabilities. By analyzing the resulting photon emission spectrum, we can draw conclusions on the spin polarization of the MBSs for different recombination processes.
[1] D. Sticlet, C. Bena and P. Simon, PRL 108, 096802 (2012)
[2] M. T. Deng et al., Science 354, 1557 (2016)
[3] E. Prada, R. Aguado and P. San-Jose, PRB 96, 085418 (2017)

TT 11.3 Mon 15:30 H4

Fano resonaces in spinfull Majorana bound state - quantum dot hybrid system — •Alexander Schuray[1] and Patrik

Recher[1,2] — [1]Institut für Mathematische Physik, TU Braunschweig — [2]Laboratory for Emerging Nanometrology Braunschweig

The emergence of Majorana bound states (MBS) as topologically protected zero energy modes in hybrid superconductor-semiconductor devices spark a lot of research activities in the last couple of years [1]. Recently, it was reported that these hybrid devices can be coupled to a quantum dot [2]. In devices in which MBS are coupled to a quantum dot (QD) on one side and a normal conducting lead on the other side Fano resonances arise. These resonances can be used to identify and quantify the couplings to the MBS [3]. Here, we want to present our recent research in which we extend our previous work on a spinless MBS-QD system [3] to the spinful case including Coulomb interaction on the QD on a mean field level. We use full counting statistics to calculate the transport properties and support our analytical findings by numerical calculations using Kwant [4].

[1] R. Aguado, Riv. Nuovo Cimento 40, 523 (2017)
[2] M.T. Deng et al., Phys. Rev. B 98, 085125 (2018)
[3] A. Schuray, L. Weithofer, and P. Recher, Phys. Rev. B 96, 085417 (2017)
[4] C. W. Groth et al., New J. Phys. 16, 063065 (2014)

Invited Talk TT 11.4 Mon 15:45 H4

Majorana states in carbon nanotubes — •Magdalena Marganska[1], Lars Milz[1], Wataru Izumida[2], Christoph Strunk[3], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93 053 Regensburg, Germany — [2]Department of Physics, Tohoku University, Sendai 980 8578, Japan — [3]Institute for Experimental and Applied Physics, University of Regensburg, 93 053 Regensburg, Germany

One of the two most popular schemes for the realization of Majorana fermions uses proximitized semiconducting nanowires with spin-orbit coupling. With proper combination of magnetic field and gate voltage they can be driven into a topological phase, hosting zero energy Majorana bound states (MBS). Carbon nanotubes have similar properties and can be used in the same setup. They are however a hundred times thinner than the nanowires, which makes them truly one-dimensional systems, with only one relevant transverse mode for spin and valley degrees of freedom. Further, this allows us to perform a full microscopic tight-binding numerical simulation. Its results then serve as the reference for the construction of effective models in the reciprocal space.

In agreement with our numerics, the topological phase diagram predicts the presence of Majorana states at magnetic fields and chemical potentials which are encouraging for the planned experiments. The MBS themselves and their spin canting angle are revealed as complex entities, with a helical spatial profile made up from contributions from six different regions in the reciprocal space. This influences the coupling of the MBS to the outside world.

TT 11.5 Mon 16:15 H4

Transport properties of nanowire networks hosting Majorana bound states in presence of Coulomb energy — •Johan Ekström[1], Patrik Recher[2], and Thomas Schmidt[1] — [1]Physics and Materials Science Research Unit, University of Luxembourg, 1511 Luxembourg, Luxembourg — [2]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany

We investigate the electron transport through Coulomb blockaded structures hosting Majorana bound states (MBS). In particular we are interested in higher-order processes beyond local and crossed Andreev reflection. A nanowire in the topologically non-trivial regime hosts a pair of MBSs, one localized on each end of the wire. In more complex wire structures, for example wire junctions, MBSs can manifest themselves at the edges as well as at crossing points. This gives rise to transport processes that are not observed in simple nanowires. We present a general way of how the different transport processes can be obtained and understood by using a master equation where the tunneling Hamiltonian is taken into account perturbatively.

TT 11.6 Mon 16:30 H4

Interacting majorana chain in presence of disorder — •Jonas Karcher[1], Michael Sonner[1], and Alexander Mirlin[1,2] — [1]KIT, Karlsruhe, Deutschland — [2]NRC Kurchatov Institute, St. Petersburg, Russia

We investigate a majorana chain model with potential applications to the description of Kitaev edges. The model exhibits various topological phases which are separated by critical lines. Since the non-interacting system belongs to class BDI one would expect these lines to remain critical in presence of disorder if the interaction is sufficiently weak . Recent numerical studies using DMRG confirm this for attractive interactions. For strong repulsive interactions, these studies find that the system localizes. Our preliminary results show localization also for weak repulsive interaction. We want to understand the mechanism that drives the system into localization despite topological protection. To reach this goal we employ both DMRG calculations and diverse analytical RG-schemes. Our results from DMRG suggest spontaneous breaking of the translation symmetry. This cannot be understood from the weak disorder and weak interaction RG around the clean noninteracting fixed point (FP), where the interaction is irrelevant. Hence we investigate the stability of the infinite randomness FP against weak interaction. The wave functions exhibit (multi)fractality. Correlators are again computed analytically using a SUSY transfer matrix techniques. This approach is augmented by results from exact diagonalization. From their scaling behaviour we want to deduce the interaction RG flow.

TT 11.7 Mon 16:45 H4

Quasiparticle poisoning in the RSJ model for Josephson Junctions — •Daniel Frombach[1] and Patrik Recher[1,2] — [1]Institut für Mathematische Physik, TU Braunschweig — [2]Laboratory for Emerging Nanometrology Braunschweig

The fractional 4π Josephson effect, a specific feature of Majorana bound states, is based on a conserved fermion parity of the junction. Effects which break the fermion parity conservation, processes known as quasiparticle poisoning, however reduce the 4π periodic effect to the usual 2π periodicity. The timescale on which these effects occur has been estimated [1] and is generally system specific.

Here we analyze the quasiparticle poisoning by directly including it into a RSJ description of the fractional Josephson junction. We discuss possible measuring schemes for the poisoning rates as well as signatures of topology even in the presence of quasiparticle poisoning.

[1] D. Rainis and D. Loss, Phys. Rev. B 85, 174533 (2012)

15 min. break.

TT 11.8 Mon 17:15 H4

Topological Mechanics from Supersymmetry — •Jan Attig[1], Krishanu Roychowdhury[2,3], Michael Lawler[2,4], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]Laboratory of Atomic And Solid State Physics, Cornell University, Ithaca, NY 14853, USA — [3]Department of Physics, Stockholm University, SE-106 91 Stockholm, Sweden — [4]Department of Physics, Binghamton University, Binghamton, NY, 13902, USA

In the field of topological mechanics, the identification of a mechanical system's rigidity matrix with an electronic tight-binding model allows to infer topological properties of the mechanical system from the associated electronic band structure. In this talk, I will provide a broader perspective on this relation by introducing an approach to systematically construct topological mechanical systems for an entire class of free Majorana fermion models through an exact supersymmetry (SUSY) that relates the bosonic (mechanical) and fermionic (e.g. electronic) degrees of freedom. As examples we discuss mechanical analogues of the Kitaev honeycomb model and of a second-order topological insulator with floppy corner modes. On a conceptual level, our SUSY construction naturally defines hitherto unexplored topological invariants for bosonic (mechanical) systems, such as bosonic Wilson loop operators that are formulated in terms of a SUSY-related fermionic Berry curvature.

TT 11.9 Mon 17:30 H4

Time-resolved Majorana-fermion dynamics in topological superconducting wires — •Riku Tuovinen[1], Michael A. Sentef[1], Robert van Leeuwen[2], Enrico Perfetto[3], and Gianluca Stefanucci[3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany — [2]Department of Physics, University of Jyväskylä, 40014 Jyväskylä, Finland — [3]Dipartimento di Fisica, Università di Roma Tor Vergata, 00133 Rome, Italy

In the emerging field of topological quantum computing, topologically protected states can be utilized to minimize quantum decoherence [1]. We use a recently developed method for time-dependent quantum transport [2], and we consider a superconducting wire - hosting

a Majorana zero mode at its edges [3] - connected to metallic leads. We investigate how the Majorana zero mode builds up in the transient regime [4], and we discuss how these ultrafast transport properties could also be observed experimentally.

[1] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011)
[2] R. Tuovinen, E. Perfetto, G. Stefanucci, and R. van Leeuwen, Phys. Rev. B 89, 085131 (2014)
[3] E. M. Stoudenmire, J. Alicea, O. A. Starykh, and M. P. A. Fisher, Phys. Rev. B 84, 014503 (2011)
[4] R. Tuovinen, M. A. Sentef, R. van Leeuwen, E. Perfetto, and G. Stefanucci, in preparation

TT 11.10 Mon 17:45 H4

Simulating topological tensor networks with Majorana qubits — •Carolin Wille[1], Reinhold Egger[2], Jens Eisert[1], and Alexander Altland[3] — [1]FU Berlin — [2]Heinrich-Heine-Universität Düsseldorf — [3]Universität zu Köln

The realization of topological quantum phases of matter remains a key challenge to condensed matter physics and quantum information science. In this work, we demonstrate that progress in this direction can be made by combining concepts of tensor network theory with Majorana device technology. Considering the topological double semion string-net phase as an example, we exploit the fact that the representation of topological phases by tensor networks can be significantly simpler than their description by lattice Hamiltonians. The building blocks defining the tensor network are tailored to realization via simple units of capacitively coupled Majorana bound states. In the case under consideration, this defines a remarkably simple blueprint of a synthetic double semion string-net, and one may be optimistic that the required device technology will be available soon. Our results indicate that the implementation of tensor network structures via mesoscopic quantum devices may define a powerful novel avenue to the realization of synthetic topological quantum matter in general.

TT 11.11 Mon 18:00 H4

Topological Ordering in the Majorana Toric Code — •Alexander Ziesen[1], Fabian Hassler[1], and Ananda Roy[1,2] — [1]JARA Institute for Quantum Information, RWTH Aachen University — [2]Institut de Physique Théorique, CEA Saclay

At zero temperature, a two-dimensional lattice of Majorana zero modes on mesoscopic superconducting islands exhibits a $\mathbb{Z}_2$ topologically-ordered phase, similar to the ground state of the toric code. Recently, a Landau field theory was proposed for the system that describes its phases and the different phase-transitions separating them. While the field theories for the different phase-transitions were obtained in the earlier work, the signatures of topological ordering in the different phases were not investigated in detail. This is the goal of the current work. We describe a lattice gauge theory of the Majorana toric code in terms of a $U(1)$ matter field coupled to an emergent $\mathbb{Z}_2$ gauge field. Subsequently, we use a generalized Wilson-loop order-parameter, namely, the equal-time Fredenhagen-Marcu order parameter, to distinguish between the different phases. Our findings confirm the previously-obtained field theory results. In contrast to the earlier work where the topological ordering of the different phases was inferred indirectly from the Landau field theory, our method directly detects the topological ordering in the system and is thus, an independent check for the earlier results.

TT 11.12 Mon 18:15 H4

Phase-dependent heat transport in topological superconductors — •Alexander G. Bauer and Björn Sothmann — Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany

Recently, phase-coherent heat transport in superconducting tunnel junctions has received great interest. On the one hand, it allows for the realization of caloritronic circuits [1]. On the other hand, this can serve as a probe of fundamental properties of quantum matter [2]. Here, we investigate heat transport in junctions made from topological superconductors. We demonstrate that the thermal conductance can probe Majorana physics and enables us to distinguish between helical and chiral superconducting pairing.

[1] F. Giazotto and M. J. Martinez-Perez, Nature **492**, 401 (2012).
[2] B. Sothmann and E. M. Hankiewicz, Phys. Rev. B **94**, 081407 (2016).

TT 11.13 Mon 18:30 H4

Chiral Majorana fermions in graphene — •Petra Högl[1], Tobias Frank[1], Denis Kochan[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Theoretical Physics and Astrophysics, Pavol Jozef Šafárik University, 04001 Košice, Slovakia

Chiral Majorana fermions are massless self-conjugate fermions which arise as propagating edge states of 2d topological superconductors. Recently, a scheme for topological quantum computation based on chiral Majorana fermions has been proposed [1]. We show the appearance of chiral Majorana edge modes in graphene by computing zigzag and armchair ribbon spectra. For this we use an effective model of graphene which takes into account proximity induced spin-orbit coupling and exchange field. This leads to a quantum anomalous Hall state which turns into a topological superconductor by adding superconducting proximity coupling. We prove the topological nature of the system by analyzing the Chern number of the 2d bulk.

This work has been supported by DFG SFB 1277 (Project B07) and EU Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] B. Lian, X.-Q. Sun, A. Vaezi, X.-L. Qi, S.-C. Zhang, PNAS 115, 10938 (2018)

TT 12: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge II (joint session O/TT/DS/CPP)

Time: Monday 15:00–17:30 Location: H9

TT 12.1 Mon 15:00 H9

Influence of structural deformations on the applicability of the Tamm-Dancoff approximation for organic molecules — •Tobias Lettmann and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

When calculating excited state properties of electronic systems within the many-body perturbation theory (MBPT), the Bethe-Salpeter equation (BSE) needs to be solved. This is often done within the Tamm-Dancoff approximation (TDA), neglecting the coupling of resonant and anti-resonant excitations.

It is generally accepted that the TDA is justified for large, extended systems e.g. bulk crystals. However it has been shown that the TDA may no longer hold for small organic molecules [1]. In this talk we discuss the applicability of the TDA for molecules of different sizes and show the transition between the two regimes. We then discuss how the applicability is influenced by deformations of the molecules, in particular by the related conjugation length of the π-system.

[1] B. Baumeier et al., J. Chem. Theory Comput. **8**, 997 (2012)

TT 12.2 Mon 15:15 H9

Momentum-Resolved Electron Energy-Loss Spectroscopy in Oxides from Many-Body Perturbation Theory — •Christian Vorwerk[1,2], Caterina Cocchi[1,2], and Claudia Draxl[1,2] — [1]Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]European Theoretical Spectroscopy Facility

Electron energy-loss spectroscopy (EELS) is a powerful tool to investigate the local electronic and structural properties of crystalline materials. The accurate determination of these spectra from first principles requires a reliable description of the electron-hole interaction, screened by the surrounding many-electron system. We perform *ab initio* many-body perturbation theory calculations of EELS through the solution of the Bethe-Salpeter equation (BSE), including the screened non-local interaction between electron and hole. Employing an implementation in the all-electron full-potential package `exciting`, we show results for a wide range of energy loss, from the optical to the hard x-ray region. We study EELS at finite momentum loss $\mathbf{q}$, from small $\mathbf{q}$ close to the dipole limit to large $\mathbf{q}$ well beyond the first Brillouin zone. This momentum resolution of EELS reveals dipole-forbidden excitations that

are invisible in absorption spectroscopy. Our calculations also yield insight into the excitonic dispersion, *i.e.* the excitonic bandstructure. We discuss the effects of momentum loss in the EELS spectra of oxide materials, including CaO, CeO_2, and the wide-gap transparent oxide Ga_2O_3, considering both the optical and x-ray energy-loss range.

TT 12.3 Mon 15:30 H9

Electron-magnon scattering in elementary ferromagnets from first principles: implementation and results — •Christoph Friedrich, Mathias C.T.D. Müller, and Stefan Blügel — Peter Grünberg Institut and Institute of Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Propagating electrons and holes can scatter with spin fluctuations and form quasiparticles as a result or more complex many-body states. To calculate this effect, a **k**-dependent self-energy describing the scattering of electrons and magnons is constructed from the solution of a Bethe-Salpeter equation for the T matrix. Partial self-consistency is achieved by the alignment of the chemical potentials. We discuss details of the implementation and illustrative results. The renormalized electronic band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy, which are strongest in Fe. The renormalization gives rise to a band anomaly at large binding energies in iron, which results from a coupling of the quasihole with Stoner excitations.

TT 12.4 Mon 15:45 H9

Dielectric function of homogeneous electron gas from Bethe-Salpeter equation — •Jaakko Koskelo[1,2], Martin Panholzer[2,3], Lucia Reining[1,2], and Matteo Gatti[1,2,4] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, F-91128 Palaiseau, France — [2]ETSF — [3]Institute for Theoretical Physics, Johannes Kepler University, Linz, Austria — [4]Synchrotron SOLEIL, France

The homogeneous electron gas (HEG) is one of the most important model systems in condensed matter physics, and it has been subject of a great number of studies. Some properties of HEG such as total energy and static correlation functions can be obtained from quantum Monte Carlo simulations with great accuracy, but for dynamical correlation functions only very few results are available.

Methods based on the Bethe-Salpeter equation (BSE) have been very succesful in semiconductors and insulators, but metals have been less studied. In this contribution, we use the BSE in its standard approximations, including a statically screened electron-hole interaction, to study the dielectric function of HEG. We find significant differences in static screening and spectra compared to other approaches. In particular, the BSE in its current approximations fails to reproduce the negative static screening in the low-density HEG, which is related to a so-called ghost exciton. We also use the time-dependent mean-density approximation [1] in order to compare our results to experimental loss spectra of sodium.

[1] M. Panholzer et al, Phys. Rev. Lett. **120**, 166402 (2018).

TT 12.5 Mon 16:00 H9

DFT study of electronic and optical properties of $SrTiO_{3-\delta}$ including many-body effects — •Vijaya Begum, Markus E Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg.

The electronic and optical properties of $SrTiO_3$ (STO), a perovskite material of key importance in the field of oxide electronics, are explored in the framework of density functional theory including many-body effects within the GW approximation and excitonic corrections by solving the Bethe-Salpeter equation (BSE). We further analyse the origin of the strong excitonic effects, in particular a peak at ≈6.5 eV, by decomposing the BSE eigenvectors obtained from GW+BSE to extract the leading electron-hole pair contribution for the particular BSE eigenstate following the approach of Bokdam *et al.* [Scientific Reports 6, 28618 (2016)]. Alternatively, we use the model-BSE (mBSE) which utilises a parametrised analytical model for the static screening. For STO, the mBSE spectrum closely reproduces the one from GW+BSE, which allows to reduce the computational effort by circumventing the intermediate time-consuming GW step. We further proceed to describe the effect of oxygen defects on the electronic and optical properties in STO.

Funding by DFG- SFB1242, project C02 is gratefully acknowledged.

TT 12.6 Mon 16:15 H9

Second-order Møller-Plesset perturbation theory and beyond for the band gap and single-particle excitations of solids — •Maria Dragoumi[1], Sergey V. Levchenko[2,1,3], Igor Ying Zhang[4,1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DE — [2]Skolkovo Innovation Center, Moscow, RU — [3]NUST MISIS, Moscow, RU — [4]Fudan University, Shanghai, CN

Calculations of the fundamental band-gap and the low-energy excitations of solids are still a challenge for electronic-structure theory. The computationally efficient Kohn-Sham (KS) density functional theory (DFT) with the widely used local or semi-local approximations provides a KS band gap which is much smaller than the fundamental gap. Many-body perturbation theory, on the other hand, addresses the fundamental gap directly. We present here an efficient scalable implementation of Møller-Plesset second order perturbation theory (MP2) for quasi-particle energies [1,2]. By solving the Dyson equation of the single-particle Green's function, considering self-energy up to second order, we go beyond MP2. The new approach shows a competitive or even superior performance in comparison to the current state-of-the-art methods such as hybrid functionals and GW approximation, where second order exchange is missing. We present numerical results for the band-gap of a wide range of semiconductors and insulators.

[1] J. Sun and R. J. Bartlett, J. Chem. Phys. 104, 8553 (1996).
[2] A. Grüneis, et.al, J. Chem. Phys. 133, 074107 (2010).

TT 12.7 Mon 16:30 H9

Accelerating *GW* Calculations within the LAPW Framework — •Sven Lubeck, Andris Gulans, and Claudia Draxl — Humboldt-Universität zu Berlin, Germany

The GW approach of many-body perturbation theory is an indispensable method for calculating the electronic band structure of solids. Its implementation in computer programs using the linearized augmented plane-wave + local orbital (LAPW+LO) method allows for obtaining numerically precise results. Unfortunately, high precision comes at the price of a large number of LAPWs and LOs. In this work, we accelerate GW calculations by optimizing the use of LAPWs and LOs in the computer package `exciting` [1]. On the one hand, we introduce a systematic way of obtaining a minimal set of LOs. On the other hand, we perform a basis transformation from the plane-wave part of the LAPWs to different types of basis functions, exploring the efficiency of numeric atom-centered orbitals, Gaussian type orbitals, and Kohn-Sham orbitals. Presenting band gaps of two exemplary materials, zincblende ZnO and hexagonal monolayer BN, we illustrate that our optimization schemes reduce the computational cost down to values as low as 15% without compromising the precision.

[1] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, and C. Draxl, J. Phys.: Condens. Matter **26**, 363202 (2014).

TT 12.8 Mon 16:45 H9

Ab-initio description of transient ion formation of NO on Au(111) — Daniel Corken, Nicholas D. M. Hine, and •Reinhard J. Maurer — Departments of Physics and Chemistry, University of Warwick, United Kingdom

Gaining a fundamental understanding of the interactions of molecules on metal surfaces is essential for the development of novel heterogeneous catalysts. An interesting feature of gas-surface reactions at metal surfaces is that the Born-Oppenheimer approximation breaks down. Vibrationally excited and translationally hot molecules can transfer energy to the electrons of a metal via excitation of electron-hole pairs (EHP). In case of NO on Au(111), [1] this nonadiabatic energy loss is believed to stem from the transient generation of charged ion species at the surface. A computationally feasible and accurate description of such a molecule-metal charge-transfer state represents a challenge and several methods have been proposed. Upon a review of existing experimental evidence, we will present our approach to this problem. We use linear expansion-Delta-Self-Consistent-Field Density Functional Theory (leΔSCF-DFT) [2] to model the anionic resonance of NO on Au(111). The leΔSCF-DFT method enforces the electronic configuration of reference molecular states while solving the Kohn-Sham equations self-consistently. By comparison to experiment and other models, we asses the methods' ability to describe the ground- and excited-states during molecular scattering. We further explore avenues to extract nonadiabatic couplings and to construct model Hamiltonians based on this method. [1] JCP 130, 174716, [2] JCP 139, 014708;

TT 12.9 Mon 17:00 H9

Luminescence of β-SiAlON:Eu^{2+} phosphors: DFT study — •Saleem Ayaz Khan[1], Ondrej Sipr[1], Robin Niklaus[2], Wolfgang Schnick[2], and Jan Minar[1] — [1]University of West Bohemia, Pilsen, Czech Republic — [2]LMU Munich, Germany

Highly efficient phosphor-converted light-emitting diodes (pc-LEDs)are popular in lighting and high-tech electronics applications[1]. Among them β-SiAlON:Eu^{2+} stands out as a promising narrow-band green phosphor for white-LEDs applications exhibiting good thermal and chemical stabilities. Photoluminescent properties of this material can be tuned by introducing the disorder at various sublattices. To understand the mechanism behind this effect, we performed a systematic study of electronic structure and photoluminescence properties of β-SiAlON:Eu^{2+}. The calculations were done within the *ab-initio* fully relativistic full-potential framework. The disorder was treated by employing both the supercell approach and the coherent potential approximation (CPA). The Stokes shifts were calculated from differences of total energies of the ground and excited states of β-SiAlON:Eu^{2+}. The main focus is on monitoring how the Al and O content and Eu^{2+} activator concentrations influence the local β-Si3N4 electronic structure and how this may be used to tune photoluminescence properties.

[1] Z. Wang, W. Ye, Iek-H. Chu, and S. P. Ong, Chem. Mater., **28**, 8622 (2016).

TT 12.10 Mon 17:15 H9

Spin fluctuations in itinerant ferromagnets: Computing the dynamic transverse spin susceptibility with TDDFT and PAW — •Thorbjørn Skovhus and Thomas Olsen — Technical University of Denmark

We present a numerical scheme for computing the dynamic transverse spin susceptibility using time-dependent density functional theory which allows us to study magnons in itinerant ferromagnets. The scheme is based on a real-space grid implementation of the projected augmented wave method and use a simple plane wave representation of the response function. Employing the adiabatic local density approximation for the exchange-correlation kernel, calculations of the magnon spectra in bulk transition metals iron and nickel are presented. In the context of the present implementation, the influence from the choice of numerical scheme on the violation of the Goldstone theorem is investigated.

TT 13: Frustrated Magnets - Spin Liquids (joint session TT/MA)

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

TT 13.1 Mon 15:00 Theater

Designer spin liquids — •Nic Shannon[1,2], Han Yan[2], Owen Benton[3], and Ludovic Jaubert[4] — [1]TUM, Garching, Germany — [2]OIST, Okianwa, Japan — [3]RIKEN, Wakoshi, Japan — [4]Universite Bordeaux, Bordeaux, France

The pyrochlore lattice has proved a rich source of spin liquids, both in theory, and in the experiment. The best known examples are "spin ices" such as $Dy_2Ti_2O_7$, which offer a concrete realisation of a U(1) lattice gauge theory, complete with magnetic monopole excitations. However many other spin liquid-materials are known, with many different types of phenomenology, motivating the question "what else is out there ?"

In this talk we show how a variety of different spin liquids on the pyrochlore lattice can be generated systematically, by exploiting the degeneracies which arise where different forms of order meet. As examples we present the tensor spin liquid found in models of pyrochlores with anisotropic exchange interactions [1]; the nematic spin liquid found in frustrated quantum spin ice [2,3]; and a rank-2 U(1) spin liquid found by perturbing a simple Heisenberg antiferromagnet [4]. In all cases, the predictions of the relevant gauge theory are compared with the results of Monte Carlo simulation. The relevance of these results to experiments on pyrochlore magnets, including $Tb_2Ti_2O_7$, is also discussed.

[1] O. Benton *et al.*, Nat. Commun. **7**, 11572 (2016)
[2] M. Taillefumier *et al.*, Phys. Rev. X **7**, 041057 (2017)
[3] O. Benton *et al.*, Phys. Rev. Lett. **121**, 067201 (2018)
[4] H. Yan *et al.*, preprint.

TT 13.2 Mon 15:15 Theater

MIEZE spectroscopy of spin dynamics and crystal field excitations in $Tb_2Ti_2O_7$ — •Andreas Wendl[1], Steffen Säubert[1,2], Christian Franz[2], Olaf Soltwedel[1,4], Johanna Jochum[2,5], Prabhakaran Dharmalingam[3], Andrew Boothroyd[3], and Christian Pfleiderer[1] — [1]Technische Universität München, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [3]Clarendon Laboratory, University of Oxford, United Kingdom — [4]Technische Universität Darmstadt, Darmstadt, Germany — [5]Bayerisches Geoinstitut, Bayreuth, Germany

The nature of the spin liquid ground state in the cubic rare earth pyrochlore oxide $Tb_2Ti_2O_7$ has been attracting great interest for many years, where recent studies suggest a prominent role of magneto-elastic crystal field - phonon interactions [1,2]. We present measurements of the spin dynamics of $Tb_2Ti_2O_7$ by means of the Modulation of IntEnsity by Zero Effort technique (MIEZE) [3], representing an implementation of high-resolution neutron spin echo suitable for depolarizing sample conditions. Our data of the intermediate scattering function cover time-scales of over seven orders of magnitude between 1 fs and 1 ns, corresponding to an energy spectrum from the meV to neV regime. We find strong paramagnetic fluctuations as well as crystal field transitions at elevated temperatures, shedding new light on the low-lying spin dynamics.

[1] Constable et al., Phys. Rev. B, 95, 020415(R) (2017)
[2] Fennell et al. Phys. Rev. Lett., 112, 017203 (2014)
[3] Franz and Schröder, J. Large-Scale Res. Facil. JLSRF 1, 14 (2015)

TT 13.3 Mon 15:30 Theater

Magnetisation Avalanches in Classical Spin Ice $Dy_2Ti_2O_7$ — •M. Kleinhans[1], C. Duvinage[1], D. Prabhakaran[2], A. T. Boothroyd[2], and C. Pfleiderer[1] — [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 [1]. We report vibrating coil magnetometry down to mK temperatures [2,3] of $Dy_2Ti_2O_7$, addressing the evidence of putative magnetisation avalanches in the spin-frozen state which depend sensitively in number and size on the magnetic field ramp rate, sample shape and quality. These avalanches have been interpreted in terms of magnetic monopole dynamics [4].

[1] Castelnovo *et al.*, Nature **451**, 7174 (2008)
[2] Krey *et al.*, PRL **108**, 257204 (2012)
[3] Legl *et al.*, PRL **109**, 047201 (2012)
[4] Slobinsky *et al.*, PRL **105**, 267205 (2010)

TT 13.4 Mon 15:45 Theater

Magnetization beyond the Ising limit of $Ho_2Ti_2O_7$ — •L. Opherden[1], T. Herrmannsdörfer[1], M. Uhlarz[1], D. I. Gorbunov[1], A. Miyata[2], O. Portugall[2], I. Ishii[3], T. Suzuki[3], and J. Wosnitza[1,4] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Laboratoire National des Champs Magnetiques Intenses (LNCMI-EMFL), Toulouse, France — [3]Department of Quantum Matter, AdSM, Hiroshima University, Japan — [4]Institut für Festkörper- und Materialphysik, TU Dresden, Germany

We report that the local Ising anisotropy in pyrochlore oxides – the crucial requirement for realizing the spin-ice state – can be broken by means of high magnetic fields. For the case of the well-established classical spin-ice compound $Ho_2Ti_2O_7$ the magnetization exceeds the angle-dependent saturation value of the Ising limit using ultra-high fields up to 120 T. However, even under such extreme magnetic fields full saturation cannot be achieved. Crystal-electric-field calculations can account for the measured magnetization dependence and reveal that a level crossing for two of the four ion positions leads to magnetization steps at 55 and 100 T. In addition, we show that by using a field-sweep rate in the range of the spin-relaxation time, the dynamics of the spin system can be probed. Exclusively at 25 ns/T a novel peak of the susceptibility appears around 2 T. We argue, this signals the

cross-over between spin-ice and polarized correlations.

TT 13.5 Mon 16:00 Theater

The Quantum Life of Worms: Quantum Spin Ice in a [100] Magnetic Field — •Olga Sikora[1], Karlo Penc[2], Frank Pollmann[3], Ying-Jer Kao[4], and Nic Shannon[5] — [1]Institute of Nuclear Physics, Polish Academy of Sciences, ul. Radzikowskiego 152, PL-31342 Kraków, Poland — [2]Wigner Research Centre for Physics, H-1525 Budapest, POB 49, Hungary — [3]Physics Department, Technical University Munich, 85748 Garching, Germany — [4]Department of Physics, National Taiwan University, Taipei 10617, Taiwan — [5]Okinawa Institute for Science and Technology Graduate University, Onna, Okinawa, 904-0495 Japan

Quantum spin ice in a magnetic field exhibits rich physics, with many open questions about possible ordered and spin–liquid states. Here we consider the case of strong [100] magnetic field, and study excitations about the maximally–polarized spin–ice state, within a model with short–range interactions. In this approach a single string of flipped spins — a "worm" — can be mapped onto an S = 1/2 XXZ chain. This mapping provides a complete understanding of a single string, exhibiting different properties in the gapped (confined) and gapless (extended) phase of the XXZ model. We further investigate the interaction between strings, using both an effective model, and large–scale variational and Green's function Monte Carlo methods previously applied to quantum spin ice in zero field [1].

[1] N. Shannon, O. Sikora, F. Pollmann, K. Penc and P. Fulde, Phys. Rev. Lett. **108**, 067204 (2012).

TT 13.6 Mon 16:15 Theater

Investigation of the Thermodynamic Properties of Insulating Pr-based Pyrochlores — •J. Gronemann[1,2], T. Gottschall[1], E.L. Green[1], H.D. Zhou[3], A. Islam[4], B. Lake[4,5], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Univ. of Tennessee, Knoxville, USA — [4]Helmholtz-Zentrum Berlin, Germany — [5]Institut für Festkörperphysik, TU Berlin, Germany

Geometrically frustrated pyrochlores exhibit novel properties at low temperatures and are well-known spin-liquid candidates. In the insulating compounds $Pr_2Sn_2O_7$ and $Pr_2Hf_2O_7$ the orientation of the spins of the Pr^{3+} ions on corner-sharing tetrahedrons show dynamics beyond the spin-ice state [1]. Due to the small magnetic moment of the Pr^{3+} ion, generating only a small dipolar interaction, transverse fluctuations may have a significant influence. The spin dynamics in these materials remains unfrozen to lowest temperatures and the possibility of quantum fluctuations makes them quantum spin-liquid candidates [2], which are expected to host a variety of emergent electrodynamic phenomena in analogy to magnetic monopoles in spin-ice. To probe the nature of the low-temperature ground state and the changes in the entropy, specific heat was measured down to 450 mK and up to 13 T.

[1] H. D. Zhou. et al., Phys. Rev. Lett. **101**, 227204 (2008)
[2] R. Sibille et al., Phys. Rev. B **94**, 024436 (2016)

TT 13.7 Mon 16:30 Theater

Giant magneto-elastic effect in d^2 pyrochlores and the formation of a spin-lattice liquid — •Andrew Smerald[1] and George Jackeli[1,2] — [1]Max Planck Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart — [2]Insitute for Functional Matter and Quantum Technologies, University of Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart

We discuss the idea of a giant magneto-elastic effect in frustrated magnets, and suggest that this may provide a good way to understand d^2 pyrochlore systems such as $Y_2Mo_2O_7$. We define magneto-elastic coupling as "giant" when it selects low-temperature spin configurations that are completely unexpected from the point of view of a pure spin model. This can be contrasted with the more usual case in which magneto-elastic coupling selects one or more of the otherwise extensively degenerate ground states of a frustrated magnet. In the case of $Y_2Mo_2O_7$ we propose that this mechanism results in a classical spin-lattice liquid at intermediate temperatures, in which spin and lattice degrees of freedom are intimately coupled together.

15 min. break.

TT 13.8 Mon 17:00 Theater

Intermultiplet transitions and long-range order in Sm-based pyrochlores — •Viviane Peçanha-Antonio[1], Erxi Feng[1], Devashibhai Adroja[2], Fabio Orlandi[2], Xiao Sun[3], Yixi Su[1], and Thomas Brückel[3] — [1]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching, Germany — [2]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, United Kingdom — [3]Jülich Centre for Neutron Science (JCNS) and Peter Grünberg Institut (PGI), Forschungszentrum Jülich GmbH, Jülich, Germany

We present bulk and neutron scattering measurements performed on the isotopically enriched $^{154}Sm_2Ti_2O_7$ and $^{154}Sm_2Sn_2O_7$ samples. Both compounds display sharp heat capacity anomalies, at 350 mK and 440 mK, respectively. Inelastic neutron scattering measurements are employed to solve the crystalline electric field (CEF) excitations scheme, which includes transitions between the ground and first excited J multiplets of the Sm^{3+} ion. To further validate those results, the single-ion magnetic susceptibility of the compounds is calculated and compared with the experimental dc-susceptibility measured in low applied magnetic fields. It is demonstrated that the inclusion of inter-multiplet transitions in the CEF analysis is fundamental to the understanding of the intermediate and, more importantly, low temperature magnetic behaviour of the Sm-based pyrochlores. Finally, the heat capacity anomaly is shown to correspond to the onset of an all-in-all-out long-range order in the stannate sample, while in the titanate a dipolar long-range order can be only indirectly inferred.

TT 13.9 Mon 17:15 Theater

Field-induced magnetic transitions in the Yb- based $J_{\text{eff}} = \frac{1}{2}$ triangular lattice antiferromagnet $NaYbO_2$ — •Kizhake Malayil Ranjith Kumar[1], Daryna Dmytriieva[2], Seunghyun Khim[1], Jörg Sichelschmidt[1], Hiroshi Yasuoka[1], Hannes Kühne[2], and Michael Baenitz[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, D-01314 Dresden, Germany

Spin-$\frac{1}{2}$ triangular lattice antiferromagnets (TLAF) are one of the active fields of research in condensed matter physics. The Yb^{3+}- based delafossite $NaYbO_2$ provides an ideal $J_{\text{eff}} = \frac{1}{2}$ triangular lattice motif with spin-orbit entanglement. We have synthesized the phase pure polycrystalline $NaYbO_2$ material and investigated the ground state properties. At zero field, $NaYbO_2$ exhibits no sign of magnetic long-range order down to 0.35 K, which proposes a spin liquid like ground state with strong persisting quantum fluctuations. In external magnetic fields above 2 T, it yields field-induced ordered phases. We investigated the magnetic properties in detail by magnetization, specific heat, nuclear magnetic resonance (NMR), and electron spin resonance (ESR) experiments down to 0.35 K. The results are discussed within the extended XXZ model for bond-dependent exchange interactions on planar triangles.

TT 13.10 Mon 17:30 Theater

Spin orbit entangled planar $J = 1/2$ triangular lattice magnet $NaYbS_2$: from a putative spin liquid to field induced magnetic order — •M. Baenitz[1], K.M. Ranjith[1], Ph. Schlender[2], J. Sichelschmidt[1], B. Schmidt[1], H. Yasuoka[1], A.P. Mackenzie[1], and Th. Doert[2] — [1]MPI for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]TU Dresden, Department of Chemistry and Food Chemistry, D-01062 Dresden, Germany

Spin orbit coupling (SOC) brought significant progress to the field of quantum spin liquids (QSLs). Having strong spin orbit entanglement promote Yb-based magnets to ideal prime candidates for QSLs and as such $NaYbS_2$ is a unique model system for planar spin 1/2 triangular lattice magnetism (TLM). In contrast to $YbMgGaO_4$ [1], which shares the same space group (R-3m) and highlighted as first SOC-TLM-QSL, $NaYbS_2$lacks inherent lattice distortions and Yb resides on a unique centrosymmetric position in the YbS_6 octahedron. Our comprehensive single crystal study combines bulk- and local- probes and identifies $NaYbS_2$ as a new spin orbit entangled TLM and putative QSL hosted on a perfect triangular lattice [2]. The application of fields along the (a,b)-plane introduces magnetic order, whereas for fields in the c-direction the system remains unaffected. We present magnetization, specific heat and NMR data down to 300 mK for both directions.

[1] J.A.M. Paddison et al., Nat. Phys. 13, 112 (2017)
[2] M. Baenitz et al.c arXiv:1809.01947 (2018)

TT 13.11 Mon 17:45 Theater

Frustrated Ising magnetism of $TmMgGaO_4$ — Yuesheng Li,

•Alexander A. Tsirlin, and Philipp Gegenwart — EP VI, EKM, University of Augsburg, Germany

Motivated by the interesting spin-liquid physics of the triangular antiferromagnet $YbMgGaO_4$, we studied its Tm-based analog. Unlike Yb^{3+}, Tm^{3+} is a non-Kramers ion that would normally feature nonmagnetic singlet as the crystal-field ground state. However, random crystal electric field (CEF) caused by the random distribution of Mg and Ga in the structure mixes two lowest-lying CEF singlets into a quasidoublet that gives rise to Ising-like pseudospins with $g_{\parallel} \simeq 13.2$ and $g_{\perp} \simeq 0$. Low-temperature thermodynamic measurements indicate three field-induced phase transitions that can be broadly understood within the $J_1^{zz} - J_2^{zz}$ Ising model on the triangular lattice, albeit with a distribution of the critical fields and underlying exchange couplings. Interestingly, only one ordered state, the $\frac{1}{3}$-plateau below 2.5 T, shows long-range order confirmed by neutron diffraction, whereas other ordered states expected in the $J_1^{zz} - J_2^{zz}$ triangular Ising antiferromagnet seem to be only short-range in nature. Moreover, no zero-point entropy is observed.

TT 13.12 Mon 18:00 Theater

Low-energy spin excitations in the triangular-lattice quantum spin liquid candidate $YbMgGaO_4$ — •Yuesheng Li, Alexander Tsirlin, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany

$YbMgGaO_4$ was first proposed as a perfect triangular-lattice rare-earth quantum spin liquid (QSL) candidate in 2015. After that, several scenarios, such as the spin-liquid mimicry, valence bond (VB) glass, and spin-glass, were reported in the presence of the site-mixing disorder between nonmagnetic Mg^{2+} and Ga^{3+}. Here, we critically test these scenarios by probing the low-energy spin excitations of $YbMgGaO_4$ based on the low-T magnetization and triple-axis inelastic neutron scattering (INS) experiments. Our magnetization data measured down to 40 mK speak against any conventional freezing and reinstate YbMgGaO4 as a QSL candidate. The low-energy ($E \leq J_0 \sim 0.2$ meV) part of the INS continuum presents at low temperatures, but *completely* disappears upon warming the system above $T \gg J_0/k_B$. In contrast to the high-energy part at $E > J_0$ that is rooted in the breaking of nearest-neighbor VBs and persists to temperatures well above J_0/k_B, the low-energy one originates from the rearrangement of the valence bonds and thus from the propagation of unpaired spins. We further extend this picture to herbertsmithite, the QSL candidate on the kagome lattice, and argue that such a hierarchy of magnetic excitations may be a universal feature of QSLs.

TT 13.13 Mon 18:15 Theater

Randomness in the quantum spin liquid candidate κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ investigated by artificial distortion of the triangular lattice — •Yohei Saito[1], Andrej Pustogow[1], Roland Rösslhuber[1], Miriam Alonso[1], Maxim Wenzel[1], Anja Löhle[1], Martin Dressel[1], Takaaki Minamidate[2], Noriaki Matsunaga[2], Kazushige Nomura[2], and Atsushi Kawamoto[2] — [1]1. Physikalisches Inst., Universität Stuttgart, Germany — [2]Department of Physics, Hokkaido University, Sappro, Japan

The organic-molecular solid κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ is recognized as a quantum spin liquid candidate as it does not show magnetic ordering regardless of the large magnetic interactions. There is a debate about the importance of spin frustration on the triangular lattice and inherent randomness in the crystals. Does a suppression of geometrical frustration change the magnetic properties? To clarify that, we artificially distorted triangular lattices of κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ by donor molecular substitution that modifies exchange interactions. As a result, geometrical frustration is suppressed locally. We performed electric conductivity, dielectric spectroscopy, infrared spectroscopy, and 13C NMR measurements. Comparing results of non-substituted and substituted samples, we found that their magnetic fluctuation was the same as opposed to the remarkable impurity substitution effect of the conductivity. Thus, the electronic state of the $(CN)_3$ salt is already disordered even in the non-substituted sample, and that not only the ideal geometrical frustration but also the disorder effect should be considered.

TT 13.14 Mon 18:30 Theater

Thermal expansion studies on the spin-liquid candidate system κ-$(BEDT\text{-}TTF)_2Ag_2(CN)_3$ — •S. Hartmann[1], E. Gati[2], Y. Yoshida[3], G. Saito[4], and M. Lang[1] — [1]Physikalisches Institut, SFB/TR 49, Goethe-Uni Frankfurt, Germany — [2]Ames Laboratory, Iowa State University, USA — [3]Division of Chemistry, Kyoto University, Japan — [4]Toyota Physical and Chemical Research Institute, Nagakute, Japan

The search for the realization of a quantum spin-liquid (QSL) is a major concern for condensed matter physicists since its proposal in 1973. The entangled QSL state lacks magnetic ordering down to lowest temperatures where spins continue to fluctuate even at $T = 0$ K [1]. One way to experimentally realize a QSL is magnetic frustration of geometric origin, inherent to the quasi-2D triangular lattice of the organic charge-transfer salts κ-$(BEDT\text{-}TTF)_2X$, known as weak Mott insulators. We present results of ultra-high-resolution thermal expansion measurements on the newly-synthesized QSL-candidate system $X = Ag_2(CN)_3$. Our main finding includes pronounced broad extrema in the thermal expansion coefficient at $T \sim 18$ K along all three crystallographic directions which we assign to the effect of strong electronic correlations. The observed anomalies are qualitatively consistent with theoretical results based on the Hubbard model on a triangular lattice [2]. The directional anisotropy of the anomalies implies a ratio of the hopping integrals $t'/t < 1$.

[1] Balents, Nature 2010
[2] Kokalj, McKenzie, PRB 2015

TT 14: Graphene

Time: Monday 15:00–19:00 Location: H22

TT 14.1 Mon 15:00 H22

The non-local hydrodynamic transport properties of graphene — •Egor Kiselev[1] and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Within a kinetic theory approach, we calculate the non-local transport properties of graphene in the hydrodynamic regime, in the limit of a small graphene fine structure constant. We find an exact solution to the kinetic equation and derive exact expressions for the non-local (i. e. finite momentum and frequency) conductivity and viscosity. Possible applications of our findings to the study of relaxation phenomena will be discussed.

TT 14.2 Mon 15:15 H22

Spin and Charge Transport in Doped Graphene — •Marie-Luise Braatz[1,2], Axel Binder[3], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz (MAINZ), 55128 Mainz, Germany — [3]BASF SE, 67056 Ludwigshafen, Germany

Graphene in its pristine form is already a remarkable material, however it has certain shortcomings in its pure form, such as no sizeable bandgap. Materials modifications allow one to better tailor its properties to specific needs such as engineering the charge carrier density or the bandgap, which is often required for electronic applications. We use chemical doping to gradually modify the graphene lattice, which has been shown to have an effect on the electronic structure [1]. Heteroatom substitution with nitrogen leads to changes in the structure as well as the electronic and magnetotransport properties. The amount of dopants is systematically varied so different dopant concentrations can be compared. The samples are then analyzed by Raman and electron microscopy to elucidate the changes in structure. Measuring the magnetoresistance at various temperatures and fields allows us to correlate the structure to the charge transport properties [2].

[1] H. Wang et al., ACS Catal. 2, 781 (2012)
[2] M. Rein et al., ACS Nano 9, 1360 (2015)

TT 14.3 Mon 15:30 H22

Transport through time dependent magnetic barriers in

graphene — •Nico Leumer[1] and Wolfgang Häusler[2] — [1]Fakultät für Physik, Universität Regensburg — [2]Fakultät für Physik, Universität Augsburg

Studies of tunneling through time dependent scalar potential barriers have a long history, starting with the seminal work by Büttiker and Landauer [1]. Since in graphene electrostatic barriers are inefficient to guide carriers, due to Klein tunneling, we study here, to our knowledge for the first time, *time dependent magnetic barriers*. We discuss the difficulty of induced electric fields. Contrary to the scalar case, the problem now becomes inherently 2-dimensional. While more involved, we employ a strategy in the spirit of [1] by using a suitable gauge. For periodic time dependence, we find analytically the transmission through side bands. Depending on parameters, however, side bands may entirely close.

[1] M. Büttiker and R. Landauer, Phys. Rev. Lett. 49, 1739 (1982)

TT 14.4 Mon 15:45 H22

Spin-orbit coupled graphene *pn*-junction in a magnetic field — •D. Bercioux[1,2] and A. De Martino[3] — [1]Donostia International Physics Center, Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain — [3]Department of Mathematics, City, University of London, London EC1V 0HB, United Kingdom

We present a theoretical investigation of the spectral and transport properties of a *pn* junction in single-layer graphene in the presence of a uniform perpendicular magnetic field. The spectrum consists of localized bulk Landau-like and unidirectional interface states [1,2]. Specifically, we consider the effects of spin-orbit interactions (SOIs) on the spectrum of the *pn* junction. We show that the Rashba SOI [3] lifts the two-fold degeneracy of the zero mode. This degeneracy lifting takes place only in the transition from *p*- to *n*-region, whereas the modes are still two-fold degenerate in the bulk. We evaluate different observables along the transition region; particularly, we find that the spin density is different for the two zero modes and exhibits an oscillatory behaviour with the period depending on the strength of Rashba SOI. Finally, we discuss also the effects of Coulomb interaction on these chiral edge states in terms of Luttinger liquid theory.

[1] D. A. Abanin & L. S. Levitov, Science **317**, 641 (2007)
[2] L. Cohnitz, A. De Martino, W. Häusler & R. Egger, Phys. Rev. B **94**, 165443 (2016)
[3] D. Bercioux & A. De Martino, Phys. Rev. B **81**, 165410 (2010).

TT 14.5 Mon 16:00 H22

Thermoelectric efficiency in three-terminal graphene nanojunctions — Zahra Sartipi[1], Amir Hayati[2], and •Javad Vahedi[1,3] — [1]Department of Physics, Sari Branch, Islamic Azad University, Sari, Iran — [2]Faculty of Mazandaran Technical and Vocational University, Technical and Vocational University, Iran — [3]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy-Pontoise, France

The thermoelectric efficiency of a thermal machine consisting of a triangular graphene nano-junction connected to three electrodes in the linear response regime is studied. Using the Onsager formalism and a combination of semi-empirical tight-binding calculations as well as Greens function theory, the efficiency at maximum output power which can be written in terms of generalized figures of merit is investigated. The results for a set temperature and chemical potential parameters have shown that adding a third terminal improves the efficiency at maximum output power compared to the two-terminal setup.

TT 14.6 Mon 16:15 H22

Interatomic forces in current-carrying graphene nanojunctions — •Susanne Leitherer, Nick R. Papior, and Mads Brandbyge — Department of Micro- and Nanotechnology, Technical University of Denmark

The interplay between the applied field, current and the atomic structure in ballistic nanoscale conductors carrying a substantial current, as seen in experiments [1,2], is still not well understood. In this contribution, we study the non-equilibrium charge transport through nanojunctions with graphene electrodes, employing first principles electronic structure and transport calculations based on density functional theory combined with non-equilibrium Greens functions (DFT-NEGF) [3]. We calculate the forces on the atoms which are induced by a finite bias voltage. The junctions are gated to increase their conductance and to allow switching between electron and hole-dominated transport [4]. We discuss the role of the potential drop in the junction, and show how the forces can be rationalized in terms of bond-currents, charge redistribution and overlap populations.

[1] C. Schirm, M. Mat, F. Pauly J.C. Cuevas, P. Nielaba and E. Scheer, Nat. Nanotechnol. 8, 645-648 (2013)
[2] H. Sadeghi, J. A. Mol, C. S. Lau, G. A. D. Briggs, J. Warner and C. J. Lambert, PNAS 112, 2658 (2015)
[3] N. Papior, N. Lorente, T. Frederiksen, A. Garcia and M. Brandbyge, Comput. Phys. Commun. 212, 8 (2017)
[4] N. Papior, T. Gunst, D. Stradi and M. Brandbyge, Phys. Chem. Chem. Phys. 18, 1025 (2016)

TT 14.7 Mon 16:30 H22

Current splitter and valley polarizer in elastically deformed graphene — •Nikodem Szpak[1] and Thomas Stegmann[2] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Instituto de Ciencias Fisicas, UNAM, Mexico

Elastic deformations of graphene can significantly change the flow paths and valley polarization of the electric currents. We investigate these phenomena in graphene nanoribbons with localized out-of-plane deformations by means of tight-binding transport calculations. Such deformations can split the current into two beams of almost completely valley polarized electrons and give rise to a valley voltage. These properties are observed for a fairly wide set of experimentally accessible parameters. We propose a valleytronic nanodevice in which a high polarization of the electrons comes along with a high transmission making the device very efficient. In order to gain a better understanding of these effects, we also treat the system in the continuum limit in which the electronic excitations can be described by the Dirac equation coupled to curvature and a pseudo-magnetic field. Semiclassical trajectories offer then an additional insight into the balance of forces acting on the ballistic electrons and provide a convenient tool for predicting the behavior of the current flow paths. The proposed device can also be used for a sensitive measurement of graphene deformations.

[1] T. Stegmann and N. Szpak, New J. Phys. 18 (2016) 053016
[2] T. Stegmann and N. Szpak, 2D Materials (in press, DOI: 10.1088/2053-1583/aaea8d)

15 min. break.

Invited Talk TT 14.8 Mon 17:00 H22

Gate-defined quantum point contacts and quantum dots in bilayer graphene — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich GmbH

Graphene and bilayer graphene (BLG) are attractive platforms for spin qubits, thanks to their weak spin-orbit and hyperfine interaction, promising long spin-coherence times. This has motivated substantial efforts in studying quantum dot (QD) devices based on graphene and BLG. The problem of edge disorder in etched graphene can be completely circumvented in BLG, thanks to a tunable band-gap in the presence of a perpendicularly applied electric field, a feature that allows introducing electrostatic confinement in BLG. However, until very recently, essentially all devices were limited by leakage currents due to shortcomings in opening a clean and homogeneous band gap. A very recent breakthrough in this field has been the introduction of graphite back-gates. Together with the technology of encapsulating BLG in hexagonal boron nitride (hBN), giving rise to high quality hBN-BLG-hBN heterostructures, the use of a graphite back gate allows for a homogeneous and gate tunable band gap in BLG. We will show that this technological improvement allows for an unprecedented quality of quantized conductance measurements and most importantly, allows realizing complete electrostatic current pinch-off. The latter finally offers the possibility of electrostatically confining carriers in BLG and allows implementing quantum dots with a high level of control and low disorder.

TT 14.9 Mon 17:30 H22

Gap opening and quantum transport in a functionalized Bernal graphene bilayer — Ahmed Missaoui[1,3], Jouda J. Khabthani[1], Didier Mayou[2], and •Guy Trambly de Laissardiere[3] — [1]Laboratoire de la Physique de la Matière Condensée, Faculté des Sciences de Tunis, Université de Tunis El Manar, Tunis, Tunisia — [2]Institut Néel, CNRS - Univ. Grenoble Alpes, France — [3]Laboratoire de Physique théorique et Modélisation, CNRS - Univ. de Cergy-Pontoise, France

We describe numerically the electronic properties in Bernal bilayer

graphene in presence of a random distribution of vacant atoms that simulate resonant adsorbates. The values of fundamental quantities such as conductivity, elastic mean free path, localization length are computed. In a Bernal graphene bilayer, carbon atoms belong to two inequivalent sub-lattices A and B of each layer. Therefore, selective functionalizations on only a sub-lattice can significantly change its electronic properties [1]. In particular, we find that for some selective functionalizations, a mobility gap of the order of 0.5 eV is formed near the Dirac energy at concentration of adatoms larger than 1
[1] A. Missaoui et al., J. Phys. : Condens. Matter 30, 195701 (2018).

TT 14.10 Mon 17:45 H22

Valley subband splitting in bilayer graphene quantum point contact — •Rainer Kraft[1], Igor V. Krainov[2], Vanessa Gall[1,3], Alexander P. Dmitriev[2], Ralph Krupke[1,4], Igor V. Gornyi[1,2,3], and Romain Danneau[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany — [2]A.F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia — [3]Institute for Condensed Matter Theory, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany — [4]Department of Materials and Earth Sciences, Technical University Darmstadt, Darmstadt, Germany

Here we present a study of the 1D confinement in a bilayer graphene quantum point contact, i.e. a system with fourfold degeneracy (spin and valley). The constriction is designed electrostatically with dual-gated nanostructures in edge-connected bilayer graphene-hexagonal boron nitride van der Waals heterostructures, employing the possibility of local band gap engineering in bilayer graphene. While quantized conductance due to size-quantization is observed in steps of $4\,e^2/h$ down to the lowest subband, the valley-degeneracy of the 1D subbands is lifted under a perpendicular magnetic field and a peculiar pattern of splitting and merging from two non-adjacent subbands arises.

TT 14.11 Mon 18:00 H22

Anisotropic Andreev reflection in twisted bilayer graphene — •Christophe De Beule[1] and Patrik Recher[1,2] — [1]Institute for Mathematical Physics, TU Braunschweig — [2]Laboratory for Emerging Nanometrology, Braunschweig

We consider Andreev reflection at a normal-superconducting interface in twisted bilayer graphene where superconductivity is introduced via proximity effect, for twist angles in the range where both valley coupling and localization are weak. Due to the anisotropic band structure, the conductance depends strongly on the orientation of the tunneling junction with respect to the twisted bilayer graphene when the Fermi energy is near the Van Hove singularity. This can be understood from the opening of a scattering channel between parts of the Fermi surface that are localized in different layers. Moreover, Andreev (normal) reflection in this interlayer channel can be specular (retroreflective) even at Fermi energies much larger than the superconducting gap.

TT 14.12 Mon 18:15 H22

Charge density wave orders in twisted bilayer graphene — •Markus Klug and Jörg Schmalian — Karlsruher Institut für Technologie, Karlsruhe, Deutschland

The observation of unconventional superconductivity in twisted bilayer graphene (TBG) at small twisting angles attracted great interest in the recent year, though the underlying mechanism remains still unknown. Instead, understanding the nature of the insulating phases neighbouring the superconducting pocket on the electron- and hole-doped side might shed light on the origin of superconductivity in TBG. In this work, we use an effective electron model, which is valid in the small twist-angle / low-temperature regime, to discuss possible candidates of the insulating phase. We present various types of charge order formations with a tendency towards Wigner crystallisation. Our results are supported by numerical simulations based on the unrestricted Hatree-Fock Method.

TT 14.13 Mon 18:30 H22

Tuning anti-Klein to Klein tunneling in bilayer graphene — •Ming-Hao Liu[1], Renjun Du[2], Romain Danneau[2], and Klaus Richter[3] — [1]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany — [3]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

More than a decade ago, monolayer and bilayer graphene pnp junctions were shown to exhibit perfect transmission and perfect reflection upon normal incidence [1], known as Klein tunneling and anti-Klein tunneling, respectively. When the bilayer graphene is gapped by breaking the layer symmetry, however, the anti-Klein tunneling has been recently shown to be broken due to the departure of the Berry phase from 2π toward π [2]. A simple question naturally arose: Is it possible to tune the Berry phase from 2π of a gapless bilayer graphene to π of a largely gapped bilayer graphene, such that the anti-Klein tunneling becomes Klein tunneling? We have given an affirmative answer to this question in our latest work [3], involving both experiment and theory.
[1] M. I. Katsnelson, et al., Nat. Phys. **2**, 620 (2006)
[2] A. Varlet et al., Phys. Rev. Lett. **113**, 116601 (2014)
[3] R. Du et al., Phys. Rev. Lett. **121**, 127706 (2018)

TT 14.14 Mon 18:45 H22

Quantum transport in graphene/hBN Moiré superlattices: A numerical aspect — •Szu-Chao Chen[1], Klaus Richter[2], and Ming-Hao Liu[1] — [1]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [2]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

Transport properties of graphene/hBN Moiré superlattices are studied by performing quantum transport simulations based on the scalable tight-binding model [1], combined with calculations of miniband structures and density of states within the continuum model. Both of the two-terminal conductance simulation and the calculated spectrum of the density of states reveal extra dips corresponding to satellite Dirac points due to the implemented model superlattice potential. Despite the simplicity of the adopted model which takes into account only the scalar potential term, our preliminary results already capture main features of the Moiré superlattice, and therefore shed light on further simulating more complicated transport experiments involving graphene/hBN samples, such as Fabry-Pérot interference [2] and transverse magnetic focusing [3] in the presence of Moiré superlattice potential.
[1] M.-H. Liu et al., Phys. Rev. Lett. 114, 036601 (2015)
[2] C. Handschin et al., Nano Lett. 17(1), 328-333 (2017)
[3] M. Lee et al., Science 353(6307), 1526-1529 (2016)

TT 15: Superconductivity: Fe-based Superconductors - Other Materials and Theory

Time: Monday 15:00–19:00 Location: H23

TT 15.1 Mon 15:00 H23

Specific heat of $RbEuFe_4As_4$ - a magnetic superconductor — •Kristin Willa[1,2], Matthew Smiley[2], Roland Willa[2,3], Alex Koshelev[2], Jin-Ke Bao[2], Mercoury Kanatzidis[2], Ulrich Welp[2], and Wai-Kwong Kwok[2] — [1]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Germany — [2]Materials Science Division, Argonne National Laboratory, USA — [3]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, Germany

We report detailed nanocalorimetric measurements on the newly discovered magnetic superconductor $RbEuFe_4As_4$. We investigated the superconducting transition at T_c=37K and extracted the phase boundary for in and out of plane magnetic fields obtaining an anisotropy ratio of 1.8. Large superconducting fluctuations are observed as well as a vortex lattice melting transition identified as a step of 4-5% of the zero field jump in specific heat. The melting line is considerably below the upper-critical-field line which is in quantitative agreement with theoretical predictions. In small fields near the magnetic transition T_m = 14.9K, we resolved a cusp-like behavior of the specific heat curve that shifts to lower temperatures for fields along the *c*-axis and a broad shoulder that shifts to higher temperatures for in-plane fields. We can reproduce our measured calorimetry data quantitatively by Monte-Carlo simulations of an anisotropic easy-plane 2D Heisenberg model that suggests that the cusp in specific heat is due to a BKT transition and the high temperature hump at higher fields marks a crossover from a paramagnetically disordered to an ordered state.

TT 15.2 Mon 15:15 H23

Magnetic order and superconductivity in $RbEuFe_4As_4$ — •Noah Winterhalter-Stocker[1], Stefan Gorol[1], Stevan Arsenijevic[2], Yurii Skourski[2], Hans-Albrecht Krug von Nidda[3], Mamoun Hemmida[3], Anton Jesche[1], Veronika Fritsch[1], and Philipp Gegenwart[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

$RbEuFe_4As_4$ is an ordered member of the class of iron based superconductors with a structure similar to half doped 122 iron based superconductors like $Ca_{0.5}Na_{0.5}Fe_2As_2$. In contrast to the latter $RbEuFe_4As_4$ shows a superstructure with distinct Eu and Rb positions. The material shows a superconducting transition at T_c=36.8 K and an onset of magnetic order of the paramagnetic Eu 4f moments at T_m=15 K [1]. This leads to a unique interplay between magnetic order and superconductivity which we study by magnetization, magnetotransport and ESR measurements. Our analysis reveals the temperature dependence of the lower and upper critical fields which we compare to appropriate theoretical models.

[1] M. P. Smylie *et al.*, Phys. Rev. B **98**, 104503 (2018)

TT 15.3 Mon 15:30 H23

Disentangling magnetism and superconductivity in LaOFeAs: A NQR study — •Piotr Lepucki[1], Igor Morozov[1,2], Ilya Silkin[2], Rhea Kappenberger[1], Sabine Wurmehl[1], Saicharan Aswartham[1], Markus Witschel[1], Bernd Büchner[1], and Hans-Joachim Grafe[1] — [1]IFW Dresden, Helmholtzstraße 20, 01069 Dresden — [2]Moscow State University, Moscow, Russia

The nature of the coexistence of magnetism and superconductivity in iron-based superconductors is still not well understood. The main discussion is whether there is a microscopic phase coexistence or phase separation (e.g. [1, 2]). We performed 75As nuclear quadrupole resonance (NQR) measurements on P- and Co-doped LaOFeAs powders in search of different behavior in magnetic and superconducting samples, and compare our results to F doped samples [3]. Our measurements show that independent of the dopant (isovalent P doping, in plane Co doping, or out of plane F doping), the electronic structure is changed only locally, leading to regions with different charge environments of the As, and therefore well separated NQR peaks. The relative weight of these regions is equal to the relative spectral weight of the corresponding NQR peaks and is a measure of the doping level [3]. Below the magnetic or superconducting transitions, these NQR peaks change differently, indicating that those regions which are largely unaffected by the doping are driving the magnetism, whereas the doped regions harbor superconductivity. These results suggest a microscopic phase separation in LaOFeAs irrespective of the dopant type.

[1] PRB 97, 224508
[2] PRB 80, 024508
[3] PRB 94, 014514

TT 15.4 Mon 15:45 H23

Tracking nematic fluctuations using the Nernst effect in Co-doped LaFeAsO — •Christoph Wuttke[1], Federico Caglieris[1], Steffen Sykora[1], Frank Steckel[1], Xiaochen Hong[1], Seunghyun Kim[1], Rhea Kappenberger[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Sheng Ran[2], Paul C. Canfield[2], Bernd Büchner[1,3,4], and Christian Hess[1,4] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — [3]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [4]Center for Transport and Devices, Technische Universität Dresden, 01069 Dresden, Germany

We use the Nernst coefficient to track the nematic fluctuations through the Co-doped phase diagram of LaFeAsO. Similarly to our previous measurements in an 122-iron based superconductor system, we obtain a significant enhancement of the signal in the nematic fluctuation regime. The doping dependence of the Nernst coefficient exhibits a non-monotonic behavior featuring a local maximum in the vicinity of optimal doping. This peculiar doping dependence is also in agreement with our theoretical prediction and hence demonstrates the universality of the sensitivity of the Nernst effect on nematic fluctuations in iron based superconductors.

TT 15.5 Mon 16:00 H23

Strain-derivative of thermoelectric coefficients: a sensitive probe for nematic fluctuations — •Federico Caglieris[1], Christoph Wuttke[1], Xiaochen Hong[1], Steffen Sykora[1], Rhea Kappenberger[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Bernd Büchner[1,2,3], and Christian Hess[1,2] — [1]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, 01069 Dresden — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

The role of nematic fluctuations in iron-based superconductors is still a strongly debated topic with many open questions concerning their origin and their relationship with the emerging superconductivity. In this work we tackle this issue with a new experimental technique, which combines the high sensitivity of the thermoelectric transport properties with the gentle strain offered by a piezoelectric device. The idea is to use the strain derivative of the Seebeck and the Nernst coefficients as a new tool to investigate the nematicity in the 1111 family of iron based superconductors, so far almost unexplored due to the lack of sizable single crystals. The main outcomes of our study are: i) nematic fluctuations are peaked at the structural transition temperature TS and not at the magnetic one; ii) not all the bands contribute to the measured anisotropy; iii) the Curie-Weiss scaling, previously found for the resistivity anisotropy for T>TS, also exists in the Seebeck and Nernst anisotropy, suggesting the existence of a common mechanism. Our results point towards an orbital origin of nematicity.

TT 15.6 Mon 16:15 H23

Nematicity in $BaFe_2As_2$ and LaFeAsO single crystals studied by elastoresistance and shear modulus measurements — •Sven Sauerland[1], Xiaochen Hong[2], Liran Wang[1], Francesco Scaravaggi[2,3], Anja U.B. Wolter[2], Rhea Kappenberger[2,3], Saicharan Aswartham[2], Sabine Wurmehl[2], Steffen Sykora[2], Federico Caglieris[2], Christian Hess[2], Bernd Büchner[2,3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Leibniz Institute for Solid State and Materials Research, IFW Dresden, Dresden, Germany — [3]Institute for Solid State Physics, TU Dresden, Germany

We report shear modulus and elastoresistivity measurements on LaFeAsO single crystals[1] and study the critical nematic response. The results are compared with corresponding data on $BaFe_2As_2$. In

both materials, softening of the shear modulus towards the structural phase transition is observed by means of the three-point-bending technique and similar Curie-Weiss-like divergence of the nematic susceptibilities deduced from both the shear modulus and the elastoresistivity are found. The data are analysed by means of a Landau approach. Comparison of the bare and the renormalized nematic susceptibilities provides the characteristic energy of the coupling between the lattice and the electronic degrees of freedom. Nematic susceptibilities obtained from shear modulus and elastoresistivity data are compared for LaFeAsO and $BaFe_2As_2$.
[1] R. Kappenberger et al., J. Cryst. Growth 483, 9 (2018)

TT 15.7 Mon 16:30 H23

Checkerboard electronic structure in $Na_{0.96}Li_{0.04}FeAs$ — •Jose M. Guevara[1], Zhixiang Sun[1], Steffen Sykora[1], Chanhee Kim[2], Aga Shahee[2], Dilipkumar Bhoi[2], Kee Hoon Kim[2], Bernd Büchner[1], and Christian Hess[1] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]CeNSCMR, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, South Korea

Electronic order recently emerged as a general ingredient of unconventional superconductivity. A prominent example is the checkerboard electronic order, present in the pseudo-gap regime of the cuprates.

Lately, a new type of electronic order, lacking magnetic order has been reported in Li doped NaFeAs. We performed spectroscopic imaging scanning tunneling microscopy to reveal this new electronic order in real space and to clarify its relation with the nematic and superconducting phases. We present here evidence of electronic order that strikingly resembles the checkerboard order in the cuprates. Our finding thus constitutes the first example of this type of order in the iron-based superconductor (IBS). We characterize the associated q-vector equal to $\sim 0.18\frac{2\pi}{a_{Fe}}$ and discuss it in the context of further evidence of electronic order in the IBS.

TT 15.8 Mon 16:45 H23

Bandwidth controlled insulator-metal transition in $BaFe_2S_3$: A Mössbauer study under pressure — •Philipp Materne[1], Wenli Bi[2,1], Jiyong Zhao[1], Michael Yu Hu[1], Maria Lourdes Amigó[3], Silvia Seiro[3], Saicharan Aswartham[3], Bernd Büchner[3,4], and Esen Ercan Alp[1] — [1]Argonne National Laboratory, Lemont, IL 60439, USA — [2]Department of Geology, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA — [3]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, D-01069, Germany — [4]Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany

$BaFe_2S_3$ is a quasi one-dimensional Mott insulator that orders antiferromagnetically below 117(5) K. The application of pressure induces a transition to a metallic state, and superconductivity emerges. The evolution of the magnetic behavior on increasing pressure has up to now been either studied indirectly by means of transport measurements, or by using local magnetic probes only in the low pressure region. Here, we investigate the magnetic properties of $BaFe_2S_3$ up to 9.9 GPa by means of synchrotron ^{57}Fe Mössbauer spectroscopy experiments, providing the first local magnetic phase diagram. The magnetic ordering temperature increases up to 185(5) K at 7.5 GPa, and is fully suppressed at 9.9 GPa. The low-temperature magnetic hyperfine field is continuously reduced from 12.9 to 10.3 T between 1.4 and 9.1 GPa, followed by a sudden drop to zero at 9.9 GPa indicating a first-order phase transition.

TT 15.9 Mon 17:00 H23

Finite electronic correlations and two-dome superconductivity across a clean nematic quantum phase transition — •Pascal Reiss[1], David Graf[2], Amir A Haghighirad[1,3], William Knafo[4], Loïc Drigo[4,5], Matt Bristow[1], Andrew J Schofield[6], and Amalia I Coldea[1] — [1]Clarendon Laboratory, University of Oxford, UK — [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, USA — [3]Institut fur Festkörperphysik, Karlsruhe Institute of Technology, Germany — [4]Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL), Toulouse, France — [5]Géosciences Environnement Toulouse (CNRS), Toulouse, France — [6]School of Physics and Astronomy, University of Birmingham, UK

In the proximity of a nematic quantum critical point, electronic nematic fluctuations have been identified as a candidate for enhancing superconductivity in various unconventional superconductors. However, the coexistence of long-range magnetic order has hindered detailed studies of nematic criticality. To address this challenge, we combine chemical pressure in $FeSe_{1-x}S_x$ to suppress long-range magnetic order, and physical pressure to study the uncovered, clean nematic quantum phase transition. Using magneto-transport and quantum oscillations measurements, we trace the strength of electronic correlations and their role played in promoting superconductivity. We demonstrate that electronic correlations remain finite, the Fermi surface suffers a Lifshitz transition, and superconductivity is weakened across the nematic quantum phase transition. We interpret these results in light of recent theoretical and experimental advances, and sample quality.

15 min. break.

Invited Talk TT 15.10 Mon 17:30 H23

Theory of superconducting pairing in iron-based superconductors — •Andreas Kreisel — Universität Leipzig, Germany

Theoretical studies of high temperature superconductivity seem to struggle with the question whether the electronic states should be treated in an itinerant approach or using a picture where electrons are almost localized. In the case of iron-based materials, both approaches can explain a number of physical effects and the appearance of various phases. Guided by recent experimental results in the superconducting phase, we use a spin-fluctuation pairing theory that also contains low-energy aspects of strong correlations. A main ingredient of this itinerant approach is to incorporate reduced coherence of quasiparticles occupying specific orbital states into the description of the Fermi liquid. It is demonstrated that this paradigm yields remarkably good agreement with the experimentally observed anisotropic gap structure in 3 different materials: Bulk and monolayer FeSe, as well as LiFeAs. The first system has created a lot of interest recently, because it shows a strong anisotropy in its nematic state. For a deeper understanding of the connection to the Fermi liquid picture, we study the magnetic excitation spectrum [1] and consequences for the vortex formation in the superconducting state and discuss these in view of recent inelastic neutron scattering data and magnetic penetration depth measurements[2].
[1] A. Kreisel, Brian M. Andersen, P. J. Hirschfeld, arXiv:1807.09482
[2] P. Biswas, et al., Phys. Rev. B 98, 180501(R) (2018)

TT 15.11 Mon 18:00 H23

Symmetry-resolved strain tuning of composite nematic order — •Roland Willa, Max Fritz, and Jörg Schmalian — Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Electronic nematicity in iron pnictide superconductors and charge order in the high-T_c cuprates are two phenomena that are associated with the appearance of composite order. The response of these systems to external strain has proven to be a powerful tool to study their symmetry properties [1,2]. We deploy a long-wavelength field theory to investigate the nematic transition temperature and excitation spectrum of a low-dimensional system under strain. In certain symmetry channels, strain lifts the degeneracy of the nematic order—similar to magnetic field lifting the degeneracy of Ising spins—and a crossover replaces the phase transition. In degeneracy-preserving strain channels, we find a quadratic dependence of the transition temperature with respect to strain. The magnitude of this effect as the system approaches the 2d limit reveals a logarithmic divergence for specific symmetry channels (B_{ng} sector), while evaluating to order unity in others (A_{ng} sector). This finding is in good agreement with the strong effects observed in the B_{1g}-channel of $Ba(Fe_{0.975}Co_{0.025})_2As_2$, as reported in Ref. [2], and underlines the importance of anisotropy in this system.
[1] H.-H. Kim *et al.*, Science (accepted)
[2] M. Ikeda *et al.*, arXiv:1803.09273 (2018)

TT 15.12 Mon 18:15 H23

Quasiparticle Interference and Symmetry of Superconducting Order Parameter in Strongly Electron-Doped Iron-based Superconductors — •Jakob Böker[1], Pavel Volkov[2], Peter Hirschfeld[3], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey, 08854, USA — [3]Department of Physics, University of Florida, Gainesville, Florida32611, USA

Motivated by recent experimental reports of significant spin-orbit coupling (SOC) and a sign-changing order-parameter in the $Li_{1-x}Fe_x(OHFe)_{1-y}Zn_ySe$ superconductor with only electron Fermi surface present, we study the possible Cooper-pairing symmetries and their quasiparticle interference (QPI) signatures. We find that each

of the resulting states - s-wave, d-wave and helical p-wave - can have a fully gapped density of states (DOS) consistent with angle-resolved photoemission experiments (ARPES) experiments and, due to spin-orbit coupling, are a mixture of spin singlet and triplet components leading to intra- and inter-band features in the QPI signal. Analyzing predicted QPI patterns we find that only the s- and d-wave pairing states with a dominant even parity triplet component can fit the experimental data with two dominant peaks in the DOS at energies roughly corresponding to the gap sizes at each pocket. Moreover, we show that pairing states with dominant triplet component may exist and can be identified using spin-resolved STM.

TT 15.13 Mon 18:30 H23

Enhanced Friedel oscillations by nematic fluctuations in an iron-based superconductor — •Steffen Sykora[1], Zhixiang Sun[1], Jose M. Guevara[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

Nematic fluctuations are known to provide an additional superconducting pairing channel which is considered as a possible explanation for the large critical temperatures in iron-based superconductors. We study its influence on the impurity scattering using a minimal microscopic model of nematic fluctuations in an effective two-band system of conduction electrons. Applying a projective renormalization method to integrate out the nematic interaction we find that the impurity scattering potential can be strongly renormalized at small scattering momentum through virtual particle-hole excitations in the d_{xz}/d_{yz} orbital channel. For the particular material LiFeAs we explicitly calculate the Fourier-transformed local density of states and find excellent agreement with recent scanning tunneling experiments* where resonantly enhanced Friedel oscillations have been attributed to the first spectroscopic evidence of nematic fluctuations in an iron-based superconductor.

[1] arXiv:1811.03489

TT 15.14 Mon 18:45 H23

Nematic fluctuations close to quantum criticality: a new method for comparing simulations and experiments — •Daniel Jost[1,2], Samuel Lederer[3], Thomas Böhm[1,2], Yoni Schattner[4,5], Erez Berg[6], Steven Kivelson[4], and Rudi Hackl[1,2] — [1]Walther-Meissner-Institute, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Cornell University, 14850 Ithaca, USA — [4]Department of Physics, Stanford University, 94305 Stanford, USA — [5]Stanford Institute of Material and Energy Science, 94025 Menlo Park, USA — [6]Department of Physics, University of Chicago, 60637 Chicago, USA

The comparison of numerical simulations and spectroscopic results is notoriously difficult due to the analytic continuation in the complex energy plane. Additionally, life times and mass enhancement factors must be extracted from the experimental spectra using, e.g., the Kramers-Kronig transformation with the well-known problems resulting from the extrapolations to low and high energies. One way out of this dilemma is a transformation of the experimental results from real to imaginary frequencies which provides us with an imaginary-time-ordered correlation function $\Lambda(\tau)$. From this transformation, one can extract the quantity $\beta\Lambda(\beta/2)$ with $\beta = 1/k_{\mathrm{B}}T$. In this contribution we derive this quantitiy from the electronic Raman spectra of the iron pnictide $Ba(Fe_{1-x}Co_x)_2As_2$ as a function of doping and temperature. Additionally, we highlight the perspectives of this method with view on quantum criticality and the comparison of experiment and theory.

TT 16: Graphene II: Excitations and Nanoribbons (joint session O/TT)

Time: Monday 15:00–18:00 Location: H24

TT 16.1 Mon 15:00 H24

Altering the lattice dynamics of graphene by hot-electron injection — •Marcel Weinhold, Sangam Chatterjee, and Peter J. Klar — Institute of Experimental Physics I and Center for Materials Research (LaMa), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen

Graphene is discussed as material for next-generation (opto-)electronic devices. Among others, this is due to its exceptional properties including a large electron mobility, vast mechanical flexibility and durability, and its matchless linear and gap-less band structure. By combining graphene with metallic nanostructures that feature plasmonic characteristics its intrinsic properties can be tuned significantly. Those nanostructures lead to a near-field confinement of the incident light due to the excitation of localized surface plasmons (LSP). Further, LSPs decay non-radiatively into energy-rich electron-hole pairs. These 'hot-carriers' may be injected into the graphene and lead to a doping. However, plasmonic properties are very sensitive to geometry and dielectric environment. Therefore, single particle measurements are crucial for gaining further insights into the underlying physics. Here, we study the injection of hot-electrons in a model system, i.e., a single gold nanoparticle on a monolayer graphene substrate. We show that the injection of hot-electrons into graphene induces a quantifiable altering of graphene's phonon dispersion relation using specially resolved micro-Raman spectroscopy. In addition, we present an analysis procedure yielding further information on occurring temperature and strain distributions solely from the measured Raman shift maps.

TT 16.2 Mon 15:15 H24

Single Spin Localization and Manipulation in Graphene Open-Shell Nanostructures — •Jingcheng Li[1], Sofia Sanz[2], Martina Corso[2,3], Deung Jang Choi[2,3,5], Diego Peña[4], Thomas Frederiksen[2,5], and Jose Ignacio Pascual[1,5] — [1]CIC nanoGUNE, 20018 Donostia-San Sebastián, Spain — [2]DIPC, 20018 Donostia-San Sebastián, Spai — [3]Centro de Física de Materiales (CSIC-UPV/EHU), 20018 Donostia-San Sebastián, Spain — [4]3CIQUS, Santiago de Compostela (Spain) — [5]Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Predictions state that graphene can spontaneously develop magnetism from the Coulomb repulsion of its π-electrons, but its experimental verification has been a challenge. Here, we report on the observation and manipulation of individual magnetic moments localized in graphene nanostructures on a Au(111) surface. Using scanning tunneling spectroscopy, we detected the presence of single electron spins localized around certain zigzag sites of the carbon backbone via the Kondo effect. Two near-by spins were found coupled into a singlet ground state, and the strength of their exchange interaction was measured via singlet-triplet inelastic tunnel electron excitations. Theoretical simulations demonstrate that electron correlations result in spin-polarized radical states with the experimentally observed spatial distributions. Hydrogen atoms bound to these radical sites quench their magnetic moment, permitting us to switch the spin of the nanostructure using the tip of the microscope.

TT 16.3 Mon 15:30 H24

Molecular Spin Excitation by Electron Injection Through a Single Graphene Nanoribbon — •Niklas Friedrich[1], Jingcheng Li[1], Néstor Merino-Díez[1,2], Dimas G. de Oteyza[2], Diego Peña[3], David Jacob[4,5], and Nacho Pascual[1,5] — [1]CIC nanoGUNE, San Sebastian (Spain) — [2]DIPC, San Sebastian (Spain) — [3]CIQUS, Santiago de Compostela (Spain) — [4]Departamento de Física de Materiales, UPV/EHU, San Sebastian (Spain) — [5]Ikerbasque, Basque Foundation for Science, Bilbao (Spain)

Graphene nanoribbons (GNRs) and GNR-hybrids can be synthesized on metal surfaces with atomic precision using on surface synthesis techniques. Previously, we constructed a system in which chiral (3,1)-GNRs act as leads contacting a magnetic porphyrin molecule on a Au(111) substrate. Characterizing the porphyrin's magnetic properties by inelastic electron tunneling spectroscopy (IETS) we showed that the porphyrin's spin survives up to 4 contacting GNRs.

As a further step towards fully functional molecular devices, we now characterize the transport properties of linear GNR-porphyrin-GNR systems. We created a transport junction by contacting the system at a GNR end with the STM tip and lifting the molecular complex partially from the surface. We investigate the porphyrin's spin state via IETS by electrons cotunneling through the semiconducting GNR. In this transport configuration inelastic tunneling excites the Fe spin with excitation energies similar to the one measured by STS on sur-

face. However, some molecular structures were found to lie in a mixed-valence state that vanished as the porphyrin was lifted from the metal.

TT 16.4 Mon 15:45 H24

Segregated transport channels in sidewall nanoribbons — •Stephen Power[1,2,3], Johannes Aprojanz[4], Pantelis Bampoulis[5,6], Stephan Roche[1,7], Antti-Pekka Jauho[8], Harold Zandvliet[6], Alexei Zakharov[9], and Christoph Tegenkamp[4,5] — [1]ICN2, Bellaterra, Spain — [2]UAB, Bellaterra, Spain — [3]School of Physics, Trinity College Dublin, Ireland — [4]Institut für Physik, Technische Universität Chemnitz — [5]Institut für Festkörperphysik, Leibniz Universität Hannover — [6]MESA+Institute, University of Twente, The Netherlands — [7]ICREA, Barcelona, Spain — [8]CNG and DTU Nanotech, Denmark — [9]MAX IV Laboratory and Lund University, Sweden

Conductance quantization is a defining feature of electronic transport in quasi-one dimensional conductors. In the absence of a magnetic field, confinement results in a sequence of transverse sub-bands with an increasing number of nodes across the device width. Graphene nanoribbons grown on the sidewalls of SiC mesa structures have previously[1] been shown to present a 1D ballistic channel at the micron scale. New 2-point measurements reveal additional quantised channels at shorter probe separations[2]. Surprisingly, these channels are localised in different regions across the ribbon width. Here we demonstrate how this distribution of channels is consistent with a model accounting for both edge zigzag magnetism and asymmetric interfaces between the SiC and nanoribbon at each edge.

[1] J. Baringhaus et al, Nature 506 (2014) 349 [2] J. Aprojanz, S.R. Power et al, Nature Communications 9 (2018)4426

TT 16.5 Mon 16:00 H24

Edge State Engineering of Graphene Nanoribbons — •Ping Yu — School of Physical Science and Technology, ShanghaiTech University

Zigzag edges of graphene nanoribbons are predicted to be spin-polarized and could have great potential for spintronics. The ability to precisely engineer the zigzag edge state is of crucial importance for realizing its full potential functionalities in device nanotechnology. Here, by combining scanning tunneling microscopy and atomic force microscopy, the zigzag edge states are found to get energy splitting upon fusing manganese phthalocyanine molecule with the short armchair graphene nanoribbon termini. Moreover, the edge state splitting can be reversibly switched by adsorption and desorption of atom hydrogen on the magnetic core of manganese phthalocyanine. The engineering mechanism is found to be due to the zigzag edge local doping level by the charge transfer process, which provides a new route to functionalize graphene-based molecular devices.

TT 16.6 Mon 16:15 H24

How Structural Defects Affect the Mechanical and Electrical Properties of Single Molecular Wires — •Matthias Koch[1], Zhi Li[2], Christophe Nacci[1,3], Takashi Kumagai[1], Ignacio Franco[2], and Leonhard Grill[1,3] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]University of Rochester, Rochester, United States — [3]University of Graz, Graz, Austria

Graphene nanoribbons (GNRs) [1] are attractive candidates for molecular wires [2]; a key component in molecular nanotechnology. In addition to inheriting the supreme electromechanical properties of graphene [3], these narrow stripes offer a tunable band gap [4], which is crucial for electronic applications. Although many studies on molecular wires exist, the role of defects in the chemical structure has not been investigated. Here, we show how individual defects affect the properties of single GNRs [5]. Scanning tunnelling and atomic force microscopy (STM/AFM) pulling experiments access their electrical and mechanical properties simultaneously. We find, with the help of atomistic simulations, that defects substantially vary the molecule-substrate coupling and drastically increase the flexibility of the graphene nanoribbons while keeping their desirable electronic properties intact. Our study suggests that defected GNRs are suitable for molecular electronics that require flexible components, in contrast to rigid architectures.

[1] Cai, J. et al. Nature 466, 470 (2010) [2] Koch, M. et al. Nat. Nanotech. 7, 713 (2012) [3] Novoselov, K. S. et al. Nature 490, 192 (2012) [4] Han, M. Y. et al. Phys. Rev. Lett. 98, 206805 (2007) [5] Koch, M. et al. Phys. Rev. Lett. 121, 047701 (2018)

TT 16.7 Mon 16:30 H24

Tailoring end states of graphene nanoribbons by magnetic dopants — •Tobias Preis, Sujoy Karan, Tobias Frank, Jaroslav Fabian, Ferdinand Evers, Dieter Weiss, Jonathan Eroms, and Jascha Repp — University of Regensburg, Faculty of Physics - Regensburg, Germany

Zig-zag edges of graphene are predicted to host spin-polarized electronic states and hold great promise for future spintronic device applications [1]. With the help of scanning tunneling microscopy (STM), we investigated the short zig-zag edges of bottom-up synthesized armchair graphene nanoribbons (GNRs), which were fabricated according to the recipe of Cai et al. [2]. We deposited single Co atoms on the surface and positioned them with the help of the STM tip underneath the GNRs. dI/dV spectra taken at the adsorption positions of embedded Co atoms show the emergence of a Kondo-like peak, being distinctly different from any Kondo features of isolated Co adatoms on the Au(111) surface. The peak exhibits a peculiar dependence on the position with respect to the short GNR edge.

[1] K. Nakada et al., PRB 54, 24 (1996)
[2] J. Cai et al., Nature 466, 470 (2010)

TT 16.8 Mon 16:45 H24

On-surface synthesis of chevron-like graphene nanoribbons — •Koen Houtsma, Mihaela Enache, Ida Delac Marion, Tuan Anh Pham, Van Bay Tran, and Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, Groningen, the Netherlands

Graphene nanoribbons (GNRs) are a novel material that has aroused much interest because of its excellent and tunable electronic properties. Using on-surface synthesis, GNRs can be produced with atomic precision. In our research, GNRs with chevron-like topology were created via Ullman-type coupling from the prochiral molecular precursor 6,12-dibromocrhysene on a Au(111) surface. The structural properties of these GNRs, also in dependence of post-deposition annealing temperature, were investigated using scanning tunneling microscopy [1]. With scanning tunneling spectroscopy, we additionally characterized their electronic properties.

[1] T.A. Pham et al., Small 13 (2017) 1603675.

TT 16.9 Mon 17:00 H24

Bottom-up fabrication of porous carbon nanoribbons on metal surfaces — •Mirunalini Devarajulu, Martin Haller, Maximilian Ammon, Min-Ken Li, Shadi Sorayya, and Sabine Maier — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

On-surface synthesis is a versatile technique to fabricate graphene-based nanoribbons from the bottom-up with high precision. We demonstrated that one-dimensional carbon nanoribbons with periodic hexagonal nanopores can be fabricated via Ullmann-type reactions on Ag(111) in combination with dehydrogenation reactions and the preprogrammed isomerization of the conformationally flexible precursor.[1] Here, we unveil the reaction mechanism and the N-doping of the porous nanoribbons in a low-temperature scanning tunneling microscopy study. We show that the rotation of *m*-phenylene units is a powerful design tool to promote structural control in the synthesis of porous covalent organic nanostructures on different metal surfaces. We find that the fabrication of porous nanoribbons proceeds on different terminations of the silver surface. However, the N-doping via triazine moieties influences the conformational selectivity of the molecular precursor, which affects the nanoribbon formation.

[1] M. Ammon, T. Sander, S. Maier, JACS, 2017, 139 (37), 12976

TT 16.10 Mon 17:15 H24

Chevron-based graphene nanoribbons and heterojunctions by direct contact printing — •Axel Enders[1], Jacob D Teeter[2], Paulo S Costa[2], Gang Li[2], and Alexander Sinitskii[2] — [1]Universität Bayreuth, Physikalisches Institut, 95440 Bayreuth — [2]University of Nebraska - Lincoln, Lincoln NE 68588, USA

Atomically precise graphene nanoribbons (GNRs) have been synthesized through a direct contact transfer (DCT) of molecular precursors on Au(111), followed by gradual annealing. This method provides an alternative to the conventional approach for the deposition of molecules on surfaces by sublimation and simplifies preparation of dense monolayer films of GNRs. We performed STM characterization of the precursors of chevron GNRs, and demonstrate that the assemblies of the intermediates of the GNR synthesis are stabilized by π - π interactions. DCT was then used to deposit a mixture of two structurally similar

but visually distinct chevron-type molecular precursors. Annealing of the deposited mix resulted in heterojunctions composed of units of chevron GNRs (cGNRs) and new laterally extended chevron GNRs (eGNRs). The electronic properties of these GNRs across the heterojunctions were studied with scanning tunneling spectroscopy. The dI/dV maps show that the impact of heterojunctions as well as structural defects is highly local and usually stays within the corresponding GNR units even if they are bonded to structurally and electronically different neighbors. It is expected that this method of DCT is highly versatile and allows to combine other chevron-type GNRs as well, such as nitrogen-doped cGNRs, into a variety of new GNR heterojunctions.

TT 16.11 Mon 17:30 H24

Expitaxially grown twisted bilayer graphene on SiC(0001) — •You-Ron Lin[1,2], Nafiseh Samiseresht[1,2], Markus Franke[1,2], Shayan Parhizkar[1,2], François C. Bocquet[1,2], F. Stefan Tautz[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology, 52425 Jülich, Germany

Layer by layer stacking of 2D-materials such as graphene, hexagonal boron nitride (hBN) and transition metal dichalcogenides (TMDCs) has been widely investigated developing a field on its own [1]. It has been shown that apart from the material used for stacking, the twist angle between two layers also has an immense effect on the band structure of the stack [2]. We report a reproducible method for large scale epitaxial growth of graphene bilayers utilizing the precursor molecule borazine. The existence of both graphene layers is confirmed by angular-resolved photoemission spectroscopy (ARPES). Spot-profile analysis low electron energy diffraction (SPA-LEED) has been used to determine a twist of $30 \pm 0.46°$.

[1] A. K. Geim *et al.*, *Nature*, **499**, 419, 2013.
[2] Y. Cao *et al.*, *Nature*, **556**, 43, 2018.

TT 16.12 Mon 17:45 H24

Dielectric engineering in twisted bilayer graphene — •Jose Pizarro[1], Malte Rösner[2], Ronny Thomale[3], and Tim Wehling[1] — [1]Universität Bremen — [2]University of Southern California — [3]Universität Würzburg

Twisted bilayer graphene (TBG) has appeared as a tunable testing ground to investigate the conspiracy of electronic interactions, band structure, and lattice degrees of freedom to yield exotic quantum many-body ground states in a two-dimensional semiconductor framework. While the impact of external parameters such as doping or magnetic field can be conveniently modified and analyzed, the lack of open accessiblity of the quasi-2D electron gas combined with its intricate internal properties pose a challenging task to characterize the quintessential nature of the different insulating and superconducting states found in transport experiments. We analyze the possible role of the dielectric environment for TBG on the internal electronic interaction profile, which could be conveniently adjusted in experiment, e.g. by varying the capping layer composition and thickness. We find that this allows to significantly modify the internal interaction strength. In doing so, we propose the experimental tailoring of the dielectric environment as a promising pursuit to provide further evidence for resolving the hidden nature of quantum many-body states in TBG.

TT 17: Poster Session: Correlated Electrons 1

Time: Monday 15:00–18:30 Location: Poster D

TT 17.1 Mon 15:00 Poster D

Investigation of magnetic ground state of CeCoSi by means of neutron scattering — •Stanislav Nikitin[1,2], Diego Franco[3], Jae Hyeon Kwon[1], Andreas Hoser[4], Michael Koza[5], Robert Bewley[6], Christoph Geibel[1], and Oliver Stockert[1] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]Technical University Dresden, Germany — [3]Centro Atomico Bariloche and Instituto Balseiro, Bariloche, Argentina. — [4]Helmholtz-Zentrum Berlin, Berlin, Germany — [5]Institut Laue-Langevin, Grenoble, France — [6]ISIS Neutron Source, Didcot, United Kingdom

Ce-based materials represent a rich playground for investigation of many exotic phenomena, such as heavy-fermion behavior, unconventional superconductivity, quantum criticality and so on. In this work, we explored magnetic properties of a metallic Ce-based antiferromagnet CeCoSi, which has an unusual $T-P$ phase diagram. Cerium moments order below $T_N = 8.8$ K, however, a very moderate hydrostatic pressure of $P \approx 1.5$ GPa, stabilizes a new pressure-induced-ordered phase with significantly higher transition temperature of $T_c \approx 40$ K. Motivated by these observation, we explored magnetic structure and excitation spectra of CeCoSi by means of elastic and inelastic neutron scattering. We found that the cerium moments orders in a simple AFM structure with $\mathbf{q} = 0$. Using the results of inelastic neutron scattering and specific heat measurements we resolved the Hamiltonian of crystalline electrical field. Furthermore, we discussed a possible influence of the hydrostatic pressure on the spectra of magnetic excitations

TT 17.2 Mon 15:00 Poster D

Thermopower evolution in $Yb(Rh_{1-x}Co_x)_2Si_2$ upon $4f$ localization — •Ulrike Stockert[1], Christoph Klingner[1], Cornelius Krellner[2], Veljko Zlatić[3], Christoph Geibel[1], and Frank Steglich[1,4,5] — [1]MPI for Chemical Physics of Solids, Dresden — [2]Physikalisches Institut, Goethe-Universität, Frankfurt/Main — [3]Department of Physics, University of Split, Croatia — [4]Center for Correlated Matter, Zhejiang University, Hangzhou, China — [5]Institute of Physics, Chinese Academy of Science, Beijing, China

$YbRh_2Si_2$ is a heavy-fermion system, which exhibits a large negative thermopower $S(T)$ with a single minimum around 80 K due to Kondo scattering from the full $4f$ multiplet. Substitution of Rh by Co leads to a strong reduction of the exchange coupling between the $4f$ and the conduction electron states and to a lowering of the Kondo scale T_K. This drives the system to a stable trivalent state in $YbCo_2Si_2$.

We performed thermopower measurements on $Yb(Rh_{1-x}Co_x)_2Si_2$ to study the evolution of $S(T)$ upon $4f$ localization. As T_K decreases with increasing x we observe the appearance of a second minimum that shifts subsequently to lower T. Simultaneously, the absolute thermopower values are strongly reduced due to the weaker exchange coupling between the $4f$ and the conduction electron states. Pure $YbCo_2Si_2$ still exhibits two minima in $S(T)$ indicative of weak residual Kondo scattering. The value at the high-T minimum is found to be proportional to the Sommerfeld coefficient for the whole series. We discuss this unexpected finding in relation to recent measurements of the valence and Fermi surface evolution with temperature.

TT 17.3 Mon 15:00 Poster D

Magnetic anisotropy in $GdRh_2Si_2$ probed by antiferromagnetic resonance — •Dieter Ehlers[1], Kristin Kliemt[2], Cornelius Krellner[2], Christoph Geibel[3], and Jörg Sichelschmidt[3] — [1]Experimentalphysik V, EKM, Universität Augsburg, 86135 Augsburg — [2]Physikalisches Institut, Goethe-Universität Frankfurt am Main, 60438 Frankfurt am Main — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden

$GdRh_2Si_2$ exhibits a complicated magnetocrystalline anisotropy [1] of well-localized Gd^{3+} moments. Below $T_N = 107$ K [2] long range magnetic order sets in with ferromagnetic layers in the ab-plane stacked antiferromagnetically along the c-axis of the tetragonal structure. Interestingly, the strong easy-plane anisotropy allows for the observation of antiferromagnetic resonance at X- and Q-band microwave frequencies. In addition to the easy-plane anisotropy we have also quantified a weaker fourfold anisotropy within the easy plane. The obtained resonance fields are modelled in terms of eigenoscillations of the two antiferromagnetically coupled sublattices. Conversely, this model provides plots of the eigenfrequencies as a function of field and the specific anisotropy constants. An interesting perspective is the application of a similar model for understanding the magnetic ground state of the Kondo system $YbRh_2Si_2$.

[1] J. Sichelschmidt et al., Phys. Rev. B 97, 214424 (2018)
[2] K. Kliemt and C. Krellner, J. Cryst. Growth. 419, 37 (2015)

TT 17.4 Mon 15:00 Poster D

$TbRh_2Si_2$: Single crystal growth and characterization — •Alexej Kraiker, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt

am Main, Germany

In the last decades, many studies on RT_2Si_2 (R = rare earth, T = transition metal) ternary silicides have been made. The compounds which crystallize in the bodycentered tetragonal $ThCr_2Si_2$ structure exhibit exceptional magnetic properties such as superconductivity, valence fluctuations or the Kondo effect. In recent years, we have started to systematically investigate the magnetic properties of RRh_2Si_2 compounds, which present exciting surface properties, strongly influenced by the 4f-magetism [1]. So far, the magnetism of $TbRh_2Si_2$ has been studied on polycrystalline samples using neutron scattering [2]. The compound shows antiferromagnetic order below T_N = 92 K with a magnetic ordering vector k = (001). In this contribution, we present the details of the crystal growth of $TbRh_2Si_2$ single crystals by Bridgman method from indium flux. We show the results of specific heat, specific resistivity and magnetization measurements, with a focus on the magnetic transition.

[1] A. Generalov et al., Nano Lett. 17, 811 (2017)
[2] S. Quezel et al., Solid State Commun. 49, 7 (1984)

TT 17.5 Mon 15:00 Poster D

Towards crystal growth process of isotope pure $^{174}YbRh_2Si_2$ — Susanna Rongstock, •Sebastian Witt, Doan-My Tran, and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt, D-60438 Frankfurt

A central question in condensed matter research concerns the interplay between quantum criticality and unconventional superconductivity in strongly correlated electron systems such as heavy-electron systems. Recently, superconductivity was also discovered in the quantum-critical material $YbRh_2Si_2$ at 2 mK [1]. So far the interplay between electronic and nuclear moments of Yb and ist impact on the superconductivity is not settled. For that reason, it is essential to investigate $YbRh_2Si_2$ samples with a well-defined Yb nuclear spin, with the simplest case of ^{174}Yb which has zero nuclear spin.

In this contribution, we report on the challenges to grow a $^{174}YbRh_2Si_2$ crystal, as the Yb-isotopes are only available as oxides and are rather expensive. We have developed a process to reduce the oxide to metallic Yb with minimal mass losses and scaled down to established crystal growth process to work with smaller total masses. The characterization of the single crystals by different methods (Laue, PXRD, resistivity, magnetization, heat capacity) partly down to low temperatures will be presented. Besides the desired compound we present the properties of a parasitic phase, (e.g. $YbRh_6Si_4$).

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

TT 17.6 Mon 15:00 Poster D

Crystal growth of the valence fluctuating system $EuPd_2Si_2$ — •Marius Peters, Eunhyung Cho, Doan-My Tran, Franz Ritter, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

The study of collective phenomena raising from enhanced coupling between electrons and phonons is focussed on materials exhibiting phase transitions involving both electronic and lattice-degrees of freedom. One system providing such a strongly coupled phase transition is $EuPd_2Si_2$ of the $ThCr_2Si_2$ structural type, showing a temperature induced valence transition of europium between the energetically vicinal valence states Eu^{2+} and Eu^{3+} at about 170K [1]. First reports on the synthesis of single crystals came up only recently [2], but a deep investigation of the valence transition in this compound is still missing. We approached the ternary Eu-Pd-Si system using differential thermal analysis to map the local composition phase diagram. We used the Bridgman and the Czochralski method fort he successful growth of mm-sized single crystals of $EuPd_2Si_2$. In this contribution we will present chemical and structural characterization of these crystals and some preliminary physical measurements around the valence transition.

[1] E. V. Sampathkumaran et al., J. Phys. **C14**, L237 (1981)
[2] Y. Onuki et al., Philosophical Magazine **97**, 3399 (2017)

TT 17.7 Mon 15:00 Poster D

$CeRu_2P_2$ and $CeCo_2P_2$: Single Crystal Growth Methods and Physical Characterization — •Fabian Feldmann, Marius Peters, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut Goethe Universität Frankfurt/Main

CeT_2P_2 (T = Co, Ru) are rare-earth ternary phosphides with tetragonal $ThCr_2Si_2$ type crystal structure. $CeRu_2P_2$ is an intermediate valent system [1] and $CeCo_2P_2$ is an antiferromagnet with a rather high Néel temperature $T_N = 440$ K [2], most likely due to an interplay of 3d and 4f magnetism.

Here, we present crystal growth methods to obtain millimeter-sized single crystals. These growths were executed with Sn-flux and self-flux with temperatures up to 1500 °C. Optical microscopy, Powder X-Ray Diffraction (PXRD), Energy Dispersive X-ray spectroscopy (EDX) and Laue method were used for chemical characterization and confirmation of single crystallinity.

In addition, we report on measurements of specific heat, magnetic susceptibility and electrical resistivity. We confirm some measurements, for instance a broad maximum in electrical resistivity at $T = 180$ K and metallic behavior at lower temperatures for $CeRu_2P_2$ [3]. We also show new measurements such as magnetic susceptibility of $CeCo_2P_2$, now relating to crystal orientation.

[1] T. Fujiwara et al., J. Phys.: Conf. Ser. **273**, 012112 (2011)
[2] Y. Tian et al. Physica B, **512**, 75-80, (2017)
[3] A. Amorese et al., Phys. Rev. B **93**, 165134 (2016)

TT 17.8 Mon 15:00 Poster D

Electrical resistivity of heavy fermion metal $YbNi_4P_2$ under high pressure — •Takaki Muramatsu[1], Owen Moulding[1], Kristin Kliemt[2], Cornelius Krellner[2], and Sven Friedemann[1] — [1]HH Wills Laboratory, University of Bristol, UK — [2]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany

Heavy-fermion metal $YbNi_4P_2$ is a characteristic compound in terms of the magnetic property. In the tetragonal $ZrFe_4Si_2$ type crystal structure ($P4_2/mnm$), Yb ions line up to chains along c-axis and each chain is well separated by other chains of edge-shared Ni tetrahedra, providing quasi-one dimensional heavy-fermion system. At ambient pressure, $YbNi_4P_2$ orders ferromagnetically (FM) below $T_C = 0.17$K [1] and the low T_C allows us to access the quantum critical point point by a combination of chemical and physical pressure [2]. In this work, we utilise physical pressure to study the interaction of magnetic moments and conduction electrons of $YbNi_4P_2$ by measuring temperature dependence of electrical resistivity.

TT 17.9 Mon 15:00 Poster D

High-field de Haas-van Alphen study of the heavy-fermion compound $CeCoIn_5$ — •J. Hornung[1,2], M. Raba[3], S. Mishra[3], D. Aoki[4], I. Sheikin[3], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL), France — [4]Institute for Materials Research (IMR), Tohoku University, Japan

We report on de Haas-van Alphen (dHvA) measurements in the heavy-fermion compound $CeCoIn_5$ in magnetic fields up to 36 T and temperatures down to 50 mK. Compared to previous investigations, we were able to observe additional dHvA frequencies and a very diverse field dependence. While some frequencies stay unaffected by magnetic fields, like usually observed and expected, others show a strong field dependence, such as a clear discontinuity at 26.5 T with a change of the measured frequency and/or the effective mass. In addition, the spin splitting of some frequencies, already reasoned from the non-trivial temperature dependence of the dHvA amplitudes in a earlier work, could be resolved directly.

TT 17.10 Mon 15:00 Poster D

^{59}Co NMR magnetometry of the heavy-fermion compound $CeCoGe_3$ — •Sven Luther[1,2], Ilya Sheikin[3], Rikio Settai[4], Jochen Wosnitza[1,2], and Hannes Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL), CNRS, Grenoble, France — [4]Department of Physics, Niigata University, Japan

The tetragonal heavy-fermion compound $CeCoGe_3$ yields, as established by thermodynamic probes, a complex magnetic phase diagram with several zero-field transitions to and between antiferromagnetically ordered phases below $T_N = 20$ K. We present a detailed, microscopic study of one of these magnetic phases via ^{59}Co ($I = 7/2$) NMR at 2 T. Here, below T_N, the symmetry breaking by magnetic order results in three inequivalent Co-sites with corresponding local sublattice magnetizations. These temperature-dependent internal fields can well be described by an Ising-type mean-field formalism. In addition to the

antiferromagnetic order, which is compatible with neutron-scattering results, the analysis yields an additional uniform part, which could be induced by an unusually high polarization of hybridized conduction electrons.

TT 17.11 Mon 15:00 Poster D

Study of the low-temperature specific heat of the locally non-centrosymmetric superconductor $CeRh_2As_2$ — •Jacintha Banda, Daniel Hafner, Seunghyun Khim, Helge Rosner, Christoph Geibel, and Manuel Brando — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Recently, we have discovered a new heavy-fermion, locally non-centrosymmetric superconductor $CeRh_2As_2$ in the $CeBe_2Ge_2$ type structure with a transition temperature $T_c \approx 0.3$ K. We present here a comprehensive study of its low-temperature specific heat and its behaviour in a magnetic field which was applied parallel and perpendicular to the crystallographic c-axis. We show that a second weak phase transition can be seen in specific heat at a temperature T_0 slightly above T_c. Its field dependence is similar to that of quadrupolar phases. After having subtracted the nuclear specific heat contribution due to the quadrupolar and Zeeman terms on the arsenic nuclear spins, we present the temperature and field dependence of the electronic specific heat coefficient $\gamma = C(T,H)/T$ down to 40 mK and up to 12 T.

TT 17.12 Mon 15:00 Poster D

Metallic 4f-electron system with a large magnetic cooling capacity — •Thomas Gruner[1], Jiasheng Chen[1], Jacintha Banda[2], Jang Dongjin[3], Manuel Brando[2], Christoph Geibel[2], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]MPI CPfS, Dresden, Germany — [3]KRISS, Daejeon, Republic of Korea

All standard cooling materials used in present day demagnetisation refrigerators for the temperature range 50 mK $< T <$ 2 K are insulators, resulting in some problems e.g. because of their very weak low-temperature thermal conductivity. Recently, we proposed and showed that some Yb based metallic materials provide attractive alternatives [1], and ideas which meanwhile has been picked up by further research groups. In a search for even more appropriate materials we have synthesised a new Yb Heusler compound and investigated its structural, magnetic, transport and magnetocaloric properties.
Susceptibility χ(T), magnetisation $M(B)$, specific heat C(T) and resistivity ρ(T) data evidence metallic behaviour, the absence of superconductivity and a stable trivalent Yb^{3+} state, without any sign for a significant Kondo interaction. Our new compound can easily be cast into rods, making preparation of cooling pills quite simple in contrast to commonly used paramagnetic salt refrigerants. By using a demagnetisation test set-up, we demonstrate the feasibility of a simple, economically priced and durable alternative for traditional cooling devices for temperatures down to roughly 100 mK.
[1] Jang, Gruner et al.; Nature Communications; **6**, 8680 (2015)

TT 17.13 Mon 15:00 Poster D

Spin-orbit interaction and quasiparticle bands in locally non-centrosymmetric heavy-fermion systems — •Évrard-Ouicem Eljaouhari[1], Gertrud Zwicknagl[1], Seunghyun Khim[2], Manuel Brando[2], and Christoph Geibel[2] — [1]Institut für Mathematische Physik, TU Braunschweig, Braunschweig, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Non-centrosymmetric heavy-fermion materials have gained much interest in the past decade. In these materials, the lack of inversion symmetry in combination with strong spin-orbit interaction and magnetic interactions can lead to novel phenomena. In this poster, we present calculations of the heavy quasiparticle bands of Ce- and Yb-based heavy-fermion compounds from the tetragonal "122"-family. This class of materials comprises compounds with the inversion-symmetric $ThCr_2Si_2$ structure as well as systems with the locally non-centrosymmetric $CaBe_2Ge_2$ structure. The calculations are performed by means of the Renormalized Band method which proceeds from a Dirac relativistic description of the electronic structure and accounts for Crystalline Electric Field effects and the mass renormalisation due to strong local correlations. We discuss results for $YbIr_2Si_2$ which crystallizes in both structures depending on preparation condition. Further on, we present our new results on the new HFS $CeRh_2As_2$.

TT 17.14 Mon 15:00 Poster D

Emergence of gauge fields in the rotating polaron problem — •Mikhail Maslov, Enderalp Yakaboylu, and Mikhail Lemeshko — Institute of Science and Technology, Klosterneuburg, Austria

In a recent article [1], it was shown that in any impurity problem a many-body environment manifests itself as an external gauge field with respect to the impurity interacting with it. Here, we apply this method to the so-called rotating polaron problem, which is a quantum impurity possessing both translational and internal rotational degrees of freedom interacting with a bosonic bath [2], and study its geometric and topological properties. We show that within the perturbation theory approach in the internal angular space of the impurity the emerging gauge field corresponds to a non-Abelian magnetic monopole. Furthermore, we are able to define the second Chern number in the total coordinate of the impurity.
[1] E. Yakaboylu, A. Deuchert, and M. Lemeshko, Phys. Rev. Lett. 119, 235301 (2017)
[2] E. Yakaboylu, B. Midya, A. Deuchert, N. Leopold, and M. Lemeshko, arXiv:1809.01204 (2018)

TT 17.15 Mon 15:00 Poster D

Modeling of single impurity scattering in correlated fermionic systems — •Banhi Chatterjee[1], Jan Skolimowski[2], and Krzysztof Byczuk[3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]Jozef Stefan Institute, Ljubljana, Slovenia — [3]Institute of Theoretical Physics,Warsaw University, Warsaw,Poland

The one-body scattering formalism was modified [1] to describe effects of electronic correlations in many-body fermionic systems with a single impurity potential. We consider a single band model with the densities of states corresponding to Bethe, cubic and square lattice. Effects of correlations are accounted for using a model self-energy satisfying the Fermi liquid properties [2]. Here, we investigate effects of correlations on the spectral functions at the impurity site, scattering phase-shifts, and resonance energies. Depending on the geometry of the system a bound state may appear outside the continuous band for a strong enough impurity potential. However, these discrete eigen-energies are broadened when correlations are present. The bound state outside a continuum becomes a resonance-like state in correlated hosts. Our simple model can be useful in qualitative understanding of in-gap energy levels in real solids, which occur due to impurity atoms or defects with correlation Coulomb potential.
[1] K. Byczuk, B. Chatterjee, D. Vollhardt, arXiv:1807.08559, accepted for publication
[2] B. Chatterjee, K. Byczuk, JPCS: 592, 012059 (2015)

TT 17.16 Mon 15:00 Poster D

Exact Diagonalization study of large Hubbard clusters — •Mikhail Danilov[1], Sergei Iskakov[2], Malte Harland[1], Sergei Brener[1], Andrei Bagrov[3], Alexander Lichtenstein[1], and Mikhail Katsnelson[3] — [1]I. Institut für Theoretische Physik Jungiusstrasse 9, 20355 Hamburg, Germany — [2]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA — [3]Institute for Molecules and Materials, Radboud University, 6525AJ Nijmegen, The Netherlands

Using efficient exact diagonalization scheme, we study electronic structure of 4x4 doped Hubbard cluster with realistic hopping parameters including next nearest neighbour hopping t′ = -0.3t, which is optimal for superconducting cuprates.

To find possible candidates for superconducting regime we calculate the spectral function and network entanglement measures for different doping and Coulomb interaction.

TT 17.17 Mon 15:00 Poster D

Hydrodynamic charge and heat transport in graphene from a microscopic perspective — •Lars Fritz, Simonas Grubinskas, and Kitinan Pongsangangan — Institute for Theoretical Physics and Center for Extreme Matter and Emergent Phenomena, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

In this poster we present a description of charge and heat transport in graphene close to the Dirac point. Our starting point is microscopic and builds on a kinetic equation description, taking into account relaxation due to both interaction and disordering equal footing. Our results connect to recent experimental findings in which a strong violation of the Wiedemann-Franz law was found. We find that close to the Dirac point there is a sizeable contribution of plasmons to the heat conductivity which had not been discussed previously.

TT 17.18 Mon 15:00 Poster D

Quantum Monte Carlo simulations of quantum critical fermions — •Carsten Bauer[1], Yoni Schattner[2], Erez Berg[3], and Simon Trebst[1] — [1]University of Cologne, Germany — [2]Stanford University, USA — [3]The Weizmann Institute of Science, Israel

While quantum critical phenomena in insulators are fairly well understood, their metallic counterparts pose a substantial theoretical challenge since the order parameter fluctuations can interact with gapless excitations on a Fermi surface. When driving a metal through a phase transition, this interplay can give rise to unconventional superconductivity and "strange metal" behavior and might therefore serve as a microscopic model for some of the rich physics of high-T_c materials.

Fortunately, certain classes of metallic quantum critical points can be analyzed by determinant quantum Monte Carlo as one can circumvent the notorious "sign problem" and retain polynomial efficiency. I will show numerically exact studies of two dimensional metals at the verge of an antiferromagnetic transition indicating Landau-damped dynamics of the order parameter and a breakdown of Fermi liquid theory. I will further demonstrate that machine learning techniques, such as quantum loop topography and convolutional neural networks, can be utilized to probe transport and identify phase transitions in such many-particle systems.

TT 17.19 Mon 15:00 Poster D

Quantum skyrmions in a triangular frustrated ferromagnet — •Vivek Lohani[1], Ciarán Hickey[1], and Achim Rosch[1,2] — [1]Institute of Theoretical Physics, University of Cologne, Germany — [2]Department of Physics, Harvard University, Cambridge MA 02138, USA

Magnetic skyrmions are magnetization textures characterized by a topological winding number, initially discovered in chiral magnets. More recently, they were also predicted by Leonov and Mostovoy in a spin-1/2 Heisenberg ferromagnet with frustrated next-nearest neighbor interactions and spin-anisotropy. Their classical model predicts energetically degenerate skyrmions and antiskyrmions, and the emergence of a new zero mode, the helicity, reflecting rotation of spins around the z axis. The size of these frustration-stabilized skyrmions is also expected to be lesser than the ones found in chiral magnets. As a result, quantum properties of skyrmions might be of interest in insulating magnets at temperatures well below the bulk gap.

We investigate the existence of frustration-stabilized quantum skyrmions within a 31 site flake on a triangular lattice through exact diagonalization. We also derive the selection rules for the skyrmions in such a system. Next, we introduce a phenomenological Hamiltonian for mobile skyrmions and study couplings of the internal modes to the lowest order. This is then extended to an analysis of tunneling between skyrmions and antiskyrmions, and how the bandstructure is modified by the presence of tunneling terms, and its dependence on the number of flipped spins comprising the skyrmion.

TT 17.20 Mon 15:00 Poster D

Exotic criticality in the dimerized spin-1 XXZ chain with single-ion anisotropy — Satoshi Ejima[1], Tomoki Yamaguchi[2], Fabian H. L. Essler[3], Florian Lange[1], Yukinori Ohta[2], and •Holger Fehske[1] — [1]Institute of Physics, University Greifswald, 17489 Greifswald, Germany — [2]Department of Physics, Chiba University, Chiba 263-8522, Japan — [3]The Rudolf Peierls Centre for Theoretical Physics, Oxford University, Oxford OX1 3NP, UK

We consider the dimerized spin-1 XXZ chain with single-ion anisotropy D. In absence of an explicit dimerization there are three phases: a large-D, an antiferromagnetically ordered and a Haldane phase. This phase structure persists up to a critical dimerization, above which the Haldane phase disappears. We show that for weak dimerization the phases are separated by Gaussian and Ising quantum phase transitions. One of the Ising transitions terminates in a critical point in the universality class of the dilute Ising model. We comment on the relevance of our results to experiments on quasi-one-dimensional anisotropic spin-1 quantum magnets.

TT 17.21 Mon 15:00 Poster D

Antiferromagnetic magnons with strain — •Mary Madelynn Nayga[1], Stephan Rachel[2], and Matthias Vojta[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

Motivated by recent results on strain-induced pseudo-Landau levels in graphene, nodal superconductors, and other fermionic systems, we analyze analogous scenarios in bosonic systems. We focus on magnons and provide a combined analytical and numerical study of strain effects in Heisenberg antiferromagnets. We discuss the results vis-a-vis to the graphene case.

TT 17.22 Mon 15:00 Poster D

Interchain mean-field theory for thermodynamic properties of a bimetallic ferromagnetic spin-chain compound — •Maheshwor Tiwari[1], Stefan Süllow[2], Matthias Bleckmann[2], Ralf Feyerherm[3], Wolfram Brenig[4], and Andreas Honecker[1] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy-Pontoise, France — [2]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [4]Institut für Theoretische Physik, Technische Universität Braunschweig, Germany

Two energy scales are observed in the field-dependent specific heat of $MnNi(NO_2)_4(en)_2$, en = ethylenediamine, containing ferromagnetically coupled chains with alternating spins of magnitude 1 and 5/2. $MnNi(NO_2)_4(en)_2$ orders antiferromagnetically at low temperatures in low magnetic fields, demonstrating relevant antiferromagnetic interchain coupling, with a suppression of this order already by a weak magnetic field.

Here we present numerical results for the specific heat obtained by exact diagonalization and Quantum-Monte-Carlo simulations for the alternating spin chain model, using parameters that have been derived from the high-temperature behavior of the magnetic susceptibility. The interchain coupling is included in the numerical treatment at the mean-field level. The observed strong effect of an applied magnetic field on the ordered state promises interesting magnetocaloric properties that we explore theoretically.

TT 17.23 Mon 15:00 Poster D

Strategies for the design of antiferromagnetically coupled organic spin-dimer systems — •Lars Postulka[1], Paul Eibisch[1], Ulrich Tutsch[1], Bernd Wolf[1], Martin Baumgarten[2], Kubandiran Kolanji[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe Universität, SFB/TR49, D-60438 Frankfurt (M) — [2]Max-Planck-Institute for Polymer Research, SFB/TR49, D-55128 Mainz

Coupled antiferromagnetic spin-dimer systems based on stable biradicals are recognized as suitable candidates for exploring critical phenomena under well-controlled conditions. Depending on the topology of the *inter*-dimer couplings, various scenarios can be observed. The work aims at the development of novel spin-dimer systems where the *intra*- and *inter*-dimer magnetic exchange interactions can be modified in specific ways. We discuss the magneto-structural correlations of materials based on the stable radical units nitronyl-nitroxides (NN) and imino-nitroxides (IN) bridged with tolan molecules. Furthermore, using low-temperature ac susceptibility and specific heat measurements we characterize the field-induced magnetic phases of these materials and discuss their critical behavior. In addition, we present a new approach for designing the *intra*- and *inter*-molecular magnetic exchange interactions based on planar π-bridges of benzo[1,2 -*b*:4,5 -*b'*] dithiophene derivatives which connect the stable NN and IN radical units. Our results demonstrate that π-stacking of the planar bridges allows a good control of the *inter*-molecular magnetic exchange.

TT 17.24 Mon 15:00 Poster D

Strain-dependent electronic and magnetic properties of Sr_2CoIrO_6 double perovskite from DFT+U+SOC calculations — •Jiongyao Wu and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg

The electronic and magnetic properties of the double perovskite Sr_2CoIrO_6 (SCIO) are explored and compared to the end members $SrIrO_3$ (SIO) and $SrCoO_3$ (SCO) in the framework of density functional theory (DFT) including a Hubbard U term and spin-orbit coupling (SOC) with the PBEsol exchange correlation functional. While bulk SIO is metallic with a quenched spin and orbital moment, strong changes are observed for SCIO which shows insulating behavior with a band gap of ~ 200 meV and an Ir spin moment of 1.62 μ_B pointing towards a $j = 1/2$ Mott insulating state in the double perovskite. We analyze the electronic reconstruction in this system and furthermore consider the effect of strain on the electronic and structural properties of SCIO by varying the lateral lattice constant from the one of $NdGaO_3$ (compressive), through $SrTiO_3$ (unstrained) to $GdScO_3$ (tensile).

We acknowledge funding by the German Science Foundation within CRC/TRR80, project G3.

TT 17.25 Mon 15:00 Poster D

Charge-carrier doping in nickelate heterostructures — •Roberto Ortiz[1], Friederike Wrobel[1], Fanni Misják[3], Benjamin Geisler[2], Katrin Fürsich[1], Martin Bluschke[1], Enrico Schierle[4], Georg Christiani[1], Gennady Logvenov[1], Yi Wang[1], Peter van Aken[1], Bernhard Keimer[1], Ute Kaiser[3], Rossitza Pentcheva[2], and Eva Benckiser[1] — [1]Max Planck Institute, Stuttgart, Germany — [2]CENIDE, University Duisburg-Essen, Germany — [3]University Ulm, Germany — [4]Helmholtz-Zentrum, Berlin, Germany

Transition-metal oxides of the 3d series show a variety of interesting properties including robust metal-to-insulator transitions, multiferroicity and high-temperature superconductivity. One way to access these properties is to modify the charge carrier concentration by doping a particular system. In bulk materials, doping is mostly accomplished by substitution of cations, but the structural and chemical disorder generated in this way can drastically modify the electronic phase behavior and/or generate mesoscopic electronic inhomogeneities. We explore two distinctive methods of charge-carrier doping of nickelate heterostructures to investigate changes in the filling of 3d electronic states: The synthesis of $LaNiO_{2+x}$ - band-insulator superlattices by ex-situ layer-selective chemical reduction and the transfer of charge across metal-oxide interfaces in nickelate-cuprate hybrid structures.

TT 17.26 Mon 15:00 Poster D

Orbital polarization of vanadate superlattices — •Padma Radhakrishnan — Max Planck Institute for Solid State Research, Stuttgart, Germany

Rare earth vanadates (RVO_3), R- rare-earth element such as La, Y, etc have a rich phase diagram with two different spin and orbital orders depending upon the size of the lanthanide rare-earth cation [1] Heterostructuring these materials alters their structure through epitaxial strain and could further introduce spatial confinement and interface effects [2].
Multilayers of yttrium vanadate (YVO_3) with $LaAlO_3$ were grown using ultra-high-vacuum pulsed laser deposition on $NdGaO_3$ substrate. X-ray diffraction, scanning transmission electron microscopy and X-ray absorption revealed that the samples are of good quality and of pure phase. From Resonant reflectometry, depth resolved XAS profiles were obtained for the YVO_3 stack, which showed a clear modulation of the electronic structure between the interfacial and inner layers. Further, application of sum rules suggests that both types of layers have altered t_{2g} orbital occupations compared to that of bulk YVO_3, which is very likely to affect the orbital ordering and spin ordering at low temperatures.
[1] S. Miyasaka, Y. Okimoto, M. Iwama, and Y. Tokura, Phys. Rev. B, 68, 2003.
[2] E. Benckiser et al., Nature Materials, 10, 2011

TT 17.27 Mon 15:00 Poster D

LDA+DMFT Approach to Resonant Inelastic X-Ray Scattering in Correlated Materials — •Mathias Winder[1], Atsushi Hariki[1], and Jan Kuneš[1,2] — [1]Institute for Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Praha 8, Czech Republic

We present a computational study of *L*-edge resonant inelastic x-ray scattering (RIXS) in 3*d* transition-metal (TM) oxides: NiO; $RNiO_3$; Fe_2O_3; $LaCuO_3$ and $NaCuO_2$ [1], where we employ a theoretical approach based on local density approximation and dynamical mean-field theory (DMFT). We use the Anderson impurity model (AIM) with DMFT hybridization function extended by inclusion of core orbitals. This approach enables us to describe both localized (*d*-*d*) and delocalized (unbound electron-hole pair) excitations in the RIXS spectra. We discuss the relationship of correlated 3*d* bands and fluorescencelike feature in the RIXS spectra. Our calculated results reproduce the experimental data well and RIXS can be used as a tool to study material-specific hybridization between x-ray excited TM ion and low-energy states.
[1] A. Hariki, M. Winder, J. Kuneš, Phys. Rev. Lett. **121**, 126403 (2018)

TT 17.28 Mon 15:00 Poster D

Two-dimensional electron gas at the $KTaO_3$ surface and $KTaO_3$/EuO interface — •Xue-Jing Zhang[1] and Bang-Gui Liu[2] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Since the discovery of a two-dimensional (2D) electron gas at the $LaAlO_3/SrTiO_3$ interface, 2D carrier gases at such oxide interfaces and surfaces have attracted great attention because they can host many important phenomena and may produce novel functional devices. Here, we show through first-principles investigations that the surface 2D electron and hole gases in a $KTaO_3$ (KTO) thin film can be tuned by applying biaxial stress. When increasing compressive in-plane strain, the 2D carrier concentrations decrease down to zero and then a new pair of surface 2D electron and hole gases appears in which the carrier types are switched to the opposite ones. Our analysis indicates that this carrier-type switching occurs because the increasing compressive strain reverses the slope of monolayer-resolved electrostatic potential along the [001] direction. In addition, through first-principles investigations, we also study the KTO/EuO interfaces with oxygen vacancies in the KTO unit cell adjacent to EuO. We find that through interlayer exchange of the Eu-5d and Ta-5d, EuO drives the neighboring TaO_2 layer into a ferromagnetic state. These phenomena should be useful to design novel functional devices.

TT 17.29 Mon 15:00 Poster D

Tailoring $LaTiO_3$ for Mottronics — •Berengar Leikert[1], Philipp Scheiderer[1], Matthias Schmitt[1], Martin Stübinger[1], Judith Gabel[1], Tien-Lin Lee[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut und Röntgen Center for Complex Materials (RCCM), Universität Würzburg, Germany — [2]DIAMOND Light Source, Beamline I09, Didcot, England

3d transition metal oxides exhibit fascinating phenomena - absent in conventional semiconductors - like Mott insulating behaviour due to pronounced electron-electron interactions. The field of Mottronics dreams of harnessing the phase transition between the correlated metal and the Mott insulating phase of such strongly correlated materials for novel electronic devices.

We have recently demonstrated that the prototypical Mott insulator $LaTiO_3$ can undergo the band filling controlled Mott transition if it is chemically *p*-doped by excess oxygen during thin film growth by pulsed laser deposition. Here we report on the influence of dimensionality in the ultrathin film limit for varying doping levels by photoelectron spectroscopy, tuning the material in the generic phase diagram (correlation strength versus band filling) close to the boundary of the phase transition. Doing so the metal-insulator transition can possibly be triggered by electric field gating.

TT 17.30 Mon 15:00 Poster D

Exploring the potential gradient in the $LaFeO_3/SrTiO_3$ heterostructure by photoemission — •Martin Stübinger[1], Matthias Schmitt[1], Berengar Leikert[1], Pardeep Kumar Thakur[2], Tien-Lin Lee[2], Christoph Schlueter[3], Michael Sing[1], and Ralph Claessen[1] — [1]Universität Würzburg, Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), 97074 Würzburg, Germany — [2]Diamond Light Source Ltd., Didcot, Oxfordshire OX11 0DE, United Kingdom — [3]DESY Photon Science, 22607 Hamburg, Germany

In the oxide heterostructure $LaFeO_3/SrTiO_3$ (LFO/STO), the polar discontinuity between the polar LFO and the non-polar STO leads to a potential gradient in the LFO film. As opposed to the famous $LaAlO_3/SrTiO_3$ system, the built-in potential is not compensated by an electron transfer to the interface and a two-dimensional electron system does not emerge. Indeed, photovoltaic effects making use of the potential gradient to separate electrons and holes have been observed. Furthermore, different terminations of the STO substrate have been reported to change the direction of the potential. Hence, we investigated TiO_2- as well as SrO-terminated substrates. Angle-dependent photoemission was used to determine the potential gradient across the LFO film. The enhanced probing depth of hard x-ray photoemission (HAXPES) gave also access to the substrate core levels to provide a complete picture of the band alignment at the interface. Our results show an upward bending of the substrate bands toward the interface and a thickness-dependent potential gradient in the LFO film.

TT 17.31 Mon 15:00 Poster D

Magnetic anisotropy of the van der Waals ferromagnet $Cr_2Ge_2Te_6$. — •Alexey Alfonsov[1], Julian Zeisner[1,2], Sebastian Selter[1,2], Saicharan Aswartham[1], Bernd Büchner[1,2], and

Vladislav Kataev[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany

$Cr_2Ge_2Te_6$ compound is a quasi-two-dimensional semiconducting magnet belonging to the family of ferromagnetic layered transition metal trichalcogenides. Ferromagnetic order surviving even in the monolayer samples of these compounds renders these materials attractive for the fundamental research and for future technological applications. Such violation of Mermin-Wagner theorem is possible due to magnetic anisotropy present in these materials. Here we report an experimental study of the magnetic anisotropy in bulk single crystals of $Cr_2Ge_2Te_6$ by means of electron spin resonance (ESR) and ferromagnetic resonance (FMR) using conventional and torque-detected ESR spectrometers. Measurements were carried out in a wide frequency and temperature range, and at various angles between magnetic field and sample plane. Angular and frequency dependent measurements in the ferromagnetic phase clearly show the easy-axis type anisotropy of $Cr_2Ge_2Te_6$. Furthermore, simulation of the measured data based on a phenomenological approach yielded a precise value for the magnetocrystalline anisotropy energy density.

TT 17.32 Mon 15:00 Poster D

Charge Carrier Dynamics at the Metal-Insulator Transition in κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl — •Tatjana Thomas, Harald Schubert, and Jens Müller — Institute of Physics, Goethe University Frankfurt, Germany

The organic charge-transfer salts κ-$(ET)_2X$ are intensively studied due to their interesting electronic ground states, which are usually described within an effective-dimer model. In contrast, κ-$(ET)_2Hg(SCN)_2Cl$ exhibits a metal-insulator transition at $T_{MI} \sim 30\,K$ due to charge ordering [1]. Dimerization of the ET molecules in combination with charge localization on one molecule within the dimer leads to a net dipole moment, so that the system exhibits ferroelectric order of electronic type [2]. Additional magnetic order would make the system even multiferroic, as it was recently discussed for κ-$(ET)_2Cu[N(CN)_2]Cl$ [3]. Previous works on the latter salt showed that fluctuation (noise) spectroscopy provides new insights into the low-frequency charge carrier dynamics. Here, we present recent results on κ-$(ET)_2Hg(SCN)_2Cl$, where the normalized noise power spectral density shows an increase at the charge ordering transition. At low temperatures in the ferroelectric phase, we observe a strong electric field dependence of the fluctuation spectra. An observed spectral wandering is usually a hint for spatially correlated fluctuations. Measurements of the so-called second fluctuation spectrum indeed reveal a frequency dependence below the transition, indicating a switching between metastable states.

[1] PRB **89**, 075133
[2] JPSJ **79**, 011010
[3] Nat. Mater. **11**, 755

TT 17.33 Mon 15:00 Poster D

One-dimensional spin chains in $NaCuFe_2(VO_4)_3$ studied by high-frequency ESR and static magnetization — •Florian Theuss[1], Changhyun Koo[1], Alexander N. Vasiliev[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany. — [2]Lomonosov Moscow State University, Moscow, Russia

We report magnetization and high-frequency electron spin resonance spectroscopy data (HF-ESR) on the metal oxide $NaCuFe_2(VO_4)_3$. The magnetically active ions Fe^{3+} and Cu^{2+} in this compound form quasi-one-dimensional spin chains [1]. Magnetization data confirm the evolution of long-range antiferromagnetic order below $T_N = 9.3 \pm 0.4\,K$. At high temperatures, the data imply a Curie-Weiss-like behaviour with the Weiss temperature $\Theta \approx 81.2\,K$. However, no AFM resonances are observed at low temperatures. Instead, the HF-ESR spectra show a single broad resonance feature without sizeable zero-field splitting. Upon heating, this resonance shifts to a smaller g-factor associated with Fe^{3+}-spins. Based on the these data, the AFM ordered phase of the compound will be discussed.

[1] A.V. Koshelev et. al., arXiv:1711.06990v1

TT 17.34 Mon 15:00 Poster D

***In−situ*-SQUID studies of Fe_3O_4 and V_2O_3 upon electrochemical lithiation** — •Lukas Deeg, Elisa Thauer, Michael Richter, and Rüdiger Klingeler — Kirchhoff Institut für Physik, Universität Heidelberg, D-69120 Heidelberg, Germany

A re-usable *in-situ*-SQUID electrochemical cell for magnetisation studies during electrochemical cycling is presented. The proof of function is demonstrated by recording reversible magnetisation changes in $Li_xFe_3O_4$ nanoparticles upon electrochemical cycling. The data imply the transition from inverse spinel structure ($x = 0$) to a rocksalt phase ($x = 2$). In addition, the setup is utilised to study the effect of lithiation on the Mott-Hubbard transition in V_2O_3.

TT 17.35 Mon 15:00 Poster D

Single-crystal growth and magnetic phase diagram of Li_2FeSiO_4 — •Waldemar Hergett[1], Christoph Neef[1], Sven Sauerland[1], Martin Jonak[1], Mahmoud Abdel-Hafiez[1], Hubert Wadepohl[2], Clemens Ritter[3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University — [2]Institute of Inorganic Chemistry, Heidelberg University — [3]Institut Laue-Langevin, Grenoble

By using the high-pressure optical floating-zone technique (FZ), mm-sized single crystals of γ_{II}-Li_2FeSiO_4 (space group $Pmnb$) were grown and characterized for the first time. Oriented cuboids were used for thermal expansion, specific heat, and magnetisation studies. High-resolution neutron powder diffraction experiments were performed to resolve the magnetic ground state and analyse the Li-Fe antisite disorder. The impact of different synthesis routes of the starting materials and of FZ growth parameters on the crystal quality was investigated. The single crystal structure of the $Pmnb$-polymorph was solved for the first time. Thermal expansion, magnetisation and specific heat data show a sharp λ-like anomaly associated with the onset of long-range antiferromagnetic order at $T_N = 17.0(5)$ K. Pulsed-field magnetisation studies up to 60 T enable constructing the magnetic phase diagram.

TT 17.36 Mon 15:00 Poster D

Static magnetic order in γ-Li_2FeSiO_4 as probed by ^{57}Fe Mössbauer spectroscopy — •Felix Seewald[1], Sascha Albert Bräuninger[1], Rüdiger Klingeler[2], Waldemar Hergett[2], and Hans-Henning Klauss[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany — [2]Kirchhoff Institute of Physics, Heidelberg University, D-69120 Heidelberg, Germany

γ-Li_2FeSiO_4 is proposed as a promising candidate material for lithium ion batteries. The Fe atoms are tetrahedrally coordinated by Oxygen. Iron has the Fe^{2+} (S=2) oxidation state and is displaced from the tetrahedron center resulting in a electric field gradient caused by the distorted tetrahedral crystal field. The Mössbauer spectrum of the powder sample shows one dominant site exhibiting magnetic order at 2.1 K and a considerable quadrupole splitting as observed at room temperature. The magnetic hyperfine field of $B = 14.7(4)$ T is oriented orthogonal to the largest principle axis of the electrical field gradient $V_{zz} = -125(3)\,V/Å^2$. The isomer shift of $\delta = 1.1(1)$ mm/s is consistent with the high spin Fe^{2+} (S=2) state. We will discuss the implications of these findings on the actual magnetic structure in this system. The observed static order is in agreement with susceptibility measurements showing a transition to antiferromagnetic order below 17 K.

TT 17.37 Mon 15:00 Poster D

The contribution of magnetic oxygen and magnetic correlations in the Mott insulator Ca_2RuO_4 — •Kevin Jenni[1], Stefan Kunkemöller[1], Yvan Sidis[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Deutschland — [2]Laboratoire Léon Brillouin, CEA, Saclay

The Ruthenate system $Ca_{2-x}Sr_xRuO_4$ exhibits a variety of interesting phenomena reaching from unconventional superconductivity in Sr_2RuO_4 to a Mott-insulating state in Ca_2RuO_4. Concerning the latter, the theoretical understanding of the Mott transition in this multi-band system with four electrons per Ru site is under debate to this day. There is consensus that the orbital ordering appearing in this strongly correlated material leads to an enhanced or fully occupation of the d_{xy} orbital and an occupation of the $d_{xz,yz}$ orbitals by the remaining two electrons. However, this orbital occupation only roughly corresponds to the measured ordered moment of 1.3 μ_B. To yield better insight in the exact distribution of the ordered magnetic moment over the orbitals we analyzed the magnetic form factor in detail. Our elastic neutron scattering study of an untwinned single crystal in combination with polarization analysis exposes the contribution of the apical oxygen to the ordered magnetic moment, similar to the results in $Ca_{1.5}Sr_{0.5}RuO_4$ where the p-d hybridization causes a sizeable amount of magnetic moment residing on the oxygen. Additionally we present the analysis of magnetic correlations and their dimensionality.

The magnetic Bragg peak intensity vanishes rather fast above T_N = 110 K indicating a 3D correlation of the magnetic order.

TT 17.38 Mon 15:00 Poster D

Nonequilibrium Green Functions for Excited Lattice Systems—A Case Study of the Artificial Damping — •Niclas Schlünzen, Jan-Philip Joost, and Michael Bonitz — CAU Kiel, Germany

The accurate description of nonequilibrium dynamics in correlated quantum-many-body systems remains to be a driving force for current research in condensed-matter physics and beyond. Among others, the nonequilibrium Green functions (NEGF) method has proven to be a powerful tool to predict quantum behavior[1], especially in the context of lattice systems[2]. Due to its two-time structure the NEGF approach gives access to two-particle and two-time observables, e.g. the double occupation and spectral properties. In 2009, von Friesen *et. al* reported the occurance of unphysical damping effects in NEGF calculations for strongly excited Hubbard clusters[3]. Since then, several ways have been proposed to overcome this deficiency by reducing the degree of selfconsistency[3,4]. Here, we focus on (time-dependent) spectral properties for finite Hubbard systems and the respective impact of both the artificial damping itself and the common methods of resolution. Furthermore, we introduce a controlled way to adjust the depth of selfconsistency based on the Dyson equation and compare its performance to previous approaches.

[1] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[2] N. Schlünzen *et al.*, Phys. Rev. B **95**, 165139 (2017)
[3] M. P. von Friesen *et al.*, Phys. Rev. Lett. **103** 176404 (2009)
[4] S. Hermanns *et al.*, Phys. Rev. B **90**, 125111 (2014)

TT 17.39 Mon 15:00 Poster D

***Ab initio* results for the dynamic structure factor of strongly correlated electrons** — Simon Groth, Tobias Dornheim, •Jan-Philip Joost, and Michael Bonitz — ITAP, CAU Kiel, Leibnizstraße 15, 24229 Kiel

The accurate description of electrons at high density and finite temperature is of paramount importance for, e.g., the understanding of astrophysical objects and correlated materials. In this context, the dynamic structure factor $S(q,\omega)$ constitutes a key quantity as it is directly measured e.g. in X-ray Thomson scattering experiments. We have recently [1] obtained the first *ab initio* results for $S(q,\omega)$ by carrying out extensive path integral Monte Carlo simulations and developing a new method for the required analytic continuation, which is based on the stochastic sampling of the dynamic local field correction $G(q,\omega)$. A particularly interesting result is the confirmation of a negative plasmon dispersion in the correlated liquid regime. This extends our recent work on the *ab initio* thermodynamic results of the warm dense electron gas [2] to dynamic quantities. These results are compared with an independent approach that is based on nonequilibrium Green functions [3].

[1] T. Dornheim, S. Groth, J. Vorberger, and M. Bonitz, Phys. Rev. Lett., in press, arxiv:1810.12776
[2] T. Dornheim, S. Groth, and M. Bonitz, Phys. Reports **744**, 1-86 (2018)
[3] N.H. Kwong and M. Bonitz, Phys. Rev. Lett. **84**, 1768 (2000)

TT 17.40 Mon 15:00 Poster D

Exact high-density limit calculation for quantum wires — •Klaus Morawetz[1,2], Vinod Ashokan[3], Renu Bala[4], and Kare Narain Pathak[3] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [3]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [4]Department of Physics, MCM DAV College for Women, 160036 Chandigarh, India

It is shown that in d-dimensional systems, the vertex corrections beyond the random phase approximation (RPA) or GW approximation scales with the power $d-\beta-\alpha$ of the Fermi momentum $\epsilon_f \sim p_f^\beta$ where the interacting potential possesses a momentum-power-law of $\sim p^{-\alpha}$. The condition $d < \beta + \alpha$ specifies systems where RPA is exact in the high-density limit. A cancellation of RPA and vertex corrections occurs up to second-order contact interaction. For finite-range potentials of cylindrical wires the structure function and correlation energy is found to be independent of the width parameter. The proposed high-density expansion agrees with diffusive Monte Carlo simulations and a fit formula is presented for the correlation energy.

[1] K. Morawetz, V. Ashokan, R. Bala, K. N. Pathak, Phys. Rev. B 97 (2018) 155147
[2] V. Ashokan, R. Bala, K. Morawetz, K. N. Pathak, Eur. Phys. J. B 91 (2018) 29, 1-7

TT 17.41 Mon 15:00 Poster D

Method for the DC-Conductance of one-dimensional correlated systems — •Jan-Moritz Bischoff and Eric Jeckelmann — Institut für Theoretische Physik, Hannover , Deutschland

We present a method for the linear DC-conductance of correlated one-dimensional lattice models[1]. Here specifically, we are interested in the conductance of Luttinger liquids. The method is based on the extrapolation of dynamical correlator functions in finite systems to the thermodynamic limit. We use a modified variant of the Density Matrix Renormalization Group(DMRG) algorithm to calculate the dynamical correlation function. We show that our method reproduces the predicted behaviour of the conductance in Luttinger liquids with impurities[1,3]. We investigate the complex behaviour of the spin and charge conductance of finite wires between leads and homogeneous electron-phonon systems.

[1] J.-M. Bischoff and E. Jeckelmann, PRB 96, 195111 (2017)
[2] C.L. Kane and M.P.A. Fisher, PRB 46, 15233 (1992)

TT 17.42 Mon 15:00 Poster D

Entanglement properties in quantum phases of the asymmetric two-leg Hubbard ladder — •Anas Abdelwahab and Eric Jeckelmann — Leibniz Universität Hannover, Institut für Theoretische Physik, Appelstr. 2, 30167 Hannover

We investigate entanglement properties of an asymmetric two-leg Hubbard ladder that consists of one Hubbard leg and one tight-binding leg[1,2]. We use the density matrix renormalization group method to study the von Neumann entropy, central charge, Schmidt gap and entanglement spectrum for different quantum phases that appear by varying the inter-leg hopping term. We can distinguish the gapless and the correlated band insulating phases[1,2] using the entanglement properties in the ground state. The differences in entanglement properties between the Kondo-Mott and the spin-gaped Mott insulating phases[1,2] are less clear.

[1] A. Abdelwahab, E. Jeckelmann, and M. Hohenadler, Phys. Rev. B 91, 155119 (2015)
[2] A. Abdelwahab and E. Jeckelmann, Eur. Phys. J. B 91, 207 (2018)

TT 17.43 Mon 15:00 Poster D

Linear-Response charge dynamics of the Hubbard model from the time-dependent Gutzwiller approximation — •Katharina Noatschk and Götz Seibold — Institut für Physik, BTU Cottbus-Senftenberg, Postfach 101344, 03013 Cottbus, Germany

The time dependent Gutzwiller approximation for the Hubbard model is obtained from the Lagrangian equation of motion for the density matrix and variational parameters. Expansion of the resulting equations up to second order in these dynamical variables yields an effective electron-boson problem where the bosons represent fluctuations of the double occupancy [1]. Within this formalism we investigate the charge excitations of the single-band Hubbard model for parameters relevant for cuprate superconducters. We also supplement the model with long-range Coulomb interaction and compare resulting excitations with experimental data from electron loss spectroscopy.

[1] J. Bünemann, M. Capone, J. Lorenzana, G. Seibold, New J. Phys., 2013

TT 17.44 Mon 15:00 Poster D

Building effective models for correlated electron systems — •Qian Zhang and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

To understand strongly correlated systems, we must confront the many-body problem. Our starting point is density functional calculations for individual atoms and ions to obtain realistic basis functions and the corresponding matrix elements. In particular, we focus on the open-shell orbitals, which have the strongest correlation effects. For individual atoms and ions, we collected the Slater-Condon and spin-orbit parameters from the resulting self-consistent radial wave functions and potentials. We analyzed the trends of the parameters systematically across the periodic table, which allowed us to calculate atomic open-shell spectra in LS-, intermediate-, and jj-coupling schemes.

While atomic orbitals are mutually orthogonal within a single atom, they are, in general, non-orthogonal for atoms on different lattice sites. We studied and developed efficient multi-center integral techniques for

evaluating orbital overlaps, which are essential for performing orbital orthogonalization. This allowed us to study atomic orbitals in various crystal structures. To orthogonalize the basis orbitals, we applied the Löwdin symmetric orthogonalization scheme, which minimizes the orbital modification. For the resulting orbitals, we studied the deformation due to orthogonalization and investigated the modification of the matrix elements compared with the atomic ones.

TT 17.45 Mon 15:00 Poster D

Real-Space DMFT with Classical Long-Range Coulomb Interactions: a Model Study — •Andreas Weh[1], Liviu Chioncel[1], Ulrich Eckern[1], and Junya Otsuki[2] — [1]Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Department of Physics, Tohoku University, Sendai, Japan

We present details of the numerical implementation of the charge self-consistent real-space dynamical mean-field theory (DMFT) for the Hubbard model considering long-range Coulomb effects at the local mean-field level. Results for spin-polarized multi-layers with different parameters are presented.

TT 17.46 Mon 15:00 Poster D

Robustness of transport and localization effects in long-range coupled spin chains — •Manuel Katzer and Alexander Carmele — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We study the transport properties of a disordered Heisenberg spin chain with long-range interaction [1] to shed light on excitation localization properties in the presence of gain and dissipation. The long-range coupled chain shows nearly ballistic transport and linear response for all potential differences of the external reservoirs. In contrast, the common isotropic nearest-neighbor coupling shows negative differential conductivity and a transition from diffusive to subdiffusive transport for a far-from-equilibrium driving. For the disordered long-range coupled XXZ chain, any change in the transport behavior is independent of the potential difference and the coupling strengths of the external reservoirs and provides a robust platform to study many-body localization properties. Furthermore, we investigate the transition from a spin chain to a network of coupled harmonic oscillators [2], with nonclassical saturation effects and emerging nonlinear behavior, leading to anomalous energy transport.
[1] L. Droenner and A. Carmele Phys. Rev. B **96**, 184421 (2017)
[2] J. Huber and P. Rabl, arXiv:1807.10189

TT 17.47 Mon 15:00 Poster D

Heat transport through 1D spin chains — •Sonja Fischer and Lars Fritz — Utrecht University, Institute for Theoretical Physics, Princetonplein 5, 3584 CC Utrecht

We investigate the steady-state energy transport through a system of two coupled 1D spin chains at different temperatures. For two identical XX or Ising chains we recover the conjectured expression $J_E = \frac{c\pi}{12}(T_L^2 - T_R^2)$ for gapless chains with a conformal charge c [1] and show how this result can be generalized to non-equal chains. In addition we also consider a system with an XX chain coupled to an Ising chain, where the conjecture [1] does not apply and show that the energy transport can be controlled via a magnetic field.
[1] C. Karrasch, R. Ilan and J. E. Moore, PRB 88 195129 (2013)

TT 17.48 Mon 15:00 Poster D

Transient dynamics of the Hubbard model with nearest- and next-nearest-neighbor hopping — •Yusuf Mohammed and Alexander I. Lichtenstein — Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany

We investigate the transient dynamics of the single orbital two-dimensional Hubbard model with nearest- and next-nearest-neighbor hopping. In equilibrium this model has provided a strong-coupling approach to the theory of high-temperature superconductivity as observed in copper oxides. We employ non-equilibrium cluster dynamical mean-field theory (CDMFT), using self-consistent strong-coupling perturbation theory, with the non-crossing approximation (NCA) being the lowest order. We report results for different quench protocols and driving fields.

TT 17.49 Mon 15:00 Poster D

Prescaling in a far-from-equilibrium Bose gas — Christian-Marcel Schmied[1], •Aleksandr Mikheev[2], and Thomas Gasenzer[3] — [1]christian-marcel.schmied@kip.uni-heidelberg.de — [2]aleksandr.mikheev@kip.uni-heidelberg.de — [3]t.gasenzer@uni-heidelberg.de

Non-equilibrium conditions give rise to a class of universally evolving low-energy configurations of fluctuating dilute Bose gases at a non-thermal fixed point (NTFP). While the fixed point and thus full scaling in space and time is generically only reached at very long evolution times, we here propose that systems can show prescaling much earlier, on experimentally accessible time scales. During the prescaling evolution, some well-measurable short-distance properties of the spatial correlations already scale with the universal exponents of the fixed point, while others still show scaling violations. Prescaling is characterized by the evolution obeying already, to a good approximation, the conservation laws which are associated with the asymptotically reached NTFP, defining its belonging to a specific universality class. In our simulations, we consider $N = 3$ spatially uniform three-dimensional Bose gases of labeled, e.g., by different hyperfine magnetic quantum numbers, with identical inter- and intra-species interactions. In this system, the approach of a NTFP is marked by low-energy phase excitations self-similarly redistributing towards smaller wave numbers. During prescaling, the full $U(N)$ symmetry of the model is broken, while the conserved transport, reflecting the remaining $U(1)$ symmetries, leads to the buildup of a rescaling quasicondensate distribution.

TT 18: Poster Session: Topological Topics (joint session TT/MA)

Time: Monday 15:00–18:30 Location: Poster D

TT 18.1 Mon 15:00 Poster D

Helical edge state interferometry in a quantum spin Hall insulator — •Raul Stühler, André Kowalewski, Felix Reis, Johannes Weis, Jörg Schäfer, and Ralph Claessen — Physikalisches Institut (EP4) der Universität Würzburg, 97074 Würzburg, Germany

Since the discovery of the quantum spin Hall (QSH) effect, two-dimensional topological insulators (2D-TI) have constituted a promising system for spintronics and ballistic electronic transport. The latter property of 2D-TIs is based on exceptional quantum coherence of helical edge state electrons in the absence of time-reversal symmetry breaking. Notwithstanding, quantum interference between helical edge state electrons becomes relevant when a multitude of helical edge state pairs are being brought into direct proximity in a nano-constriction. Here we present the realization of a helical edge state nano-constriction embedded in the high-temperature 2D-TI bismuthene [1], formed by an anti-phase domain boundary of limited extent. Via STS, we prove quantum interference between counter propagating helical electrons and make use of an analogy to a Fabry-Pérot electronic resonator. Such interplay between quantum coherence and interference might be further exploited, e.g., as a controllable charge and spin current switch operated with gate voltages instead of magnetic fields [2].
[1] F. Reis et al., Science 357, 287-290, (2017)
[2] P. Sternativo, F. Dolcini, Phys. Rev. B 89, 035415 (2014).

TT 18.2 Mon 15:00 Poster D

Potassium-Induced n-Doping of the High-Temperature Quantum Spin Hall System Bismuthene on SiC(0001) — •Johannes Weis, André Kowalewski, Felix Reis, Raul Stühler, Felix Spriestersbach, Lenart Dudy, Victor Rogalev, Jörg Schäfer, and Ralph Claessen — Physikalisches Institut und Röntgen Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany

Bismuthene, a monolayer of Bi-atoms bonded onto a SiC(0001) substrate in a honeycomb lattice, has recently been experimentally realized [1]. This 2D system has a large band gap of approx. 0.8 eV and is a most promising candidate for the realization of the quantum spin Hall effect at room-temperature. Theoretical tight-binding and DFT calcu-

lations consistently predict the existance of helical edge states forming Dirac branches. While Reis et al. [1] showed proof for 1D metallic edge states spanning the 2D bulk band gap by means of STM and STS, up to date a direct experimental observation of the linear electron dispersion has not been reported and ARPES would be highly desirable.

One major obstacle here is the Fermi level being too close to the 2D bulk valence band maximum. Here we present the adsorption of potassium as a tool to shift the Fermi level above the predicted Dirac point in a controlled way. The effect of the dopant has been investigated both on an atomic level by STM and STS and spacially integraged by ARPES.

[1] F. Reis *et al.*, Science 357,287-290 (2017)

TT 18.3 Mon 15:00 Poster D

Electronic correlation effects on double Dirac semimetals — •Niklas Wagner[1], Domenico Di Sante[1], Sergio Ciuchi[2], and Giorgio Sangiovanni[1] — [1]Institut fuer Theoretische Physik und Astrophysik, Universitaet Wuerzburg, Germany — [2]Department of Physical and Chemical Sciences, University of L'Aquila, Italy

Particles without a high-energy analog, namely special multiple-degeneracy points in the electronic bandstructure of solids protected by fundamental symmetries of the underlying lattice, have been recently postulated in condensed matter physics [1]. A particularly interesting example is that of space groups Nr. 130 and 135, whose Brillouin zones host double Dirac points at high-symmetry points [2]. We study tight-binding models for these two space groups and look at the influence of electronic correlation on the eightfold degeneracies at the touching points of their valence and conduction bands. To this aim, we use methods ranging from simple approaches like the Hubbard-I and Hubbard-III approximations, to more sophisticated ones including DMFT and cluster extensions thereof [3].

[1] B. Bradlyn, et al., Science 353, aaf5037 (2016)
[2] B. Wieder, et al., PRL 116, 186402 (2016)
[3] D. Di Sante, et al., PRB 96, 121106(R) (2017)

TT 18.4 Mon 15:00 Poster D

Bychkov-Rashba Spin-Orbit Coupling Effects in a Multi-Band Tight-Binding Model of Graphene — •Thorben Schmirander, Marta Prada, and Daniela Pfannkuche — I. Institut für theoretische Physik - Universität Hamburg, Hamburg, Deutschland

The description of Dirac electrons in the band structure of graphene is commonly performed using effective tight binding models [1]. These effective models use single-orbital Hamiltonians with modified hopping parameters in order to account for the influence of the higher energy orbitals in graphene. We go beyond such effective models by including d-orbitals in an atomistic tight-binding model. The inclusion of the Bychkov-Rashba spin-orbit coupling splits each of the two Dirac cones into four distinct ones [2]. When considering a finite graphene sample, edge states occur, which cross the band gap and connect the Dirac cones at the K and K' point. These edge states are the key to the topological properties of graphene. The crossing of the edge states under the influence of Bychkov-Rashba spin-orbit coupling is examined by computing the winding number around each of the cones.

[1] van Miert, G., Juricic, V. and Morais Smith, C. Phys. Rev. B 90, 195414 (2014)
[2] van Gelderen, R. and Morais Smith, C., Phys. Rev. B 81, 125435 (2010)

TT 18.5 Mon 15:00 Poster D

Surface currents in Weyl semimetal nanowires — •Patrick Grössing, Daniel Hernangómez-Pérez, and Ferdinand Evers — Institute of Theoretical Physics, Regensburg University, D-93053 Regensburg (Germany)

We investigate the transport properties of thin wires made of a Weyl semimetal within the framework of a tight-binding model. Our focus is on bias induced surface currents in materials where time-reversal symmetry is broken because of magnetisation [1, 2]. Depending on the crystallographic growth direction, the current flow exhibits different patterns; in particular, large transverse (wrapping) currents can be observed. We perform a careful finite size analysis that reveals,. e. g., the interplay between quantum size effects and the Fermi arcs, which are a hallmark of the topological nature of the material [3, 4].

[1] P. Baireuther et al., New J. Phys. 18, 045009 (2016)
[2] A. Igarashi et al., Phys. Rev. B 95, 195306 (2017)
[3] F. D. M. Haldane, arXiv:1401.0529 (2014)
[4] Y. Chen et al., Phys. Rev. B 88, 125110 (2013)

TT 18.6 Mon 15:00 Poster D

Anomaly transport ingraphene and Weyl semimetals — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

Based on the quantum kinetic equations for systems with SU(2) structure, regularization-free density and pseudospin currents are calculated in Graphene and Weyl-systems realized as the infinite-mass limit of electrons with quadratic dispersion and a proper spin-orbit coupling. Correspondingly the currents possess no quasiparticle part but only anomalous parts. The intraband and interband conductivities are discussed. The optical conductivity agrees well with the experimental values using screened impurity scattering and an effective Zeeman field. The universal value of Hall conductivity is shown to be modified due to the Zeeman field. The chiral anomalous terms are shown to be derivable from a conserving transport theory and their usually believed origin is questioned.

[1] arXiv:1809.01547, arXiv:1806.06214, Phys. Rev. B 94 (2016) 165415, Phys. Rev. B 92 (2015) 245425, errata: Phys. Rev. B 93 (2016) 239904(E), Phys. Rev. B 92 (2015) 245426

TT 18.7 Mon 15:00 Poster D

Edge currents as a probe of the strongly spin-polarized topological noncentrosymmetric superconductors — •M. Biderang[1,2], M.H. Zare[3], H. Yavari[2], P. Thalmeier[4], and A. Akbari[1,5] — [1]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Korea — [2]Department of Physics, University of Isfahan, Isfahan, Iran — [3]Department of Physics, Faculty of Science, Qom University of Technology, Qom, Iran — [4]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [5]Department of Physics, POSTECH, Pohang, Korea

Recently the influence of antisymmetric spin-orbit coupling has been studied in novel topological superconductors such as half-Heusler compounds and artificial heterostructures. We investigate the effect of Rashba and/or Dresselhaus spin-orbit couplings on the band structure and topological properties of a two-dimensional noncentrosymmetric superconductor. For this goal, the topological helical edge modes are analyzed for different spin-orbit couplings as well as for several superconducting pairing symmetries. To explore the transport properties, we examine the response of the spin-polarized edge states to an exchange field in a superconductor-ferromagnet heterostructure. The broken chiral symmetry causes the unidirectional currents at opposite edges[1].

[1] M. Biderang et al., Phys. Rev. B 98, 014524 (2018)

TT 18.8 Mon 15:00 Poster D

Decoherence of Majorana edge modes under adiabatic drives — •Zihao Gao, Yuval Vinkler-Aviv, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, D-50937 Cologne, Germany

We study how Majorana edge modes behave under adiabatic movement in the presence of disorder, interactions and thermal fluctuations. In a 1D Kitaev chain, zero-energy Majorana bound states are formed at the edges of the topological region. Such Majorana edge modes are robust due to protection by an energy gap and their spatial separation. Therefore they can effectively encode a qubit, and are believed to be useful for quantum computation. By controlling the chemical potential we have the ability to adiabatically move these Majorana edge modes. However, during this process, disorder, interactions and thermal fluctuations can be harmful to the fidelity of the Majorana qubit. We numerically calculate the time-evolution of a Majorana qubit in such a setup in order to measure the decoherence from different sources, applying approximations based on exploiting the adiabatic nature of the movement and the protection by the gap.

TT 18.9 Mon 15:00 Poster D

Anyonic statistics of quantum impurities in two dimensions — •Enderalp Yakaboylu and Mikhail Lemeshko — IST Austria (Institute of Science and Technology Austria)

We demonstrate that identical impurities immersed in a two-dimensional many-particle bath can be viewed as flux-tube-charged-particle composites described by fractional statistics. In particular, we find that the bath manifests itself as an external magnetic flux tube with respect to the impurities, and hence the time-reversal symmetry is broken for the effective Hamiltonian describing the impurities. The

emerging flux tube acts as a statistical gauge field after a certain critical coupling. This critical coupling corresponds to the intersection point between the quasiparticle state and the phonon wing, where the angular momentum is transferred from the impurity to the bath. This amounts to a novel configuration with emerging anyons. The proposed setup paves the way to realizing anyons using electrons interacting with superfluid helium or lattice phonons, as well as using atomic impurities in ultracold gases [1].

[1] E. Yakaboylu and M. Lemeshko, Phys. Rev. B 98, 045402 (2018)

TT 18.10 Mon 15:00 Poster D

Truncation of lattice fractional quantum Hall Hamiltonians derived from CFT — •Srivatsa N. S[1], Dillip Nandy[2], and Anne E. B. Nielsen[3] — [1]MPIPKS, Dresden, Germany — [2]Aarhus University, Aarhus, Denmark — [3]MPIPKS, Dresden, Germany

Conformal field theory has recently been applied to derive few-body Hamiltonians whose ground states are lattice versions of fractional quantum Hall states. The exact lattice models involve interactions over long distances, which is difficult to realize in experiments. It seems, however, that such long-range interactions should not be necessary, as the correlations decay exponentially in the bulk. This poses the question, whether the Hamiltonians can be truncated to contain only local interactions without changing the physics of the ground state. Previous studies have in a couple of cases with particularly much symmetry obtained such local Hamiltonians by a combination of guesswork and numerical optimization. Here, we propose a different strategy to construct truncated Hamiltonians, which does not rely on optimization, and which can be applied independent of the choice of lattice. We test the approach on models with bosonic Laughlin-like ground states and find that the overlaps per site between the states constructed from conformal field theory and the ground states of the truncated models are higher than 0.98 for all the studied lattices.

TT 18.11 Mon 15:00 Poster D

Effects of topological line defects on two-dimensional electronic transport — •Nico Bassler and Kai Schmidt — Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

We investigate the effect of topological line defects on the transport properties of two-dimensional electronic systems. Experimentally, this is mostly motivated by bilayer graphene which is known to host a superstructure of line defects separating AB- and BA-stacking domains. More concretely, we study microscopically specific arrangements of such line defects by calculating the conductance, local densities, and topological invariants using an effective one-particle description for bilayer graphene in a magnetic field. In addition, we compare our findings to the well-known Haldane model on the honeycomb lattice, which is exactly solvable in the absence of line defects and displays a topologically non-trivial band structure.

TT 18.12 Mon 15:00 Poster D

Robustness of Haah's code in a magnetic field — •Matthias Walther and Kai Phillip Schmidt — Institut für Theoretische Physik I FAU Erlangen-Nürnberg, Erlangen, Deutschland

Haah's cubic code is an exactly solvable three-dimensional quantum spin model realizing topological fracton order. It is a promising candidate for self correcting quantum memory due to its macroscopic energy barrier between different ground states. Here we analyse the quantum robustness of this topological fracton order in a homogeneous magnetic field at zero temperature. Technically, this is achieved by applying the method of perturbative continuous unitary transformations and a mean-field approach. In all cases studied, we find strong first-order phase transitions separating the topological fracton phase and the polarized phase.

TT 18.13 Mon 15:00 Poster D

Quantum phase transitions to topological Haldane phases in spin-one chains studied by linked-cluster expansions — •Patrick Adelhardt[1], Julian Gritsch[1], Marvin Hille[2], David Anselm Reiss[1], and Kai Phillip Schmidt[1] — [1]Institute for Theoretical Physics, FAU Erlangen-Nürnberg, Germany — [2]Lehrstuhl für Theoretische Physik 1, TU Dortmund, Germany

We use linked-cluster expansions to analyze the quantum phase transitions between symmetry-unbroken trivial and topological Haldane phases in two different spin-one chains. The first model is the spin-one Heisenberg chain in the presence of a single-ion anisotropy, while the second one is the dimerized spin-one Heisenberg chain. For both models, we determine the ground-state energy and the one-particle gap inside the nontopological phase as a high-order series using perturbative continuous unitary transformations. Extrapolations of the gap series are applied to locate the quantum critical point and to extract the associated critical exponent. We find that this approach works unsatisfactorily for the anisotropic chain, since the quality of the extrapolation appears insufficient due to the large correlation length exponent. In contrast, extrapolation schemes display very good convergence for the gap closing in the case of the dimerized spin-one Heisenberg chain.

TT 19: Poster Session: Disordered Quantum Systems

Time: Monday 15:00–18:30 Location: Poster D

TT 19.1 Mon 15:00 Poster D

Weak localization corrections to the thermal conductivity in disordered conventional superconductors — •Lucía González[1,2], Gianluigi Catelani[1], and Fabian Hassler[2] — [1]JARA-Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

Particle diffusion in a disordered system is affected by quantum interference between self intersecting paths giving rise to weak localization and weak anti-localization effects, which respectively decrease or increase the probability of diffusion.

We study the corrections to the thermal conductivity in conventional superconductors due to such effects using semiclassical Green's functions. We analyze the repercussions of time reversal symmetry breaking by including a supercurrent flow.

TT 19.2 Mon 15:00 Poster D

Direct Probing of the Nuclear Quadrupole Impact onto Tunnelling Systems in Glasses at Low Temperatures — •Aljoscha Auer, Lukas Münch, Benedikt Frey, Andreas Schaller, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University

The low temperature behaviour of amorphous solids are often well described with the phenomenological standard tunneling model (STM), which assumes a distribution of two level systems (TLS) inside the glass. However, several experiments like polarisation echo experiments and dielectric measurements on glasses containing large nuclear quadrupole moments have shown significant deviation from the STM. Thus over the years several extensions revolving around the coupling of Nuclear Quadrupole Moments (NQM) to local electric field gradients were proposed.

To get a better understanding of this mechanism we measured the TLS dynamics via the dielectric permittivity. Hereby we tune the frequency to the nuclear quadrupole frequency. In the second experiment we measured the low frequency dielectric permittivity using a superconducting interdigital capacitor surrounded by a single-loop coil. This coil enables us to apply a radio-frequency magnetic field at the dominant quadrupole splitting frequency to the sample, while directly measuring the dielectric response. We will present this new approach as well as current data from both experiments.

TT 19.3 Mon 15:00 Poster D

Influence of Nuclear Quadrupole Moments on the Dielectric Properties of Amorphous Solids in the MHz-regime at Low Temperatures — •Lukas Münch, Timothy Jay Herbst, Alexander Werner, Benedikt Frey, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, D-69120 Heidelberg

The low temperature behavior of amorphous solids is mainly governed by atomic tunneling systems and can be described in many cases by the phenomenological standard tunneling model (STM). Acoustic and dielectric measurements however have also revealed deviations from the

STM. These led to a number of refinements of the STM, among others for glasses containing elements with large nuclear quadrupole moments. In order to further investigate the influence of nuclear quadrupole moments, we performed dielectric measurements in the MHz regime, using an LC resonator filled with the samples as dielectric material.
In a first attempt, we performed measurements on two brominated samples with a well known quadrupole splitting of about 12 mK, which is thermally accessible in our experiment. For both samples we observe slight deviations towards the quadrupole splitting energy. In a second experiment we stimulated the quadrupole moments of As_2S_3 directly by tuning the resonance frequency of the LC resonator to the sample's quadrupole splitting of 72 MHz. Comparing the result to a measurement with a slightly detuned excitation frequency, we are able to relate existing deviations to the nuclear quadrupole moments.

TT 20: Dynamics in many-body systems: Equilibration and localization II (joint session DY/TT)

Time: Monday 15:30–18:00 Location: H19

TT 20.1 Mon 15:30 H19

Environment induced pre-thermalization in the Hubbard dimer — •Nikodem Szpak[1], Eric Kleinherbers[1], Friedemann Queisser[2], Jürgen König[1], and Ralf Schützhold[2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Institut für Theoretische Physik, Technische Universität Dresden

We study a strongly interacting two-site Fermi-Hubbard model representing two coupled quantum dots and couple them to Markovian baths. We compare the real-time diagrammatic technique derived within the Keldysh formalism with a simplified model in the form of a Lindblad master equation for the reduced density matrix based on the Born-Markov approximation. Solving it exactly, we observe equilibration at different time-scales corresponding to thermalization and pre-thermalization processes.

TT 20.2 Mon 15:45 H19

Prethermalization and typical response of weakly perturbed quantum many-body systems — •Lennart Dabelow and Peter Reimann — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld

We explore the temporal relaxation of quantum many-body systems under the influence of weak-to-moderate perturbations. Situations we have in mind include, for instance, a sudden quench from one Hamiltonian to a related but different second Hamiltonian. Another example are integrable systems subject to a small integrability-breaking perturbation, commonly leading to prethermalization. Using a typicality approach, we show that the perturbed dynamics resembles the unperturbed time evolution modulated by an exponential decay towards the (possibly modified) long-time limit. We support our theory by comparison with both experimental and numerical data.

TT 20.3 Mon 16:00 H19

How to teach equilibration to the Boltzmann equation: a noisy relaxation time approximation — •Philipp Weiss and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

Equilibration of closed systems is controlled by diffusive transport of conserved quantities. After a quench these systems approach thermal equilibrium only slowly, hydrodynamic long-time tails emerge. As an analog in space one expects long-distance tails to appear when the system is perturbed only locally. A natural example for this situation is a current-carrying wire coupled to leads. We expect the connections to induce long-distance tails which show up as correction in the voltage drop.

The Boltzmann equation is widely used for tackling transport problems. However, it predicts exponential relaxation as it does not capture fluctuations of the hydrodynamic modes. Close to equilibrium a fluctuation-dissipation relation restores the missing piece of information, giving rise to a stochastic Boltzmann-Langevin equation.

Here, we present a simplified version, a "noisy relaxation time approximation", which we derive from a conserving relaxation time approximation supplemented with a suitably correlated noise term. We use our new tool to track the equilibration of a one-dimensional wire after a quench. Our prime goal is to detect long-time tails and long-distance tails indicating the diffusive built-up of the equilibrium correlations.

TT 20.4 Mon 16:15 H19

Boltzmann relaxation dynamics in strongly interacting quantum lattice systems — •Friedemann Queisser[2,3] and Ralf Schützhold[1,2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, Duisburg 47057, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

To the best of our knowledge, we present the first derivation of the Boltzmann equations for strongly interacting spinless fermions on a lattice in higher dimensions. Our derivation is based on a hierarchy of correlations [1]. For a large repulsive nearest neighbor interaction, the ground state at half filling is given by a charge density wave state. In this limit, we find that the collisions between particles and holes dominate over particle-particle and hole-hole scattering. Furthermore we shall discuss the validity of the η-theorem and the dependence of the thermalization dynamics on the type of excitation (particles or holes).

[1] P. Navez and R. Schützhold, Phys. Rev. A **82**, 063603 (2010)

TT 20.5 Mon 16:30 H19

Effect of anisotropic diffusion on spinodal decomposition — •Abhinav Sharma[1], Hidde Vuijk[1], and Joseph Brader[2] — [1]Leibniz Institute for polymer research, Dresden, Germany — [2]University of Fribourg, Fribourg, Switzerland

We study the phase transition dynamics of a fluid system in which the particles diffuse anisotropically in space. The motivation to study such a situation is provided by systems of interacting magnetic colloidal particles subject to the Lorentz force. The Smoluchowski equation for the many-particle probability distribution then acquires an anisotropic diffusion tensor. Using the method of dynamical density functional theory we predict that the intermediate-stage decomposition dynamics can be slowed down significantly by anisotropy; the coupling between different Fourier-modes is strongly reduced. Numerical calculations are performed for a model (Yukawa) fluid that exhibits gas-liquid phase separation.

15 min break

TT 20.6 Mon 17:00 H19

Cooperative efficiency boost for quantum heat engines — David Gelbwaser-Klimovsky[1], Wassilij Kopylov[2], and •Gernot Schaller[2] — [1]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, USA — [2]Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

The power and efficiency of many-body single-stroke heat engines can be boosted by performing cooperative non-adiabatic operations in contrast to the commonly used adiabatic implementations. The key property relies on the fact that non-adiabaticity allows for cooperative effects, that can use the thermodynamic resources only present in the collective non-passive state of a many-body system. In particular, we discuss an analytic formula for the efficiency of a quantum Otto cycle, which increases with the number of copies used and reaches a many-body bound, which we discuss analytically.

[1] D. Gelbwaser-Klimovsky, W.Kopylov, and G. Schaller, *Cooperative efficiency boost for quantum heat engines*, arXiv:1809.02564.

TT 20.7 Mon 17:15 H19

Light-induced Hall current in Graphene: beyond the high-frequency limit — •Marlon Nuske[1] and Ludwig Mathey[1,2,3] — [1]Zentrum für optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging, 22761 Hamburg, Germany

In the high-frequency limit driving graphene with circularly-polarized light leads to a quantized Hall effect. In experiment, however, this idealized theoretical limit is often not achievable. We therefore investigate the effects of a finite-frequency circularly-polarized pulse on the Hall conductivity of graphene. For such a setup it is crucial to include decay processes in the theoretical model. We analyze the additional resonant contributions to the Hall current that arise from finite frequency driving. We explore different regimes, where either the resonant or the effective high-frequency contributions dominate the Hall current.

TT 20.8 Mon 17:30 H19

Environment induced pre-thermalization in the Mott-Hubbard model — •Friedemann Queisser[2,3], Ralf Schützhold[1,2,3], Nikodem Szpak[1], and Patrick Navez[2] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, Duisburg 47057, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

Using a hierarchy of correlations, we discuss the strongly interacting Fermi-Hubbard model in the Mott insulating regime coupled to a Markovian environment [1,2]. The environment is chosen such that the particle number is constantly monitored at each lattice site. As expected, the environment induces a decay rate of γ the quasi-particles frequencies and tends to diminish the correlations between lattice sites. Surprisingly, the environment does also steer the state of the system on intermediate time scales $\mathcal{O}(1/\gamma)$ to a pre-thermalized state very similar to a quantum quench. The full thermalization and the approach to an infinite temperature state occurs via local on-site heating and takes much longer.

[1] P. Navez and R. Schützhold, Phys. Rev. A **82**, 063603
[2] F. Queisser and R. Schützhold, arXiv:1808.09906

TT 20.9 Mon 17:45 H19

Laser driven ultrafast crystallization of phase-change material Ge1Sb2Te4 — •Jingyi Zhu[1], Shuai Wei[2], Julian Merten[2], Christoph Persch[2], Lin Yang[1], Matthias Wuttig[2], and Paul H. M. van Loosdrecht[1] — [1]Physics institute 2, University of Cologne, 50937, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Aachen, 52074, Germany

Rapid and reversible switching between amorphous and crystalline phases of the phase-change materials are either used or very promising in a wide range of applications in the electronic, optoelectronic, and photonic memory devices. Here we use time-resolved spontaneous Raman spectra to monitor the ultrafast process of melting, bond softening and crystallization in the phase changing material Ge1Sb2Te4 upon laser excitation. We demonstrate ultrafast crystallization on a ps timescale by monitoring the transient formation of a well-defined phonon mode signaling the crystalline state emerging from a broad vibrational continuum typical for the amorphous state.

TT 21: Focus Session: Quantum Dynamics of Kinetically Constrained Many-Body Systems (joint session TT/DY)

Over the past few years it has been shown that quantum many-body systems far from equilibrium can exhibit very rich and exciting physics, including the emergence of thermodynamics in closed quantum systems, dynamical quantum phase transitions, and many-body localization. This topic became of particular relevance as closed quantum many body states can now be prepared experimentally and coherent quantum dynamics can be observed over long time scales. Strongly correlated systems that are subject to a kinematic constraints receive currently a lot of attention. Such constrained quantum matter is characterized by a Hilbert space structure that is different from a conventional tensor product structure. Well known examples are frustrated quantum magnets described by effective dimer models, fractional quantum Hall liquids, and so called fracton models with excitations that are only mobile in certain directions. In a recent experiment, constrained models have also been realized in synthetic quantum matter in which Rydberg excitations of one-dimensional ultracold atoms are energetically forbidden to occupy neighbouring sites*a constrained model that can be mapped onto a 1D quantum dimer model. While the equilibrium properties of constrained systems have been studied in depth over the past decades in the context of frustrated magnetism and gauge theories, we just begin to understand the rich non-equilibrium physics of these systems. The proposed session aims to give an overview ofrecent developments and point towards the open questions.

Organized by: Michael Knap (Technical University of Munich), Frank Pollmann (Technical University of Munich), Roderich Moessner (Max-Planck-Institute for the Physics of Complex Systems)

Time: Tuesday 9:30–13:00 Location: H2

Invited Talk TT 21.1 Tue 9:30 H2

Quantum dynamics, scars, and integrability in constrained Rydberg systems — •Vedika Khemani[1], Christopher Laumann[2], and Anushya Chandran[2] — [1]Harvard University, Cambridge, Massachusetts, USA — [2]Boston University, Boston, Massachusetts, USA

A recent experiment on a 51-atom chain of Rydberg atoms observed anomalously long-lived temporal oscillations of local observables after quenching from an antiferromagnetic initial state. This coherence is surprising as the initial state should have thermalized rapidly to infinite temperature. I will describe the novel dynamics of this system using various diagnostics, and provide some insights into the underlying causes for the unusual dynamical properties of this system.

Invited Talk TT 21.2 Tue 10:00 H2

DMRG investigation of constrained models: from quantum dimer and quantum loop ladders to hard-boson and Fibonacci anyon chains — •Natalia Chepiga[1] and Frederic Mila[2] — [1]University of California, Irvine, USA — [2]EPFL, Lausanne, Switzerland

Motivated by the presence of Ising transitions that take place entirely in the singlet sector of frustrated spin-1/2 ladders and spin-1 chains, we study two types of effective dimer models on ladders, a quantum dimer model and a quantum loop model. We further show that both models can be mapped rigorously onto a hard-boson model first studied by Fendley, Sengupta and Sachdev [Phys. Rev. B 69, 075106 (2004)]. Building on a density-matrix renormalization group algorithm that takes full advantage of the dimers constraints, we study systems with up to 9'000 sites and calculate the correlation length and the wave-vector of the incommensurate short-range correlations with unprecedented accuracy. We discuss the full phase diagram of these models, with special emphasis on the phase transitions. In particular, we provide strong numerical evidence that there is an intermediate floating phase far enough from the integrable Potts point, while in its vicinity, our numerical data are consistent with a unique transition in the Huse-Fisher chiral universality class. Moreover, using conformal field theory, we fully characterize the tricritical Ising point, with a com-

plete analysis of the boundary-field correspondence including partially polarized edges.

Invited Talk TT 21.3 Tue 10:30 H2

Localization in Fractonic Random Circuits — Shriya Pai, •Michael Pretko, and Rahul Nandkishore — University of Colorado Boulder

In this talk, I will describe a new mechanism for many-body localization, making use of ideas drawn from the field of fractons. Specifically, I will present results on the spreading of initially local operators under random unitary evolution in spin chains subject to fracton conservation laws, such as conservation of dipole moment. We find that fractons remain permanently localized at their initial positions, providing a crisp example of a non-ergodic dynamical phase of random unitary evolution. These results can be interpreted as a consequence of the properties of low-dimensional random walks. This mechanism for localization remains robust in one and two dimensions, but breaks down in three-dimensional fracton systems. We argue that these results extend to Floquet and Hamiltonian time evolution, even in the absence of disorder, thereby providing a mechanism for many-body localization in a translationally invariant system.

15 min. break.

Invited Talk TT 21.4 Tue 11:15 H2

Many-body localization dynamics from gauge invariance — •Markus Heyl — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

In this talk I will show how lattice gauge theories can display many-body localization dynamics in the absence of disorder as a consequence of local constraints induced by gauge invariance. The starting point is the observation that, for some generic homogeneous initial conditions, the time-evolved state can be decomposed into different superselection sectors as a consequence of Gauss law in such a way that it realizes an effective disorder average. By carrying out extensive exact simulations on the real-time dynamics of a lattice Schwinger model, describing the coupling between U(1) gauge fields and staggered fermions, it is shown that the dynamics can become nonergodic leading to a slow, double-logarithmic entanglement growth. These findings are immediately relevant to cold atoms and trapped ion experiments realizing dynamical gauge fields and suggest a new and universal link between confinement and entanglement dynamics in the many-body localized phase of lattice models.

Invited Talk TT 21.5 Tue 11:45 H2

Slow dynamics due to kinetic constraints, from classical to quantum — •Juan Garrahan — School of Physics and Astronomy, University of Nottingham

Classical many-body systems that display slow collective relaxation - the canonical example being those that form glass - often do so due to effective constraints in the their dynamics. The simplest manifestation of this principle is in so-called kinetically constrained models (KCMs) where dynamical constraints are explicit. After reviewing the basic properties of constrained dynamics in classical systems, I will dis- cuss how similar ideas can be made relevant for quantum many-body systems. I will describe quantum KCMs which display slow thermalization and even in certain cases (apparent) non-ergodicity in the absence of disorder. Like in the classical case, I will show how slow relaxation goes together with spatially fluctuating dynamics, giving rise to heterogeneous growth of entanglement. I will also discuss connections with other quantum systems with complex dynamics such as fracton models. My main aim will be to highlight links between concepts and methods of classical and quantum non-equilibrium.

TT 21.6 Tue 12:15 H2

Dynamical Phase Transitions in a 2D Quantum Dimer Model — •Johannes Feldmeier, Michael Knap, and Frank Pollmann — Technische Universität München

The study of dynamical properties in systems with local constraints has attracted a lot of interest, spurred by experiments with Rydberg blockaded atoms, that naturally implement constrained many-body models. We study the quench dynamics in a 2D quantum dimer model to identify dynamical phase transitions in constrained models by means of exact diagonalization on systems of sizes up to 8x8 sites. We find that the quenched quantum system thermalizes efficiently by determining the relaxation dynamics of both the order parameter (OP) and local correlation functions. The observed fast relaxation to thermal expectation values allows us to study the underlying thermal BKT-transition between a columnar ordered valence bond solid (VBS) and a symmetric liquid (VBL) phase in the form of a dynamical phase transition. The existence of this finite-temperature transition in the dynamics is confirmed by the long-time averaged values of the OP. Moreover, upon quenching across the VBS-VBL phase boundary, the dynamical transition can be shown to be manifest in the Loschmidt-echo, whose rate-function displays kinks at the zero-crossings of the columnar OP.

TT 21.7 Tue 12:30 H2

Hamiltonian systems with charge and dipole conservation far from equilibrium — •Pablo Sala, Tibor Rakovszky, Ruben Verresen, Michael Knap, and Frank Pollmann — Technische Universität München, Physics Department T42, 85747 Garching, Germany

Recently so-called fracton phases, which are characterized by excitations with restricted mobility, have been discovered. The mobility constraints are related to the conservation of a U(1) charge and its associated dipole moment. Motivated by results on random unitary circuits [1], we study one dimensional spin-1/2 and spin-1 Hamiltonian systems conserving these two intertwined quantities and consider the implications of a U(1) local gauge invariance. We investigate the effects of these conservation laws on the dynamics, and the implications for higher dimensional systems following the same construction. [1] S. Pai, M. Pretko and R. M. Nandkishore. arXiv:1807.09776 [cond-mat.stat-mech]

TT 21.8 Tue 12:45 H2

Apparent slow dynamics in the ergodic phase of a driven many-body localized system without extensive conserved quantities — •Talía Lezama Mergold Love[1], Soumya Bera[2], and Jens H. Bardarson[1,3] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India — [3]Department of Physics, KTH Royal Institute of Technology, Stockholm, 106 91 Sweden

One of the distinguishing features of the ergodic phase in systems exhibiting many-body localization (MBL) is a slowing down of the dynamics as they approach the MBL transition. Using a fast Walsh-Hadamard transform, we numerically study the former scenario in a Floquet model with no global conservation laws. In this model, the ergodic-MBL transition can be tuned by the disorder strength within a region of the frequency-amplitude space. Similarly to models with conserved quantities, our data is consistent with a subballistic spread of entanglement and a stretched-exponential decay of an autocorrelation function, with their associated exponents reflecting slow dynamics near the transition for a fixed system size. However, with access to larger system sizes, we find a clear flow of the exponents towards faster dynamics. We further observe examples of non-monotonic dependence of the exponents with time, consistent with the slow dynamics being a crossover phenomena with a localized critical point.

TT 22: Superconductivity: Theory

Time: Tuesday 9:30–12:30 Location: H7

TT 22.1 Tue 9:30 H7

Doping induced superconductivity in compressed hydrides, an *ab-initio* investigation — •Antonio Sanna[1] and José A. Flores-Livas[2] — [1]Max Planck Institute of microstructure physics, Halle (Saale), Germany — [2]University of Basel, Department of Physics, Basel, Switzerland

Under pressure hydrides have reached extremely high superconducting critical temperatures rekindling the dream of a room temperature superconductor.

Unfortunately, many (if not most) chemical compounds containing hydrogen only metallize at extreme pressures. A possible solution to this issue could be to use a heavy chemical doping, that can render metallic and even superconducting a semiconducting system.

Following this idea we have investigated, by *ab initio* methods, if doping can be used to obtain high-T_C superconductivity in hydrides. We have considered three examples: H_2O [1], as one of the most abundant, and best studied, hydrides; polyethylene [2] a polymeric hydrocarbon, as representative of the immense family of organic compounds; and the (6,0) graphene nanotube [3] with exohedral hydrogenation.

[1] J.A. Flores-Livas et al., Scientific Reports **7**, 6825 (2017)
[2] J.A. Flores-Livas et al., Eur. Phys. J. B **91** 176(2018)
[3] A. Sanna et al., Eur. Phys. J. B **91** 177 (2018)

TT 22.2 Tue 9:45 H7

Investigating the effect of impurities on the superconducting state — •Tom Saunderson[1], Gábor Csire[2], James Annett[1], Balázs Úfalussy[2], and Martin Gradhand[1] — [1]HH Wills Laboratory, University of Bristol, UK — [2]Wigner Research Centre for Physics, PO Box 49, H-1525 Budapest, Hungary

Our understanding of the superconducting state in real materials is still very limited. Not only are the driving mechanisms for many unconventional superconductors poorly understood but also the coupling to magnetic layers or the effect of impurities represent major conceptual challenges [1]. Furthermore, the effects of interfaces, impurities and spin orbit coupling on spin dependent transport, properties well established in the normal state, attract more and more interest [2]. Here we present the implementation of the Bogoliuobov-de Gennes (BdG) equation into a Green′s function (KKR) first principles method [3]. Due to it being a Green′s function method, it is possible to model bulk materials including impurities and interfaces without the need of artificial supercells. We parameterise the pairing potential but solve the BdG equation self-consistently incorporating the microscopic properties of real materials. Here we are going to present calculations for various test cases of simple superconductors and will investigate the influence of impurities on the superconducting state with a particular future interest in the influence of magnetic impurities.

[1] G. R. Stewart, Adv. in Phys., **66**, 75 (2017)
[2] M. Eschrig, Rep. Prog. Phys,, **78**, 104501 (2015)
[3] G. Csire *et al*, Phys. Rev. B,, **91**, 165142 (2015)

TT 22.3 Tue 10:00 H7

Reduced Density Matrix Functional Theory for Superconductors — Jonathan Schmidt, •Carlos Benavides Riveros, and Miguel Marques — Martin-Luther Universität Halle Wittenberg

We present a new ab-initio theory for superconducting systems with nonlocal external potentials based on the one-particle reduced density matrix $\rho(r, r')$, the anomalous density $\chi(r, r')$ and the nuclear density $D(r, r')$. We prove that all the system's equilibrium properties are determined uniquely by these three quantities and deduce a variational principle for the grand canonical potential in terms of them. By replacing the local electronic density, which is used in density functional theory for superconductors (SC-DFT), with the non-local one-particle reduced density matrix, our theory is able to solve difficulties which arise in SC-DFT through the combination of local and non-local quantities.

Analogue to the Kohn-Sham system in DFT, we prove the existence of a Kohn-Sham system that is able to reproduce ρ, χ and D of an interacting system at finite temperature. On the basis of the Kohn-Sham system, we obtain a set of Bogoliubov-De Gennes-like single particle equations. Finally, we derive a first exchange-correlation functional through the Sham-Schlüter connection.

TT 22.4 Tue 10:15 H7

Feasible model for light-induced interband pairing — Sergio Porta[1,2], •Lorenzo Privitera[2], Niccolò Traverso Ziani[1,2], Fabio Cavaliere[1], and Björn Trauzettel[2] — [1]Dipartimento di Fisica, Università di Genova, 16146 Genova, Italy — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

Recent theoretical works [1,2] have highlighted the existence of a purely electronic mechanism for the appearance of non-equilibrium superconductivity in a resonantly driven semiconductor with repulsive interband interactions. The original proposals relied anyway on the existence of a specific fermionic dissipation mechanism and the careful simultaneous tailoring of the electronic dispersion relation and the electron-electron interaction.

In this work we show that this mechanism is actually more general and does not need any special tuning of the parameters. When considering a pair of bands with the same sign of concavity, we indeed demonstrate that interband pairing emerges under the natural assumptions of the presence of phononic baths and radiative recombination. In light of these findings, we show how the appearance of superconductivity can be understood in terms of standard equilibrium interband BCS theory. Finally, we conclude by presenting a phase diagram for the steady state of the model.

[1] G. Goldstein, C. Aron, and C. Chamon, Phys. Rev. B 91, 054517 (2015)
[2] O. Hart, G. Goldstein, C. Chamon and C. Castelnovo, arXiv:1810.12309

TT 22.5 Tue 10:30 H7

Higgs spectroscopy for periodically driven unconventional superconductors — •Lukas Schwarz and Dirk Manske — Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Higgs spectroscopy for superconductors in nonequilibrium is a new method to obtain phase-sensitive information about the underlying gap symmetry [1]. One experimental setup to observe the Higgs mode is third-harmonic generation (THG), where the driving frequency of a multicycle THz pulse is brought in resonance with the Higgs mode. This was already successfully demonstrated for s-wave superconductors [2]. We show that THG can be used to observe also additional Higgs modes predicted to occur in d-wave superconductors [3]. They show up as a second resonance in the THG response. Such an additional resonance was found in recent THG experiments on cuprates and can be explained by our theory [4]. This theory is not limited to d-wave superconductors but applies in general to any gap symmetry where multiple Higgs modes are possible. Thus, THG experiments extend the repertoire of Higgs spectroscopy experiments and can be used for the identification of gap symmetries of unconventional superconductors.

[1] B. Fauseweh et al., arXiv:1712.07989 (2017)
[2] R. Matsunaga et al., Science 345, 1145 (2014)
[3] L. Schwarz et al., Higgs spectroscopy for periodically driven unconventional superconductors, arXiv
[4] H. Chu et al., New collective mode in superconducting cuprates uncovered by Higgs spectroscopy, arXiv

15 min. break.

TT 22.6 Tue 11:00 H7

Hall coefficient in two-dimensional metals with spiral magnetic order and application to cuprate high-T_c superconductors — •Johannes Mitscherling and Walter Metzner — Max Planck Institute for Solid State Research, Stuttgart, Germany

Charge transport measurements in high magnetic fields recently shed new light on the non-superconducting ground state in cuprate high-T_c superconductors [1]. In particular, Hall measurements yield a drop of the Hall number indicating a phase transition associated with a Fermi surface reconstruction. On the theoretical side, spiral magnetic order (or quasi-order) remains a hot candidate for the Fermi surface reconstruction mechanism. The electromagnetic response of spiral magnetic states has already been analyzed for small relaxation rates [2]. However, the relaxation rate in the cuprate samples studied experimentally

is sizable. We have, thus, derived, for the first time, a complete formula (including all interband contributions) for the Hall conductivity in the low field limit $\omega_c\tau \ll 1$ [3]. We use the complete expressions to study the importance of a sizable relaxation rate and show that the observed Hall number drop in cuprates can be fitted with realistic parameters.
[1] Badoux *et al.*, Nature **531**, 210 (2016)
[2] Voruganti *et al.*, PRB **45**, 13945 (1992)
[3] Mitscherling and Metzner, PRB **98**, 195126 (2018)

TT 22.7 Tue 11:15 H7

Unconventional superconductivity in the 2D Hubbard model: weak-coupling renormalization group — •Sebastian Wolf[1], Thomas Schmidt[2], and Stephan Rachel[1] — [1]School of Physics, University of Melbourne, Parkville, VIC 3010, Australia — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511, Luxembourg

We employ the weak-coupling renormalization group approach to study unconventional superconducting phases emerging in the extended, repulsive Hubbard model on paradigmatic two-dimensional lattices. Repulsive interactions usually lead to higher-angular momentum Cooper pairing. By considering not only longer-ranged hoppings, but also nonlocal electron-electron interactions, we are able to find superconducting solutions for all irreducible representations on the square and hexagonal lattices, including extended regions of chiral topological superconductivity. For paradigmatic 2D lattices, we provide detailed superconducting phase diagrams as well as the coupling strengths which quantify the corresponding critical temperatures depending on the bandstructure parameters, band filling, and interaction parameters.

TT 22.8 Tue 11:30 H7

Kohn-Luttinger superconductivity and chirality in twisted bilayer graphene — •Tobias Stauber[1], Jose Gonzalez[2], Tony Low[3], and Guillermo Gomez-Santos[4] — [1]Departamento de Teoria y Simulacion de Materiales, Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049 Madrid, Spain — [2]Instituto de Estructura de la Materia, CSIC, E-28006 Madrid, Spain — [3]Department of Electrical & Computer Engineering, University of Minnesota, Minneapolis, Minnesota 55455, USA — [4]Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Twisted bilayer graphene has attracted much attention due to its novel electronic and optical properties. Here, we will present our recent theoretical results on the superconducting instability and also on the inherent chirality of the system. In particular, we will show that the Kohn-Luttinger mechanism might be active in TBL [1]. Furthermore, we find a paramagnetic response around the neutrality point, a longitudinal Hall effect and longitudinal plasmonic excitations which are accommodated by a longitudinal magnetic moment [2,3].
[1] J. Gónzalez and T. Stauber, arXiv:1807.01275
[2] T. Stauber, T. Low, and G. Gómez-Santos, Phys. Rev. Lett. 120, 046801 (2018)
[3] T. Stauber, T. Low, and G. Gómez-Santos, Phys. Rev. B 98, 195414 (2018)

TT 22.9 Tue 11:45 H7

Analytic study of dissipative phase transitions in a driven nonlinear resonator model — •Mikhail Pletyukhov — RWTH Aachen University, Institute for Theory of Statistical Physics, 52074 Aachen, Germany

The Kerr nonlinearity model plays an important role in circuit QED. At strong microwave drive and weak nonlinearity it is known to feature a bistable behavior, which can be interpreted as a dissipative phase transition. In this talk, I show on the basis of the analytical solution for the steady state of this model that some effective limiting procedure (mimicking the thermodynamic limit) does lead to a jump in observables - the property of the first order transition, and I give a full analytic charaterization of this transition. In the two-photon driven Kerr model, a similar consideration allows one to characterize a second-order transition occurring in it, and this issue is also addressed in the talk.

Invited Talk TT 22.10 Tue 12:00 H7

Superconducting films and interfaces: Novel features from spin imbalance and Rashba spin-orbit coupling — •Gertrud Zwicknagl — Institut f. Mathemat. Physik, TU Braunschweig, Braunschweig, Germany

In recent years, the manufacturing of controlled ultra-thin superconducting films has made impressive progress.Important examples are monoatomic or monomolecular layers on a substrate, superconducting layers in a superlattice, or superconducting interfaces and surfaces. These systems have in common the absence of inversion symmetry and hence the presence of Rashba-type spin-orbit energy λ. The latter can be modified to some extent by varying the thickness, the number of layers, or by applying an electric voltage. The subtle interplay of spin imbalance created by a magnetic field and the Rashba spin-orbit interaction gives rise to novel phenomena in quasi-2D superconductors which, in turn, could provide new functionalities. I discuss the results of a microscopic theory of superconducting films with population imbalance which are subject to Rashba spin- orbit interaction. The full range from small to large spin-orbit interaction is covered. A quantum phase transition at a critical value of the spin-orbit energy λ_c is predicted where abrupt changes in the superconducting state are expected. It is tempting to speculate, that this feature might give rise to novel phenomena. For example, the Josephson interference effects should change dramatically near this point. These and other open issues together with recent work and promising future directions will be discussed.

TT 23: Frustrated Magnets - General 1 (joint session TT/MA)

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

TT 23.1 Tue 9:30 Theater

Ground state properties of the sawtooth chain — •Alexandros Metavitsiadis and Wolfram Brenig — Institute for Theoretical Physics, TU Braunschweig, 38106 Braunschweig, Germany

Recent experimental and theoretical studies on the natural mineral Atacamite [$Cu_2Cl(OH)_3$] have revealed that it might be one of the few true cases where a sawtooth chain, a minimal one-dimensional frustrated system, is materialized. Prompted by these recent results, we revisit the low energy properties of the sawtooth chain presenting a comprehensive theoretical study of its ground state properties using numerical techniques (full diagonalization, Lanczos, and matrix product states), as well as analytical field theory calculations.

TT 23.2 Tue 9:45 Theater

Magnetization plateau in the frustrated quantum sawtooth chain atacamite, $Cu_2Cl(OH)_3$ — •Leonie Heinze[1], Xiaxin Ding[2], Vivien Zapf[2], Franziska Weickert[2], Marcelo Jaime[2], Gaël Bastien[3], Anja U.B. Wolter[3], Manfred Reehuis[4], Jens-Uwe Hoffmann[4], Ralf Feyerherm[4], Dirk Menzel[1], Kirrily C. Rule[5], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig, Braunschweig, Germany — [2]NHMFL, Los Alamos, USA — [3]IFW Dresden, Dresden, Germany — [4]HZB, Berlin, Germany — [5]ANSTO, Kirrawee, Australia

The frustrated nature of the quantum magnet atacamite, $Cu_2Cl(OH)_3$, is displayed by its magnetic properties [1]. Band structure calculations [2] suggest that the magnetic coupling scheme can essentially be understood in terms of a quantum sawtooth chain with a dominant coupling along the chain of about $J_1 \sim 100\,\mathrm{K}$, and a secondary coupling about $J_2 \sim 30\,\mathrm{K}$.

Here, we present new insights into the magnetic phase diagram of atacamite. We discuss the long-range ordered magnetic ground state below $T_\mathrm{N} = 8.6\,\mathrm{K}$ and present high field magnetization data revealing a 1/2-magnetization plateau. Magnetic saturation is estimated to be attained in fields between 75 to 80 T.
[1] L. Heinze, *et al.*, Physica B **536**, 377 (2018)
[2] H. O. Jeschke and R. Valentí, private communication.

TT 23.3 Tue 10:00 Theater

Phase diagram of the pseudo-Kagome francisite $Cu_3Bi(SeO_3)_2O_2Cl$ studied by high-resolution dilatometry — •Sven Spachmann[1], Liran Wang[1], Alexander Vasiliev[2], and

Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Lomonosov Moscow State University, Moscow, Russia

Single crystals of the layered Kagome-like francisite $Cu_3Bi(SeO_3)_2O_2Cl$ have been studied by high-resolution thermal expansion and magnetostriction as well as by bulk magnetization measurements. At $B = 0$ T, in addition to a well-known structural phase transition at $T_s = 120$ K, long range antiferromagnetic order of the ferromagnetically coupled layers develops around $T_N = 26.4$ K. The ordering is associated with pronounced anomalies in the uniaxial thermal expansion coefficients. Magnetic fields yield a suppression of T_N. In plane, a sign change of the uniaxial pressure dependencies (at $B > 2$ T for $B\|a$) signals a change in the nature of the phase transition. At $T = 2$ K, metamagnetic transitions are observed for B parallel to the (in-plane) a-, b-, and (out-of-plane) c-axes at $B_C = 5.4$ T, 1.6 T, and 0.9 T, respectively. The transitions are associated with sharp magnetization jumps. The magnetic phase diagram for all three crystal axes is constructed and discussed.

TT 23.4 Tue 10:15 Theater

Magnetic excitations in the correlated paramagnetic state of the frustrated quantum antiferromagnet Cs_2CuCl_4 — •Bernd Wolf, Paul Eibisch, Lars Postulka, Franz Ritter, Cornelius Krellner, and Michael Lang — Physikalisches Institut, Goethe Universität, SFB/TR49, D-60438 Frankfurt (M)

We present a magnetoelastic investigation of the frustrated triangular-lattice S = 1/2 antiferromagnet Cs_2CuCl_4 by studying the longitudinal modes c_{11}, c_{22} and c_{33}. The measurements were performed in magnetic fields up to 10 T and down to 0.032 K to cover the the long range order and the spin-liquid regime. At the lowest temperatures of our experiment the field dependence of the c_{33} mode can be well described using a Landau free energy model which combines the elastic constant with the magnetic susceptibility data, measured independently. From fits to the experimental c_{33} data we obtain a very small magnetoelastic coupling constant $G/k_B = 2.8$ K for Cs_2CuCl_4 consistent with the results of susceptibility measurements under hydrostatic pressure. Remarkably, we find that the classical approach provides an excellent description of the data at lowest temperatures, i.e., close to the putative quantum critical point at B = 8.5 T of this material. However, at somewhat higher temperatures, there are deviations between the experimental data and the theoretical curves. At these temperatures we also observe anomalies in the ultrasonic attenuation α and χ'', the imaginary part of the magnetic susceptibility. We discuss these losses with respect to the peculiarities of the magnetic excitation spectrum for this low dimensional spin system.

TT 23.5 Tue 10:30 Theater

Thermodynamics of the 2D $S = 1/2$ Shastry-Sutherland Model and $SrCu_2(BO_3)_2$ — Alexander Wietek[1], Philippe Corboz[2], Frédéric Mila[3], Bruce Normand[4], Stefan Wessel[5], and •Andreas Honecker[6] — [1]Center for Computational Quantum Physics, Flatiron Institute, New York, USA — [2]Institute for Theoretical Physics and Delta Institute for Theoretical Physics, University of Amsterdam, The Netherlands — [3]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland — [4]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Switzerland — [5]Institut für Theoretische Festkörperphysik, RWTH Aachen University, Germany — [6]Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, France

Reliable computation of the low-temperature thermodynamic properties of highly frustrated quantum magnets such as the 2D $S = 1/2$ Shastry-Sutherland model is a considerable challenge. Notwithstanding recent progress with QMC simulations in the dimer basis, the parameter regime relevant to $SrCu_2(BO_3)_2$ has remained inaccessible [1]. Here we present accurate results obtained from two other methods, namely Thermal Pure Quantum (TPQ) states and infinite Projected Entangled Pair States (iPEPS). We observe the emergence of a low-temperature peak in the specific heat C and relate it to the large number of bound states that emerge close to the first-order transition from the dimer to the plaquette phase.

[1] S. Wessel, I. Niesen, J. Stapmanns, B. Normand, F. Mila, P. Corboz, A. Honecker, Phys. Rev. B **98**, 174432 (2018)

TT 23.6 Tue 10:45 Theater

Theory of the intermediate phase of $SrCu_2(BO_3)_2$ under pressure — •Carolin Boos[1,2], Schelto Crone[3], Ido Niesen[3], Philippe Corboz[3], Frédéric Mila[2], and Kai Phillip Schmidt[1] — [1]FAU Erlangen-Nürnberg, Germany — [2]EPF Lausanne, Switzerland — [3]University of Amsterdam, Netherlands

Building on the NMR evidence that two different Cu sites are present in the intermediate phase of $SrCu_2(BO_3)_2$ under pressure, we investigate the nature of the intermediate phase in an orthorhombically distorted Shastry-Sutherland model. We show that a few percent difference between nearest-neighbor couplings is sufficient to destabilize the plaquette phase in favor of a one-dimensional phase in which bonds around half the full plaquettes become stronger. This phase is adiabatically connected to the Haldane phase that is stabilized when next-nearest neighbor couplings take different values, and the excitations in this one-dimensional phase are shown to agree qualitatively with neutron scattering results.

TT 23.7 Tue 11:00 Theater

Electron spin resonance studies on the frustrated tripod-Kagome compound $Mg_2Gd_3Sb_3O_{14}$ — •Christoph Wellm[1,2], Julian Zeisner[1,2], Mihai Sturza[1], Gaël Bastien[1,2], Sebastian Gass[1], Anja U.B. Wolter[1], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 — [2]Institut für Festkörper-und Materialphysik, TU Dresden, D-01062

As an example of a class of geometrically frustrated magnetic systems, the so-called tripod Kagome materials have been suggested as an interesting target of experimental investigation due to the frustrated nature and the question of dimensionality of the magnetic interactions. In our work we performed high-field electron spin resonance measurements on a powder sample of $Mg_2Gd_3Sb_3O_{14}$, a representative of a quasiclassical Heisenberg magnet, where the effect of spin-orbit coupling of Gd^{3+} ions vanishes to first order. Measurements were conducted over a frequency range of 70-420 GHz and temperatures ranging from 3-50 K. The Gaussian lineshape is consistent with a model of dominant dipolar spin-spin interactions, while the growing asymmetry of the lineshape upon decrease of temperature signifies an increase of an effective internal field, an indication of increasing short-range spin-spin-correlations. Such a behavior is typical for frustrated systems, making our studies one of the first to reveal such significant features in this family of materials. Furthermore, temperature dependent critical broadening of the linewidth and increase of the internal field strength provide insights into the dimensionality of the spin-spin correlations.

15 min. break.

TT 23.8 Tue 11:30 Theater

Frustrated magnetism of S=5/2 moments on a coupled triangular lattice in $Cs_3Fe_2Br_9$ — •Daniel Brüning[1], Tobias Fröhlich[1], Markus Braden[1], Ladislav Bohatý[2], Petra Becker[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Deutschland — [2]Abteilung Kristallographie, Institut für Geologie und Mineralogie, Universität zu Köln, Deutschland

$Cs_3Fe_2Br_9$ is a hexagonal material consisting of Fe^{3+} ions with S=5/2 in face-sharing Fe_2Br_9 bi-octahedra, which form hexagonal double layers of the Fe ions. The triangular arrangement of the magnetic ions in the individual layers causes magnetic frustration. The type of magnetic ground state depends on the ratio between the magnetic exchange couplings: the intradimer coupling J, the intralayer (or in-plane) coupling J_p, and the interlayer coupling J_c. The magnetic ground state of $Cs_3Fe_2Br_9$ is not a singlet-dimer state as in isostructural $Cs_3Cr_2Br_9$ and $Cs_3Cr_2Cl_9$, but there is evidence for antiferromagnetic order with $T_N = 13.5$ K. However, our measurements up to 17 T on large single crystals reveal a very unusual magnetic field vs. temperature phase diagram. For an in-plane field, we find linear M(H) curves, whereas a field H‖c causes multiple phase transitions including a magnetization plateau of 1/3 $M_{sat} = 10\mu_B$. Neutron diffraction resolved the magnetic structure of two phases which indicate an increasing intralayer coupling. Additionally, we present pulsed-field magnetization measurements revealing further transitions, before reaching saturation around 40 T for H‖c.

This work was supported by the DFG through CRC 1238.

TT 23.9 Tue 11:45 Theater

Importance of biquadratic exchange for a new Ni-based quantum magnet of frustrated $S = 1$ isolated spin-triangles — •B Lenz[1], S Chattopadhyay[2], S Kanungo[3], NA Sushila[4], S K Panda[1], S Biermann[1,5], W Schnelle[6], K Manna[2], R Kataria[4], M Uhlarz[2], Y Skourski[2], S A Zvyagin[2], A Ponomaryov[2], T Herrmannsdörfer[2], R Patra[4], and J Wosnitza[2,7] — [1]CPHT,

Ecole Polytechnique, Palaiseau, France — [2]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, Germany — [3]School of Physical Sciences, IIT Goa, India — [4]Department of Chemistry and Centre for Advanced Studies in Chemistry, Panjab University, India — [5]Collège de France, Paris, France — [6]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [7]Institut für Festkörper- und Materialphysik, TU Dresden, Germany

The new metal-organic framework BHAP-Ni_3 is comprised of essentially isolated spin-1 triangle centers, which renders this quantum magnet an ideal system to study the magnetism of a frustrated spin-triangle unit. Pulsed-field magnetometry and AC-susceptibility measurements of single-crystalline samples allow to identify a disordered magnetic ground state and a peculiar pronounced 2/3 magnetization plateau between 7T and 20T. Here, we show how theoretical modeling guided by ab initio calculations identifies the interplay of Heisenberg and biquadratic spin-spin interactions to be responsible for the stabilization of an exotic state that manifests itself in form of the 2/3 magnetization plateau.

TT 23.10 Tue 12:00 Theater

Estimating the density of states of frustrated spin systems — •Martin Weigel[1], Lev Barash[2], Jeffrey Marshall[3], and Itay Hen[3] — [1]Applied Mathematics Research Centre, Coventry University, Priory Street, Coventry, CV1 5FB, UK — [2]Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia — [3]Department of Physics and Astronomy, and Center for Quantum Information Science & Technology, University of Southern California, Los Angeles, California 90089, USA

Estimating the density of states of systems with rugged free energy landscapes is a notoriously difficult task of the utmost importance in many areas of physics ranging from spin glasses to biopolymers. Density of states estimation has also recently become an indispensable tool for the benchmarking of quantum annealers when these function as samplers. Some of the standard approaches suffer from a spurious convergence of the estimates to metastable minima, and these cases are particularly hard to detect. Here, we introduce a sampling technique based on population annealing enhanced with a multi-histogram analysis and report on its performance for spin glasses. We demonstrate its ability to overcome the pitfalls of other entropic samplers, resulting in some cases in orders of magnitude scaling advantages that can result in the uncovering of new physics. To do that we devise several schemes that allow us to achieve exact counts of the degeneracies of the tested instances.

TT 23.11 Tue 12:15 Theater

Ground states of the transverse-field long-range Ising model on infinite-cylinder triangular lattices — •Jan Koziol, Sebastian Fey, and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

To gain a better understanding of the interplay between frustrated long-range interactions and zero-temperature quantum fluctuations, we investigate the ground-state phase diagram of the transverse-field Ising model with algebraically-decaying long-range Ising interactions on quasi one-dimensional infinite-cylinder triangular lattices. Technically, we apply various approaches including low-field and high-field series expansions. For the classical long-range Ising model, we investigate cylindric triangular lattice configurations, i.e. a triangular lattice with an even finite length periodic boundary condition ($4 - 40$ lattice sites) in one direction and infinite extension in the other direction. We show the occurrence of new columnar-ordered phases differing from the infinitely degenerate nearest-neighbour Ising ground-state manifold on the two-dimensional triangular lattice. The existence of these columnar phases is connected to the long-range nature of the Ising interaction. For the full quantum model, we concentrate on cylinders with extensions four and six. The ground-state phase diagram consists of several quantum phases in both cases including a polarised phase, columnar-ordered phases, and ordered phases which emerge from an order by disorder scenario already present in the nearest-neighbour model.

TT 23.12 Tue 12:30 Theater

Quantum-criticality in two-dimensional transverse-field Ising models with frustrated long-range interactions — •Sebastian Fey, Sebastian C. Kapfer, and Kai P. Schmidt — FAU Erlangen-Nürnberg, Germany

Quantum-critical behavior is found in many quantum systems displaying universal properties such as critical exponents. In the past, most investigations of strongly correlated quantum many-body systems have tackled short-range interactions because long-range interacting systems are notoriously difficult to treat. Nevertheless, important examples of long-range interactions exist in nature, e.g. dipolar interactions in spin ice or long-range forces between cold atoms in optical lattices. Here, we present results for the frustrated long-range transverse-field Ising model (lrTFIM) with antiferromagnetic interactions on two-dimensional lattices obtained via linked-cluster expansions extended by classical Monte-Carlo integrations. It is found that the nature of the phase transition crucially depends on the lattice geometry: On the square lattice, the lrTFIM remains in the nearest-neighbor universality class for all algebraically-decaying interactions studied. In contrast, on the triangular lattice, the nature of the quantum phase transition changes from 3D XY universality to a first-order transition due to the presence of a stripe-ordered phase for very slowly-decaying Ising interactions.

TT 23.13 Tue 12:45 Theater

Magnetism of the N = 42 kagome lattice antiferromagnet — •Jürgen Schnack[1], Jörg Schulenburg[2], and Johannes Richter[3] — [1]Fakultät für Physik, Universität Bielefeld, Postfach 100131, D-33501 Bielefeld, Germany — [2]Universitätsrechenzentrum, Universität Magdeburg, D-39016 Magdeburg, Germany — [3]Institut für Physik, Universität Magdeburg, P.O. Box 4120, D-39016 Magdeburg, Germany and Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

For the paradigmatic frustrated spin-half Heisenberg antiferromagnet on the kagome lattice we performed large-scale numerical investigations of thermodynamic functions by means of the finite-temperature Lanczos method for system sizes of up to N = 42 [1]. We present the dependence of magnetization as well as specific heat on temperature and external field and show in particular that a finite-size scaling of specific heat supports the appearance of a low-temperature shoulder below the major maximum. This seems to be the result of a counterintuitive motion of the density of singlet states towards higher energies. Other interesting features that we discuss are the asymmetric melting of the 1/3 magnetization plateau as well the field dependence of the specific heat that exhibits characteristic features caused by the existence of a flat one-magnon band. By comparison with the unfrustrated square-lattice antiferromagnet the tremendous role of frustration in a wide temperature range is illustrated.
[1] Phys. Rev. B 98, 094423 (2018)

TT 24: Molecular Electronics and Photonics

Time: Tuesday 9:30–12:15 Location: H22

TT 24.1 Tue 9:30 H22

Heat transport through single-atom and single-molecule junctions — •Fabian Pauly — Okinawa Institute of Science and Technology Graduate University, Okinawa, Japan

In this presentation, I will discuss our present theoretical understanding of heat transport at the atomic scale. Starting from results of a collaboration with experimentalists [1], I will elicidate the importantance of phonons for the thermal conductance of atomic-size contacts made of different metals [2] and will examine the validity of the Wiedemann-Franz law, which relates the electrical and the thermal conductance. Next, I will present a newly developed procedure to determine transmission eigenchannels for coherent phonon transport in nanoscale devices using the framework of nonequilibrium Green's functions [3]. To illustrate its value, I will study phonon eigenchannels in various systems ranging from metallic atomic-size contacts to different single-molecule junctions.

[1] L. Cui et al., Science 355, 1192 (2017)
[2] J. C. Klöckner et al., Phys. Rev. B 96, 205405 (2017)
[3] J. C. Klöckner et al., Phys. Rev. B 97, 155432 (2018)

TT 24.2 Tue 9:45 H22

Large Conductance Variations in a Mechanosensitive Single-Molecule Junction — •Maxim Skripnik[1,2], Davide Stefani[3], Kevin J. Weiland[4], Chunwei Hsu[3], Mickael L. Perrin[3,5], Marcel Mayor[4,6,7], Herre S. J. van der Zant[3], and Fabian Pauly[1,2] — [1]Okinawa Institute of Science and Technology, Japan — [2]University of Konstanz, Germany — [3]Delft University of Technology, The Netherlands — [4]University of Basel, Switzerland — [5]Swiss Federal Laboratories for Materials Science and Technology, Switzerland — [6]Karlsruhe Institute of Technology, Germany — [7]Sun Yat-Sen University, China

Using quantum-chemistry calculations we show that the conductance of a spring-like molecule can be mechanically controlled by several orders of magnitude by compressing or elongating it. [1] The calculations indicate that the large conductance variations are the result of a destructive quantum interference between the frontier orbitals. Furthermore, oscillations in the conductance occur when the stress built up in the molecule is high enough to allow the anchoring groups to move along the surface in a stick-slip-like fashion. Theoretical results are very well supported by break-junction measurements which demonstrate that the large conductance variations are also present at room temperature. This may open the door for applications in, e.g., a nanoscale mechanosensitive sensing device that does not rely on cryogenic cooling.

[1] D. Stefani et al., Nano Lett. 18, 5981 (2018).

TT 24.3 Tue 10:00 H22

High Magnetoresistance and Kondo Resonance in Radical Molecular Junctions — •Gautam Mitra[1], David Weber[1], Jonathan Low[2], Sujun Wei[2], Karol Francisco[2], Luis Campos[2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Department of Chemistry, Columbia University, Newyork, United States

The presence of an unpaired electron in organic radical molecules gives rise to intrinsic magnetic properties when coupled to nonmagnetic electrodes. In the present study, we report on the magnetic behavior of polychlorotriphenylmethyl radical molecule [1] junctions using the mechanically controlled break junction technique. The transport measurements were carried out at low temperatures down to 1.5K. We have observed very high positive and negative magnetoresistance up to 140% for a magnetic field of 6T applied perpendicular to the current direction. Alongside, we also observe significant zero bias anomalies corresponding to Kondo temperatures around 9K, originates from a spin flipping Kondo mediated transport channel as observed for a similar molecule contacted by rigid electrodes before [2]. Meanwhile the exact origin of magnetoresistance behavior from this molecule is still unknown and open for further investigation. By changing the inter-electrode spacing, we follow the development of the Kondo resonance and magnetoresistance which further opens up the relation between coupling of electrodes with molecule.

[1] Armet, O. et.al. J. Phys. Chem. 1987, 91, 5608-5616
[2] Frisenda, R. et.al. Nano Lett. 2015, 15, 3109-3114

TT 24.4 Tue 10:15 H22

Conductance switching by CO adsorption in Ag point contacts — Atasi Chatterjee[1], Frederik Edler[1,2], Christoph Tegenkamp[1,2], and •Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Institut für Physik, TU Chemnitz, Germany

We demonstrate that atomic point contacts can be generated at well-defined locations with extreme reliability in ultra-thin (5 nm) and ultra-small (minimum width 16 nm) Ag nanostructures, grown on hydrogen terminated low-doped Si (100) samples using the process of electro-migration at 100K inside a 4-tip SEM/STM UHV chamber. Single contacts were always obtained once the smallest constriction of the structures was below the average grain size of the Ag films and competing thermal migration was suppressed. Conductance histograms exhibit characteristic conductance values that were assigned to the different metastable configurations prior to atomic point contact formation. In-situ chemisorption of CO strongly altered the conductance from $0.9\,G_0 < \sigma < 1.3\,G_0$ to a stable value close to $0.1\,G_0$, suggesting adsorption of single CO molecules within the contact. In the presence of CO, current versus voltage curves showed a slightly rectifying behavior indicating preferential binding of CO to one side of the electrode. Furthermore, time resolved current measurements at 100 K demonstrate voltage-induced bi-stable conductance at 0.08 and 0.14 G_0 with stability of the 0.14 G_0 value below 0.1 V and of the lower conductance above 0.25 V, whereas at intermediate voltages switching between these values was observed.

TT 24.5 Tue 10:30 H22

Molecular junctions and molecular motors: Inclusion of electron-electron interactions in the electronic friction — •Miroslav Hopjan[1,2], Gianluca Stefanucci[3,4], Enrico Perfetto[3,5], and Claudio Verdozzi[2] — [1]current: Condensed Matter Theory, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Physics, Lund University, S-22100 Lund, Sweden — [3]Dipartimento di Fisica, Università di Roma Tor Vergata, Via della Ricerca Scientifica 1, I-00133 Rome, Italy — [4]INFN, Sezione di Roma Tor Vergata, Via della Ricerca Scientifica 1, I-00133 Roma, Italy — [5]CNR-ISM, Division of Ultrafast Processes in Materials (FLASHit), Area della Ricerca di Roma 1, Via Salaria Km 29.3, I-00016 Monterotondo Scalo, Italy

A semi-classical Ehrenfest (or Langevin) dynamics of current-induced forces in molecular junctions with electron-electron interactions will be presented. For the regime of slow nuclear dynamics we derive a general formula of the Markovian electronic friction, described within the one-particle non-equilibrium Green's function formalism. The proposed framework is approximations-free but at the same time it enables the direct use of many-body perturbation theory to include the interactions, thus it is suitable for practical calculations. Using a paradigmatic model and by benchmarking to non-Markovian dynamics we demonstrate the validity and numerical efficiency of the proposed scheme. We observe that the interactions can dramatically reduce the possibility of a negative friction coefficient, thus the self-sustainable current induced motion (i.e. molecular motor) can be suppressed by the interactions.

15 min. break.

TT 24.6 Tue 11:00 H22

Electron Transport through single Mn-salen molecule: Theoretical Study — •Lokamani Lokamani[1], Filip Kilibarda[1,2], Torsten Sendler[1], Peter Zahn[1], Michael Mortensen[3], Kurt Vesterager Gothelf[3], Artur Erbe[1,2], and Sibylle Gemming[1,4] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, 01328 Dresden, Germany — [2]Dept. of Physics, Universität Konstanz, 78457 Konstanz, Germany — [3]iNANO and Dept. of Chemistry, University Aarhus, 8000 Aarhus, Denmark — [4]Institute of Physics, Technische Universität, 09107 Chemnitz, Germany

Metal-salen complexes, formed by the coordination of a metal cation and a N,N'-bis(salicylidene)ethylenediamine-based ligand, are promising candidates for molecular electronics, because of possible modulations of transport channels using different metal cations. One such candidate is Mn-salen complex.

Here, we first explore the electronic structure of single molecules using wave function (MS-CASSCF) and density-functional (DFT+U) methods. We then employ the non-equilibrium Green's function (NEGF) technique to study electron transport through single molecules attached to gold electrodes under finite bias. We explore various docking configurations for the single molecule between the gold electrodes.

A comparison with experimental coupling constants and energy levels, obtained using mechanically controllable break junction (MCBJ) technique is also presented.

TT 24.7 Tue 11:15 H22

Electron Transport through single Mn-salen molecule: Experimental Study — •Filip Kilibarda[1,4], Lokamani Lokamani[1], Torsten Sendler[1], Michael Mortensen[2], Kurt Gothelf[2], Peter Zahn[1], Sibylle Gemming[1,3], and Artur Erbe[1,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]iNANO and Dept. of Chemistry, University Aarhus, 8000 Aarhus, Denmark — [3]Institute of Physics, Technische Universität, 09107 Chemnitz, Germany — [4]Dept. of Physics, Universität Konstanz, 78457 Konstanz, Germany

Molecular electronics offers new ways for scaling down nanoelectronic components and making their production and operation more energy efficient. Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junction (MCBJ).
Here, we perform measurements on salen molecule and metal-salen complexes in liquid environments. They are explored as candidates for "chemical doping", because they provide the possibility to fine-tune electrical properties by using different molecular inclusions. We measure both constant voltage vs. distance and IV characteristic of our metal-molecule-metal junctions.
Measurements are then fitted to a theoretical model, which takes the contribution of a single molecular level into account. From this model the energy of the molecular level and the coupling to the electrodes can be extracted and compared to first principles calculations.

TT 24.8 Tue 11:30 H22

Proximity effects of a STM tip on the magnetic properties of Fe-porphyrin on Au(111) — Laëtitia Farinacci[2], •Sumanta Bhandary[1], Reecht Gael[2], Silke Biermann[1], and Katharina Franke[2] — [1]Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau, France — [2]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We have investigated the adsorption of Fe-porphyrin (FeP) molecules on a Au (111) surface. By means of Scanning Tunnelling Microscopy (STM), we show that the FeP molecules are preferentially adsorbed on the fcc and hcp areas of the surface. Density functional calculations suggest the top-site to be the most stable adsorption site for FeP monomers. The electronic and magnetic features of adsorbed molecules depend largely on the hybridization with the Au surface as well as with the STM tip, and can only be modeled by taking into account the large effective Coulomb interactions, crystal field and spin-orbit coupling at the Fe centre. The tip-molecule, as well as surface-molecule hybridizations are tuned by approaching the STM tip, revealing changes in the magnetic fingerprints of molecules in the STM spectra. Based on density functional theory and many-body theory, we show that the ground state electronic configuration is changed as the tip approaches the molecule, changing the magnetic anisotropy and hence the STM spectra, while the spin state remains unchanged.

TT 24.9 Tue 11:45 H22

On surface formation of 1D polyferrocenylene chains on metal surfaces with unique structural and electronic properties — •Vijai Meena Santhini[1], Oleksandr Stetsovych[1], Martin Ondracek[1], Martin Svec[1], Jesus Mendieta[1], Bruno De La Torre[1,3], Irena G.Stara[2], Ivo Stary[2], Radek Zboril[3], and Pavel Jelenik[1] — [1]Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic — [2]Institute of Chemistry and Biochemistry, Czech Academy of Sciences, Praha, Czech Republic — [3]Regional Centre of Advanced Materials and Technologies, Olomouc, Czech Republic

We present a novel way of generation of long flexible 1D polyferrocenylene chains on metal surface with lengths up to 50 nm, representing the longest homo-coupled polyferrocenylene up to our knowledge. We employ on surface Ullman coupling polymerization of 1,1*-diiodobiferrocene molecules, deposited at room temperature under ultra-high vacuum conditions. The product are analysed using the low temperature scanning tunnelling microscope/atomic force microscopy (LT-STM/AFM). We observe two distinct 2D well-ordered polymer islands after annealing, with different electronic structure, due to the different packing of 1D molecular nanowires within the islands. We identified the internal molecular arrangement of island with help of high-resolution STM/AFM imaging with functionalized tips. We also succeeded in pulling out the 1D PFc chains from the islands to form free-standing 1D chains. We have identified a transition in the electronic behaviour, from semiconducting polymer 2D islands to metallic 1D chains using scanning tunneling spectroscopy.

TT 24.10 Tue 12:00 H22

Tunable quantum interference in ferrocene-based molecular junctions — •María Camarasa-Gómez[1], Daniel Hernangómez-Pérez[1], Michael S. Inkpen[2], Giacomo Lovat[2], Latha Venkataraman[2], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, Regensburg University, D-93053 Regensburg (Germany) — [2]Department of Applied Physics and Chemistry, Columbia University, New York, NY 10027 (USA)

Ferrocene is a well-known organo-metallic compound comprising a single iron atom 'sandwiched' between two cyclopentadiene rings. However, not many of the transport properties of an isolated ferrocene have actually been measured [1] or calculated [2, 3]. We here present a computational study of ferrocene and ferrocene moieties employing density functional theory-based quantum transport calculations inspired by recent experimental scanning-transport break junction measurements. Our results suggest that ferrocene-derived species exhibit interesting quantum interference properties: we find Fano-type resonances due to the localized d-states of the ferrocene metal, as well as mechanically-tunable anti-resonances. The latter can change dramatically the conductance at the Fermi level by orders of magnitude in a relatively controlled manner. Our numerical findings are rationalized by an effective three-level tight-binding model which explains the key role of the symmetries of frontier molecular orbitals in the position and shape of the quantum interference.

[1] S. A. Getty, et al., Phys. Rev. B 71, 241401 (2005)
[2] K. Kanthasamy et al., Small 12, 4849 (2016)
[3] X. Zhao, et al., Phys. Rev. B 96, 085421 (2017)

TT 25: Disordered Quantum Systems

Time: Tuesday 9:30–11:00 Location: H23

TT 25.1 Tue 9:30 H23

Ab-initio typical-medium single-site theory for disordered systems — •Liviu Chioncel[1], Andreas Östlin[2], Levente Vitos[3], Voicu Popescu[4], Krzysztof Byczuk[5], Hanna Terletska[6], Yi Zhang[7], Mark Jarrell[7], and Dieter Vollhardt[2] — [1]ACIT, Uni-Augsburg,Germany — [2]EKM, TP III, Uni-Augsburg,Germany — [3]KTH, Stockhom, Sweden — [4]LMU, Muenchen, Germany — [5]Uni Warsaw, Poland — [6]Middle Tennessee State University, USA — [7]Louisiana State University, USA

We introduce a self-consistent method to perform electronic structure calculations of disordered systems. The approach employs the single-site typical medium theory and is formulated in the language of multiple scattering. We present the formalism, implementation details and applications for realistic materials in which we find characteristics of Anderson localization, i.e., extended states and localized levels in different regions of the impurity bands.

TT 25.2 Tue 9:45 H23

Generalized Dynamical Mean-Field Theory for the Hubbard model with Off-Diagonal Disorder — Yi Zhang[1], •Liviu Chioncel[2], Hanna Terletska[3], Ka Ming Tam[1], Krzysztof Byczuk[4], Mark Jarrell[1], and Dieter Vollhardt[2] — [1]LSU, Baton Rouge, USA — [2]EKM, TP III, Uni-Augsburg,Germany — [3]MTU, Murfreesboro, USA — [4]Uni Warsaw, Poland

We generalize dynamical mean-field theory to describe systems with

off-diagonal (hopping) disorder. Our approach is based on the BEB formalism [1], which is an extension of the coherent potential approximation to study alloy systems with off-diagonal disorder. Here, within a cavity method [2] we show that the Hubbard model with bimodal off-diagonal disorder can be mapped onto an effective 2-band model coupled to two independent single impurity Anderson problems. Preliminary numerical results for spectral functions are presented. This method is formally exact in the infinite dimension. It can be extended to model multicomponent alloy systems with diagonal and off-diagonal disorders where electronic correlations are important.

[1] J. A. Blackman, D. M. Esterling, N. F. Berk, Phys. Rev. B 4, 2412 (1971)
[2] A. Georges, G. Kotliar, W. Krauth, M.J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996)

TT 25.3 Tue 10:00 H23

Dynamic Structure Factor of Disordered Coupled-Dimer Heisenberg models — •Max Hörmann and Kai Schmidt — Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen

We investigate the impact of quenched disorder on the zero-temperature dynamic structure factor of coupled-dimer Heisenberg models on the two-leg ladder and the two-dimensional square lattice bilayer. Using perturbative continuous unitary transformations, huge effects on individual quasiparticles but also on composite bound states and two-quasiparticle continua are observed [1]. This leads to intriguing quantum structures in dynamical correlation functions well observable in spectroscopic experiments.

[1] M. Hörmann, P. Wunderlich, K. P. Schmidt, Phys. Rev. Lett. 121, 167201 (2018)

TT 25.4 Tue 10:15 H23

Exceptional points and nodal-lines in disordered superconductors — •Alexander Zyuzin[1] and Pascal Simon[2] — [1]Aalto University, Espoo, Finland — [2]University Paris Sud, Orsay, France

We consider the effect of disorder on the spectrum of quasiparticles in the point-node and nodal-line superconductors. We show that the interplay of disorder, band-structure anisotropy, and the supercurrent might give rise to the non-Hermitian superconducting phase, where depending on the dimensionality of the system, the nodes in the spectrum are replaced by the bulk Fermi arc or area bounded by the exceptional points or lines, respectively. We first consider a model of the proximity-induced superconductivity in the anisotropic two-dimensional Dirac semimetal. It is shown that disorder leads to a non-Hermitian self-energy contribution resulting in a bulk Fermi arc in the gap function bounded by the exceptional points. We then consider three-dimensional nodal superconductors in the presence of the supercurrent and show that disorder scattering transforms the nodes in the spectrum of quasiparticles into a Fermi area bounded by the exceptional lines.

TT 25.5 Tue 10:30 H23

Microstructured Superconducting Resonator Technique for Measurements of Dielectric Polarization Echoes at Very Short Pulse Separation Times — •Andreas Schaller, Marcel Haas, Robert Haase, Anna Pollithy, Sergey Tsurkan, Matthias Sinnwell, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, D-69120 Heidelberg

The anomalous properties of amorphous solids at low temperatures are governed by tunneling systems, which are described as two-level systems in the phenomenological standard tunneling model. However, measurements of the dielectric constant, sound velocity, and dielectric polarization echoes of glasses containing atoms carrying large nuclear quadrupole moments revealed unexpected characteristics, such as magnetic field dependencies, which are not observed in glasses without nuclear quadrupole moments.

We present results of dielectric two-pulse polarization echo measurements carried out on different multicomponent glasses and polymers containing large nuclear quadrupole moments. For all these samples the two-pulse-echo decay occurs on a comparably short timescale. In order to investigate those echo decays on sub-μs times we developed planar microfabricated superconducting resonators. We were able to measure dielectric polarization echoes at unprecedentedly small pulse separation times and could see the flattening off of the polarization amplitude of N-BK7 towards small pulse separation times, as predicted by spectral diffusion theory.

TT 25.6 Tue 10:45 H23

Studying the Dielectric Low Temperature Properties of Amorphous Solids using Biased Resonators — •Benedikt Frey, Diana Körner, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, D-69120 Heidelberg

The low temperature properties of amorphous solids are governed by atomic tunneling systems, often described as two-level systems (TLS) with the energy splitting E. Besides the recent interest in these systems, due to their diverse impact on microfabricated quantum devices, such tunneling systems have been studied for many years in amorphous solids and are successfully described in many cases by the phenomenological standard tunneling model.

We use microfabricated superconducting resonators in a bridge-type setup to study the dielectric rf-response of the amorphous substrate in the presence of an electrical bias field. This bias field modifies the energy splitting E of a TLS by coupling to its dipole moment. Consequently, a sweep of the bias field constantly pushes different TLS in resonance with the resonator. We see a correlation between the dielectric function and the bias field sweep rate, which is compared to the simulation results of a Monte Carlo Method approach.

TT 26: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge III (joint session O/CPP/DS/TT)

Time: Tuesday 10:30–13:00 Location: H9

Topical Talk TT 26.1 Tue 10:30 H9

Addressing the structure and dynamics of weakly-bonded interfaces — •Mariana Rossi — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin

Interfaces between different materials constitute the basis of technological devices. Incorporating organic components within different architectures opens the path for creating more versatile interfaces with a wide range of properties at a reduced cost. However, the large conformational space that organic components can explore at finite temperatures and the inherent anharmonicity of their intra and intermolecular interactions brings further challenges to first-principles simulations. In this talk, I will discuss our recent efforts to address these challenges, based on developments within density functional theory an ab initio (path integral) molecular dynamics. I will present strategies for conformational space sampling of organic/inorganic interfaces, discuss the relationship between atomic and electronic structure including the effect of different functionals, present techniques to include anharmonicity in vibrational fingerprints and machine learning tools to calculate these at reduced costs, and our recent methodological developments that allow the inclusion of quantum nuclear effects in high-dimensional systems (especially weakly bonded interfaces) using path integral molecular dynamics.

TT 26.2 Tue 11:00 H9

Elucidating the Nuclear Quantum Dynamics of Intramolecular Double Hydrogen Transfer in Porphycene — •Yair Litman[1], Jeremy O. Richardson[2], Takashi Kumagai[1], and Mariana Rossi[1] — [1]Fritz Haber Insitute of the Max Planck Society, Berlin, Germany — [2]ETH, Zurich, Switzerland

We address the double hydrogen transfer (DHT) dynamics of the porphycene molecule: A complex paradigmatic system where the making and breaking of H-bonds in a highly anharmonic potential energy surface requires a quantum mechanical treatment not only of the electrons but also of the nuclei[1]. We combine density-functional theory calculations, employing hybrid functionals and van der Waals corrections, with recently proposed and optimized path-integral ring-polymer

methods for the calculation of vibrational spectra and reaction rates. Our simulations predict the position and width of the N-H stretching band of porphycene and DHT rates in excellent agreement with experiments, thus confirming our determination of the tunneling pathways and the anharmonic mode couplings that play a role in this reaction. They also provide quantitative information about the usually ignored competition between concerted and stepwise DHT pathways at different temperature. These results show that our theoretical approach can describe hydrogen transfer dynamics in different environments, for example when porphycenes are adsorbed on surfaces in prototype molecular switch architectures[2]. [1] Y. Litman, Richardson, J. O., Kumagai, T., Rossi, M. *arXiv*:1810.05681. [2] T. Kumagai, et al., *J. Chem. Phys.,* **148,** 102330 (2018).

TT 26.3 Tue 11:15 H9

Interplay of quantum nuclear fluctuations and the electronic structure of the cyclohexane/Rh(111) interface — •Karen Fidanyan and Mariana Rossi — Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, Berlin

Cyclohexane (C_6H_{12}) adsorbed on metal surfaces can participate in catalytic dehydrogenation reactions, which show good potential for hydrogen storage. It has been observed experimentally that C_6H_{12} adsorbed on the Rh(111) surface shows an isotope effect on the work function change and the adsorption energy upon deuteration [1]. The physical origin of this puzzling isotope effect on the electronic structure has not been fully resolved. We employ density-functional theory (PBE functional with van der Waals corrections) and *ab initio* path-integral molecular dynamics at 150 K to characterize the underlying physics of this phenomenon. We perform these simulations almost at classical-nuclei cost by making use of the spatially-localized ring-polymer contraction scheme proposed in Ref. [2]. The harmonic approximation to zero-point-energy in the adsorption energy is not able to capture the isotope effects observed experimentally. We thus include anharmonic corrections through the dynamics and identify the temperature-dependent electronic level broadening and renormalization due to the interaction with phonons in this system.
[1] T. Koitaya and J. Yoshinobu, *Chem. Rec.* **14** 848-856 (2014).
[2] Y. Litman, D. Donadio, M. Ceriotti and M. Rossi, *J. Chem. Phys.* **148** 102320 (2018).

TT 26.4 Tue 11:30 H9

Quantum-Nuclear Effects in Anharmonic Thermal Transport of Organic Materials — •Hagen-Henrik Kowalski, Mariana Rossi, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

To date, an accurate computational assessment of thermal transport in organic compounds still constitutes a considerable challenge for first principles theory, since the vibrations in such compounds are to a large extent governed by quantum-nuclear (QN) ***and*** strongly anharmonic (SA) effects [1]. Perturbative approaches account for QN, but not for SA effects, whereas Molecular Dynamics (MD) approaches [2] with classical nuclei account for SA, but neglect QN effects. To overcome this limitation, we here present a framework capable of accounting for both QN and SA effects by sampling the vibrational motion via Thermostatted Ring Polymer Molecular Dynamics (TRPMD). The lattice thermal conductivity is assessed through the Green-Kubo formalism and the auto-correlation of the heat flux. To obtain this quantity, we extend the *ab initio* heat-flux definition proposed in Ref. [2] from MD to TRPMD, in order to include QN effects. We critically discuss the approach, its accuracy, and numerical cost for several materials, ranging from toy-models, e.g., solid Argon, to recently discussed organic materials, in which both QN and SA effects are non-negligible.
[1] M. Rossi, P. Gasparotto, M. Ceriotti, *Phys. Rev. Lett.* **117**, 115702, (2016).
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901, (2017).

TT 26.5 Tue 11:45 H9

Electronic Conduction in Metal Junctions with Multi-Heme Proteins — •Zdenek Futera[1], Xiuyun Jiang[1], Jan Elsner[2], and Jochen Blumberger[1,3] — [1]Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom — [2]University of Cambridge, Robinson College, Grange Road, Cambridge CB3 9AN, United Kingdom — [3]Institute for Advanced Study, Technische Universität München, Lichtenbergstrasse 2 a, D-85748, Garching, Germany

Multi-heme proteins such as STC or MtrF are membrane proteins facilitating long-range electron transfer (ET) across cell membrane in metal-reducing bacteria. We have used classical molecular dynamics (MD) together with electronic-structure calculations based on density functional theory (DFT) to show that in native environment the conducted electrons are transferred by incoherent hopping between the heme cofactors. However, recent experimental measurements of current-voltage (I-V) curves suggested that the ET mechanism changes to coherent electron tunneling in vacuum when the protein is electronically coupled with metal electrodes. To investigate such conditions, we performed MD simulations in accurate gold/protein interaction force field to identify adsorption of STC and MtrF between two gold electrodes. By large-scale DFT calculations of the whole interfacial structure we identified the conduction channels formed predominantly by delocalized heme iron states. Finally, we apply Landauer formalism to compute I-V curves on STC junction using the DFT electronic states corrected for band alignment and discuss the ET mechanism.

TT 26.6 Tue 12:00 H9

Elastic and lattice-dynamical properties of titanium-based compounds — •Peter Weber, Pasquale Pavone, and Claudia Draxl — Humboldt-Univeristät zu Berlin, Physics Department and IRIS Adlershof, Germany

Titanium is the basic element of a variety of compounds with very different electronic, mechanical, and thermal properties. While, for instance, the rocksalt crystals TiC and TiN are well known for their hardness, allotropes of TiO_2 show much softer elastic behaviour. In this work we present the results of an *ab-initio* investigation of the elastic and lattice-dynamical properties of these compounds under pressure. The elastic-constant tensor is calculated up to the third order. Pressure effects on the lattice-dynamical properties of these compounds are evaluated in terms of the mode Grüneisen parameter at the Brillouin zone center. The calculations are performed using density-functional theory as implemented in the full-potential all-electron software package `exciting` [1]. Linear and nonlinear elastic constants are obtained using the `ElaStic` tool [2].

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202
[2] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184** 1861 (2013)

TT 26.7 Tue 12:15 H9

Understanding the electron transport through $NiSi_2$-Si interfaces — •Florian Fuchs[1,2,3,4], Sibylle Gemming[1,2,3], and Jörg Schuster[2,4] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Dresden, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [4]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Metal-semiconductor interfaces are of huge importance for applications and can be found in various field-effect transistors. We study the interface between $NiSi_2$ and silicon on the basis of density functional theory and the NEGF formalism. Different crystal orientations and strain states are investigated systematically.

We focus on the tunneling phenomena of carriers through the Schottky contact at the interface, which are crucial for the on-current in transistors. The on-current is found to be strongly dependent on strain and orientation. It will be shown that the height of the Schottky barrier determines the tunneling current. However, not all changes in the current can be traced back to the barrier height. The modification of the electronic structure matter as well, which can be modeled based on the effective mass of the tunneling carriers. We have also extracted work functions of the isolated materials which we relate to the extracted Schottky barrier heights. It will be shown that the Schottky-Mott model fails for this material system. Better approaches will be discussed in our contribution.

TT 26.8 Tue 12:30 H9

Impact of Lattice Screening on Wannier-Mott Excitons — •Claudia Rödl — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Optical properties of materials are most relevant for a large variety of technological applications, ranging from photovoltaics over various spectroscopy techniques to LEDs and displays. In optical spectra, microscopic quantum many-body effects like excitons, i.e. coupled electron-hole-pair excitations, are measurable at a macroscopic scale and crucially determine the materials properties. Hence, a deep understanding of exciton physics constitutes an indispensable driving force

for innovation in optics and optoelectronics.

The state-of-the-art parameter-free theoretical description of excitons is based on the Bethe-Salpeter equation of many-body perturbation theory. The present theoretical standard approach takes only the static electronic screening of the electron-hole-pair interaction into account. The coupling of excitons to phonons and, hence, polaronic screening contributions are omitted. However, the exciton-phonon coupling is crucial for the qualitative and quantitative understanding of exciton spectra in materials with strong polaronic effects, such as many technologically highly relevant oxides. We will tackle this problem and explore routes towards the inclusion of the polaronic screening contributions into the Bethe-Salpeter framework. As test systems, we study simple two-atomic bulk semiconductors and insulators.

TT 26.9 Tue 12:45 H9

Discovering a novel nanometric cubic phase in monochalcogenide semiconductors - Theory meets experiment — •Guy Makov[1,2], Uri Argaman[1], Elad Segev[2], Ran Abutbul[1,2], and Yuval Golan[1,2] — [1]Dept. of Materials, Ben-Gurion University, Beer-Sheva, Israel — [2]Ilse Katz Institute of nanoscience, Ben-Gurion University, Beer-Sheva, Israel

A new nanometric cubic binary phase with a low-symmetry 64-atom cubic structure was recently discovered in tin monosulfide. Subsequently, this phase was synthesized and identified in tin monoselenide and posited to exist in germanium monosulfide and monoselenide based on density functional theory total energy calculations. A series of computational and experimental studies have identified promising optical properties due to the larger bandgap and non-centrosymmetric structure of the crystal. The structure, atomic positions, band gaps and vibrational spectra of these phases were determined by ab-initio density functional calculations and found to be in very good agreement with experimental measurements. The phases were determined to be mechanically stable from ab-initio phonon spectra and energetically close to competing structures such as rhombohedral and orthorhombic. Surface energy calculations indicate that the particles must be stabilized by ligand adsorption. Ligand surface properties are explored to explain the nanocrystal growth mechanisms. This talk will focus on the results of our calculations on surface and bulk properties and their interplay with experimental studies.

TT 27: Focus Session: Designer Quantum Systems I (joint session O/TT)

Toy models are simplistic theoretical constructs, meant to capture the basic principles of complex phenomena observed in experiment. Recent amazing advances in condensed matter physics have enabled the reverse, namely the realization of basic theoretical models in well-controlled artificial experimental systems. Such solid state or molecular realizations of models allow us to tune their parameters, thus they may be termed designer quantum systems and can substantially deepen our understanding. Some talks in this session explore the insights offered by the already famous designer quantum systems; others propose or even report new quantum simulators. Moreover, these designer systems are not limited to single-particle physics but extend to many-body phenomena, such as superconducting correlations.

Organizers: Magdalena Marganska and Jascha Repp (University of Regensburg).

Time: Tuesday 10:30–12:45 Location: H15

Invited Talk TT 27.1 Tue 10:30 H15

Imaging Electronic Correlations in Twisted Bilayer Graphene — •Stevan Nadj-Perge — California Institute of Technology, Pasadena, CA, USA

Twisted bilayer graphene with a twist angle close to 1° features isolated flat electronic bands that form a strongly correlated electronic system. Here we investigate properties of this system by probing local tunneling density of states using scanning tunneling microscopy and spectroscopy. We show that the flat bands get deformed when they are aligned with the Fermi level using electrostatic gating. Careful characterization of the bands allows us to estimate energy scale of electron-electron interactions. Our results provide basis for microscopic understanding of correlated quantum phases in small angle twisted bilayer graphene.

Invited Talk TT 27.2 Tue 11:00 H15

Designing Electronic Quantum Matter: Fabrication and Characterization with Atomic Scale Precision — •Ingmar Swart — Debye Institute for Nanomaterials Science

In a visionary colloquium nearly sixty years ago, Richard Feynman proposed to study complex and elusive quantum systems using more controllable analogues, an approach known as quantum simulation [later published, 1]. Although quantum simulation based on ultracold atoms in optical lattices, nanophotonic systems, trapped ions and superconducting circuits has been very fruitful, electronic quantum simulators have been lacking behind [2].

In this talk, I will demonstrate that electron gases on well-defined metal surfaces form an excellent platform for quantum simulation. By patterning the surface with atomic scale precision using a scanning tunneling microscope, the electrons can be corralled into artificial lattices of nearly any geometry. The same microscope can then be used to measure the local density of states at all positions of interest and to probe the spatial extend and shape of the wave functions. I will show several examples of how we exploit the tunability of this platform. Particular emphasis will be given to our recent efforts to create and study electronic higher-order topological insulators.

References: 1. Richard P. Feynman, International Journal of Theoretical Physics, 21, 467 (1982). 2. Nature Physics Insight on Quantum Simulation, Volume 8 (2012).

TT 27.3 Tue 11:30 H15

Characterisation of pure s- and p-orbital bands in electronic honeycomb lattices — •Thomas Gardenier[1], Jette van den Broeke[2], Ingmar Swart[1], Cristiane Morais Smith[2], and Daniel Vanmaekelbergh[1] — [1]Debye Institute for Nanomaterials Science, Utrecht, The Netherlands — [2]Institute for Theoretical Physics, Utrecht, The Netherlands

Honeycomb systems have generated much interest in experimental and theoretical physics due to their interesting band structures. The architypical example of a honeycomb lattice is graphene. The electronic structure of graphene close to the Fermi level can be understood by only considering C 2pz orbitals. Bands due to coupling of sp2 hybrid orbitals are either much higher or lower in energy. It has been shown that in the absence of hybridisation, the band structure of honeycomb lattices features a topologically non-trivial flat band, as well as Dirac cones formed by px and py orbitals.

We patterned a Cu(111) surface with CO molecules to confine the surface state electrons into a honeycomb geometry. By careful tuning of the lattice parameters, we created a honeycomb lattice where s- and p-orbital bands are separated. Scanning tunneling spectroscopy and wavefunction mapping are used to determine the band structure and visualise the electron densities. The results are complemented by theoretical muffin-tin and tight-binding calculations.

TT 27.4 Tue 11:45 H15

Constructing a Topological Insulator Atom-by-Atom — •Saoirsé Freeney — Condensed Matter and Interfaces, Princetonplein 1, 3584 CC Utrecht, The Netherlands

In a honeycomb lattice with alternating hopping strengths (Kekulé lattice), a gap in the energy dispersion is opened. Depending on the ratio of hopping parameters and the shape of the boundary, the band structure is either topologically trivial or non-trivial. Using scanning tunnelling microscopy, we realize Kekulé lattices through the coupling of artificial atoms, created by the careful arrangement of electron scat-

terers (carbon monoxide molecules) on a 2D electron gas (Cu(111) surface state). The electronic properties were probed using scanning tunnelling spectroscopy and differential conductance mapping. We show that the topologically non-trivial lattice features a robust edge state whereas the trivial equivalent does not. The experimental outcomes align well with results from tight binding and muffin tin calculations.

TT 27.5 Tue 12:00 H15

Eu-doped NaI scintillators: Point defects and EuI_2 sheets. — •Martin Setvin[1], Manuel Ulreich[1], Igor Sokolovic[1], Michele Reticcioli[3], Lynn Boatner[2], Flora Poelzleitner[1], Cesare Franchini[3], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institute of Applied Physics, TU Wien, Vienna, 1040, Austria — [2]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831, USA — [3]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Vienna, Austria

Activator impurities and their distribution in the host lattice play a key role in scintillation phenomena. A combination of cross-sectional noncontact atomic force microscopy (nc-AFM) and X-ray photoelectron spectroscopy (XPS) was used to study the distribution of Eu^{2+} dopants in a NaI scintillator activated by 3% of EuI_2. Two types of precipitate structures were identified. First, a single-sheet of EuI_2 layered precipitate is a favoured configuration at the surface. Second, precipitates with a cubic crystal structure and a size below 4 nm were found in the bulk material. A surprisingly low concentration of point defects was detected in all of the investigated samples. The relation between the atomic structure and scintillation will be discussed.

The work was supported by the FWF Wittgenstein Prize Z-250.

TT 27.6 Tue 12:15 H15

Machine learning the 3D shape of non-planar molecules from AFM images — •Prokop Hapala[1], Fedor Utirev[1], Niko Oinonen[1], Ondřej Krejčí[1], Filippo Federici Canova[1], Benjamin Alldritt[1], Juho Kannala[2], Peter Liljeroth[1], and Adam Foster[1] — [1]Department of Applied Physics, Aalto University — [2]Department of Computer Science, Aalto University

In recent decade Atomic Force Microscopy with tip functionalized by carbon monoxide (CO) provided unique tool to experimentally image sub-molecular details of individual organic molecules [1]. Yet up to now most experiments are limited to flat aromatic molecules, due to difficulties with interpretation of highly distorted images originating from non-planer molecules due to mechanical relaxation of tip or sample. These problems can be partially overcome using a simple mechanical model [2] which can reproduce those distortions, therefore simulate AFM images for given molecular structure. Testing many possible candidate structures is, however, laborious. Instead we attempt to develop automatic tool to conduct inverse task - i.e. to recover molecular structure from given set of AFM images. Preliminary results suggests that convolutional neural network (CNN) [3] trained on simulated AFM images can learn this inverse mapping rather easily. Yet application of the method on real experimental data, and identification of atomic species remains to be a challenge. [1] Gross, L., et al., Science, 325(5944), 1110-1114 (2009). [2] Lecun, Y., et al., Proceedings of the IEEE, 86(11), 2278-2324 (1998). [3] Hapala, et al. PRB, 90(8), 085421 (2014).

TT 27.7 Tue 12:30 H15

Spectral Properties of the Herringbone lattice — M. A. Jimenez Herrera[1], O. Dutta[2], A. Iniguez[3], G. Giedke[2,4], and •D. Bercioux[2,4] — [1]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain — [2]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [3]University of the Basque Country, UPV/EHU, Bilbao, Spain — [4]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain

We investigate the spectral properties of a two-dimensional lattice system described by a non-symmorphic symmetry; specifically, we look at the herringbone lattice that is characterised by two glide symmetries. We model the system via a tight-binding model with horizontal and vertical hopping terms. We evaluate the spectrum of the system in the presence of a perpendicular magnetic field: we show how the Hofstadter's butterfly presents characteristics inherited by the honeycomb and square lattice butterflies. Furthermore, we investigate the appearance of edge states in the system when dimerizing the hopping parameters on the horizontal and vertical direction. We analyse the topological properties of these bands in a similar way to the analysis presented for the case of a symmorphic lattice [1]. Finally, we present a possible implementation in terms of CO atoms placed on the top of a Cu(111) surface [2].

[1] F. Liu, & K. Wakabayashi Phys. Rev. Lett. **118**, 076803 (2017). [2] K. K. Gomes, W. Mar, W. Ko, F. Guinea, & H. C. Manoharan Nature, **483**, 306 (2012).

TT 28: Cryotechnique: Refrigeration and Thermometry

Time: Tuesday 11:15–12:45 Location: H23

TT 28.1 Tue 11:15 H23

A small scale 4 K pulse tube cryocooler suitable for geophysical measurements — •Bernd Schmidt[1,2], Jack Schmidt[1,2], Jens Falter[1], Günter Thummes[1,2], and André Schirmeisen[1,2] — [1]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany — [2]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Although pulse tube cryocoolers (PTCs) reaching liquid Helium temperature were already presented in the 1990s [1], they are still subject to vivid development in many directions. For instance, PTCs with cooling powers up to 2 W, capable of competing with large LHe cryostats, have been presented recently [2]. For such high cooling power, an input power of > 11 kW is needed. We here present a development in miniaturization of a small PTC providing 70 mW @ 4.2 K with low input power [3]. This PTC works with an air-cooled, single phase 1 kW Helium compressor and is suitable for sensitive low-temperature applications, such as SQUIDs, SNSPDs or TES. The working principle and design challanges of this cold head are discussed. The performance of cooling sensitive measurements is demonstrated with a proof-of-concept experiment of a dc SQUID in a geophysical setup [4].

[1] Wang, C., Thummes, G., et al. Cryogenics, 37, 159-164 (1997)
[2] Wang, C. A. , Cryocoolers, 19, 299-305 (2016)
[3] Schmidt, B., Vorholzer, M., Dietrich, M., Falter, J., Schirmeisen, A., & Thummes, G., Cryogenics, 88, 129-131 (2017)
[4] Schmidt, B., Falter, J., Schirmeisen, A., & Mück, M., Superconductor Science and Technology, 31, 075006 (2018)

TT 28.2 Tue 11:30 H23

Analysis of intrinsic variations of a small scale low input power 4 K pulse tube cryocooler driven by smart Helium compressor — •Jack-Andre Schmidt[1,2], Bernd Schmidt[1,2], Jens Falter[2], Stefano Spagna[3], Günter Thummes[1,2], and André Schirmeisen[1,2] — [1]Justus-Liebig-Universität Gießen — [2]TransMIT GmbH — [3]Quantum Design, inc.

Today's research often exceed the available measurement time with liquid helium cryostats. Closed cycle cryocooler offer the possibility of almost nonstop cooling around 4 Kelvin, but suffer from intrinsic temperature and mechanical variations due to their working principle with high and low pressure phases. Among the regenerative cryocoolers, pulse tube cold heads stand out because of the absence of moving parts at the cooled parts, which is a preferable choice for sensitive applications. Here we present an experimental study of the intrinsic effects of a minimized 4 K pulse tube [1]. For the first time a broad parameter set can be studied by using a smart energy compressor [2]. The results show potential aspects that should be considered to reduce intrinsic effects in future cryostat designs.

[1] Schmidt B., et al., Cryogenics 88 (2017) 129-131.
[2] Chialvo, C., et al., Proceedings of Cryocoolers 18 (2014).

TT 28.3 Tue 11:45 H23

Cross Correlated Noise Thermometer for Milli-Kelvin Temperatures — •Christian Ständer, Andreas Reifenberger, Felix Mücke, Marius Hempel, Sebastian Kempf, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University.

Within our search for easy-to-use and reliable thermometers for milli-Kelvin and micro-Kelvin temperatures we developed a noise thermometer, where the Johnson noise of a massive cylinder of high purity silver is monitored simultaneously by two current sensing dc-SQUIDs. Operating both SQUIDs in voltage biased mode in a 2-stage configurations allows to reduce the power dissipation as well as the noise of the SQUIDs to a minimum. By cross-correlating the two SQUID signals, the noise contribution of the read-out electronics is suppressed to a marginal level even at micro-Kelvin temperatures. To further reduce the correlated amplifier noise we fabricated SQUIDs with minimal coupling of input and feedback coil. We compare two thermometers of this type to each other within the temperature range from 1 K down to 5 mK. Statistical uncertainties below 0.25 % are achieved within 10 s of measurement time. No significant systematic deviation between the two thermometers was observable. According to readout noise and a detailed thermal model the thermometers could be used down to 0.5 μK.

TT 28.4 Tue 12:00 H23

Measuring temperature gradients with superconducting sensors — •Sandra Sandra Gottwals[1], Thierry Crozes[2], and Georg Schmidt[1,3] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Fachgruppe Nanostrukturierte Materialien, Halle — [2]Institut Néel, CNRS, Grenoble — [3]Martin-Luther-Universität Halle-Wittenberg, Interdisziplinäres Zentrum für Materialwissenschaften, Halle

For the investigation of spin caloric phenomena it is necessary to know the local temperature of the investigated material or even determine local temperature gradients. We intend to investigate the spin Nernst effect [1] in Pt which creates a spin Accumulation from a temperature gradient in a normal metal. Because we want to measure this spin accumulation using micro-SQUIDS [2] it is necessary to create and measure a temperature gradient over a distance of a few micrometer at cryogenic temperatures. The gradient is created by a resistive heater and the temperature gradient is determined using superconducting stripe sensors. The temperature dependence of the critical current in superconductors allows us to calibrate the sensors and to reliably measure the temperature. All structures are fabricated by e-beam lithography and reactive ion etching. We present details of the fabrication process and performance tests of individual sensors and sensor pairs.

[1] S.-G.Cheng, et al.: Phys. Rev. B 78 045302 (2008)
[2] W. Wernsdorfer: Supercond. Sci. Technol. 22 (2009) 064013

TT 28.5 Tue 12:15 H23

Crossover of dominant energy relaxation mechanism in normal metal films — •Libin Wang and Jukka Pekola — QTF Centre of Excellence, Department of Applied Physics, Aalto University, FI-00076 Aalto, Finland

For normal metals at low temperature, the electrons are known to be well decoupled from the phonons. When a constant heating is applied to the normal metal, the electron temperature will be elevated above the phonon temperature, which leads to the hot electron effect. For thin normal metal films at low temperature, the high thermal resistance (R_{ep}) between electrons and phonons in the metal films will dominate over the thermal boundary resistance (R_d) between the metal film and insulating substrate, and become the bottleneck for energy relaxation in the films. By increasing the film thickness or temperature, the ratio of R_{ep}/R_d will increase and to some point the dominant energy relaxation constrain will be the thermal boundary resistance between films phonons and substrate phonons. Here we will present the experimental observation of this crossover in normal metal films on the silicon substrate at temperature below 0.2K, where phonons in metal films are supposed to be two dimensional (2D). The derived thermal boundary resistance between 2D phonons and the substrate is a few times higher than that when the phonons are in the three dimensional (3D). The observed crossover for the dominant energy relaxation mechanism in normal metal films has significant benifit in understanding of thermal behavior of nanoelectronic devices at low temperature.

TT 28.6 Tue 12:30 H23

Development of a liquid hydrogen moderator with a free adjustable ortho/para ratio for the provision of specific cold neutron spectra — •Johannes Baggemann[1], Tobias Cronert[1], Ulrich Rücker[1], Paul Zakalek[1], Paul-Emmanuel Doege[1], Thomas Gutberlet[1], Sarah Boehm[2], Marcel Klaus[3], Sebastian Eisenhut[3], and Thomas Brückel[1] — [1]Forschungszentrum Jülich GmbH — [2]RWTH Aachen University — [3]TU Dresden

Neutron scattering as a method for studying structure and dynamics of condensed matter offers unique opportunities for a wide field of application. Under the frame of the High Brilliance Neutron Source (HBS) project, the Jülich Centre for Neutron Science is developing a new type of scalable accelerator driven pulsed neutron source. One of the projects objectives is to make the scattering method more accessible in regards to costs, lead times and restrictions. The design of the source enables an optimization along the whole neutron production chain towards the needs of each scattering experiment and fully offset the low neutron production.

One of the key components of this optimization is the development of a novel low dimensional liquid hydrogen neutron moderator with a variable ortho/para ratio. By adjusting this ratio, an optimal neutron energy spectrum could be delivered to a particular scattering experiment. After a brief introduction to the project, the fundamentals of the liquid ortho/para mixture as neutron moderator will be presented. The state of the development of the hydrogen moderator as well as its potential that must be determined experimentally will be outlined.

TT 29: Nanotubes and Nanoribbons

Time: Tuesday 14:00–16:00 Location: H2

Invited Talk TT 29.1 Tue 14:00 H2

Mesoscopic quantum electrodynamics with carbon nanotubes — •Takis Kontos — CNRS/ENS, Paris, France

Cavity quantum electrodynamics techniques have turned out to be instrumental to probe or manipulate the electronic states of nanoscale circuits. Recently, cavity QED architectures have been extended to quantum dot circuits. These circuits are appealing since other degrees of freedom than the traditional ones (e.g. those of superconducting circuits) can be investigated. I will show how one can use carbon nanotube based quantum dots in that context. In particular, I will focus on how to engineer a coherent spin/photon coupling in a double quantum dot spin-valve and to use this interface to manipulate the electronic spin with cavity photons. Quantum dots also exhibit a wide variety of many body phenomena. The cQED architecture could also be instrumental for understanding them. One of the most paradigmatic phenomenon is the Kondo effect which is at the heart of many electron correlation effects. I will show that a cQED architecture has allowed us to observe the decoupling of spin and charge excitations.

Invited Talk TT 29.2 Tue 14:30 H2

Nanomechanical characterization of the Kondo charge dynamics in a carbon nanotube — Karl J. G. Götz, Daniel R. Schmid, Felix J. Schupp, Peter L. Stiller, Christoph Strunk, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Suspended single wall carbon nanotubes are at cryogenic temperatures both extraordinary nanomechanical systems and prototypical clean and defect-free single electron devices. This allows for many interesting studies. In particular, by measuring the gate voltage dependence of the transversal vibration frequency, the evolution of the charge on a quantum dot embedded in the nanotube can be precisely evaluated.

We apply this technique to the case of strong Kondo correlations between a quantum dot and its contacts. The current through the nanotube displays a clear odd-even pattern, with a zero-bias conductance anomaly at odd electron number. The time-averaged charge on the quantum dot, however, shows no odd-even pattern, and can be well modelled via sequential tunneling only. We conclude that the Kondo current is carried via virtual occupation of the quantum dot alone.

In addition, the simultaneous detection of charge and current signal allows us to compare the gate potentials where on one hand the current is maximal and on the other hand the charge in the quantum dot increases. Here, a distinct relative shift is observed, decreasing logarithmically with temperature. Our observations agree very well with models for Kondo-correlated quantum dots.

[1] K. J. G. Götz *et al.*, PRL **120**, 246802 (2018)

TT 29.3 Tue 15:00 H2

Oscillator induced phase transition in a quantum dot Josephson junction — •Robert Hussein, Daniel Reger, and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, Germany

We investigate the Josephson transport through a suspended carbon nanotube quantum dot—acting likewise as a mechanical resonator—in the presence of an external magnetic field. At sufficiently low temperatures, the transport properties are characterized by the ground state of the electronic subsystem being either in a singlet, doublet, or current suppressing triplet state. We show that the triplet blockade can be lifted by the coupling to the resonator and study the emergence of a triple point, where all three ground states coexist. Furthermore, we demonstrate that this oscillator induced phase transition also manifests in the critical current.

TT 29.4 Tue 15:15 H2

Quantum transport through carbon nanotube $NbSe_2$ hybrid devices for Majorana Fermion detection — •Christian Bäuml[1], Michaela Eichinger[1], Brecht Simon[1,2], Maria-Teresa Handschuh[1], Lorenz Bauriedl[1], Anh-Tuan Nguyen[1], Nicola Paradiso[1], and Christoph Strunk[1] — [1]University of Regensburg, Regensburg, Germany — [2]Delft University of Technology, Delft, Netherlands

The initial proposals for the realization of Majorana fermions (MFs) were based on one-dimensional semiconductors proximitized by a superconductor (SC) in the presence of spin-orbit interaction and of perpendicular magnetic field. More recently, it was suggested that MFs can also occur in carbon nanotubes (CNTs) in proximity to an ultrathin superconductor in large parallel fields [1,2].

In this work, we demonstrate first building blocks of the device proposed by Marganska et al. As a SC we chose a bilayer $NbSe_2$ crystal, which is so thin that its electron density and chemical potential can be tuned by a gate. Such tunability is crucial to enter the topological phase of the proximitized CNT. We show that the $NbSe_2$-CNT contact transparency can be drastically improved by exfoliating and stamping the flake in N_2 atmosphere. Finally, we present a first proof-of-principle device, whose transport characteristics are measured as a function of temperature and magnetic field.

[1] R. Egger et al. Phys. Rev. B **85**, 235462 (2012)
[2] M. Marganska et al. Phys. Rev. B **97**, 075141 (2018)

TT 29.5 Tue 15:30 H2

Transport properties of MoS_2 and WS_2 nanotubes — •Simon Reinhardt[1], Luka Pirker[2], Christian Bäuml[1], Maja Remškar[2], and Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany — [2]Solid State Physics Department, Institute Jožef Stefan, Ljubljana, Slovenia

While synthesis procedures for nanotubes based on layered materials other than graphene are well-known [1, 2, 3], their transport properties are so far largely unexplored [4]. Here, we introduce transition metal dichalcogenide (TMDC) nanotubes as a new material platform for transport spectroscopy. We present results on optimized nanotube synthesis, first device fabrication, and electrical characterization. MoS_2 and WS_2 nanotubes are synthesized using a chemical transport reaction. Optimized growth parameters lead to thin nanotubes with diameters down to 7nm, lengths up to several millimeters, and an extremely low number of structural defects. Field effect devices based on individual nanotubes are characterized in low temperature transport measurements.

[1] R. Tenne *et al.*, Nature **360**, 444 (1992)
[2] M. Remškar *et al.*, Appl. Phys. Lett. **69**, 351 (1996)
[3] M. Remškar *et al.*, Advanced Materials **10**, 246 (1998)
[4] F. Qin *et al.*, Nature Communications **8**, 14465 (2017)

TT 29.6 Tue 15:45 H2

Coexistence of superconductivity and quantum Hall states in InSb Nanosheets — •Ning Kang — Department of Electronics, Peking University, China

Hybrid superconducting devices based on high-mobility two-dimensional electron gases with strong spin-orbit coupling are considered to offer a flexible and scalable platform for topological quantum computation. Here, we report the realization and electrical characterization of hybrid devices based on high-quality InSb nanosheets and superconducting Nb electrodes. The high critical magnetic field of Nb combined with high-mobility InSb nanosheets allows us to exploit the transport properties in the exotic regime where the superconducting proximity effect coexists with quantum Hall effect. Transport spectroscopy measurements in such a regime reveal an enhancement of the conductance at the quantum Hall plateaus, accompanied by a pronounced zero-bias peak in the differential conductance. We discuss that these features originate from the formation of Andreev edge states at the superconductor-InSb nanosheet interface in the quantum Hall regime.

TT 30: Correlated Electrons: 1D Theory

Time: Tuesday 14:00–15:45 Location: H4

TT 30.1 Tue 14:00 H4

Static properties of an atomic Luttinger liquid superimposed on a linear ion chain — •Andreas B. Michelsen[1,2,3], Manuel Valiente[4], Nikolaj T. Zinner[1,5], and Antonio Negretti[6] — [1]Department of Physics and Astronomy, Aarhus University, DK-8000 Aarhus C, Denmark — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg — [3]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom — [4]SUPA, Institute of Photonics and Quantum Sciences, Heriot-Watt University, Edinburgh EH14 4AS, United Kingdom — [5]Aarhus Institute of Advanced Studies, Aarhus University, DK-8000 Aarhus C, Denmark — [6]Zentrum für Optische Quantentechnologien and The Hamburg Centre for Ultrafast Imaging, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany

We investigate the one-dimensional physics of a linear chain of ions immersed in a Luttinger liquid (LL) of spin-polarized fermionic atoms. Such systems have recently become experimentally realizable and host an interesting interplay between atom-atom interactions and atom-ion interactions. We compute the LL parameter and the speed of sound as a function of the quantum defect parameters, the latter of which can be controlled e.g. by manipulating the ions' internal state. We find a strong dependence of the LL parameter and the speed of sound on the quantum defect parameters, enabling us to modify the static properties of the quantum liquid via external driving of the ionic impurities.

TT 30.2 Tue 14:15 H4

Dynamical and entanglement properties of a one-dimensional many-body-localized system coupled to a bath — •Elisabeth Wybo, Michael Knap, and Frank Pollmann — Technische Universität München

Interactions and disorder can lead to a novel many-body localized phase provided the disorder is strong enough. We study how a dephasing bath destroys many-body localization by investigating interferometric protocols known from nuclear magnetic resonance. We determine the time scale, governed by the dephasing rate, at which the localization will be destroyed. We also investigate various measures of entanglement in these systems, and study how their typical behavior is modified by the presence of a bath. For this research we develop exact Krylov methods and tensor-network techniques, to exactly address the effect of the environment on the quantum dynamics.

TT 30.3 Tue 14:30 H4

Dimensional phase transitions from 1D quantum liquids to 3D condensates — •Polina Matveeva[1], Imke Schneider[1], Sebastian Eggert[1], Axel Pelster[1], Denis Morath[1], and Dominik Strassel[1,2] — [1]Technical University of Kaiserslautern, Kaiserslautern, Germany — [2]Competence Center for High Performance Computing, Fraunhofer ITWM, Kaiserslautern,Germany

We consider weakly coupled strongly interacting quantum chains, such as quantum wires, anisotropic ultracold gases, or quasi-1D spin-chain compounds. It is known that a phase transition from the 1D Luttinger liquid behavior to a 3D ordered states can be qualitatively descibed by a chain mean field theory to determine the critical temperature, but the quantitative corrections and the range of validity is not well estab-

lished. We therefore simulate the transition using a fully 3D microscopic model with very large scale quantum Monte Carlo calculations and compare with theoretical prediction including higher order terms in the chain mean field theory. We not only determine the very strong quantitative corrections, but also find a new regime of low density behavior where long range quantum correlations between the chains dominate the behavior, which leads qualitatively different powerlaws as a function of interchain couplings.

TT 30.4 Tue 14:45 H4

Effective narrow ladder model for quantum multi-wires on a semiconducting substrate — •Anas Abdelwahab and Eric Jeckelmann — Leibniz Universität Hannover, Institut für Theoretische Physik, Appelstr. 2, 30167 Hannover

We propose a lattice model for quantum multi wires on a three dimensional substrate and map them onto effective two-dimensional lattice using the Block-Lanczos algorithm. This mapping is a generalization of the mapping introduced in [1] for single-wire system. Then, we approximate the resulting two-dimensional lattice by taking only a limited number of legs to form a narrow ladder model. We investigate the validity of this approximation and discuss the influence of the wire-substrate hybridization on the wire-wire coupling using noninteracting two-wire systems. We discuss the possibility to realize Luttinger liquid properties in correlated two-wire systems.

Support from the DFG through the Research Units FOR 1700 is gratefully acknowledged.

[1] A. Abdelwahab, E. Jeckelmann, and M. Hohenadler, Phys. Rev. B 96, 035445 (2017)

TT 30.5 Tue 15:00 H4

Phase diagram of spin-1 chains with Dzyaloshinskii-Moriya interaction — •Hugo Tschirhart[1], Ernest Teng Siang Ong[2], Pinaki Sengupta[2], and Thomas L. Schmidt[1] — [1]University of Luxembourg, Luxembourg, Luxembourg — [2]Nanyang Technological University, Singapore, Singapore

We investigate an antiferromagnetic spin-1 Heisenberg chain in the presence of Dyzaloshinskii-Moriya interactions (DMI) and an external magnetic field. We study the resulting spin chain using a combination of numerical and analytical techniques. Using DMRG simulations to determine the spectral gap and the entanglement spectrum, we map out the phase diagram as a function of magnetic field strength and DMI strength. We provide a qualitative interpretation for these numerical findings by mapping the spin-1 chain on a spin-1/2 ladder and using a bosonization approach.

TT 30.6 Tue 15:15 H4

Understanding the Difference between a Hole in the 1D and 2D Antiferromagnet: Crucial Role of Magnon-Magnon Interactions — •Piotr Wrzosek[1], Krzysztof Bieniasz[2,3], Andrzej Michał Oleś[2,4], and Krzysztof Wohlfeld[1] — [1]Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, Prof. S. Łojasiewicza 11, PL-30348 Kraków, Poland — [3]Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z4 — [4]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

We determine the spectral function of a hole for the one-dimensional (1D) Ising t-J_z model using the variational approximation which converges to the exact result with increasing magnon number, however only when the magnon-magnon interactions are properly included. Surprisingly, although the creation of subsequent magnons beyond the first one does not cost any energy, a (modified) self-consistent Born approximation requires also infinite number of magnons to reproduce the exact 1D spectrum. This demonstrates that a single spinon is reproduced by infinite number of magnons. In contrast, in two dimensions magnon-magnon interactions do not change the spectral function qualitatively, explaining why the hole is subject to the string potential, absent in the 1D model.

TT 30.7 Tue 15:30 H4

The spin Drude weight of the XXZ chain and generalized hydrodynamics — •Yahya Öz[1], Andrew Urichuk[2], Andreas Klümper[1], and Jesko Sirker[2] — [1]Bergische Universität Wuppertal, Deutschland — [2]University of Manitoba, Canada

Based on a generalized free energy we derive exact thermodynamic Bethe ansatz formulas for the expectation value of the spin current, the spin current-charge, charge-charge correlators, and consequently the Drude weight. These formulas agree with recent conjectures within the generalized hydrodynamics formalism. They follow, however, directly from a proper treatment of the operator expression of the spin current. The result for the Drude weight is identical to the one obtained 20 years ago based on the Kohn formula and TBA. We numerically evaluate the Drude weight for anisotropies $\Delta = \cos\gamma$ with $\gamma = \frac{\pi n}{m}$, $n \leq m$ integer and coprime. We prove, furthermore, that the high-temperature asymptotics for general $\gamma = \frac{\pi n}{m}$ obtained by analysis of the quantum transfer matrix eigenvalues agrees with the bound which has been obtained by the construction of quasi-local charges.

TT 31: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge IV (joint session O/CPP/DS/TT)

Time: Tuesday 14:00–16:45 Location: H9

Topical Talk TT 31.1 Tue 14:00 H9

The Data Revolution in Materials Science, Through the Lens of the Materials Project — •Kristin Persson — University of California, Berkeley, USA

Advanced materials are essential to economic and societal development, with applications in multiple industries, from clean energy, to national security, and human welfare. Historically, novel materials exploration has been slow and expensive, taking on average 18 years from concept to commercialization. Due to the tremendous improvements in computational resources, coupled with software development during the last decades, real materials properties can now be calculated from quantum mechanics much faster than they can be measured. A new era of computational materials prediction and design has been born. A result of this paradigm change are databases like the Materials Project which is harnessing the power of supercomputing together with state of the art quantum mechanical theory to compute the properties of all known inorganic materials and beyond, design novel materials and offer the data for free to the community together with online analysis and design algorithms. We leverage the rich data from the Materials Project for machine learning; accelerating materials design, characterization and finally synthesis of materials. This talk will survey this rapidly evolving and exciting paradigm in science, showcasing the possibilities and iteration between ideas, computations, insight and new materials development.

TT 31.2 Tue 14:30 H9

High-throughput simulations of complex band structure — •Emanuele Bosoni and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2

The Complex Band Structure (CBS) generalizes the conventional band structure of a material by considering wave-vectors with complex components. The CBS extends the description of the allowed states of a material beyond the bulk propagating states, including in the picture the evanescent wave-functions that grow or decay from one unit cell to the next. Even though these latter states are forbidden by translational symmetry, they become important when this is broken via, for example, an interface. In the past, many studies made use of CBS calculations in order to confirm or motivate experimental findings, but only recently we see some efforts to give an unified prospective to the study of this quantity [1]. Moreover, the growth in recent years of high-performance computational resources available at relatively low cost opens the possibility to make a systematic, high-throughput, study of the CBS within the Density Functional Theory (DFT) framework.

In this contribution we will present our implementation of the Transfer Matrix Method [1] for the calculation of the CBS within the DFT code Siesta [2] and we will explain challenges and benefits of the high-throughput approach. We will present a proof of concept example in which we calculated the CBS for a set of materials and we will conclude explaining the relevance of our project in the field of spintronics.

[1] Reuter M. G., J. Phys.: Condens. Matt. 29, 053001 (2017)
[2] J. M. Soler et al., J. Phys.: Condens. Matt. 14, 2745 (2002)

TT 31.3 Tue 14:45 H9

Computational Screening of 2D Materials for Solar Cells Application — •Anders Christian Riis-Jensen and Kristian Sommer Thygesen — Institute for Physics, Technical University of Denmark

Two-dimensional (2D) materials have attracted great attention in recent years, not least due to their extremely strong coupling to light and pronounced excitonic effects. This makes 2D materials an ideal playground for studying light-matter interaction in nano-scale materials for applications within e.g. solar cells and photo-detectors. In this work, we present a large-scale computational study of a wide variety of 2D materials with the aim of identifying novel candidates with strong light-matter interaction. Specifically, we calculate the absorption spectrum of almost 2000 materials at the level of the Random Phase Approximation (RPA) and/or by solving the Bethe-Salpeter Equation (BSE). This enables us of calculating the Power Conversion Efficieny (PCE) for all these materials fully ab-initio. Based on this we identify specific 2D semiconductors for both single- and tandem solar cells. The best candidates present power densities (PCE per unit mass) of several orders of magnitude larger than both Si and GaAs. Lastly, we also show a detailed analysis of a few 2D materials, in which we find exciton states with exceptionally strong coupling to light and large exciton binding energies.

TT 31.4 Tue 15:00 H9

First-principles Modelling of Solid-Solid Interfaces in all Solid-State Batteries — •Bora Karasulu[1], James P. Darby[1], Clare P. Grey[2], and Andrew J. Morris[3] — [1]Dept. of Physics, Univ. of Cambridge, UK — [2]Dept. of Chemistry, Univ. of Cambridge, UK — [3]School of Metallurgy and Materials, Univ. of Birmingham, UK

All solid-state batteries (ASSBs) can potentially mitigate the safety issues known for conventional Li-ion batteries, and provide enhanced energy densities, by replacing the organic electrolyte solutions with solid inorganic equivalents. Mechanical and (electro)chemical incompatibilities between the ASSB solid components, however, lead to high resistances, curtailing the Li-ion transport at their interfaces. In this talk, we introduce a high-throughput ab initio modelling approach towards the rational design of electrolyte/electrode interfaces in ASSBs. First, we obtain phase diagrams of sulfide-based electrolytes with diverse compositions, phases, vacancies and doping using the Ab Initio Random Structure Searching (AIRSS) method. Next, the stable and low-lying metastable phases are screened for their ionic conductivity using ab initio molecular dynamics simulations. Finally, diverse surfaces of the selected electrolyte phases are interfaced with the surfaces of electrodes or other interfacial (e.g. solid electrolyte interphase, SEI) layers to determine the stable combinations using an automated procedure (INTERFACER). The devised approach will be demonstrated in action for a collection of interfaces, e.g. Li-P-S electrolytes with LiCo2, Li-metal electrodes and alike.

TT 31.5 Tue 15:15 H9

New Insights into Amorphous Materials and their Surfaces by Combining Machine Learning and DFT — •Volker Deringer — University of Cambridge, Cambridge, UK

Understanding links between atomic structure, chemical reactivity, and physical properties in amorphous solids is a long-standing challenge. DFT-based atomistic simulations have played important roles in this, but come at high computational cost. Novel interatomic potentials based on machine learning (ML) achieve close-to DFT accuracy, but require only a small fraction of the cost. In this talk, I will argue that such ML-based potentials are particularly useful for studying amorphous solids.

First, I will describe a Gaussian Approximation Potential (GAP) for amorphous carbon, which we recently used to simulate the deposition of tetrahedral amorphous carbon (*ta*-C) films, one atom at a time. These simulations reproduced the experimentally observed count of sp^3 atoms and gave new insight into the microscopic growth mechanism. I will then discuss how ML-based potentials can be combined with density-functional methods to yield new insights into surface functionalization (specifically, hydrogenation and oxidation) of *ta*-C. Finally, I will present recent work on amorphous silicon, another prototypical non-crystalline material that ML-driven simulations can describe with high accuracy. Looking ahead, these studies suggest that ML-based potentials may become more widespread tools for the realistic modelling and understanding of the amorphous state.

TT 31.6 Tue 15:30 H9

Harvesting from unbiased sampling of open systems: phase diagrams and property maps of surfaces and clusters in reactive atmosphere — •Yuanyuan Zhou, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Numerous processes that occur at surfaces of materials play a critical role in the manufacture and performance of functional materials, e.g., electronic, magnetic, and optical devices, sensors, catalysts, and coatings. A prerequisite for analyzing and understanding the electronic properties and the function of surfaces is detailed knowledge of the atomic structure, i.e., the surface composition and geometry under realistic condition. We introduce a Replica-Exchange (RE) Grand-Canonical (GC) Monte-Carlo algorithm. By means of the coupled sampling at several chemical potentials (i.e., partial pressures) of a reactive gas atmosphere and temperatures, the REGC scheme enables the unbiased calculation of (p, T) phase diagrams of surfaces, nanoparticles, or clusters in contact with reactive atmosphere, where all anharmonic contributions are included. Moreover, the multi-canonical sampling yields the temperature-pressure dependence (map) of all equilibrium observables that can be measured within the given model Hamiltonian. For instance, structural parameters such as the radial distribution function, or the fundamental electronic gap. This allows for rational design, where *operando* condition are taking fully into account. We demonstrate the approach for model Lennard-Jones surfaces as well as Si clusters and surfaces in a hydrogen atmosphere.

TT 31.7 Tue 15:45 H9

Crystal structure prediction for high capacity battery materials — •Angela F Harper[1] and Andrew J Morris[2] — [1]Department of Physics, University of Cambridge, JJ Thomson Ave, Cambridge CB3 0HE, UK — [2]School of Metallurgy and Materials, University of Birmingham, Edgbaston, Birmingham, UK

The future of large-scale energy storage relies heavily on the ability of Li-ion batteries to have high capacity and long-term stability. At present, graphite anodes limit the overall capacity of Li-ion batteries to a theoretical maximum of 372 mAh/g, and thus there is a need for higher capacity anodes such as phosphorus. We have studied lithiation in phosphorus using a combination of *ab initio* random structure searching (AIRSS) and density-functional theory calculations. In the Li-P system we found a novel phase of $P2_12_12_1$ Li_4P_3, which showed stable 0K phonon modes [1]. We further showed, using defect AIRSS searches, that doping the known Li-P phases with aluminium improved their electronic density of states at the Fermi level, and could improve conductivity in phosphorus anodes. To improve the cyclability of these phosphorus anodes, which break down after several cycles due to volume expansion of over 200%, in this talk we will investigate the phase diagrams and voltage profiles of several ternary compounds of Li-P-M where M is a metallic element which maintains the conductivity of aluminium doping and adds stability to the anode.

[1] Mayo, M. et al. Chem. Mater. 2016, 28, 2011*2021

TT 31.8 Tue 16:00 H9

Constructing Accurate Machine Learning Force Fields for Flexible Molecules — •Valentin Vassilev-Galindo, Igor Poltavsky, and Alexandre Tkatchenko — Physics and Material Science Research Unit, University of Luxembourg, Luxembourg

State-of-the-art machine learning (ML) models can reproduce potential energy surfaces (PES) for molecules containing up to a few tens of atoms with the accuracy comparable to the most exact ab initio methods. This provides a unique tool for computing different thermodynamic properties that would require millions of CPU years otherwise. For instance, a recently developed sGDML[1,2] model predicts forces and energy with CCSD(T) accuracy using just a few hundreds of configurations for training. However, up to now ML has been mainly applied to rather rigid molecules. In this regard, our objective is to test ML for flexible molecules and out-of-equilibrium configurations along transition paths. For this, we select molecules (e.g. azobenzene, stilbene) with relatively complex transition paths, which result from an interplay between long- and short-range interactions. Then, different paths connecting PES minima are tested using sGDML. This allows us to define optimal descriptors and the most appropriate strategies for choosing the training sets, which is crucial for ML models relying on a limited number of training points. Our results open an avenue for efficiently calculating transport pathways, transition rates and other

out-of-equilibrium properties with previously unattended accuracy.

[1] Chmiela, S. et al., Sci. Adv. 3, e1603015 (2017).
[2] Chmiela, S. et al., Nat. Commun. 9, 3887 (2018).

TT 31.9 Tue 16:15 H9

Calculating critical temperatures for magnetic order in two-dimensional materials — •Daniele Torelli — CAMD, Department of Physics, Technical University of Denmark, 2820 Kgs. Lyngby, Denmark

Recent observation of ferromagnetic out-of-plane order in two-dimensional (2D) CrI_3 highlights the importance of a microscopic understanding of magnetic anisotropy (MA) in ground state magnetic systems. Single-ion anisotropy and anisotropic exchange coupling comprise crucial ingredients to escape the Mermin-Wagner theorem which implies that rotational symmetry cannot be spontaneously broken at any finite temperature in 2D and thus prevents magnetic order.

In the present work we investigate the variation of critical temperature in Heisenberg model systems using classical Metropolis Monte Carlo simulations. A fit for square, hexagonal and honeycomb lattices leads to a simple expression for the critical temperatures as a function of MA and exchange coupling constants.

Based on a new developed computational 2D materials database, we predict 2D structures with high critical temperatures and high thermodynamic and dynamic stability for future experimental investigations. As testing system, relevant Heisenberg exchange couplings and MA energies in mono-layer CrI_3 are obtained from first principle calculations and energy mapping analysis, yielding to an estimation of Curie temperature in good agreement with experimental results.

TT 31.10 Tue 16:30 H9

Amino-acids on metallic surfaces: searching conformational space — •Dmitrii Maksimov, Carsten Baldauf, and Mariana Rossi — Fritz-Haber-Institut der Max-Planck- Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Organic-inorganic interfaces are challenging for computational modeling, in particular regarding the prediction of stable configurations at the interface, which determine the electronic properties of the system as a whole. The amino acid arginine is a flexible molecule in the gas phase and experiments show its self-assembly into dimers, rings, and chains on Ag(111) and Au(111) surfaces. For two protonation states (neutral Arg and charged $ArgH^+$), we perform systematic structure searches by placing known gas-phase minima in different orientations on top of the surfaces, followed by full relaxation within long-range dispersion corrected density-functional theory (DFT). In the analysis, we aim at understanding the alterations of the conformational space from the gas phase to surface adsorption by means of a dimensionality-reduced representation based on a combination of the Smooth Overlap of Atomic Positions (SOAP) and the Sketchmap techniques [1]. The favorable interaction with the metallic surface reduces the number of accessible conformations for neutral Arg. For the adsorption of charged $ArgH^+$, the number of local minima increases due to surface-dependent partial charge screening. [1] S. De et al., *J. Cheminform.*, **9**:6 (2017)

TT 32: Focus Session: Designer Quantum Systems II (joint session O/TT)

Time: Tuesday 14:00–15:45 Location: H15

Invited Talk TT 32.1 Tue 14:00 H15

Topological quantum phases in atomically precise graphene nanoribbons — •Oliver Gröning[1], Shiyong Wang[2], Qiang Sun[1], Akimitsu Narita[3], Müllen Klaus[3], Pascal Ruffieux[1], and Roman Fasel[1] — [1]Empa Materials Science and Technology, Dübendorf, Switzerland — [2]School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai, China — [3]Max Planck Institute for Polymer Research, Mainz, Germany

Topological materials have attracted great interest in solid state physics due to their ability to support robust, yet exotic quantum states at their boundaries or interfaces such as spin-momentum locked transport channels or Majorana fermions. Very recently, it has been found theoretically by Louie et al., that localized zero energy modes can be obtained at the junctions of topologically dissimilar graphene nanoribbons (GNR). We have experimentally realized such GNR junctions using on-surface synthesis, i.e. by the polymerization of molecular precursors rationally designed to yield the desired final GNR on single crystal surfaces. By creating well defined periodic sequences of these topological electronic modes, one-dimensional electronic bands can be created, which are described by the Su-Schrieffer-Heeger (SSH) Hamiltonian representing the dimerized atomic chain. By manipulating the intra- and inter-cell coupling strength we could further create SSH analogs with different winding number and therefore topological class. The topological class distinction is evidenced by presence, respectively absence of zero energy end states at the termini of the corresponding GNR or their junctions to structurally dissimilar GNRs.

Invited Talk TT 32.2 Tue 14:30 H15

Electronic properties of twisted graphene layers: bands, interactions and superconductivity. — •Francisco Guinea — Imdea Nanscience, Faraday , 28049 Madrid, Spain — School of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK

Twisted graphene bilayers show an unusual band structure, with very narrow bands. In these bands, states with different momenta show significant variations in their charge density. A change in the number of carriers leads to inhomogeneous charge distributions, which, in turn, modify significantly the shape of the bands. This effect can be described in terms of emergent assisted hopping interactions. These couplings tend to favor superconductivity.

TT 32.3 Tue 15:00 H15

Symmetry breaking in Molecular Artificial Graphene — •Linghao Yan[1,2], Muqing Hua[2], Qiushi Zhang[2], Tsz Ue Ngai[2], Zesheng Guo[2], Tsz Chun Wu[2], Tong Wang[2], and Nian Lin[2] — [1]Aalto University, Finland — [2]The Hong Kong University of Science and Technology, Hong Kong, China

Artificially-assembled molecular lattices on metal surfaces, known as molecular designers (Nature 483, 306, 2012), have been used as simulators to explore exciting physics that are extremely challenging to access in real materials. For example, gauge field, edge states and flat band are demonstrated in artificial grahpene, graphene nanoribbons, and Lieb lattice. In this work, we exploit the unique tunability of the molecular designers to break the symmetry of Dirac quasiparticles. The importance of symmetry breaking in graphene for applications has been widely recognized. Several schemes have been proposed, including breaking sublattice symmetry and applying uniaxial strain. Here we report the realization of both of these schemes by designing isotropic molecular potentials and isotropic lattices, respectively. The spatially-resolved local density of states acquired using scanning tunneling spectroscopy confirm that in both cases the local density of states undergo characteristic changes.

TT 32.4 Tue 15:15 H15

On-Surface Synthesis and Characterization of Cycloarenes: a C108 Graphene Quantum Ring — •Qitang Fan[1], Daniel Martin Jimenez[2], Simon Werner[1], Daniel Ebeling[2], André Schirmeisen[2], Jörg Sundermeyer[1], Wolfgang Hieringer[3], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Institute of Applied Physics (IAP), Justus Liebig University Gießen, Germany — [3]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Cycloarenes, such as kekulene, are a unique class of polycyclic aromatic hydrocarbons (PAHs). They enclose a cavity by circularly annulated benzene rings. In a modern view, they can thus be considered as nanorings cut-out from graphene with atomic precision. These graphene rings could serve as useful model quantum materials for the exploration of geometry-dependent electronic properties of nanographenes, e.g., the Aharonov-Bohm effect in graphene quantum rings. However, the synthesis and characterization of cycloarenes with more than one band of benzene rings is still challenging due to their special ring-shaped geometry and low solubility. Here, we employed the high-dilution principle both on a metal surface and in solution to synthesize a novel hexagonal cycloarene with two bands of annulated benzene rings, containing 108 sp2 carbons, by hierarchical Ullmann coupling and cyclodehydrogenation reaction of dibrominated aromatic precursors. The structure

and properties of this C108 cycloarene molecule has been unambiguously clarified by various techniques including STM/STS, nc-AFM, UV-vis spectroscopy, and DFT calculations.

TT 32.5 Tue 15:30 H15

Nonlinear optical Hall effect in BC_2N — •Julen Ibañez-Azpiroz[1], Ivo Souza[1,2], and Fernando de Juan[2,3] — [1]Materials Physics Center, CSIC-UPV/EHU, 20018 Donostia-San Sebastián, Spain — [2]Ikerbasque Foundation, 48013 Bilbao, Spain — [3]Donostia International Physics Center (DIPC), 20018 Donostia, Spain

The bulk photovoltaic effect is a nonlinear optical response that yields a net photocurrent in noncentrosymmetric crystals. Its interband contribution under linearly polarized light, known as the *shift current*, involves a subtle Berry-phase-like quantity that makes this effect very sensitive to wavefunction properties. Here we show that the relative parity of valence and conduction bands under mirror reflection determines whether the shift current flows parallel or perpendendicular to the applied electric field. The former situation is realized in GeS and similar monolayers [1,2] while the later, which corresponds to a nonlinear optical Hall effect, is far less common. Based on a recently developed *ab-initio* method [3], we show that this novel effect is realized in layer-structured graphitic BC_2N. Furthermore, our calculations reveal an enhanced shift-current absorption in the visible range, which makes BC_2N a prime candidate for future experimental studies.

[1] A. Cook, B. M. Fregoso, F. de Juan et. al., Nat. Commun. **8**, 14176 (2017).

[2] T. Rangel, B. M. Fregoso, B. S. Mendoza et. al., Phys. Rev. Lett. **119**, 067402 (2017).

[3] J. Ibañez-Azpiroz, S. S. Tsirkin and I. Souza, Phys. Rev. B **97**, 245143 (2018)

TT 33: Frustrated Magnets - General 2 (joint session TT/MA)

Time: Tuesday 14:00–16:00 Location: Theater

TT 33.1 Tue 14:00 Theater

Strong quantum interactions prevent quasiparticle decay — •Ruben Verresen[1,2], Roderich Moessner[1], and Frank Pollmann[2] — [1]Max-Planck-Institute for the Physics of Complex Systems — [2]Technical University of Munich

Quantum states of matter typically exhibit collective excitations known as quasiparticles. Known to be long-lived at the lowest energies, common wisdom says that quasiparticles become unstable when they encounter the inevitable continuum of many-particle excited states at high energies. Whilst correct for weak interactions, we show that this is far from the whole story: strong interactions generically stabilise quasiparticles by pushing them out of the continuum. This general mechanism is straightforwardly illustrated in an exactly solvable model. Using state-of-the-art numerics, we find it at work also in the spin-1/2 triangular lattice Heisenberg antiferromagnet (TLHAF) near the isotropic point—this is surprising given the common expectation of magnon decay in this paradigmatic frustrated magnet. Turning to existing experimental data, we identify the detailed phenomenology of avoided decay in the TLHAF material Ba3CoSb2O9, and even in liquid helium—one of the earliest instances of quasiparticle decay.

TT 33.2 Tue 14:15 Theater

Spin-1/2 Heisenberg antiferromagnet on the star lattice: Competing valence-bond-solid phases studied by means of tensor networks — •Saeed Jahromi and Roman Orus — Donostia International Physics Center (DIPC) Paseo Manuel de Lardizabal 4 20018 Donostia - San Sebastian (Guipuzkoa), Spain

Using the infinite projected entangled pair states algorithm, we study the ground-state properties of the spin-1/2 quantum Heisenberg antiferromagnet on the star lattice in the thermodynamic limit. By analyzing the ground-state energy of the two inequivalent bonds of the lattice in different unit-cell structures, we identify two competing valence-bond-solid (VBS) phases for different antiferromagnetic Heisenberg exchange couplings. More precisely, we observe (i) a VBS state which respects the full symmetries of the Hamiltonian, and (ii) a resonating VBS state which, in contrast to previous predictions, has a six-site unit-cell order and breaks C3 symmetry. We also studied the ground-state phase diagram by measuring the ground-state fidelity and energy derivatives, and further confirmed the continuous nature of the quantum phase transition in the system. Moreover, an analysis of the isotropic point shows that its ground state is also a VBS as in (i), which is as well in contrast with previous predictions.

TT 33.3 Tue 14:30 Theater

Quantum Monte-Carlo simulation of SU(2N) Spin systems — •Jonas Schwab, Francesco Parisen Toldin, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We consider the spin-S, SU(2N) Heisenberg model corresponding to the irreducible representation of SU(2N) consisting of a Young tableau of N rows and 2S columns. In the large-S limit the spin wave approximation leads to spin ordering, whereas in the large-N limit a saddle point approximation favors dimerization. We show that this generalized SU(2N) spin model can be solved with sign-problem free determinantal quantum Monte-Carlo methods on any bipartite lattice so that the phase diagram in the S versus N plane can in principle be mapped out.

TT 33.4 Tue 14:45 Theater

Doping a 2d Mott insulator - Study of a quantum dimer model — •Sebastian Huber[1], Fabian Grusdt[2,3], and Matthias Punk[1] — [1]Arnold Sommerfeld Center, Ludwig-Maximilians University, 80333 Munich, Germany — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA — [3]Department of Physics and Institute for Advanced Study, Technical University of Munich, 85748 Garching, Germany

Experiments with quantum gas microscopes have started to explore the antiferromagnetic phase of the Fermi-Hubbard model and effects of doping with holes away from half filling [1]. We show in this talk that the system averaged local two-spin density matrix enables to distinguish magnetically ordered and interesting topologically ordered spin-liquid phases, which might occur in the Hubbard model close to half filling.

Fractionalized Fermi liquids (FL*) are a promising candidate for this parameter regime. The generalized quantum dimer model introduced in Ref. [2] is an effective lattice realization of such an FL* with a Hilbert space spanned by configurations of fermionic and bosonic short-range bound states. We construct a rather unconventional dynamical cluster approximation (DCA) by making explicit use of the dimer Hilbert space and show first results of spectral data for a minimal cluster of two lattice sites.

[1] A. Mazurenko, C. Chiu et al., Nature 545, 7655 (2017)

[2] M. Punk, A. Allais and S. Sachdev, PNAS 112, 31 (2015)

TT 33.5 Tue 15:00 Theater

The evolution of spin – orbital entanglement in the approximate SU(2)⊗SU(2) model — •Dorota Gotfryd[1,2], Ekaterina Paerschke[3], Andrzej M. Oles[2,4], and Krzysztof Wohlfeld[1] — [1]Institute of Theoretical Physics, University of Warsaw, Warsaw, Poland — [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland — [3]Department of Physics, University of Alabama at Birmingham, Birmingham, USA — [4]Max Planck Institute for Solid State Research, Stuttgart, Germany

In insulating states of transition metal oxides with orbital degeneracy spin – orbital superexchange describes the effective interactions [1]. In such a frustrated environment the quasi – empirical Goodenough – Kanamori rules may be violated leading to inter – site spin – orbital entanglement [2]. In this talk we analyse the phase diagram of an SU(2)⊗SU(2) symmetric model [3, 4] perturbed with a less symmetric term. Even though such conditions create more complicated type of entanglement, interestingly the underlying physics becomes much simpler. We present extensive numerical studies supported also by analytical calculations.

This work is supported by Narodowe Centrum Nauki (NCN, Poland) under Projects No. 2016/23/B/ST3/00839 and No. 2016/22/E/ST3/00560.

[1] A.M. Oles, J. Phys.: Condensed Matter **24**, 313201 (2012)

[2] A.M. Oles *et al.*, Phys. Rev. Lett. **96**, 147205 (2006)

[3] S.K. Pati, R.R.P. Singh, D. Khomskii, Phys. Rev. Lett. **81**, 5406

(1998)
[4] W.-L. You, P. Horsch, A.M. Oles, Phys. Rev. B **92**, 054423 (2015)

TT 33.6 Tue 15:15 Theater

Asymptotical high-field saturation in spin-1/2 systems with XYZ spin-anisotropy and/or Dzyaloshinskii Moriya interactions — •Stefan-Ludwig Drechsler[1], Rolf Schumann[2], Richter Johannes[3], Ullrich Roessler[1], Roman Kuzian[4], Helge Rosner[5], Alexander Tsirlin[6], and Satoshi Nishimoto[1,2] — [1]ITF at the IFW-Dresden, Dresden, Germany — [2]TU Dresden, Theoret. Phys., Germany — [3]Universität Magdeburg, Inst. Theo. Phys. — [4]Inst. f. Material Sciences, Kyiv, Ukraine — [5]MPI-CPfS. Dresden, Germany — [6]Exp. Physik, Augsburg, Germany

We consider the high-field saturation of longitudinal and transversal magnetizations $M(B)$ of a wide class of spin-1/2 systems with low lattice symmetry leading to XYZ spin anisotropy and/or the presence of Dzyaloishnskii-Moriya (DM) interaction between nearest neighbor (NN) spins. Exact analytical, exact doagonalization and DMRG results are presented for small and large clusters as well as extended 1D and 2D systems. Above the last inflection point of the longitudinal magnetization only a power-law universal magnetization $\propto 1/B^2$ in leading order is found. We provide also higher order terms and focus on the influence of boundary conditions and the cases of staggered magnetizations and transversal DM components. Applications to various spin-chain compounds such as linarite and qubit/qutrit quantum dots being of interest in the field of quantum computing are discussed and compared critically with results published so far. Fitting experimental data within improper spin-symmetries, such as XXZ, may lead to unphysical large DM terms overestimated by an order of magnitude.

TT 33.7 Tue 15:30 Theater

Nonlocal probes for topological phase transitions from worldline braiding in path-integral quantum Monte Carlo — •Wei Wang[1], Fabio Lingua[2], Liana Shpani[2], and Barbara Capogrosso-Sansone[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Physics, Clark University, Worcester, U.S.A.

We propose non-local probes to study quantum and topological phase transitions in bosonic lattice spin-1/2 models. These probes can be explained as certain properties of braids of bosons' world-lines in configurations of path-integral quantum Monte Carlo (PIQMC). These new probes have been demonstrated to be good alternatives to order parameters for topologically trivial quantum phase transitions, and also have been shown to be efficient methods in studying topologically nontrivial phase transition. Furthermore, numerical results indicate that the world-line braids in configurations of PIQMC give a concrete meaning of so called "patterns" of short and long-range entanglement.

TT 33.8 Tue 15:45 Theater

Multi-loop contributions in the pseudo-fermion functional renormalization group for quantum spin systems: implementation and consequences — •Tobias Müller[1], Yasir Iqbal[2], Johannes Reuther[3,4], and Ronny Thomale[1] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilians University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Department of Physics, Indian Institute of Technology Madras, Chennai 600036, India — [3]Dahlem Center for Complex Quantum Systems and Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [4]Helmholtz-Zentrum für Materialien und Energie, Hahn-Meitner-Platz 1, 14019 Berlin, Germany

We extend the pseudo-fermion functional renormalization group (PFFRG) treatment of quantum spin systems by including diagrammatic higher loop contributions into the renormalization group flow. This allows us to consistently account for all contributions of parquet-type diagrams in the two-particle vertex and self-energy derivatives within the two-particle truncated PFFRG flow. We will discuss the impact of these corrections in different quantum spin models within PFFRG, especially in the light of the Mermin-Wagner theorem.

TT 34: Nonequilibrium Quantum Many-Body Systems 2

Time: Tuesday 14:00–16:00 Location: H22

TT 34.1 Tue 14:00 H22

Thermalization and Bose-Einstein condensation dynamics of photons coupled to a dye-molecule bath — •Michael Kajan and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Discrete electronic or spin excitations in molecules or atoms coupled to vibrations are often described by the Jaynes-Cummings or the spin-boson models. When, in addition, the electronic excitations are coupled to the electromagnetic environment via photon emission and absorption, the system becomes not exactly solvable due to the non-canonical dynamics of the (pseudo)spins. Experimentally, by the emission of photons from a reservoir of laser-pumped dye molecules into an optical cavity with a non-zero lower band cutoff or with a discrete mode spectrum, thermalization and Bose-Einstein condensation of the photon gas has been realized [1]. We develop a novel slave boson representation for the molecule dynamics which accounts for all molecular states, electronic and vibrational, on the same footing. It makes the dynamics of photons coupled to the non-Markovian bath of molecule excitations tractable by standard diagrammatic techniques. We extend the method to describe Bose-Einstein condensation of the photons. It can be generalized in a straight-forward way to non-equilibrium time-dependent dynamics using the Keldysh technique.
[1] J. Klaers, J. Schmitt, F. Vewinger, M. Weitz, Nature **468**, 545 (2010)

TT 34.2 Tue 14:15 H22

Quantum thermalization in isolated ultracold gases — •Marvin Lenk[1], Anna Posazhennikova[2], Tim Lappe[1], and Johann Kroha[1] — [1]Physikalisches Institut, Universität Bonn, Germany — [2]Royal Holloway, University of London, United Kingdom

Quantum thermalization, i.e., how an isolated quantum system can dynamically reach thermal equilibrium behavior, is a long-standing problem of quantum statistics. The eigenstate thermalization hypothesis (ETH) poses that, under certain conditions, the long-time expectation value w.r.t. a typical energy eigenstate is indistinguishable from a microcanonical average. By contrast, thermal behavior is reached generally in a non-integrable quantum many-body system alone due to the vast size of the Hilbert space dimension D. In any realistic experiment, only a small subset of the quantum numbers defining a pure state can be measured, if D is sufficiently large. The Hilbert space spanned by the undetermined quantum numbers is traced over and dynamically forms a grand-canonical bath [Ann. Phys. **530**, 1700124 (2018)]. We identify this mechanism in a generic system of N interacting bosons in M single-particle levels by computing numerically exactly the time evolution of the reduced densitiy matrix, the entanglement entropy for the observed subsystem as well as expectation values, fluctuations, thermalization times and the distribution function. The thermalizing quantities are, thus, defined by the measurement itself and not restricted to local observables. For $N \approx 25$ and $M \approx 5$, D is large enough for thermalization to occur dynamically. By contrast, ETH requires microcanonical initial conditions implying stationary time dependence.

TT 34.3 Tue 14:30 H22

Exact long-time evolution of spinless fermion systems from a highly correlated state — •Kristof Harms, Lorenzo Cevolani, Stefan Kehrein, and Salvatore Manmana — Institute for Theoretical Physics, University of Göttingen

We investigate the dynamics of a one-dimensional system of spinless fermions, which is initially prepared in a highly correlated groundstate of an interacting Hamiltonian. In particular, for a global quench that turns off the interaction, we evolve the initial state obtained via density matrix renormalisation group (DMRG) using analytical solutions of the equations of motion. This allows us to reach arbitrary times. We examine features of the dynamics of density-density correlations and susceptibilities on several time scales. Shortly after the quench, we identify, in addition to the typical lightcone-behavior, periodic recurrences of the initial correlations outside the lightcone. At very long times, we use our approach to investigate the Fluctuation-Dissipation theorem in this strong nonequilibrium situation.

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Forschungsgemeinschaft (DFG) is gratefully acknowledged.

TT 34.4 Tue 14:45 H22

Stabilizing a dissipative discrete time crystal — Leon Droenner[1], •Regina Finsterhölzl[1], Markus Heyl[2], and Alexander Carmele[1] — [1]Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

Experimental evidence of time reversal symmetry breaking in many-body Floquet systems has led to the discovery of a new phase of matter out-of-equilibrium, the so called discrete time crystal (DTC) [1]. The DTC shows periodic oscillations with an integer number of the Floquet period. Here, an essential ingredient is random disorder such that the system is many-body localized (MBL) to remain out-of-equilibrium due to the suppression of entanglement growth within the isolated many-body system.
However, in case of an open quantum system, dissipation naturally melts the DTC [2]. To create a stable DTC in the presence of dissipation, we propose to structure the external reservoirs such that non-Markovian effects are non-negligible. Similar to MBL for the isolated system, the idea is to suppress entanglement growth with external degrees of freedom. We show that such feedback dynamics stabilize the DTC and its oscillations become independent of the coupling to the environment.
[1] J. Zhang et al, Nature 543, 217-220 (2017).
[2] A. Lazarides and R. Moessner, Phys. Rev. B 95, 195135 (2017).

TT 34.5 Tue 15:00 H22

Preparation of Floquet-topological states with shortcuts of adiabaticity — •Tobias Gulden and Netanel Lindner — Technion - Israel Institute of Technology

A major obstacle in the experimental realization of Floquet topological insulators is the preparation of the desired initial state. Fast protocols for state preparation with high fidelity are needed. We develop a modification of shortcuts to adiabaticity for Floquet systems. This allows to create a desired Floquet eigenstate out of the ground state of the undriven system within a short time. Despite crossing the topological phase transition while turning on the drive we obtain the ground state of the Floquet system with high fidelity. This approach can more generally be used in different Floquet systems.

TT 34.6 Tue 15:15 H22

Engineering Feshbach resonances by time-periodic driving — •Christoph Dauer, Axel Pelster, and Sebastian Eggert — Physics Department and Research Centre OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger Straße 46, 67663 Kaiserslautern, Germany

Magnetic Feshbach resonances are a powerful tool in order to control the scattering length in ultracold gas experiments [1], but are limited to given atomic species or applied magnetic field strengths. Here we investigate a periodically driven two-channel model describing magnetic Feshbach resonances using the Floquet formalism [2-4]. Position and width of the resulting resonances, which appear in the scattering length, turn out to be tunable by both driving strength and frequency. An extension of our two-channel model also allows to describe the corresponding case of an optical Feshbach resonance [5], where either the Rabi frequency or the detuning is modulated periodically in time. The goal of these investigations is to check whether the variability of the accessible s-wave scattering lengths can be increased by the time-periodic modulation.
[1] C. Chin et al. Rev. Mod. Phys. 82 1225 (2010)
[2] D.H. Smith. Phys. Rev. Lett. 115, 193002 (2015)
[3] A.G. Sykes, H. Landa, and D.S. Petrov. PRA 95, 062705 (2017)
[4] S.A. Reyes et al. New J. Phys. 19, 043029 (2017)
[5] O. Thomas et al. Nature Comm. 9, 2238 (2018)

TT 34.7 Tue 15:30 H22

Exploring in the dynamical quantum phase transition theory the presence of a quantum critical region close to the critical time — •Daniele Trapin and Markus Heyl — Max Planck Institute for the Physics of Complex Systems Nöthnitzer Straße 38 D-01187 Dresden

The presence of dynamical quantum phase transitions(DQPTs) with properties resembling those of the continuous phase transitions, suggests to investigate the existence of a quantum critical region in the proximity of the critical time. This region plays a fundamental role in the theory of quantum phase transition, since it allows to prove experimentally the presence of the quantum critical point. This is achieved because the physical features at the critical point are extended to nonzero temperature and for a small range of the control parameter around the critical point. In the out-of-equilibrium regime, we study the presence of a dynamical quantum critical region close to the critical time. In this context, to get an analogous picture with the equilibrium case, we have to substitute the control parameter with time, and temperature with the energy density.

TT 34.8 Tue 15:45 H22

Entanglement properties of continuous many-body systems via machine learning — •Fabio Hernandez-Hernandez[1,2] and Matthias Rupp[2] — [1]Universidade Estadual de Campinas (UNICAMP), Campinas, Brazil — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Quantum entanglement plays an important role in strongly correlated systems and new quantum technologies. However, computing entanglement properties of continuous systems such as atoms, molecules and materials is challenging. One of the most successful techniques for this, variational quantum Monte Carlo, requires a suitable parametrization of the wave function to identify a systems' ground state. The structure of this variational wave function determines which phenomena can be accessed. It should therefore be both general and efficiently computable. Building on recent work for discrete model systems, such as Ising and Hubbard models, [1] we propose to parametrize the ground state wave function of continuous systems via a Gaussian-Bernoulli Restricted Boltzmann Machine [2]. We demonstrate feasibility of this approach by calculating the linear entropy, a bipartite quantum entanglement measure, for two model systems, Hooke's atom and the helium atom. We discuss the utility of this approach to study critical phenomena and other exotic physical properties in strongly-correlated continuous systems.
[1] Carleo & Troyer, Science **355**, 602 (2017),
Nomura et al., Phys Rev B **96**, 205152 (2017)
[2] Melchior et al., PLoS One **12**, e0171015 (2017)

TT 35: Spintronics (joint session TT/MA/DY)

Time: Tuesday 14:00–16:00 Location: H23

TT 35.1 Tue 14:00 H23

Long-lived chirality states in low-temperature strongly-coupled Rashba systems — •Philipp C. Verpoort, James R. A. Dann, Gareth J. Conduit, and Vijay Narayan — Department of Physics, University of Cambridge, J.J. Thomson Avenue, Cambridge CB3 0HE, UK

We observe ultra-slow magnetoresistance dynamics at sub-Kelvin temperatures in various systems that display strong Rashba spin-orbit coupling. These dynamics display a striking magnetoresistance curve that follows different traces depending on direction and speed of a magnetic field sweep. This novel effect cannot be explained by magnetisation or magnetocaloric effects. We suggest that the dynamics arise from detuning of the Fermi levels of the two Rashba bands and the slowness of their relaxation into equilibrium due to the suppression of inter-band scattering mechanisms that would be expected in conventional systems. Surprisingly, the relaxation timescale of this non-equilibrium state is 10 seconds so exceeds typical electronic relaxation timescales by several orders of magnitude, which makes this effect intriguing to study and relevant for potential applications in information processing.

TT 35.2 Tue 14:15 H23

Channel analysis of atomic Pd contacts by Andreev Reflections — •Martin Prestel[1], Torsten Pietsch[1,2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]now at: Carl Zeiss AG, 73447 Oberkochen, Germany

For the strong paramagnetic material palladium (Pd) theoretical calculations predicted a local magnetic ordering [1]. In transport measurements a strong non-monotonic magneto-transport behaviour as well as indications for Kondo resonances have been reported for atomic contacts in Pd [2]. To get a more detailed view of the nature of this magnetic ordering we want to investigate the transport channel distribution and their spin polarisation in such contacts. Therefore we add superconducting leads to apply the method of multiple Andreev reflections [3, 4, 5]. In this talk I will present first experimental superconducting current-voltage characteristics revealing superconducting proximity effect into Pd depending on the exact atomic configuration.

[1] Delin et al., Phys. Rev. Lett. 92, 057201 (2004)
[2] Strigl et al., Phys. Rev. B 94, 144431 (2016)
[3] Scheer et al., Nature 394, 154 (1998)
[4] Andersson et al., Physica C 367, 117-122 (2002)
[5] Martin-Rodero et al., Physica C 352, 67-72 (2001)

TT 35.3 Tue 14:30 H23

Quasiparticle cooling using a Topological insulator-Superconductor hybrid junction — •D. Bercioux[1,2] and P. Lucignano[3,4] — [1]Donostia International Physics Center, Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain — [3]CNR-SPIN, Monte S.Angelo, via Cinthia, I-80126 Napoli, Italy — [4]Dipartimento di Fisica "E. Pancini", Universitá di Napoli "Federico II", Monte S.Angelo, I-80126 Napoli, Italy

We investigate the thermoelectric properties of a hybrid junction realised coupling surface states of a three-dimensional topological insulator with a conventional *s*-wave superconductor. We focus on the ballistic devices and study the quasiparticle flow, carrying both electric and thermal currents, adopting a scattering matrix approach based on conventional Blonder-Tinkham-Klapwijk formalism [1]. We calculate the cooling efficiency of the junction as a function of the microscopic parameters of the normal region (*i.e.* the chemical potential etc.). The cooling power increases when moving from a regime of Andreev specular-reflection to a regime where Andreev retro-reflection dominates. Differently from the case of a conventional N/S interface [2], we can achieve efficient cooling of the normal region, without including any explicit impurity scattering at the interface, to increase normal reflection [3].

[1] Blonder, Tinkham & Klapwijk, Phys. Rev. B **25**, 4515 (1982).
[2] Bardas & Averin, Phys. Rev. B **52**, 12873 (1995).
[3] Bercioux & Lucignano, arXiv:1804.07170, EPJ ST, *in press* (2018).

TT 35.4 Tue 14:45 H23

Magnetism in atomic Gd contacts: Noise and transport measurements — •Marcel Strohmeier, Martin Prestel, and Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Materials with partially filled f shells bear interesting electronic and magnetic properties, wich have been intensively studied in bulk. Yet, on the atomic scale they are still a widely unexplored topic. For gadolinium (Gd) first transport measurements and theoretical calculations on the influence of f electrons on the electronic transport have been carried out [1]. To get a deeper insight into the magnetic ordering at the atomic scale we use the mechanically controllable break junction (MCBJ) technique at low temperatures to produce tunable atomic-size contacts. Here we present first measurements on magnetic transport behavior as well as shot noise measurements. Shot noise is known to reveal the exact channel configuration [2] and is even sensitive to spin polarization [3].

[1] Olivera et al., Phys. Rev. B 95, 075409 (2017)
[2] Kumar et al., Phys. Rev. Lett. 108, 146602 (2012)
[3] Burtzlaff et al., Phys. Rev. Lett. 114, 016602 (2015)

TT 35.5 Tue 15:00 H23

Magnetoconductance in Bi quantum well states: coupling of interfaces — •Doaa Abdelbarey and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover

Ultrathin epitaxial Bi films are governed by strongly spin-polarized bands that determine to a large extent their magneto-transport properties. Magneto-conductance of films grown epitaxially on Si(111) with a thickness of 10 to 100 bilayers (BL) was measured mostly at T= 8 K in magnetic fields up to 4T and with orientations both perpendicular and parallel to the surface plane. For B-fields normal to the surface weak anti-localization (WAL) was observed. Analysis within the theory by Hikami et al. [1] indicates strong coupling of the interfaces up to 50 BL, whereas above 80 BL two independently conducting channels were observed. For the in-plane B-field orientation, the magneto conductivity turned out to be anisotropic. Whereas for in-plane B-fields parallel to the current direction and for films up to 70 BL mainly weak localization is seen, it switches to WAL for larger thicknesses. For in-plane B-fields perpendicular to the current only WAL was observed irrespective of thickness. Both curves merge close to 100 BL, i.e. WAL becomes independent of B-field direction. These phenomena are explained within the framework of interface scattering, including superimposed effects of band structure and spin polarization due to the Rashba effect.

[1] Hikami S., et al., Prog. Theor. Phys. 63, 707 (1980)

TT 35.6 Tue 15:15 H23

Manipulating orbitals with magnetic fields — xionghua liu, •chun-fu chang, alexander komarek, steffen wirth, and liu hao tjeng — Max Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, 01187 Dresden, Germany

Magnetite (Fe_3O_4) is one of most controversially discussed materials in solid state physics due to its enigmatic Verwey transition, while being heavily studied as thin film for spintronic applications. Here, we report on our study of the Verwey transition under magnetic fields in Fe_3O_4 thin films on spinel substrates $Co_{2-x-y}Mn_xFe_yTiO_4$ and non-magnetic Mg_2TiO_4. The Verwey transition of these films is highly tunable and anisotropic with applied magnetic fields. The strong magnetostriction evidences an active spin-orbit effect of the Fe^{2+} (d^6) ions in Fe_3O_4 which allows one to manipulate the Fe^{2+} orbital occupation via magnetic fields. Remarkably, the high magnetic tunability of the Verwey transition results in a closed magnetoresistance (MR)-loop with an MR as large as 88% at 0.5 Tesla, which is up to 2 order larger than the reported values of Fe_3O_4 films.

TT 35.7 Tue 15:30 H23

Noise of charge current generated by a precessing itinerant ferromagnet — •Tim Ludwig[1], Igor S. Burmistrov[2,3,1,4], Yuval Gefen[5], and Alexander Shnirman[1,4] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [2]L.D. Landau Institute for Theoretical Physics RAS, Kosygina street 2, 119334 Moscow, Russia — [3]Laboratory for Condensed Matter Physics, National Research University Higher School of Economics, 101000 Moscow, Russia — [4]Institut für Nan-

otechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [5]Department of Condensed Matter Physics, Weizmann Institute of Science, 76100 Rehovot, Israel

We determine the zero frequency noise of charge current that is generated by a precessing small itinerant ferromagnet which is tunnel-coupled to two normal metal leads. We assume the leads to be in equilibrium with each other, i.e. neither voltage nor thermal bias is applied. In this situation, the average charge current vanishes. However, the noise of charge current remains. While at high temperatures, we obtain the standard thermal noise; for low temperatures we find the noise of charge current to be governed by the precession frequency of the magnetization and the angle between magnetization and precession axis. We propose that this result can be used in FMR-type experiments to gain additional information about the magnetization dynamics.

TT 35.8 Tue 15:45 H23

Time stable remanence in Dzyaloshinskii Moriya Interaction driven canted antiferromagnets — Namrata Pattanayak[1], AAkanksha Kapoor[1], Arun kumar Nigam[2], and •Ashna Bajpai[1] — [1]Indian Institute of Science Education and Research, Pune, India — [2]Tata Institute of Fundamental Research , India

We report remanence measurements conducted on a number of magnetic oxides which are Dzyaloshinskii-Moriya Interaction (DMI) driven canted antiferromagnets or weak ferromagnets (WFM). All these systems are also symmetry allowed piezomagnets (PzM). We consistently observe an ultra-slow magnetization dynamics with a counter-intuitive magnetic field dependence in these WFM or PzM. This ultra- slow magnetization dynamics manifests itself in the form of a time-stable remanence and appears exclusive to these WFM. Though the effect is tunable with nano scaling, it is intrinsic in nature as these features are also observed in bulk single crystal. We further demonstrate that the magnitude of this unique remanence can be significantly enhanced at the room temperature by encapsulation of these WFM inside carbon nanotubes. These results illustrate why encapsulation of these functional magnetic oxides within carbon nanotubes is interesting from fundamental point of view and it can lead to nano spintronic devices tunable by electric field, magnetic field and possibly by stress.

TT 36: Fluctuations, Noise and Quantum Coherence

Time: Wednesday 9:30–10:30 Location: H7

TT 36.1 Wed 9:30 H7

Factorial cumulants of charge fluctuations: correlations vs. spin relaxation — •Philipp Stegmann[1], Annika Kurzmann[1,2], Jens Kerski[1], Rüdiger Schott[3], Arne Ludwig[3], Andreas Wiek[3], Axel Lorke[1], Martin Geller[1], and Jürgen König[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Solid State Physics Laboratory, ETH Zurich, 8093 Zurich, Switzerland — [3]Chair for Applied Solid State Physics, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum, Germany

We use factorial cumulants to study the charge fluctuations between a single self-assembled quantum dot and a charge reservoir [1]. Measurements are performed by means of a new optical technique allowing to resolve higher-order cumulants up to 25th order. The factorial cumulants, in contrast to ordinary ones, are most suited to reveal correlations between the tunneling events of electrons [2,3]. Moreover, they turn out to be less demanding on the time resolution of the charge detector. We are able to quantify accurately how spin-relaxation destroys correlations.

[1] A. Kurzmann, P. Stegmann, J. Kerski, R. Schott, A. Ludwig, A. D. Wieck, J. König, A. Lorke, and M. Geller, Optical detection of single electron transport dynamics, submitted.
[2] P. Stegmann and J. König, Phys. Rev. B **92**, 155413 (2015).
[3] E. Kleinherbers, P. Stegmann, and J. König, New J. Phys. **20**, 073023 (2018).

TT 36.2 Wed 9:45 H7

Higher order moments, cumulants, and spectra of continuous quantum measurements — •Fabian Schefczik and Daniel Hägele — AG Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, Deutschland

We provide general quantum expressions for the multi-time moments $\langle z(t_n)\cdots z(t_1)\rangle$, cumulants, and spectra of the detector output $z(t)$ of a continuous quantum measurement with applications in spin noise spectroscopy and transport theory [1]. The expressions are correct in all orders of the measurement strength, i.e. they cover both the case of spin noise experiments where Gaussian background noise dominates and of transport measurements that usually exhibit quantum jump behavior (telegraph noise). The expressions follow from a rigorous treatment of the so-called stochastic master equation in terms of Ito-calculus. The quantum expressions for the cumulants can be formulated in a way to appear as compact as those for the mult-time moments. We shortly discuss a connection of higher order moments to the celebrated full counting statistics of transport theory.

[1] Daniel Hägele and Fabian Schefczik, Phys. Rev. B 98, 205143 (2018)

TT 36.3 Wed 10:00 H7

Revealing attractive electron-electron interaction in a quantum dot by full counting statistics — •Eric Kleinherbers, Philipp Stegmann, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, Lotharstr. 1, 47048 Duisburg

Recent experiments [1,2] have presented evidence for electron pairing in a quantum dot beyond the superconducting regime. An electron-electron attraction can effectively arise due to the surrounding solid state environment (e.g. coupling to bosonic modes as polarons, excitons or plasmons) and can be phenomenologically described by the negative-U Anderson model.

In my talk, I will discuss that an attractive interaction, compared to a repulsive one, does generate pronounced correlations in sequential electron transport [3]. In particular, these correlations are revealed by a sign change of higher-order current correlators (generalized factorial cumulants) which can be obtained from the full counting statistics of electron transfer. Remarkably, those correlations are robust against a fast spin relaxation and, most importantly, are detectable even when typical experimental limitations of a charge detector are considered.

[1] G. Cheng et al., Nature **521**, 196 (2015)
[2] G. Prawiroatmodjo et al., Nat. Commun. **8**, 395 (2017)
[3] E. Kleinherbers, P. Stegmann, and J. König, New J. Phys. **20**, 073023 (2018)

TT 36.4 Wed 10:15 H7

Optimal synchronization deep in the quantum regime: resource and fundamental limit — •Martin Koppenhöfer and Alexandre Roulet — Department of Physics, University of Basel, Basel, Switzerland

In this talk, we present an analytical framework to study the synchronization of a quantum self-sustained oscillator to an external signal. Our unified description allows us to identify the resource on which quantum synchronization relies, and to compare quantitatively the synchronization behavior of different limit cycles and signals. We focus on the most elementary quantum system that is able to host a self-sustained oscillation, namely a single spin 1. Despite the spin having no classical analogue, we first show that it can realize the van der Pol limit cycle deep in the quantum regime, which allows us to provide an analytical understanding of recently reported numerical results. Moving on to the equatorial limit cycle, we then reveal the existence of interference-based quantum synchronization blockade and extend the classical Arnold tongue to a snake-like forked tongue. Finally, we derive the maximum synchronization that can be achieved in the spin-1 system, and construct a limit cycle that reaches this fundamental limit asymptotically.

TT 37: Topological Semimetals - Theory (joint session TT/MA)

Time: Wednesday 9:30–12:30 Location: H22

TT 37.1 Wed 9:30 H22

Semiclassical transport theory in Weyl semimetals beyond the relaxation time approximation — •Tobias Meng — Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

Transport is a frequently used tool to study the properties of topological semimetals. In Weyl semimetals, the negative magnetoresistance proportional to the square of the magnetic field is a famous example of such a transport property. However, experimental semimetals usually are multi band systems containing disorder. It is essential to further develop the description of transport in Weyl semimetals in order for theory to match the experimental progress. We report on some first steps towards this goal by extending the Boltzmann approach towards a more realistic description of disorder scattering, which in turn allows us to identify novel signatures of Berry phase physics in transport.

TT 37.2 Wed 9:45 H22

Topological crossings in magnetic space groups — •Darshan G. Joshi[1], Yang-hao Chan[2], and Andreas P. Schnyder[1] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan

Non-symmorphic symmetry is known to enforce topological crossings in crystals. Using the elementary band irreducible representations nontrivial crossings in the form of hour-glass or accordian spectrum have been discovered in certain space groups. Here we extend such an analysis to a wider domain of magnetic space groups (MSGs). We show that the magnetic co-representations (coreps), which are derived from the non-magnetic irreducible representations, can be used to detect non-symmorphic symmetry enforced topological crossings in MSGs. We demonstrate this with two examples, where we find magnetic Weyl points and hour-glass dispersions. DFT band-structure calculation of corresponding magnetic materials confirms our findings. Furthermore, we compute the surface states and discuss other experimental consequences of the hourglass dispersion in magnetic materials.

TT 37.3 Wed 10:00 H22

Chiral anomaly in Weyl semimetals within a Fermi surface harmonics approach — •Annika Johansson[1,2], Jürgen Henk[2], and Ingrid Mertig[2,1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

In Weyl semimetals, external nonorthogonal magnetic and electric fields lead to nonconservation of the chiral charge, known as chiral anomaly [1-4]. This quantum phenomenon manifests itself in a negative longitudinal magnetoresistance. Using a Fermi surface harmonics approach [5] for solving the semiclassical Boltzmann equation, we calculate transport properties of type-I Weyl semimetals, including influences of chiral anomaly, Lorentz force as well as momentum-dependent scattering. Respecting a modified phase-space volume, we identify additional contributions to the chiral charge conductivity which can change the sign of the magnetoresistance in systems with broken inversion symmetry. Considering momentum-dependent scattering modifies the energy-dependence of the transport properties. On top of this, we show for TaAs that a misalignment of an applied magnetic field with the crystal axes can destroy the negative longitudinal magnetoresistance.

[1] S. Adler, Phys. Rev. **177**, 2426 (1969)
[2] J. S. Bell and R. Jackiw, Nuovo Cimento A **60**, 47 (1969)
[3] H. B. Nielsen and M. Ninomiya, Phys. Lett. B **130**, 389 (1983)
[4] D. T. Son and B. Z. Spivak, Phys. Rev. B **88**, 104412 (2013)
[5] P. B. Allen, Phys. Rev. B **13**, 1416 (1976)

TT 37.4 Wed 10:15 H22

Symmetry-Protected Nodal Phases in Non-Hermitian Systems — •Jan Carl Budich[1], Johan Carlström[2], Flore K Kunst[2], and Emil J Bergholtz[2] — [1]Institute of Theoretical Physics, TU Dresden, 01062 Dresden, Germany — [2]Department of Physics, Stockholm University, AlbaNova University Center, 106 91 Stockholm, Sweden

Non-Hermitian (NH) Hamiltonians have become an important asset for the effective description of various physical systems that are subject to dissipation. Motivated by recent experimental progress on realizing the NH counterparts of gapless phases such as Weyl semimetals, here we investigate how NH symmetries affect the occurrence of exceptional points (EPs), that generalize the notion of nodal points in the spectrum beyond the Hermitian realm. Remarkably, we find that the dimension of the manifold of EPs is generically increased by one as compared to the case without symmetry. This leads to nodal surfaces formed by EPs that are stable as long as a protecting symmetry is preserved, and that are connected by open Fermi volumes. We illustrate our findings with analytically solvable two-band lattice models in one and two spatial dimensions, and show how they are readily generalized to generic NH crystalline systems.

TT 37.5 Wed 10:30 H22

Evolution of surface states of the Luttinger semimetal under strain and inversion symmetry breaking: Dirac and Weyl semimetals — •Benedikt Mayer, Maxim Kharitonov, and Ewelina Hankiewicz — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

Luttinger semimetal, the quadratic-node semimetal for $j = 3/2$ electrons under full cubic symmetry, is the parent highest-symmetry minimal model for a variety of topological and/or strongly correlated materials, such as HgTe, α-Sn, and iridate compounds. Recently, Luttinger semimetal has been demonstrated to exhibit surface states of topological origin that can be attributed to approximate chiral symmetry. In the present work, we theoretically study the effect of the symmetry-lowering perturbations on these surface states within an analytical model. Under compressive strain lowering rotational symmetry, Luttinger semimetal becomes a Dirac semimetal with a pair of double-degenerate linear nodes. Breaking further inversion symmetry, the system turns into a Weyl semimetal, with each Dirac node split into four Weyl nodes. We analyze the corresponding evolution of the surface states, connecting the surface-state structures in the linear regime near the nodes and in the quadratic regime of the Luttinger semimetal away from the nodes. In particular, we demonstrate agreement of the Chern numbers with the chiralities of the surface states.

TT 37.6 Wed 10:45 H22

Photo-induced anomalous Hall effect in nodal-line semimetals — •Andreas Leonhardt and Andreas P. Schnyder — Max Planck Institute for Solid State Research

Spatial symmetries like reflection or PT-symmetry are able to protect band crossings along closed lines in the Brillouin zone at momenta left invariant by the symmetry. These nodal-lines carry a topological charge, characterized by a quantized Berry phase. This implies a divergent Berry curvature at these topological defects.

In semi-classical transport theory, a non-vanishing Berry curvature is associated with an anomalous velocity. In most cases however, the contributions from opposite points in the Brillouin zone cancel exactly, such that no anomalous Hall effect can be observed. Since circular polarized light couples differently to positive and negative momenta, the cancellation of anti-symmetric terms can be lifted, leading to a non-vanishing Hall current that changes direction with switching the polarization.

We describe the lattice model of a nodal-line semimetal driven by circular polarized light in the Floquet formalism. Coupling this system to leads with a potential difference allows us to calculate the Hall current in the Keldysh formalism. We investigate the relation of the photo-induced Hall conductivity to material characteristics and light amplitude and frequency and provide estimates for the required intensities and magnitude of the effect for some known nodal-line compounds.

15 min. break.

TT 37.7 Wed 11:15 H22

Tuning the anomalous Hall effect in topological magnets via the Berry curvature design — •Kaustuv Manna, Lukas Muechler, Ting Hui Kao, Rolf Stinshoff, Nitesh Kumar, Jürgen Kübler, Chandra Shekhar, Yan Sun, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

For a long time anomalous Hall effect (AHE) has been considered as

one of the characteristic signature of finite spontaneous magnetization in a material. It was considered to scale with sample's magnetization. However, the recent realization of the connection between the intrinsic AHE and the Berry curvature predicts other possibilities. AHE is an excellent method to understand the effect of various topological states and the Berry phase on the physical properties of material. Depending on the details of the band structure, the Hall conductivity can take a colossal value or even zero, independent of the corresponding magnetization of the sample. As a case study, we illustrate the situation in the Heusler compounds where one can easily tune the band structure by engineering the crystal symmetry and composition. With experimental evidences, we demonstrate how the Hall conductivity can be tuned from 0 to 2000 Ω-1cm-1 without disturbing sample's magnetization. With the help of the theoretical band structure calculations and ARPES data, we discover the first topological magnet with giant anomalous Hall conductivity (˜ 1700 Ω-1cm-1) and an exceptionally high anomalous Hall angle up to 12% in a topological magnetic Heusler.

TT 37.8 Wed 11:30 H22

Disorder-driven exceptional lines and Fermi ribbons in tilted nodal-line semimetals — •Kristof Moors[1], Alexander A. Zyuzin[2,3], Alexander Yu. Zyuzin[3], Rakesh P. Tiwari[4], and Thomas L. Schmidt[1] — [1]University of Luxembourg, Luxembourg, Luxembourg — [2]Aalto University, Aalto, Finland — [3]Ioffe Physical-Technical Institute, St. Petersburg, Russia — [4]McGill University, Montréal, Québec

We consider the impact of disorder on the spectrum of three-dimensional nodal-line semimetals. We show that the combination of disorder and a tilted spectrum naturally leads to a non-Hermitian self-energy contribution that can split a nodal line into a pair of exceptional lines. These exceptional lines form the boundary of an open and orientable bulk Fermi ribbon in reciprocal space on which the energy gap vanishes. We find that the surface of such a disorder-induced bulk Fermi ribbon in general lies orthogonal to the direction of the tilt, which can be exploited to realize a bulk Fermi ribbon with nontrivial topology by means of a tilt vector that twists along a nodal loop. Our results put forward a new paradigm for the exploration of non-Hermitian topological phases of matter.

TT 37.9 Wed 11:45 H22

Hopf-link topological nodal-loop semimetals — •Feng Xiong[1,2] and Yao Zhou[2] — [1]Institute for Theoretical solid state physics, RWTH Aachen. — [2]National Laboratory of Solid State Microstructures, Department of Physics, Nanjing University, Nanjing 210093, China

We construct a generic two-band model which can describe topological semimetals with multiple closed nodal loops. All the existing multi-nodal-loop semimetals, including the nodal-net, nodal-chain, and Hopf-link states, can be examined within the same framework. Based on a two-nodal-loop model, the corresponding drumhead surface states for these topologically different bulk states are studied and compared with each other. The connection of our model with Hopf insulators is also discussed. Furthermore, to identify experimentally these topologically different semimetal states, especially to distinguish the Hopf-link from unlinked ones, we also investigate their Landau levels. It is found that the Hopf-link state can be characterized by the existence of a quadruply degenerate zero-energy Landau band, regardless of the direction of the magnetic field.

TT 37.10 Wed 12:00 H22

Access to Weyl point properties revealed by anomalous Nernst effect — •Steffen Sykora[1], Christoph Wuttke[1], Federico Caglieris[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

In Weyl semimetals the Nernst coefficient is dominated by anomalous contributions to the thermal particle transport which originate from a specific property of the conduction electrons, the Berry curvature. Here we extend our recently developed theoretical approach of the anomalous Nernst effect to find explicit expressions for the temperature dependence of the thermal and electrical conductivity components. We apply these findings to fit experimental curves of recent Nernst effect measurements in a Weyl semimetal where it could be shown that signatures of Weyl physics are dominating the Nernst signal. From this analysis we determine fundamental properties of the Weyl points, such as their energy and distance in k-space.

TT 37.11 Wed 12:15 H22

Anomaly transport normally explained — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics - UFRN, Campus Universitário Lagoa nova, 59078-970 Natal, Brazil

The anomalous term $\sim \vec{E}\vec{B}$ in the balance of the chiral density can be rewritten as quantum current in the classical balance of density. Therefore it does not violate classical conservation laws as it is claimed to be caused by quantum fluctuations. Moreover this term is derived from the quantum kinetic equations for systems with SU(2) structure within a completely conserving approach. Therefore the origin of this term is not a unique signal of symmetry-breaking terms in the field-theoretical Lagrangian. Regularization-free density and pseudospin currents are calculated in Graphene and Weyl-systems realized as the infinite-mass limit of electrons with quadratic dispersion and a proper spin-orbit coupling. The intraband and interband conductivities are discussed. The optical conductivity agrees well with the experimental values using screened impurity scattering and an effective Zeeman field. The universal value of Hall conductivity is shown to be modified due to the Zeeman field.

[1] arXiv:1809.01547, arXiv:1806.06214, Phys. Rev. B 94 (2016) 165415, Phys. Rev. B 92 (2015) 245425, errata: Phys. Rev. B93 (2016) 239904(E), Phys. Rev. B 92 (2015) 245426

TT 38: f-Electron Systems and Heavy Fermions

Time: Wednesday 9:30–12:45 Location: H23

Invited Talk TT 38.1 Wed 9:30 H23

A new heavy-fermion superconductor $CeRh_2As_2$ with Rashba and quadrupolar interactions — •Seunghyun Khim, Jacintha Banda, Daniel Hafner, Ulrike Stockert, Manuel Brando, and Christoph Geibel — Max Planck Institut für Chemische Physik fester Stoffe, Dresden, Germany

One of the hot topic in the field of superconductivity is the effect of breaking inversion symmetry in the presence of strong spin-orbit interactions. This leads to a spin-splitted Fermi surface with unique momentum-locked spin polarization. Superconductivity appearing from such polarized bands is robust against Zeeman pair-breaking effect and can host mixed-parity pairing providing exotic superconducting states. Here, we report the discovery of heavy-fermion superconductivity in $CeRh_2As_2$ with $T_c \sim 0.25$ K. This compound crystallizes in the $CaBe_2Ge_2$-type structure where inversion symmetry is locally broken at the Ce site. We observe a huge upper critical field of $\gtrsim 12$ T for the out-of-plane direction surpassing the Pauli-paramagnetic limit of ~ 0.5 T. This provides a clear signature of a Rashba-type in-plane spin polarization arising from an alternating asymmetric potential due to the broken local inversion symmetry. In addition, our results indicate this system to be very close to a quantum critical point (QCP) with a further transition at $T_o \sim 0.4$ K, likely of quadrupolar nature. Therefore, $CeRh_2As_2$ is a promising candidate for studying how heavy-fermion superconductivity behaves under the influence of Rashba-type interactions and a possible multipolar QCP.

TT 38.2 Wed 10:00 H23

Study of the low-temperature resistivity of the locally non-centrosymmetric heavy-fermion superconductor $CeRh_2As_2$ — •Daniel Hafner, Jacintha Banda, Seunghyun Khim, Christoph Geibel, and Manuel Brando — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

$CeRh_2As_2$ is a novel locally non-centrosymmetric heavy fermion superconductor with a transition temperature $T_c \approx 0.3$ K. A second weak transition has been observed in specific heat at a temperature T_0 just above T_c and it is suspected to be of quadrupolar nature. We present a comprehensive study of the low temperature resistivity of $CeRh_2As_2$ in

which we could observe signatures of both phase transitions. We have investigated the evolution of T_c and T_0 and the resistivity exponent n, with $\rho(T) = \rho_0 + AT^n$, in magnetic field parallel and perpendicular to the crystallographic c-axis up to 18 T. The resulting phase diagrams are presented. We then discuss the evolution of the observed phases in relation to the lack of local inversion symmetry in the Ce sites, quadrupolar order and quantum criticality.

TT 38.3 Wed 10:15 H23

The high-field/high-pressure relationship of magnetic order and nematicity in the heavy-fermion superconductor $CeRhIn_5$ — •Toni Helm[1,2], Audrey Grockowiak[4], Fedor Balakirev[5], John Singleton[5], Kent R. Shirer[2], Markus König[2], Eric D. Bauer[6], Filip Ronning[6], Stanley W. Tozer[4], and Philip J.W. Moll[2,3] — [1]High Magnetic Field Laboratory Dresden (HLD-EMFL), HZDR, Germany — [2]MPI for Chemical Physics of Solids, Dresden, Germany — [3]Institute of Materials, EPFL, Lausanne, Switzerland — [4]Tallahassee NHMFL, FL, USA — [5]Los Alamos NHMFL, NM, USA — [6]Los Alamos National Laboratory, NM, USA

Recently, a nematic signature, i.e., a sudden resistivity anisotropy above a critical field $B^* = 28$ T, has been observed in $CeRhIn_5$. This heavy-fermion antiferromagnet ($T_N = 3.85$ K) superconducts under pressure above $p_c = 23$ kbar, associated with an antiferromagnetic quantum critical point (QCP). The reported nematic behavior survives at ambient pressure only until magnetic order is suppressed at a critical field of $B_c = 51$ T, associated with a second QCP. An open question is if and how the two QCPs, B-induced nematicity and p-induced superconductivity (SC) are related. Here we report high-field (up to 65 T) / high-pressure (up to 40 kbar) studies of magnetotransport in $CeRhIn_5$. The combination of plastic diamond-anvil-cells, pulsed magnets, and focused-ion-beam microstructures enables us to investigate this region in the (p, T, B) phase diagram. We show that nematicity and SC reside in distinct regions. Our experiments reveal an unexpected enhancement of magnetic order in high fields with pressure.

TT 38.4 Wed 10:30 H23

Spin-dependent Masses in High Magnetic Field: Minimal Model for $CeCoIn_5$ — •Andrzej P. Kadzielawa[1,2], Dominik Legut[2], Maciej Fidrysiak[1], and Józef Spałek[1] — [1]Insytut Fizyki, Uniwersytet Jagielloński, Kraków, Poland — [2]IT4Innovations, Vysoká škola báňská - Technická univerzita Ostrava, Ostrava, Czech Republic

The intertwinement of superconductivity **[1]** and magnetism **[2]** in $CeCoIn_5$ is an arduous problem, often approached by accurate but time-consuming methods like Dynamical Mean-Field Theory **[3]**. In contrast, we provide a minimal, two-dimensional (after **[4]**), model to understand the mechanism of spin-split masses in this heavy-fermion system. Using the band Hubbard U technique (DFT+U calculations), we retrieve the precise energy scale for the strong correlations. To account for this we use a minimal model of the Periodic Anderson Lattice solved using the so-called Statistically-consistent Gutzwiller Approximation. We obtain the proper, experimentally confirmed, qualitative behavior of the spin-dependent masses, as well as overall half-metallic nature of the heavy fermion behavior in this compound.

The work was supported by Grant MAESTRO No. DEC-2012/04/A/ST3/00342 from National Science Centre and Path to Exascale project No. CZ.02.1.01/0.0/0.0/16_013/0001791 by Min. of Edu. of Czechia.

[1] C. Petrovic *et al.*, J. Phys. Condens. Matter **13**, L337 (2001)
[2] I. Sheikin *et al.*, Phys. Rev. Lett. **96**, 077207 (2006)
[3] K. Haule *et al.*, Phys. Rev. B **81**, 195107 (2010)
[4] A. Gyenis *et al.*, Nat. Comm. **9**, 549 (2018)

TT 38.5 Wed 10:45 H23

Switching the propagation vector of the hidden-order phase in $Ce_3Pd_{20}Si_6$ with a magnetic field — •Pavlo Y. Portnichenko[1], Stanislav E. Nikitin[2], Andrey Prokofiev[3], Silke Paschen[3], Jean-Michel Mignot[4], Jacques Ollivier[5], Andrey Podlesnyak[6], Siqin Meng[7,8], Zhilun Lu[8], and Dmytro S. Inosov[1] — [1]IFMP, TU Dresden, Germany — [2]MPI-CPfS, Dresden, Germany — [3]Vienna Univ. of Technology, Austria — [4]LLB, France — [5]ILL, France — [6]SNS, Oak Ridge, USA — [7]CIAE, Beijing, China — [8]HZB, Berlin, Germany

Hidden-order phases that occur in a number of correlated f-electron systems are among the most elusive states of electronic matter. The heavy-fermion compound $Ce_3Pd_{20}Si_6$ exhibits magnetically hidden order that occurs at subkelvin temperatures, known as phase II. Additionally, only in a magnetic field applied parallel to the [001] cubic axis, another field-induced phase II′ was observed in magnetization measurements, yet the nature of the II-II′ phase transition has remained a mystery. Here we use inelastic neutron scattering to demonstrate that this transition is associated with a switching in the propagation vector of the antiferroquadrupolar order from (111) to (100) with a simultaneous change in the type of the ordered quadrupole from O_2^0 to O_{xy}. Despite the absence of magnetic Bragg scattering in the phase II′, its propagation vector was revealed by the location of an intense soft mode in the excitation spectrum along the (100) direction, orthogonal to the applied field. Our experiment also reveals collective excitations in the field-polarized paramagnetic phase, after phase II′ is suppressed.

15 min. break.

TT 38.6 Wed 11:15 H23

Probing Fermi-surface evolution and crystal-field excitations in heavy-fermion systems by THz time-domain spectroscopy — •Shovon Pal[1], Christoph Wetli[1], Farzaneh Zamani[2], Oliver Stockert[3], Hilbert v. Loehneysen[4], Manfred Fiebig[1], and Johann Kroha[2] — [1]ETH Zurich, Switzerland. — [2]Bonn University, Germany. — [3]MPI-CPFS Dresden, Germany. — [4]KIT, Germany.

An enlarged Fermi volume ratifies the existence of heavy quasiparticles (QPs) in heavy-fermion (HF) compounds. The energy scale for the heavy QP formation is believed to be the Kondo lattice temperature. However, recent observations of large Fermi volume at temperatures much higher than the Kondo lattice temperature raised controversies on the validity of this long-known scale. We measure the QP weight in the HF compound $CeCu_{6-x}Au_x$ ($x = 0, 0.1$) by time-resolved THz spectroscopy for temperatures from 2 K to 300 K. This method distinguishes contributions from the heavy Kondo band and from the crystal-electric-field (CEF) split satellite bands by different THz response delay times [1]. We find that an exponentially enhanced, high-energy Kondo scale controls the formation of heavy bands, once the CEF states become thermally occupied [2]. We corroborate these observations by temperature-dependent, high-resolution dynamical mean-field calculations for the multi-orbital Anderson lattice model and discuss its relevance for quantum critical scenarios.

[1] C. Wetli, S. Pal *et al.*, Nat. Phys. **14**, 1103 (2018)
[2] S. Pal *et al.*, arXiv:1810.07412 (2018)

TT 38.7 Wed 11:30 H23

Exploring quantum criticality in strain-tuned heavy fermion thin films by THz spectroscopy — •C.-J. Yang[1], S. Pal[1], F. Zamani[2], M. Trassin[1], H. v. Loehneysen[3], J. Kroha[2], and M. Fiebig[1] — [1]ETH Zurich, Switzerland. — [2]Bonn University, Germany. — [3]KIT, Germany.

Quantum phase transition (QPT) refers to a second-order phase transition between the ground states of a many-body system occurring around T = 0 K, governed by critical fluctuations. In heavy fermion compounds, $CeCu_{6-x}Au_x$, Cu-substitution by Au expands the lattice thereby inducing a QPT from a paramagnetic Fermi-liquid state to an antiferromagnetically ordered ground state at $x = 0.1$. In this contribution, we take a novel approach, replacing the role of Au by strain-tuning in $CeCu_6$ epitaxial thin films. Films of various thicknesses are sputtered from a pure $CeCu_6$ target onto single-crystal substrates. The crystallinity and orientation of the thin films are investigated by X-ray diffraction. To understand the dynamic evolution of Kondo quasiparticle weight and of optical properties, we perform time-resolved THz measurements as function of temperature. For the sample of a 30 nm thick $CeCu_6$ film, our results show similar temperature-dependent Kondo response as observed in bulk samples [1]. We find a logarithmic onset of the Kondo spectral weight at 100 K. This behavior is further corroborated by the temperature-dependent mass enhancement ratio and the inverse scattering rate. We also observe a non-linear temperature-dependence of the optical resistivity.

[1] C. Wetli, S. Pal *et al.*, Nat. Phys. **14**, 1103 (2018)

TT 38.8 Wed 11:45 H23

Thermal Transport Measurement on Heavy Fermion Compound LiV_2O_4 — •Mohammad Pakdaman, Yosuke Matsumoto, Masahiko Isobe, Jan Bruin, and Hidenori Takagi — Department of Quantum Materials,Max Planck Institute for Solid State Research,Heisenbergstraße 1, 70569 Stuttgart

LiV_2O_4 is the only d-electron heavy fermion compound. The HF state in this compound was proved using different experimental techniques. However the mechanism for heavy fermion is still unknown. We per-

formed the thermal transport measurement in order to reveal the mechanism for HF behavior.

TT 38.9 Wed 12:00 H23

Development of microstructure strain rig and investigations into PrV_2Al_{20} — •Po-Ya Yang[1], Jack Bartlett[1,2], and Clifford Hicks[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews, St. Andrews, United Kingdom

Uniaxial stress is a powerful method to explore the electronic states of materials. By lifting the symmetry of a lattice, it enables direct probing of symmetry-related phenomena. Reducing the size of the sample and improving surface quality are expected to improve the achievable precision and the maximum achievable stress before the sample fractures. Here, I will present methods and apparatus for applying uniaxial stress to samples that have been microstructured with a focused ion beam, and demonstrate with measurements on PrV_2Al_{20}.

TT 38.10 Wed 12:15 H23

Electronic structure and valence-to-core RIXS of europium sulfide — •Jindrich Kolorenc[1] and Lucia Amidani[2,3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]Institute of Resource Ecology, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]ESRF, Grenoble, France

We investigate the electronic structure of europium sulfide (EuS) with the aim to understand the valence-to-core resonant inelastic x-ray scattering (RIXS) spectra measured at the europium L_3 edge. We employ LDA+DMFT for the theoretical modeling of the valence-band electronic structure as well as the RIXS spectra. More specifically, we use a generalization of the method described recently in [1].

We show that the main signal comes from the direct RIXS: an Eu 2p core electron is excited to an empty Eu 5d band above the Fermi level, and then another electron from an Eu 5d state hybridized with the S 3p bands (located below the Fermi level and hence occupied) fills back the Eu 2p core hole. Besides this straightforward channel, the measured RIXS spectra display a number of satellite features that we attempt to identify with indirect RIXS processes where additional excitations are induced by the Coulomb potential of the core hole.
[1] J. Kolorenč, Physica B **536**, 695–700 (2018).

TT 38.11 Wed 12:30 H23

Electronic structure, magnetism, lattice dynamics and thermodynamic stability of fcc UH_2 — •Lukas Kyvala[1], Ladislav Havela[2], and Dominik Legut[1] — [1]VSB - Technical University of Ostrava, 17. listopadu 15, 70833 Ostrava-Poruba, Czech Republic — [2]Charles University, Ke Karlovu 5, 12116 Prague, Czech Republic

Uranium metal is known to form two different hydrides with the stoichiometry 1:3 (α and β UH_3). Although the other 5 f-elements as Pu, Np or Th exist in dihydride form, UH_2 was not reported for very long time. Hovewer, recent work [1] showed that *fcc* uranium dihydride can exist, if it is synthetized as a thin film.

Using the density funcitonal theory calculations employing VASP code we investigated electronic structure, mechanical and magnetic properties, lattice dynamics and thermodynamic stability of *fcc* uranium dihydride. The change of the magnetic order as well the thermodynamic stability vs. parent structure of UH3 is discussed.

A detailed comparison of thermodynamics and electronic structure of UH_2 with UH_3 shed on the light on the question why UH_2 can be stabilized as thin film and not in a bulk form.
[1] L. Havela, M. Paukov, M. Dopita, L. Horak, D. Drozdenko, M. Divis, I. Turek, D. Legut, L. Kyvala, T. Gouder, A. Seibert, and F. Huber, Inorganic Chemistry (2018)

TT 39: Focus Session: Direct-Write Nanofabrication and Applications I (Electron Beam Induced Processing) (joint session DS/TT)

Part I: Advances in Focused Particle Beam Processing & New Approaches

Focused electron beam induced deposition (FEBID) and focused electron beam induced etching (FEBIE) are direct-write approaches for the fabrication of 2D- and 3D-nanostructures made from different materials, such as superconductors, magnetic materials, alloys and intermetallic compounds, as well as meta-materials in which suitable materials combinations result in a desired functionality for various application fields (strain / magnetic / dielectric sensing, multi-functional scanning probe sensors, 3D plasmonic structures, 3D magnetic structures etc).

The Focus Session aims at providing a concentrated presentation of various new developments of the most versatile direct-write techniques for functional nanostructures to a broader audience within the condensed matter community.

Organizers:
- Michael Huth, Physikalisches Institut, Goethe-Universität, Frankfurt, Germany
- Harald Plank, FELMI-ZFE, TU Graz, Austria

Time: Wednesday 9:30–12:30 Location: H32

Invited Talk TT 39.1 Wed 9:30 H32

3D-Nanoprinting with Focused Electron Beams. Advances and Applications — •Robert Winkler[1], Jason D Fowlkes[2,3,4], Jürgen Sattelkow[1], Philip D Rack[2,3,4], and Harald Plank[1,5] — [1]Christian Doppler Laboratory - DEFINE, Institute of Electron Microscopy, Graz University of Technology, 8010 Graz, Austria — [2]Bredesen Center for Interdisciplinary Research, The University of Tennessee, Knoxville, 37996, USA — [3]Nanofabrication Research Laboratory, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, 37831, USA — [4]Materials Science and Engineering Department, The University of Tennessee, Knoxville, 37996, USA — [5]Graz Centre for Electron Microscopy, 8010 Graz, Austria

While 3D printing of objects down to the micrometer scale is well established, techniques for controlled additive manufacturing at the nanoscale are only few. Based on the progress in recent years, Focused Electron Beam Induced Deposition (FEBID) has evolved into a 3D nano-printing technology, allowing mask-less direct-write fabrication of complex 3D nano-architectures on almost any substrate. The growing availability of different precursor types expand the functionalities of those FEBID structures from electrically over magnetically towards optically active purposes, enabling applications, which have been very challenging in the past. Here, we introduce the technology and sketch possibilities and limitations for a comprehensive FEBID portfolio picture. We focus on recent advances in accuracy and predictability based on local heating effects and finally present selected applications of such 3D-nanoprinted structures in research and industry.

TT 39.2 Wed 10:00 H32

Modeling FEBID frequency maps: Lateral deposit resolution

and surface diffusion — Jakub Jurczyk[1,2], Czeslaw Kapusta[2], and •Ivo Utke[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Feuerwerkstrasse 39, CH-3602 Thun, Switzerland — [2]AGH University of Science and Technology Krakow, Al. Mickiewicza 30, 30-059 Kraków, Poland

Focused electron beam induced deposition (FEBID) is governed by four main processes: adsorption, desorption, surface diffusion and dissociation of precursor molecules on the sample surface [1],[2]. All of them influence growth rate, lateral resolution and shape of deposited structures; hence we can distinguish four different deposition regimes: reaction-rate limited, mass transport limited, diffusion enhanced and the combination of the two latter [3]. In their recent work, Sanz-Hernandez et al. [4] visualized these regimes based on characteristic frequencies for every process, creating frequency maps for the growth rates and coverage [4]. In this contribution we expand this approach to include the lateral deposit resolution and the influence of surface diffusion into the frequency maps. Results of simulations will be discussed in the context of their physical basis and future designed experiments. [1] I. Utke et al., J. Vac. Sci. Technol. B, 26, (2008), 1197-1276; [2] M. Toth et al. Beilstein J. Nanotech., 6, (2015), 1518*1540[3]; A. Szkudlarek et al., Appl. Phys. A, 117, (2014), 1715*1726;[4] D. Sanz-Hernandez et al., Beilstein J. Nanotechnol., 8, (2017), 2151*2161

TT 39.3 Wed 10:15 H32

On the reduction of proximity effects by exploring (metal-) organic materials as substrates/resists for gas-assisted electron beam lithography — Chrisatian Preischl, Elif Bilgilisoy, Florian Vollnhals, and •Hubertus Marbach — Physikalische Chemie II, FAU Erlangen-Nürnberg

We investigated organic and metal-organic materials as substrates/resists in different Focused Electron Beam Induced Processing (FEBIP) techniques. Here, FEBIP methods rely on the local decomposition of the volatile precursors $Fe(CO)_5$ and $Co(CO)_3NO$, by the direct impact of the focused electron beam (Electron Beam Induced Deposition, EBID) or through the interaction of the precursor with pre-irradiated/activated surface areas (Electron Beam Induced Surface Activation, EBISA).[1−3] The investigated materials range from porphyrin layers [1,2] over surface anchored metal-organic frameworks (SURMOFs)[3] to self-assembled monolayers (SAMs).[4] Application of our surface science approach, i.e. working in an ultra-high vacuum environment, allows to obtain chemically well-defined deposits. A major advantage of the used materials are reduced electron proximity effects, i.e. reduced electron scattering and quenching of secondary electrons within the latter materials.[1−3] An illustrative example is the fabrication of test structures with $Fe(CO)_5$ on a SURMOF with an average line width value below 10 nm.[3]

[1] Marbach, H., Appl. Phys. A, 117 (2014) 987-995. [2] Drost, M., et al., Small methods, 1(2017)1700095. [3] Drost, M., et al., ACS Nano. 12 (2018) 3825 . [4] Turchanin, A., et al., Adv. Mater. 28 (2016) 6075.

TT 39.4 Wed 10:30 H32

FEBIP on Self-Assembled-Monolayers and Carbon Nanomembranes — •Christian Preischl[1], Elif Bilgilsoy[1], Florian Vollnhals[1], Le Hoang Linh[2], Sascha Koch[2], Armin Gölzhäuser[2], and Hubertus Marbach[1] — [1]Physik. Chemie II, FAU Erlangen-Nürnberg, GER — [2]PSS, Bielefeld University, GER

In our approach, we investigate two different FEBIP methods in UHV on Self-Assembled-Monolayers (SAM) and on nanometer thick Carbon Nanomembranes (CNM). These thin CNM sheets can be produced out of SAMs by electron-induced crosslinking.[1] The two FEBIP methods of choice are EBID[2] and Electron-Beam-Induced-Surface-Activation (EBISA). In EBISA, the surface is locally activated by an electron beam and the subsequently dosed precursor is catalytically decomposed at the activated sites and forms a deposit.[3] These two approaches were explored on 1,1´,4´,1´´-terphenyl-4-thiol (TPT) and the corresponding cross-linked CNM with $Fe(CO)_5$ and $Co(CO)_3NO$. Whereas EBID works with both precursors on both substrates, EBISA can only be driven successfully on the non cross-linked TPT with $Fe(CO)_5$. Regarding this result, we observe a chemical selectivity in EBISA between the two precursors, which was already reported in previous studies on different substrates.[4] Furthermore upon crosslinking, TPT loses its catalytic activity towards the EBISA process.

[1] A. Turchanin, A. Gölzhäuser, Adv. Mater. 28 (2016), 6075 [2] W. van Dorp, C.W. Hagen, J. Appl. Phys. 104 (2008), 081301 [3] H. Marbach, Appl. Phys. A 117 (2014), 987 [4] Drost et al., Small Methods 1 (2017), 1700095; M. Drost et al., ACS Nano. 12 (2018), 3825

TT 39.5 Wed 10:45 H32

Fabrication of Photonic and Optomechanics Devices in hBN by Electron Beam Induced Etching — •Johannes Froech[1], Sejeong Kim[1], Prasoon Shandilya[2], Bishnupada Behera[2], Chris Healy[2], James Bishop[1], Matthew Mitchell[2], David Lake[2], Paul Barclay[2], Igor Aharonovich[1], and Milos Toth[1] — [1]University of Technology Sydney, Ultimo, NSW, 2007, Australia — [2]University of Calgary, Calgary, AB, T2N 1N4, Canada

Exceptional efforts have been undertaken in recent years to identify suitable platforms for solid state quantum photonic technologies. Several schemes exploit materials that typically host on-demand single photon emitters and can be easily processed in a robust and reliable manner to yield functional nanostructures. A potential material for applications in this field is hexagonal Boron Nitride (hBN), based on the discovery of room-temperature, stable, ultra-bright quantum emitters. However, until recently, fabrication of complex hBN geometries was not viable. Here, we demonstrate new processing approachess for the fabrication of complex photonic and optomechanics nanostructrues in suspended hBN and hBN/ Si hybrid systems using the technique of Electron Beam Induced Etching (EBIE). It is minimally invasive and allows for post fabrication editing to tune optical properties. In combined systems, the etching technique is highly selective and allows for precise and maskless fabrication. Overall, our methodology and results set the foundation for cavity quantum electrodynamics experiments and further work in integrated optomechanics systems to be performed utilizing hBN quantum emitters.

TT 39.6 Wed 11:00 H32

Energy from Green House Gas Stored in Nanogranular Material — •Hans Koops — HaWilKo GmbH, Ober-Ramstadt, Germany

Light energy from the sky having Ultra-Violet to 10 μm wavelengths is stored as Bosons in nano-granular material. The upper atmosphere of the earth contains layers of green-house material and this emits infrared radiation with 380 W/ m^2, as measured by NASA in 2009. Nanogranular compound material, Platinum nanocrystals in Fullerene crystals layers, can absorb the IR-radiation and stores it in electron-hole-Bosons with parallel spin. There the electrons can tunnel to the close by conductor, which carries a potential higher than the Boson-layers. Experiments at KNMF in KIT delivered from a Pt/C ribbon of 150 nm thickness and 1 μm width a 4 V a current of 0,6 A without melting the nano-granular Pt/C ribbon. The stored charge can be moved using a field gradient, which shifts the Bosons to the end of the material. There the electrons can tunnel to the close by conductor, which carries a potential higher than the Boson-layers. Experiments at KNMF in KIT delivered from a Pt/C ribbon of 150 nm thickness and 1 μm width a 4 V a current of 0,6 A without melting the nano-granular Pt/C ribbon.

15 min. break.

Invited Talk TT 39.7 Wed 11:30 H32

Resist-free fabrication of graphene devices using focused ion beam patterning and direct-write ALD — •Ageeth Bol — Eindhoven University of Technology, Eindhoven, the Netherlands

Graphene has long been proposed as ideal candidates to replace silicon in future nanoelectronic devices and has therefore attracted considerable attention from the scientific community. Regardless, graphene struggles to leave the lab as many challenges for large-scale integration still exist. This presentation addresses one of these challenges: the resist-free fabrication of graphene devices. For the fabrication of graphene devices, graphene sheets must be patterned into individual devices, and then contacted to form electrical connections. The conventional approach involves lithography using resist films. To avoid contamination by resist residues as much as possible, a direct patterning and contacting approach was developed. We showed that a focused ion beam (FIB) is able to directly etch graphene from a substrate. By optimizing the pressure as well as reducing the amount of ions used, ion scattering could be minimized, making FIB patterning a feasible alternative to conventional lithography. Next, the FIB-patterned graphene was used to fabricate and characterize electrical devices. For the first time, Pt contacts were deposited by using a combination of electron-beam induced deposition and area-selective Pt which further avoids the use of resist films. The ALD-contacted devices show remarkable improvements compared to conventionally deposited Pt contacts.

TT 39.8 Wed 12:00 H32

Atomic layer deposition on electron beam written nanostructures — Caspar Haverkamp[1], Hanno Kröncke[1], Patryk Kusch[2], Felix Oertel[1], Catherine Dubourdieu[1,3], Stephanie Reich[2], and •Katja Höflich[1] — [1]Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin — [3]Freie Universität Berlin, Institut für Chemie und Biochemie, Takustr. 3, 14195 Berlin

The uniform coverage of complex three-dimensional structures is highly beneficial for the process of direct electron beam writing. Thereby, crucial issues in thermal and chemical stability of electron beam written structures can be successfully addressed, while in other cases the desired material response may be realized. Atomic layer deposition (ALD) is a self-limited deposition technique, that allows to deposit conformal ultrathin films on surfaces. The deposition consists of an iterative growth sequence of four steps. First, precursor molecules bind to the surface forming a monolayer. Then, excess precursor molecules and volatile byproducts are purged from the reactor. In a third step, the co-reactant is introduced to react with the chemisorbed precursor molecules. Finally, all volatile products are purged again. While mostly known for the deposition of oxides, other materials and especially metals are available for ALD as well. Therewith, atomic layer deposition constitutes an ideal counterpart to trigger various applications of direct electron beam writing. Examples are demonstrated for plasmonic antennas of different types, optimized for chiroptical interaction, tip-enhanced Raman scattering or nonlinear interactions.

TT 39.9 Wed 12:15 H32

Towards all-metallic nano-structures using FEBID and ALD — •Peter Gruszka and Michael Huth — Goethe Universität, Frankfurt am Main, Deutschland

In recent years, conventional methods of nano-structuring are slowly reaching their lower limits. A novel bottom-up and maskless approach emerged[1], which combines focused electron beam induced deposition (FEBID) and area-selective atomic layer deposition (AS-ALD).FEBID is a serial, bottom-up and direct-write technique yielding structures with superior lateral resolution ($<$ 10 nm), but with poor material quality. In contrast, ALD and especially AS-ALD are parallel bottom-up approaches with exceptional thickness control in the sub-nm regime resulting in high purity films.

We successfully performed the AS-ALD process in our custom ALD micro-reactor on ultra-thin platinum seed layers prepared in a Nova 600 Dual Beam scanning electron microscope by FEBID. The seed layers were purified with a technique developed by Sachser et al.[2]. Additionally, we monitored the AS-ALD process via in-situ conductance measurements which enabled us to tune the resistance to a desired value. Low-temperature measurements on standard four-probe structure show metallic behaviour with an RRR of about 2.6 and a Debye temperature of about 230K. First results on high-resolution nanostructure fabrication by FEBID/AS-ALD and their low-temperature transport characteristics are presented.

[1] Mackus, et al., J. Appl. Phys 107 (2010), 116102
[2] Sachser, et al., ACS Appl. Mater. Interfaces 6 (2014), 15868

TT 40: Superconductivity: Qubits 1

Time: Wednesday 9:30–13:00 Location: H48

TT 40.1 Wed 9:30 H48

Coherence of a transmon qubit under in-plane magnetic fields — •Andre Schneider[1], Alexey V. Ustinov[1,2], and Martin Weides[1,3] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]National University of Science and Technology MISIS, Moscow, Russia — [3]University of Glasgow, Glasgow, United Kingdom

Superconducting quantum circuits are versatile building elements for quantum technologies, with applications ranging from computing and simulation to sensing and metrology. The extreme sensitivity of SQUIDs to magnetic fields is used in many technological applications, and new quantum sensing schemes like the detection of amplitude and frequency of microwave signals by a superconducting transmon qubit [1] are being developed.

To identify possible fields of application, we investigate the environmental magnetic conditions for the usability of such a qubit. By placing a transmon qubit in a magnetic field, we analyze its transition frequency and coherence properties. We find that the transition frequency strongly depends on the flux penetrating the $Al/AlO_x/Al$ Josephson junction and can be modeled precisely as function of the in-plane magnetic field. We demonstrate quantum coherence up to field values of 40 mT with qubit lifetimes of $T_1 \gtrsim 0.5\mu$s and find corresponding T_2 times resulting in a constant pure dephasing rate at any field. The possibility to operate superconducting qubits in magnetic fields far beyond the critical field of the bulk superconductor opens new avenues, for instance in quantum sensing and metrology.

[1] A. Schneider *et al.*, Phys. Rev. A **97**, 062334 (2018)

TT 40.2 Wed 9:45 H48

What Can Be Learned from Measuring Quantum Jumps of a Transmon Qubit? — •Dennis Rieger[1], Patrick Winkel[1], Ivan Takmakov[1,2], Luca Planat[3], Farshad Foroughi[3], Wiebke Hasch-Guichard[3], Kiril Borisov[2], Julian Ferrero[1], Lukas Grünhaupt[1], Daria Gusenkova[1], Fabio Henriques[1], Nataliya Maleeva[1], Alexey V. Ustinov[1], Wolfgang Wernsdorfer[1,2,3], Nicolas Roch[3], and Ioan M. Pop[1,2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [3]Institut Néel, CNRS and Université Joseph Fourier, Grenoble, France

Resolving quantum jumps of superconducting qubits requires fast, high-fidelity readout, which can be enabled by a superconducting parametric amplifier as a first amplifier stage for the readout signal. We use the Dimer Josephson Junction Array Amplifier (DJJAA) to measure quantum jump traces of a transmon qubit dispersively coupled to a readout resonator and placed inside a 3D waveguide.

The measured coherence times of the transmon are sufficiently long compared to the integration time needed for qubit state discrimination. The quantum jumps follow Poisson statistics and we find that the T_1 during readout is significantly reduced compared to the free evolution T_1. Also, the effective qubit temperature saturates at approximately 50 mK even though the qubit is thermally anchored to the mixing chamber stage of a dilution refrigerator at 20 mK.

TT 40.3 Wed 10:00 H48

Tuning decoherence sources in Transmon qubits by electric fields — •Jürgen Lisenfeld[1], Alexander Bilmes[1], Georg Weiss[1], Rami Barends[2], Anthony Megrant[2], Julian Kelly[2], John M. Martinis[2], and Alexey V. Ustinov[1,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Google Inc., Santa Barbara — [3]Russian Quantum Center, National University of Science and Technology MISIS, Moscow 119049, Russia

A major part of decoherence in superconducting quantum bits arises from their interaction with microscopic material defects forming parasitic two-state quantum systems, so-called TLS. For the further advancement of quantum processors, it is thus vital to gain a better understanding of TLS properties and how they are formed.

Here we demonstrate a new technique to tune the resonance frequencies of defects by exposing a transmon qubit circuit to a DC-electric field generated by electrodes surrounding the sample chip.

Our experiments indicate that about 50% of over 200 individually observed TLS are tuned by the electric field, as it is expected from defects residing on qubit circuit electrodes or at substrate interfaces. In comparison, practically all TLS respond to mechanical strain that is generated by a piezo actuator. Our statistical analyses of the defect's coupling strengths to the qubit, strain, and electric field reveal two distinguishable defect classes whose probable origins will be discussed.

TT 40.4 Wed 10:15 H48

Resolving the Positions of Parasitic Defects in Superconducting Qubits — •Alexander Bilmes[1], Anthony Megrant[2], Julian Kelly[2], Rami Barends[2], John M. Martinis[2], Weiss Georg[1], Alexey V. Ustinov[1,3], and Jürgen Lisenfeld[1] — [1]Karlsruhe Institute of Technology, 76137 Karlsruhe, Germany — [2]Google Inc., Santa Barbara, USA — [3]Russian Quantum Center, National University of Science and Technology MISIS, Moscow 119049, Russia

We demonstrate a new technique to identify the spatial positions of decoherence-inducing material defects known as Two-Level-Tunneling systems (TLS) in superconducting qubits. For this, we operate a transmon qubit circuit in a DC-electric field that is generated by several electrodes surrounding the sample chip, and study the TLS response by monitoring their resonance frequencies using qubit swap spectroscopy. By comparing measured and simulated coupling strengths of TLS to each DC-electrode, we obtain information about the possible locations and hosting interfaces of observed surface TLS. This method is applicable to any ready-made transmon qubit, and opens a path for the optimization and verification of qubit fabrication procedures by directly indicating which circuit interfaces must be improved in order to enhance qubit coherence.

TT 40.5 Wed 10:30 H48

A Two-Level-System sensor derived from a superconducting qubit. — •Alexander Bilmes[1], Ioan Pop[1], Martin Weides[2], Alexey V. Ustinov[1,3], and Jürgen Lisenfeld[1] — [1]Karlsruhe Institut für Technologie, Wolfgang-Gaedestr. 1, 76131 Karlsruhe — [2]University of Glasgow, Schottland — [3]Russian Quantum Center, MISIS, Moscow 119049, Russia

Since the first experimental realization of superconducting qubits in the 2000s, Two-Level-Systems (TLS) are a main and yet unsolved source of noise and decoherence in quantum circuits. The microscopic origin of TLS in the microfabricated devices is manifold. Tunnelling ions, impurities, trapped electrons and adsorbates are the most common and competeng models explaining formation of TLS in dielectrics and interfaces of the circuits. While examination of TLS in ready-made qubits [1,2] is a useful method to improve the sample geometry and fabrication, another complementary approach is to actively study the TLS nature in specially tailored quantum circuits [3,4]. A novel TLS-sensor has been derived from a transmon-qubit architecture where the Josephson junction is shunted by a small capacitor containing a sample dielectric. This allows for exploring of TLS hosted in dielectric films, bulks and at circuit surfaces. Here, we present the proof of principle for TLS-detection in amorphous AlOx films using such a TLS-sensor, which opens up further possibilities for TLS-studies. [1] J. Lisenfeld et al., Sci. Rep. 6 (23786) (2016) [2] A. Bilmes et al., Phys. Rev. B 96, 064504 (2017) [3] B. Sarabi et al., Phys. Rev. Lett. 116, 167002 (2016) [4] J. Brehm et al., Appl. Phys. Lett. 111, 112601 (2017)

TT 40.6 Wed 10:45 H48

Time-resolved tomography of a compact 3D quantum memory — •Michael Renger[1,2], Edwar Xie[1,2,3], Frank Deppe[1,2,3], Qi-Ming Chen[1,2], Michael Fischer[1,2,3], Stefan Pogorzalek[1,2], Kirill G. Fedorov[1,2], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther- Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

We realize a quantum memory by coupling a transmon qubit to a rectangular 3D cavity resonator [1]. Exploiting the multimode structure of the 3D cavity enables us to use single resonator for storage and readout purposes, thereby significantly enhancing scalability. Compared to the bare qubit, the T_1-time of the memory is 6 times longer. We accurately characterize the loss of quantum information during the storage and retrieval process by performing quantum process tomography on our memory system and find a process fidelity of 88%. A detailed error budget analysis enables us to estimate the fidelity losses caused by decoherence, thermal excitations, state leakage and inaccurate state preparation. We investigate the dynamical behavior of our system with time-resolved tomography and a master equation approach.

We acknowledge support by the German Research Foundation through FE 1564/1-1 and the Excellence Cluster MCQST, the Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (Grant No 820505).

[1] E. Xie *et al.*, Appl. Phys. Lett. **112**, 202601 (2018)

TT 40.7 Wed 11:00 H48

Dispersive Readout of AC-Driven Qubits — •Sigmund Kohler — Instituto de Ciencia de Materiales de Madrid, CSIC

We present a unified picture of dispersive readout of quantum systems in and out of equilibrium. A cornerstone of the approach is the backaction of the measured system to the cavity obtained with non-equilibrium linear response theory. It provides the dispersive shift of the cavity frequency in terms of a system susceptibility [1] as well as resonance conditions that relate the cavity transmission to spectral properties and Berry phases [2]. Examples are the readout of detuned qubits and thermally excited multi-level systems. For ac-driven quantum systems, we identify the relevant Fourier component of the susceptibility and introduce a computational scheme based on Floquet theory. The theory is applied to Landau-Zener-Stückelberg-Majorana interference in Si/SiGe double quantum dots, where the interference patterns exhibit a harp-like stemming from the valley degree of freedom [3]. The theoretical and experimental interference patterns show a striking agreement.

[1] S. Kohler, Phys. Rev. A **98**, 023849 (2018).
[2] S. Kohler, Phys. Rev. Lett. **119**, 196802 (2017).
[3] X. Mi, S. Kohler, J. R. Petta, Phys. Rev. B **98**, 161404(R) (2018).

15 min. break.

TT 40.8 Wed 11:30 H48

Coherence of a granular aluminum fluxonium qubit — •Martin Spiecker, Lukas Grünhaupt, Daria Gusenkova, Nataliya Maleeva, Sebastian T. Skacel, Ivan Takmakov, Francesco Valenti, Patrick Winkel, Hannes Rotzinger, Alexey V. Ustinov, and Ioan M. Pop — Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

A promising alternative for the implementation of superinductors, compared to the predominantly used mesoscopic Josephson junction arrays, is granular aluminum (grAl), with a microstructure consisting of pure aluminum grains embedded in an AlOx matrix, effectively forming a self-assembled Josephson junction network [1]. This material offers a large kinetic inductance, while its non-linearity is orders of magnitude smaller than that of Josephson junction arrays [2]. We present a fluxonium qubit employing a granular aluminium superinductor with coherence times T up to 23 μs and T up to 30 μs at the flux bias sweet spot. The measured T approaches the limit 2 * T [3]. These coherence times recommend granular aluminum for increasingly complex protected superconducting quantum circuits, while they also evidence the need to further investigate and mitigate loss mechanisms in high impedance circuits.

[1] Grünhaupt et al., Phys. Rev. Lett. 121, 117001 (2018)
[2] Maleeva et al., Nat. Commun. 9, 3889 (2018)
[3] Grünhaupt and Spiecker et al., arXiv:1809.10646 (2018)

TT 40.9 Wed 11:45 H48

Design and fabrication of a granular aluminum fluxonium qubit — •Lukas Grünhaupt[1], Martin Spiecker[1], Daria Gusenkova[1], Nataliya Maleeva[1], Sebastian T. Skacel[1,2], Ivan Takmakov[1,2,3], Francesco Valenti[1,4], Patrick Winkel[1], Hannes Rotzinger[1], Alexey V. Ustinov[1,3], and Ioan M. Pop[1,2] — [1]Physikalisches Institut, KIT, Karlsruhe, Germany — [2]Institute of Nanotechnology, KIT, Karlsruhe, Germany — [3]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia — [4]Institute for Data Processing and Electronics, KIT, Karlsruhe, Germany

Superconducting materials with low microwave losses and high kinetic inductance are a valuable resource in quantum circuit design, enabling the design of so-called superinductors, which can provide electromagnetic environments with characteristic impedance larger than the resistance quantum $R_Q = 6.5\,\mathrm{k}\Omega$. To implement superinductors, a promising alternative to the predominantly used mesoscopic Josephson junction arrays is granular aluminum (grAl). Its microstructure consists of pure aluminum grains embedded in an AlO_x matrix, effectively forming a compact self-assembled Josephson junction network. We present a superconducting fluxonium qubit employing a superinductor with impedance $Z > R_Q$, fabricated from a grAl thin film, in-situ integrated with a conventional $Al/AlO_x/Al$ Josephson junction. The measured qubit spectrum is in good agreement with the fluxonium Hamiltonian.

TT 40.10 Wed 12:00 H48

Coherent Revival of Ramsey Oscillations in the Fluxonium Qubit Coupled to a bath of Harmonic Oscillators — •Farshad Foroughi[1], Mattia Mantovani[2], Karthik Bharadwaj[1], Remy Dassonneville[1], Luca Planat[1], Sebastien Leger[1], Etienne Dumur[4], Yuriy Krupko[1], Wolfgang Belzig[2], Cecile Naud[1], Olivier Buisson[1], Nicolas Roch[1], Gianluca Rastelli[2,3], and Farshad Foroughi[1] — [1]Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, Grenoble, France — [2]Fachbereich Physik, Universität Konstanz, Konstanz, D-78457 , Germany — [3]Zukunftskolleg, Universität Konstanz, D-78457, Konstanz, Germany — [4]The institute for Molecular Engineering, University of Chicago, Chicago, IL, United

States

We realized a 2D fluxonium qubit coupled to 12 on-chip lumped element resonators. The oscillators are composed of chain of SQUIDs in series with an interdigited capacitor. Careful choice of number of SQUIDs let putting the 12 resonators equally spaced around the qubit frequency. Moreover by applying a global DC external magnetic field to the loop of SQUIDs one can fine tune the resonant frequencies of the modes. We used a fast flux line to control the frequency of the fluxonium qubit and hence coupling between it and and the resonators. We have studied theoretically the emerging spin-boson Hamiltonian for this particular circuit with the perspective of measuring revival effects in the coherent oscillations of the qubit. We implemented the measurements, revealing the effect on the qubit dynamics of a non-dissipative bath formed by a discrete set of harmonic oscillators.

TT 40.11 Wed 12:15 H48

FPGA-based Platform for Control and Readout of Superconducting Qubits — •Richard Gebauer[1], Nick Karcher[1], Oliver Sander[1], Martin Weides[2,3], Alexey V. Ustinov[2,4], and Marc Weber[1] — [1]Institute for Data Processing and Electronics, KIT, Karlsruhe, Germany — [2]Physikalisches Institut, KIT, Karlsruhe, Germany — [3]School of Engineering, University of Glasgow, Glasgow, United Kingdom — [4]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

A typical measurement setup for superconducting qubits consists of arbitrary waveform generators, signal recorders, and vector network analyzers. Although sufficient for simple experiments, this approach is limited due to long communication delays, poor scalability, and static pulse sequences. A faster, more integrated and more flexible solution for qubit readout and control is FPGA-based custom hardware. It not only reduces costs and space requirements but also simplifies measurements and enables many-qubit experiments as well as advanced control schemes like quantum feedback where a low response time is critical.

We developed a flexible FPGA-based integrated platform to control and read out superconducting qubits which also enables fast feedback loops to manipulate qubits depending on their measured state. The platform allows arbitrary X and Y rotations around the Bloch sphere and enables the user to perform all standard measurements needed for single qubit characterization. We will give a short overview about the platform features and capabilities. Furthermore, we present different experimental applications including results on quantum feedback.

TT 40.12 Wed 12:30 H48

Qubit Measurement by Multichannel Driving — Joni Ikonen[1], •Jan Goetz[1], Jesper Ilves[1], Aarne Keränen[1], Andras M. Gunyho[1], Matti Partanen[1], Kuan Y. Tan[1], Dibyendu Hazra[1], Leif Grönberg[2], Visa Vesterinen[1,2], Slawomir Simbierowicz[2], Juha Hassel[2], and Mikko Möttönen[1] — [1]QTF Centre of Excellence, Department of Applied Physics, Aalto University, P.O. Box 15100, FI-00076 Aalto, Finland — [2]VTT Technical Research Centre of Finland, QTF Center of Excellence, P.O. Box 1000, FI-02044 VTT, Finland

We theoretically propose and experimentally implement a method of measuring a qubit by driving it close to the frequency of a dispersively coupled bosonic mode [1]. The separation of the bosonic states corresponding to different qubit states begins essentially immediately at maximum rate, leading to a speedup in the measurement protocol. Also the bosonic mode can be simultaneously driven to optimize measurement speed and fidelity. We experimentally test this measurement protocol using a superconducting qubit coupled to a resonator mode. For a certain measurement time, we observe that the conventional dispersive readout yields close to 100 % higher average measurement error than our protocol. Finally, we use an additional resonator drive to leave the resonator state to vacuum if the qubit is in the ground state during the measurement protocol. This suggests that the proposed measurement technique may become useful in unconditionally resetting the resonator to a vacuum state after the measurement pulse.

[1] Ikonen, et al., arXiv 1810.05465

TT 40.13 Wed 12:45 H48

Low frequency excess flux noise in dc-SQUIDs — •Anna Ferring, Andreas Fleischmann, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

Low frequency excess flux noise strongly impairs the performance of superconducting quantum devices (SQDs) such as SQUIDs and Qubits. It is, for example, the dominating mechanism causing decoherence in flux or phase Qubits and makes SQUID based measurements of low frequency signals rather challenging. Recent experiments strongly hint for surface adsorbates as an origin of this noise contribution. But even though more and more information on its origin and physical properties are gathered, a lot of open questions remain such as whether additional sources of low frequency excess flux noise exist.

In this contribution, we show indications for a correlation between the noise amplitude of dc-SQUIDs and the dc-magnetization of material layers used for device fabrication. This suggests that low-frequency excess flux noise is to some extend caused by the conditions of the fabrication process. We further present a SQUID setup which allows for temperature dependent cross-correlation measurements of the magnetic flux noise of a sample SQUID. Finally, we discuss the scaling of low frequency excess flux noise of simple washer SQUIDs with device inductance showing that the energy sensitivity rather than the magnetic flux noise is the more appropriate figure of merit for describing low frequency excess flux noise.

TT 41: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge V (joint session O/CPP/DS/TT)

Time: Wednesday 10:30–13:15 Location: H9

Topical Talk TT 41.1 Wed 10:30 H9

Theoretical Investigations of Electrochemical CO2 Reduction — •Karen Chan — Department of Physics, Technical University of Denmark

The electroreduction of CO_2 has the potential to store energy from intermittent renewable sources and to produce carbon-neutral fuels and chemicals; In this talk, I will discuss new developments in modeling the electrochemical interface. I will then present the application of these models of the interface to CO_2 reduction: the determination of reaction pathways and kinetics on transition metals, field and solvation effects, pH effects on C_2 product selectivity, and implications for catalyst design.

Topical Talk TT 41.2 Wed 11:00 H9

First-principles approach to model electrochemical reactions at the solid-liquid interface — •Mira Todorova, Sudarsan Surendralal, and Jörg Neugebauer — MPI für Eisenforschung, Düsseldorf

Processes at solid-liquid interfaces are at the heart of many present day technological challenges related to the improvement of battery materials, electro-catalysis, fuel cells, corrosion and others. Describing and quantifying the underlying fundamental mechanisms is equally challenging for experimental and theoretical techniques.

Utilizing concepts from semiconductor physics, we have developed a novel potentiostat design, which enables us to perform ab initio calculations under controlled bias conditions. Easily applied in standard density functional theory codes, it controls the electrode potential of the system by tuning the excess charge of the working electrode and allows us to obtain direct insight into key mechanisms of electrocatalysis and corrosion. As a prototype example, we consider one of the most corrosive systems under wet conditions - Mg. Using the new approach we solve a 150-year-old problem, which links H-evolution under anodic conditions to Mg dissolution [1].

[1] S. Surendralal, M. Todorova, M.W. Finnis and J. Neugebauer, Phys. Rev. Lett. 120, 246801 (2018).

TT 41.3 Wed 11:30 H9

Towards out of the box implicit solvation at liquid-liquid interfaces — •Jakob Filser[1], Markus Sinstein[1], Christoph Scheurer[1], Sebastian Matera[2], Karsten Reuter[1], and Harald Oberhofer[1] — [1]Technische Universität München — [2]Freie Universität Berlin

Implicit solvation models are widely used to incorporate solvent effects in electronic structure theory. Treating the solvent as a structureless dielectric continuum, they lift the necessity to explictly sample solvent degrees of freedom. However, even state of the art models currently cannot treat solvation at technically highly important dielectric interfaces, e.g. between two immiscible liquids.

As a remedy, we modify the multipole expansion (MPE) model to also account for liquid-liquid interfaces, specifically focusing on the electrostatics of mutually interacting dielectric regions. Non-electrostatic free energy contributions thereby are treated with a simple linear model, fitted to experimental free energies of solvation in the two liquids. We demonstrate the efficacy of this approach for small molecules at a water–1-octanol interface, which show the correct qualitative behaviour with respect to orientation and position at the interface.

Future, quantitative applications of our new implicit solvation interface methods are clearly possible but will necessitate both improvements to the non-electrostatic free energy terms and a more exhaustive parameterization effort for a wide range of solvents.

TT 41.4 Wed 11:45 H9

Continuum models of the electrochemical diffuse layer in electronic-structure calculations — •Francesco Nattino[1], Oliviero Andreussi[2], and Nicola Marzari[1] — [1]Theory and Simulations of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Department of Physics, University of North Texas, Denton, TX 76207, USA

The electrical diffuse layer is a structure that spontaneously forms at essentially any solvated interface, such that its presence in electrochemistry is ubiquitous. While first-principles methods are desirable to describe any process occurring at the surface, fully-atomistic models of electrolyte solutions suffer from computational limitations. In this context, continuum models represent a practical tool to bypass these difficulties and to account for the presence of the diffuse layer at electrified interfaces. However, despite the increasing popularity of continuum models in the field of materials science, even relatively simple observables such as the differential capacitance (DC) of single-crystal electrode surfaces remain challenging to model quantitatively. I will present and discuss the performance of a hierarchy of continuum diffuse-layer models that we have implemented and coupled to an atomistic first-principles description of a charged metal surface. In particular, I will compare computed DC values for the prototypical Ag(100) surface in an aqueous solution to experimental data, and validate in this way the accuracy of the models considered.

TT 41.5 Wed 12:00 H9

***Ab initio* molecular dynamics of Pt(111)/H_2O interfaces in an electrolytic cell setup** — •Sudarsan Surendralal, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany.

Recently, we developed a novel scheme to perform density functional theory (DFT) simulations of electrochemical interfaces under conditions of constant applied voltage utilizing charge transfer from a semiconductor counter electrode [1]. We use a fractionally doped Ne counter electrode because of its inertness, wide band gap, and low deformation potential. Our DFT based molecular dynamics calculations of the Pt(111)/H_2O interface in this setup reveals that we are able to accurately reproduce macroscopic observables like the potential of zero charge (PZC). We discuss the work function drop at the interface at the PZC, due to the charge polarization by the non-dissociative chemisorption of water molecules at the Pt surface. Possible pitfalls due to the choice of the DFT exchange-correlation functional, non-converged computational parameters and confinement effects due to the presence of the counter electrode will also be discussed.

[1] S. Surendralal, M. Todorova, M. W. Finnis, and J. Neugebauer, Phys. Rev. Lett. 120, 246801 (2018).

TT 41.6 Wed 12:15 H9

Swipe left for water molecules? - Implicit vs explicit descriptions of liquid water at interfaces. — •Nicolas Hörmann[1], Oliviero Andreussi[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, CH-1015 Lausanne, Switzerland — [2]Department of Physics, University of North Texas, Denton, TX 76207, USA

We present a study of relevant electrochemical interfaces, such as semiconductor-water and metal-water interfaces based on periodic density functional theory (DFT) calculations with the interface modelled with different degrees of complexity. Water at metallic surfaces is modelled within the self-consistent continuum solvation scheme (SCCS) [1] with explicit application of a potential which allows the comparison of pH dependent properties with experimental results [2,3]. In the case of semiconductors, different amounts of interfacial water are substituted with implicit solvent and observables such as the measured band alignment are obtained from thermal averaging over molecular dynamics snapshots. We find that it is necessary and sufficient to include strongly bound interfacial water molecules (dissociated or not) explicitly and replace the rest with an implicit model, in order to obtain consistent results with all-explicit simulations [4]. Based on these result we simulate the surface Pourbaix diagrams of the most stable surfaces of GaAs, GaN, GaP, CdS and anatase and rutile TiO_2.

[1] *J. Chem. Phys.* **136**, 064102 (2012); [2] *Nat Commun.* **9**, 3117 (2018). [2,3] NH (2018) submitted

TT 41.7 Wed 12:30 H9

Transition metal oxide nanoparticles as efficient catalysts for proton exchange membrane electrolyzers: morphology, activity and stability — •Daniel Opalka, Yonghyuk Lee, Jakob Timmermann, Christoph Scheurer, and Karsten Reuter — Technische Universität München

Transition metal oxides such as RuO_2 and IrO_2 are currently the best known electrocatalysts for the oxygen evolution reaction from liquid water in proton exchange membrane (PEM) electrolyzers. However, dynamic load operation of PEM cells induces transformations of the catalyst morphology leading to metal dissolution and catalyst degradation. We present a computational model to predict the morphology, activity and stability from *ab initio* electronic structure theory and fundamental thermodynamic principles. Based on this model, we have explored novel strategies to reduce material expenses and improve catalyst stability while preserving high catalytic activity via nanoparticles with a core-shell design. From an analysis of different surface coverages with oxygen, hydroxyl and hydroxo species, voltage-dependent phase diagrams for catalyst surfaces are presented which correlate with characteristic features observed in cyclovoltammetric measurements. Results from atomistic models of selected nanoparticles on the basis of Wulff's Theorem show negligible size effects, but a strong influence of the facet terminations on the surface relaxation.

TT 41.8 Wed 12:45 H9

Modelling the fingerprint of chemical reactions on catalytic surfaces in core-electron binding energies — •Johannes Lischner and Juhan Matthias Kahk — Imperial College London

Core-electron X-ray photoemission spectroscopy is a powerful experimental technique to gain information about chemical reactions on catalytic surfaces. Interpreting experimental spectra, however, is often challenging and theoretical modelling of core-electron binding energies is required to meaningfully assign peaks to adsorbate species. In this talk, I will present a novel first-principles modelling strategy to calculate core-electron binding energies of molecules on metallic surfaces. Specifically, we combine plane-wave/pseudoptential DFT calculations of surface slab models for geometry optimizations with all-electron Delta-SCF calculations on cluster models for determining accurate core-electron binding energies. This approach is computationally efficient and yields good agreement with experimental measurements for a wide range of adsorbates on copper(111) surfaces.

TT 41.9 Wed 13:00 H9

What Makes a Successful Photoanode? - The Role of the Semiconductor–Catalyst Interface — •Franziska Simone Hegner[1], Benjamin Moss[2], James Durrant[2], Sixto Gimenez[3], José-Ramón Galán-Mascarós[1], and Núria López[1] — [1]Institute of Chemical Research of Catalonia (ICIQ) — [2]Imperial College London — [3]Institute of Advanced Materials, Castellón

A large scale implementations of artificial photosynthesis is still limited by the low efficiencies of the employed photoelectrochemical systems. A common strategy to improve performance is to deposit a co-catalyst on the light-harvesting photoanode. However, the role of the catalyst is controversial; is it acting as a true catalyst, i.e. transferring charges, or is it merely influencing the electronic structure of the semiconductor?[1]

The semiconductor-catalyst interface is key to catalytic performance, but its accurate description is limited since linear scaling re-

lationships no longer apply. Herein the function of the co-catalyst (cobalt hexacyanoferrate) is discussed on two photoanode interfaces, Fe2O3 and BiVO4. Density Functional Theory and time-resolved spectroscopy were used to shed light on the underlying charge-transfer processes. Taking into account the advantages and disadvantages of all applied techniques, a relationship between electronic structure alignment, interface morphology, and photocatalytic efficiency is proposed.[2]

[1] D. R. Gamelin, Nat. Chem., 4 (2012), 965-967. [2] F. S. Hegner, D. Cardena-Moscoros, S. Gimenez, N. López, J. R. Galán-Mascarós. ChemSusChem, 10 (2017) 4552-4560.

TT 42: Nano- and Optomechanics

Time: Wednesday 10:45–12:30 Location: H7

TT 42.1 Wed 10:45 H7

Optomechanics of a suspended carbon nanotube quantum dot coupled to a coplanar microwave resonator, part 1: theory — Stefan Blien, Patrick Steger, Niklas Hüttner, Richard Graaf, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

A clean, suspended single wall carbon nanotube is the ultimate limit of a nanomechanical beam resonator, where the fundamental transversal vibration mode reaches resonance frequencies on the order of 100MHz – 1 GHz and mechanical quality factors up to 10^6. Placing a nanotube next to a coplanar resonator at cryogenic temperatures results in a microwave optomechanical system with dispersive coupling. This system, however, has a fundamentally new property: the nanotube is also a quantum dot, and the interaction of motion and single electron tunneling dominates its behaviour.

We demonstrate how Coulomb blockade leads to an enhanced optomechanical coupling g that is also tuneable by the gate potential. The inherent electronic nonlinearity acts as amplifier, leading to values up to $g \simeq 10\,\mathrm{kHz}$ already at moderate cavity occupation. With the combined optomechanical system in the far resolved sideband limit, many interesting experiments become feasible.

TT 42.2 Wed 11:00 H7

Optomechanics of a suspended carbon nanotube quantum dot coupled to a coplanar microwave resonator, part 2: experiment — •Stefan Blien, Patrick Steger, Niklas Hüttner, Richard Graaf, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

A clean, suspended single wall carbon nanotube is the ultimate limit of a nanomechanical beam resonator. We have implemented a transfer technique to integrate such a nanotube into a superconducting circuit, and present measurements on a combined device coupling a suspended carbon nanotube quantum dot to a coplanar microwave resonator mode at millikelvin temperatures.

Nanotube vibration and microwave cavity form a dispersively coupled optomechanical system, which we characterize via two-tone spectroscopy (red side band photon upconversion) as well as optomechanically induced transparency (OMIT). The interaction of charge transport and vibration, via Coulomb blockade and single electron tunneling, leads to a strongly enhanced, tunable optomechanical coupling.

TT 42.3 Wed 11:15 H7

In situ tunable string resonators in a network — •Daniel Schwienbacher[1,2,3], Thomas Luschmann[1,2], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Nanosystems Initiative Munich (NIM), München, Germany

Mechanical resonator networks are currently discussed in the context of model systems giving insight to condensed matter problems including topology[1]. Here, we discuss networks based on three high-Q nanomechanical string resonators (nanostrings) made from highly tensile stressed Si_3N_4. The strings are strongly coupled via shared support structures and thus can form a fully mechanical, classical multi-level system. Moreover, the individual strings are tunable in frequency [2], which allows to investigate their coupling dynamics using continuous wave and time domain techniques. In particular, such systems allow the experimental explorations of quantum classical analogies such as Landau-Zener dynamics[3,4]. We extend the previous work performed on two coupled strings to three resonators and discuss the additional features of the inter string dynamics, such as the classical analog of Landau-Zener dynamics in a three mode system and the observation of dark states.

[1] Brendel et al., Phys. Rev. B **97** 020102(R) (2018)
[2] Pernpeintner et al., Phys. Rev. App. **10** 034007 (2018)
[3] Faust et al., Nat. Phys. **9**, 485-488 (2013)
[4] Seitner et al., Phys. Rev. B **84**, 245406 (2016)

TT 42.4 Wed 11:30 H7

Nano-strings in circuit QED — •Philip Schmidt[1,2,3], Daniel Schwienbacher[1,2,3], Natalie Segercrantz[1], Mohammad T. Amawi[1,2], Christoph Utschick[1,2], Matthias Pernpeintner[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Departement, Technische Universität München, Garching, Germany — [3]Nanosystems Initiative Munich, München, Germany

In nano-electromechanics, quantum mechanical phenomena can be studied in the literal sense. For example, the coupling of a nanomechanical element to a superconducting resonator allows to cool the mechanical mode to its ground state and to squeeze its motion. Replacing the linear microwave resonator with a nonlinear one enables the preparation of more complex non-classical mechanical states.

Here, we discuss such a realization, based on Josephson junctions in superconducting circuit environments. In particular, we envisage the scenario of a mechanically compliant tensile-strained nanostring embedded into a microwave resonator combined with Josephson junctions circuits. We present experimental data of such ciruits and critically highlight limitations imposed by the embeded Jospheson junctions regarding the device performance.

Such hybrid systems open new perspectives in the field of optomechanics ranging from sensing applications to the use of quantum states.

TT 42.5 Wed 11:45 H7

Circuit electromechanical hybrid system featuring three-body interactions — •Natalie Segercrantz[1], Daniel Schwienbacher[1,2,3], Philip Schmidt[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Germany — [2]Physik-Departement, Technische Universität München, Garching, Germany — [3]Nanosystems Initiative Munich, München, Germany

Nanomechanical resonators coupled to a microwave cavity are promising candidates for both sensing applications and quantum experiments including the preparation and transfer of non-classical states. The control and manipulation of these quantum circuits can be extended by adding a non-linear element, such as a transmon qubit, to the system. Recently, an architecture involving embedding a nanobeam into the shunt capacitance of a transmon was proposed [1]. This hybrid system with the nanomechanical transmon coupled capacitively to the microwave resonator includes three-body interactions between the mechanical and the electrodynamical degrees of freedom. Ground-state cooling and the preparation of mechanical Fock- and cat-states was theoretically predicted for the system.

We present a design on the three-body hybrid system consisting of a superconducting coplanar waveguide resonator, a transmon and a nanomechanical resonator. Using finite element simulations, the device parameters are optimized with respect to the coupling strengths and resonance frequencies.

[1] M. Abdi *et al*, Phys. Rev. Lett. 114, 173602 (2015)

TT 42.6 Wed 12:00 H7

SiN nanomechanical resonators for cavity-optomechanics — •Felix Rochau, Irene Sánchez Arribas, Alexandre Brieussel, and Eva Weig — Universität Konstanz, Konstanz, Germany

We study a high-finesse fiber-based micro-cavity with small mode volume. Similar to the membrane-in-the-middle approach to cavity-optomechanics, silicon nitride (SiN) stripes are used as 1D mechanical resonators, or to introduce nano-objects inside the cavity. To understand the system, the interaction between the cavity mode and the

transverse flexural modes of the SiN stripe resonators are studied. Optomechanical coupling strength and mechanism can be tuned by changing the resonator position with respect to the cavity mode. First attemps to observe dynamical backaction are presented.

TT 42.7 Wed 12:15 H7

Modelling of coupled molecular rotors — Huang-Hsiang Lin[1,2], Alexander Croy[1], •Rafael Gutiérrez[1], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01069 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany

The possibility of creating molecular gears able to transfer motion has opened novel routes to implement true molecule-based mechanical analogs of computational machine. Here, we use a classical description of rigid molecules to investigate the dynamics of coupled gears for different arrangement and in presence of disorder. To be specific, we consider two gears and many gears problem; Then we demonstrate the solution analytically and numerically. In particular, we focus on the question of transfer of angular momentum acting on assembly of gears, which is relevant in light of recent experiments.

TT 43: Focus Session: Topology in 3D Reciprocal Space: Beyond Dirac and Weyl Quasiparticles (joint session TT/MA)

Topological Dirac and Weyl semimetals are currently in focus of condensed-matter research. The ultra-relativistic electrons in these systems manifest themselves in experimental probes in many very unusual ways, such as chiral currents, hydrodynamic electron flows, and chiral optical response. Theory and experiment go further and offer even more exotic topological phases, which have no analogies in high-energy physics. Among the recent discoveries are Lorentz-invariance breaking quasiparticles, multi-Weyl semimetals, and topological phases in non-electronic systems.

Organized by: Artem Pronin (Universität Stuttgart), Claudia Felser (MPI-CPfS Dresden), Martin Dressel (Universität Stuttgart)

Time: Wednesday 15:00–18:15 Location: H2

Invited Talk TT 43.1 Wed 15:00 H2

Novel optical and electrical responses in topological semimetals — •Joel Moore — University of California, Berkeley, USA — Lawrence Berkeley National Laboratory, Berkeley, USA

Several new classes of topological materials have been confirmed to exist in experiments over the past decade. Many of these materials support unique electromagnetic properties that affect transport and optical responses in potentially useful ways. For example, topological insulators support a particular electromagnetic coupling known as "axion electrodynamics", and understanding this leads to an improved understanding of magnetoelectricity in all materials. The main focus of this talk is on how topological Weyl and Dirac semimetals can show unique electromagnetic responses; we argue that in linear response the main observable property solves an old problem about optical rotation via the orbital moment of Bloch electrons. Nonlinear responses such as magnetoconductivity can reveal more surprising behavior. Nonlinear optical response (second-harmonic generation) is already known to be remarkably strong in existing Weyl materials, and may show an unexpected strength and quantization in Weyl materials without mirror symmetries.

Talk includes results obtained with Fernando de Juan, Adolfo Grushin, Takahiro Morimoto, Joseph Orenstein, Daniel Parker, Ivo Souza, and Shudan Zhong.

Invited Talk TT 43.2 Wed 15:30 H2

Beyond the elementary particles and the 10-fold classification of non-interacting topological phases — •Alexey Soluyanov — Physics Institute, University of Zurich, Zurich, Switzerland

One of the research directions in string theory is the separation of important theoretical problems into distinct classes based on their similarities. Electronic structure problem is usually not considered to be important in the string theory community. In this talk I will show that the electronic structure theory in fact allows not only for theoretical analysis of problems in quantum field theory and general relativity, but also for their cheap (on the LHC scale) experimental tests, and also provides many hints to other problems in physics, often considered to be of bigger importance than the study of material properties. In particular, I will show that even weakly-interacting crystalline materials realize a collection of topologically-protected quasiparticle excitations that can either be direct analogs of relativistic elementary particles, or due to the absence of Lorentz-symmetry constraint realize completely novel quasiparticles not present in the high-energy standard model. Materials that host such quasiparticles exhibit special transport properties. I will give a detailed description of several families of such materials. Finally, I will show that even the simplest elemental compounds hide physical phenomena that provide very accessible analogies to complicated theoretical physics theories, and illustrate that the current understanding of even the simplest non-correlated crystalline materials is far from complete.

Invited Talk TT 43.3 Wed 16:00 H2

Direct optical detection of Weyl fermion chirality in a topological semimetal — •Nuh Gedik — Department of Physics, Massachusetts Institute of Technology, Cambridge, MA USA

A Weyl semimetal is a novel topological phase of matter, in which Weyl fermions arise as pseudo-magnetic monopoles in its momentum space. The chirality of the Weyl fermions, given by the sign of the monopole charge, is central to the Weyl physics, since it serves as the sign of the topological number and gives rise to exotic properties such as Fermi arcs and the chiral anomaly. In this talk, I will present our recent measurements in which we directly detect the chirality of the Weyl fermions by measuring the photocurrent in response to circularly polarized mid-infrared light. The resulting photocurrent is determined by both the chirality of Weyl fermions and that of the photons. Beyond Weyl semimetals, these experiments establish nonlinear photocurrent spectroscopy as a powerful tool for studying the geometrical properties of the electronic wavefunction in quantum materials. To this end, I will also discuss how we used this method to reveal electrically switchable Berry curvature dipole in the monolayer topological insulator WTe2.

15 min. break.

Invited Talk TT 43.4 Wed 16:45 H2

Evidence for an axionic charge density wave in the Weyl semimetal $(TaSe_4)_2I$ — •Johannes Gooth — Max Planck Institut für Chemische Physik fester Stoffe

An axion insulator is a correlated topological phase, predicted to arise from the formation of a charge density wave in Weyl semimetals. The accompanying sliding mode in the charge density wave phase, the phason, is an axion. It is expected to cause anomalous magneto-electric transport effects. However, this axionic charge density wave has so far eluded experimental detection. In this paper, we report for the first time the observation of a large, positive contribution to the magneto-conductance in the sliding mode of the charge density wave Weyl semimetal $(TaSe_4)_2I$ for collinear electric and magnetic fields (E||B). The positive contribution to the magneto-conductance originates from the anomalous axionic contribution of the chiral anomaly to the phason current, and is locked to the parallel alignment of E and B. By rotating B, we show that the angular dependence of the magneto-conductance is consistent with the anomalous transport of an axionic charge density wave.

Invited Talk TT 43.5 Wed 17:15 H2

Investigations of Dirac/Weyl semimetals under external stimuli — •Ece Uykur — 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany

Dirac/Weyl semimetals acquire 3D linearly dispersive electronic bands, as opposed to the parabolic bands, with band crossings near the Fermi energy, where the low energy excitations are described by the relativistic Weyl or Dirac equations. Optical spectroscopy is one of the strongest methods to probe these low energy responses. Moreover, it can be coupled to an external tuning mechanism such as magnetic fields, pressure, etc. Additional tuning parameters can be used to create a Dirac/Weyl state and/or to provide valuable information about the nature of the observed topological state. A peculiar magnetic field dependence of the Landau-level transitions, for instance, would hint the existence of the massless Dirac/Weyl fermions in the studied system. In this talk, I will summarize our efforts on different Weyl/Dirac semimetals and their optical responses under an external tuning parameter.

TT 43.6 Wed 17:45 H2

Optical conductivity studies of topological nodal semimetals — •Artem V. Pronin[1], David Neubauer[1], Micha B. Schilling[1], Felix Hütt[1], Martin Dressel[1], Alexander Yaresko[2], Leslie M. Schoop[3], Chandra Shekhar[4], and Claudia Felser[4] — [1]1. Physikalisches Institut, Universität, Stuttgart, 70569 Stuttgart, Germany — [2]MPI für Festkörperforschung, 70569 Stuttgart, Germany — [3]Princeton University, Princeton, NJ 08544, USA — [4]MPI für Chemische Physik fester Stoffe, 01187 Dresden, Germany

We have studied a large number of different topological nodal semimetals (TNSMs) by means of optical spectroscopy [1]. Theory predicts that the optical conductivity of TNSMs is not only distinct from the response of "ordinary" semiconductors and metals, but also very sensitive to the TNSM's band structure and band dimensionality [2]. In real TNSMs, free-electron absorption and contributions from topologically trivial parabolic bands are essential. Both effects may mask the predicted behavior. Some of the studied materials are indeed affected by the aforementioned effects quite substantially. In the others, the low-energy optical response, related to the linear electronic bands, is clearly observed. In the course of the presentation, optical conductivity of the studied TNSMs will be discussed alongside the theory predictions.

[1] PRB **93**, 121202 (2016); PRL **119**, 187401 (2017); PRL **121**, 176601 (2018); PRB **98**, 195203 (2018); JPCM **30**, 485403 (2018).
[2] PRL **108**, 046602 (2012).

TT 43.7 Wed 18:00 H2

Thin-film investigations of 3D Dirac fermions in antiperovskite compounds — •Dennis Huang[1], Hiroyuki Nakamura[1], Eslam Khalaf[1,2], Pavel Ostrovsky[1,3], Kathrin Müller[1], Ulrich Starke[1], Alexander Yaresko[1], and Hidenori Takagi[1,4,5] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Department of Physics, Harvard University, Cambridge MA 02138, USA — [3]L. D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia — [4]Department of Physics, University of Tokyo, 113-0033 Tokyo, Japan — [5]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, 70569 Stuttgart, Germany

Topological semimetals hosting Dirac or Weyl fermions lie at the forefront of research in condensed matter physics. Recently, a class of antiperovskite compounds (A_3BO: A = Ca, Sr, Ba; B = Sn, Pb) have been predicted to possess both massive 3D Dirac fermions and topological surface states protected by crystal symmetry. Using molecular beam epitaxy, we grow thin films of the antiperovskite compounds Sr_3PbO and Sr_3SnO. We report ongoing efforts to elucidate the exotic electronic properties of these compounds using transport and spectroscopic probes.

TT 44: Correlated Electrons: Method Development

Time: Wednesday 15:00–19:00 Location: H7

TT 44.1 Wed 15:00 H7

Dynamical susceptibility in DMFT: a sparse QMC sampling approach — •Dominique Geffroy[1,2], Hiroshi Shinaoka[3], Jan Kuneš[2], Junya Otsuki[4], Markus Wallerberger[5], Emanuel Gull[5], and Kazuyoshi Yoshimi[6] — [1]Department of Condensed Matter Physics, MU Brno, Czech Republic — [2]Institute for Solid State Physics, TU Wien, Austria — [3]Department of Physics, Saitama University, Japan — [4]Department of Physics, Tohoku University, Japan — [5]University of Michigan, Ann Arbor, USA — [6]Institute for Solid State Physics, University of Tokyo, Japan

We discuss a new technique for the efficient sampling of two-particle correlation functions in the framework of dynamical mean-field theory. The approach is based on the expansion of the two-particle Green's function, based on the recently introduced "intermediate representation" basis [1,2]. We demonstrate that both the complex low-frequency structure, and the high-frequency tails are correctly described.

This sparse sampling can be used for the calculation of dynamic susceptibilities, after inversion of the Bethe-Salpeter equation. We present results in the context of the BEC to BCS crossover [3, 4] in the vicinity of the excitonic condensation in the two-band Hubbard model [5].

[1] H. Shinaoka, J. Otsuki et. al., Phys. Rev. B 96, 035147 (2017)
[2] H. Shinaoka, J. Otsuki et al., Phys. Rev. B 97, 205111 (2018)
[3] B. Zenker, D. Ihle et al., Phys. Rev. B 85, 121102(R) (2012)
[4] J. Kuneš, J. Phys.: Cond. Mat. 27, 333201 (2015)
[5] D. Geffroy, J. Kaufmann et al., arXiv 1808.08046 (2018)

TT 44.2 Wed 15:15 H7

Self-Consistent Ladder Dynamical Vertex Approximation — •Josef Kaufmann[1], Anna Kauch[1], Oleg Janson[1,2], and Karsten Held[1] — [1]Institute for Solid States Physics, TU Wien — [2]IFW Institute for Theoretical Solid State Physics, Dresden

The dynamical vertex approximation (DΓA) is a diagrammatic extension [1] of the dynamical mean-field theory (DMFT). In the so-called ladder-DΓA, one treats the irreducible vertex in the particle-hole channel as completely local and builds nonlocal ladder diagrams from it, which are then used as corrections to the DMFT self-energy. The local vertex is extracted from two-particle Green's functions, calculated by using continuous-time quantum Monte Carlo for an effective Anderson impurity model [2,3].

Traditionally, self-consistency has been mimicked by a so-called λ-correction. In this talk, we go a considerable step beyond and present a self-consistent formulation and solution of the DΓA equations, naturally fulfilling physical constraints, such as the asymptotics of the self-energy. The applicability is demonstrated in calculations for the Hubbard model on a square lattice and on a (geometrically frustrated) Kagome lattice.

[1] G. Rohringer *et al.*, Rev. Mod. Phys. 90, 025003 (2018)
[2] P. Gunacker *et al.*, Phys. Rev. B 92, 155102 (2015)
[3] J. Kaufmann *et al.*, Phys. Rev. B 96, 035114 (2017)

TT 44.3 Wed 15:30 H7

Predicting exact Green functions from perturbative solutions by a neural network — •Patryk Kubiczek and Alexander Lichtenstein — I. Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany

Green functions are building blocks for a plethora of many-body theories. While in many cases quantum Monte Carlo methods allow for a reliable calculation of Green functions for large interacting systems, they can still be hindered by the sign problem, especially in the real-time formulation. However, it is usually relatively inexpensive to get approximate solutions from a perturbation theory. We propose a new calculation scheme, in which a neural network is trained to predict exact Green functions from complementary perturbative solutions, as long as there exists an efficient method to generate a sufficiently large training set of exact solutions. We employ this scheme as an imaginary-time impurity solver for the dynamical mean field theory (DMFT) for the Hubbard model on a Bethe lattice.

TT 44.4 Wed 15:45 H7

Slave rotor approach to impurity models with ligand orbitals — •Jakob Steinbauer[1] and Silke Biermann[1,2,3] — [1]Ecole Polytechnique, Palaiseau, France — [2]Collège de France, Paris, France —

[3]European theoretical spectroscopy facility, Europe

We propose a slave (spin/rotor) method for the solution of many-orbital quantum impurity problems, which maps the original problem with correlated and ligand orbitals onto one with an effective correlated shell only. This is particularly useful for the dynamical mean field theory treatment of transition metal oxides where the interactions between ligand states and d-states are all too often simply neglected. We derive a general formalism relying on an optimized effective model obtained from the variational principle of Feynman and Peierls and apply our method to a minimal 2-band model with orbitals of d and p character.

TT 44.5 Wed 16:00 H7

Fermion-boson vertex within Dynamical Mean-Field Theory — •Erik van Loon[1,2], Friedrich Krien[3,4], Hartmut Hafermann[5], Alexander Lichtenstein[3], and Mikhail Katsnelson[1] — [1]Radboud University, Nijmegen, the Netherlands — [2]University of Bremen, Bremen, Germany — [3]University of Hamburg, Hamburg, Germany — [4]SISSA, Trieste, Italy — [5]Huawei Technologies, Paris, France

In the study of strongly interacting electrons, correlations on the two-particle level are becoming accessible. These correlation functions are generally rather complicated and cumbersome objects that lack a clear physical intuition. In this work, we study a particular two-particle correlation function that does have a clear intuition: the fermion-boson vertex. It describes the response of the Green's function (self-energy) when an external field is applied. As such, it displays interesting behaviour when the metal-insulator transition is approached. We provide several perspectives on this object, including Ward identities, sum rules, analytical continuation, and its role in diagrammatic extensions of Dynamical Mean-Field Theory.

TT 44.6 Wed 16:15 H7

Spektra: An Online Tool for Analytic Continuation — •Khaldoon Ghanem — Max Max Planck Institute for Solid State Research, Stuttgart, Germany

The stochastic sampling method (StochS) is used for the analytic continuation of quantum Monte Carlo data from the imaginary axis to the real one. Due to its lack of explicit parameters and its potential of resolving sharp features, StochS provides a promising alternative to the commonly used maximum entropy method.

In earlier DPG talks, we presented an efficient algorithm of stochastic sampling that reduces the computational cost by orders of magnitude. We also showed that StochS has an implicit default model given by the discretization grid and provided a recipe for choosing this grid. We extended StochS into a gridless method (gStochS) by sampling the grid points from a default model and then extend gStochS to sample over a whole class of default models with different widths (eStochS).

In this talk, we review the aforementioned developments in a unifying framework where stochastic sampling methods are organized as a hierarchy of increasing power and cost. We present a highly-optimized implementation of all three methods: StochS, gStochS and eStochS, and make it accessible through an online interface. The user can simply upload data in a convenient format and submit calculations with few clicks. The computation is done remotely and results are available in seconds/minutes. The interface also facilitates comparing different results in order to apply our recipe for choosing the optimal hyperparameters, if needed.

TT 44.7 Wed 16:30 H7

Quantum Monte Carlo simulation of the chiral Heisenberg Gross-Neveu-Yukawa phase transition with a single Dirac cone — •Thomas C. Lang and Andreas M. Läuchli — University of Innsbruck, Austria

We present quantum Monte Carlo simulations for the chiral Heisenberg Gross-Neveu-Yukawa quantum phase transition of relativistic fermions with $N = 4$ Dirac spinor components subject to a repulsive, local four fermion interaction in $2+1d$. Here we employ a two dimensional lattice Hamiltonian with a single, spin-degenerate Dirac cone, which exactly reproduces a linear energy-momentum relation for all finite size lattice momenta in the absence of interactions. This allows us to significantly reduce finite size corrections compared to the widely studied honeycomb and π-flux lattices. A Hubbard term dynamically generates a mass beyond a critical coupling of $U_c = 6.76(1)$ as the system acquires antiferromagnetic order and SU(2) spin rotational symmetry is spontaneously broken. At the quantum phase transition we extract a self-consistent set of critical exponents $\nu = 0.98(1)$, $\eta_\phi = 0.53(1)$, $\eta_\psi = 0.18(1)$, $\beta = 0.75(1)$. We provide evidence for the continuous degradation of the quasi-particle weight of the fermionic excitations as the critical point is approached from the semimetallic phase. Finally we study the effective "speed of light" of the low-energy relativistic description, which depends on the interaction U, but is expected to be regular across the quantum phase transition. We illustrate that the strongly coupled bosonic and fermionic excitations share a common velocity at the critical point.

TT 44.8 Wed 16:45 H7

Critical energy spectrum of the chiral Ising Gross-Neveu-Yukawa field theory on the torus — •Michael Schuler[1], Stephan Hesselmann[2], Thomas C. Lang[1], Stefan Wessel[2], and Andreas M. Läuchli[1] — [1]Institute for Theoretical Physics, University of Innsbruck, Austria — [2]Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University, 52056 Aachen, Germany

We investigate the critical torus low-energy spectrum of the chiral Ising universality class with $N = 4$ component Dirac spinors in $2 + 1d$ from the strongly interacting t-V model of spinless fermions, which serves as a universal fingerprint of the associated critical Gross-Neveu-Yukawa field theory. We employ a combination of exact diagonalization and quantum Monte Carlo simulations to compute the critical energy spectra on finite-size clusters and extrapolate them to the thermodynamic limit. We show that the strong interaction between the spinor field and the scalar order-parameter field strongly influences the critical energy levels on the torus. Furthermore, we highlight the effect of different cluster shapes on the critical torus spectrum and illustrate that they can be interpreted by adding non-zero flux around the torus. In addition we estimate the renormalization of the Fermi velocity in the semimetallic (Dirac) phase from the behavior of the energy spectrum and extrapolate the observed linear renormalization to the critical point. Our investigation shows that precise knowledge of the spectrum even on small clusters already provides valuable insight into the properties of critical systems.

15 min. break.

TT 44.9 Wed 17:15 H7

News on tensor network algorithms — •Roman Orus — Donostia International Physics Center (DIPC)

In this talk I will make an overview of recent developments concerning the simulation of quantum lattice systems with tensor networks, focusing on systems in the thermodynamic limit. In particular, I will flash developments concerning: (i) results from infinite-PEPS for different models in the ruby, triangle-honeycomb and star lattices; (ii) a simple PEPS algorithm for arbitrary lattices; (iii) PEPO algorithms for 2d dissipative and finite-temperature systems, and (iv) the implementation of SU(2) symmetry via fusion trees and the study of a chiral Heisenberg ladder.

TT 44.10 Wed 17:30 H7

Tensor network algorithms for simulating real quantum materials — •Augustine Kshetrimayum[1], Matteo Rizzi[2], Roman Orus[3], Bella Lake[4], and Jens Eisert[1] — [1]Dahlem Center for Complex Quantum Systems, Physics Department, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [3]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

In this talk, I will present some results on how tensor network algorithms can be used to simulate real quantum materials. In particular, I will first talk about how PEPS can be used to simulate two-dimensional thermal states based on an annealing mechanism. I will give the examples of the Ising and the Bose Hubbard model on a square lattice. In the second part, I will discuss about the material $Ca_{10}Cr_7O_{28}$ that was recently discovered in the lab to be a quantum spin liquid. We study this material using a variant of PEPS known as the Projected Entangled Simplex State. We show that our numerical results nicely fit with the previously obtained experimental results.

TT 44.11 Wed 17:45 H7

Quantum dynamics via universal quantum gates emulated with matrix product states — •Constantin Meyer[1], Sebas-

tian Paeckel[1], Robert Schade[2], Salvatore R. Manmana[1], and Thomas Köhler[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Institut für Theoretische Physik, Technische Universität Clausthal, Germany

As quantum-computation devices are currently under development, but have only a small number of qubits, it is interesting to ask whether one can emulate gate-based quantum computations for certain simple cases using a classical computer. Often, approaches based on exact diagonalizations and a complete representation of the states are used, which severely restrict the number of emulated qubits. Here, we use matrix-product states, which allow for the treatment of significantly more qubits. We implement the time evolution of a many-body Hamiltonian in this setup by formulating the Trotter decomposition via universal gates. The matrix-product operators of these gates are represented as finite-states machines. This allows us to test the reliability of the implemented emulator by comparing time evolutions to exact results.

TT 44.12 Wed 18:00 H7

Simulations in 2D using isometric Projected Entangled Pair States — •Sheng-Hsuan Lin and Frank Pollmann — Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany

Projected Entangled Pair States (PEPS) have been proposed as a generalization of matrix-product states (MPS) to two-dimensional systems. However, numerical algorithms based on PEPS tend to be unstable due to the lack of a proper canonical form. This problem can be addressed by introducing a gauge fixing or constraint on local tensors. In our approach, we consider PEPS consisting of isometric tensors which then allow for efficient simulations. First, we benchmark an algorithm that variationally minimizes the energy within the manifold of isometric tensors by comparing to exact results. Second, we consider real time evolution and focus on dynamical correlations in a quantum spin system.

TT 44.13 Wed 18:15 H7

An fRG library for high performance computing — •Jannis Ehrlich[1,2], Daniel Rohe[3], and Carsten Honerkamp[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen, Germany — [3]Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

The functional renormalization group (fRG) is a versatile tool to investigate different aspects of correlated electron systems, for example the emergence and competition of ordering tendencies and their energy scales. Although the fRG enables an unbiased investigation of correlations without favouring a specific channel in contrast to Bethe-Salpeter equations, numerical implementations of the fRG easily become intricate and require sufficient testing. Hence the fRG has not been as widely used as other numerical schemes for correlated electrons. In order to facilitate an easier application, we present a fRG-library which can be used readily by simply specifying the model for investigation. The calculation of the fRG flow is done inside the fRG-library, which is parallelized by MPI and OpenMP. As a first example, we present the code performance obtained for the 2D Hubbard model with and without the recently developed Truncated Unity formalism. In addition, as a demonstration of the code versatility, we present the phase diagram of the 3D Hubbard model and first results of a Rashba model with Zeeman splitting.

TT 44.14 Wed 18:30 H7

Leading logarithmic approximation to the X-ray-edge model from a single-loop functional renormalization group approach — •Jan Diekmann and Severin Georg Jakobs — Institut für Theorie der Statistischen Physik, RWTH Aachen University, 52056 Aachen

Numerous models for low-dimensional correlated systems (e.g. X-ray-edge model, Kondo model, one-dimensional metals) have logarithmic divergencies in different diagrammatic channels of the four-point function. Then the sum of all parquet diagrams with bare lines contains all leading logarithmic divergencies, cf. Ref. [1]. The functional renormalization group (FRG) in a single-loop truncation does not reproduce all parts of all parquet diagrams; recently, it was shown how a multi-loop extension of the FRG can achieve this [2]. However, in this talk we present a (purely Fermionic) single-loop FRG that reproduces identically the leading logarithmic result of Ref. [1] for the four-point function of the X-ray-edge model. Our FRG approximation accounts for the leading contribution of every parquet diagram and is closely related to the parquet approach of Ref. [1]. Indeed, certain technical steps in Ref. [1] can be understood as introducing an RG cut-off and solving the very single-loop FRG flow equation. We expect that our findings can be transferred to other models with logarithmic divergencies.

[1] B. Roulet, J. Gavoret, P. Nozières, Phys. Rev. **178**, 1072 (1969)
[2] F. B. Kugler, J. von Delft, Phys. Rev. Lett. **120**, 057403 (2018)

TT 44.15 Wed 18:45 H7

Learning multiple order parameters with interpretable machines — •Jonas Greitemann, Ke Liu, and Lode Pollet — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München

Machine learning shows promise for studying phase transitions many-body systems. However, most studies are tied to situations involving only one phase transition and one order parameter. Systems that accommodate multiple phases of coexisting and competing orders, which are common in condensed matter physics, remain largely unexplored from a machine learning perspective. We investigate the multiclassification of phases using Support Vector Machines (SVMs) and present a generic protocol for detecting hidden spin and orbital orders to learn multiple phases and their analytical order parameters. Our focus is on multipolar orders and their tensorial order parameters whose analytical form is extracted for tensors up to rank 6. Furthermore, we discuss an intrinsic parameter of SVM, the bias, which allows for a special interpretation in the classification of phases, and its utility in diagnosing the existence of phase transitions. We show that it can be exploited as an efficient way to explore the topology of unknown phase diagrams where the supervision is entirely delegated to the machine.

TT 45: Frontiers of Electronic-Structure Theory: Focus on the Interface Challenge VI (joint session O/DS/CPP/TT)

Time: Wednesday 15:00–17:45 Location: H9

TT 45.1 Wed 15:00 H9

First-principles quantum transport simulations including strong correlation effects — •Andrea Droghetti[1], Wilhelm Appelt[2], Liviu Chioncel[2], Milos Radonjić[3], Enrique Muñoz[4], Stefan Kirchner[5], David Jacob[1], Dieter Vollhardt[2], Angel Rubio[6], and Ivan Rungger[7] — [1]University of the Basque Country (Spain) — [2]University of Augsburg (Germany) — [3]University of Belgrade (Serbia) — [4]Pontificia Universidad Católica de Chile — [5]Zhejiang University (China) — [6]Max Planck Institute for the Structure and Dynamics of Matter (Germany) — [7]National Physical Laboratory (UK)

When magnetic molecules are brought into contact with metals the electron-electron interaction leads to the appearance of the correlated Kondo state. In this talk we will present the results of first-principles calculations for the electronic structure and the linear-response conductance of radical molecules adsorbed on metallic surfaces in the Kondo regime [Phys. Rev. B 95, 085131 (2017), Nanoscale 10, 17738 (2018)]. In particular we will outline the methodological approach as implemented in the Smeagol electron transport code and we will benchmark the results against experiments. The method relies in the first place on the combination of Density Functional Theory with the Green's functions technique. We will explain how a molecular devices is projected onto an effective Anderson impurity problem, which is then solved either by continuum time quantum Monte Carlo or numerical renormalization group. Finally, we will describe some work-in-progress aimed at computing transport properties beyond linear-response.

TT 45.2 Wed 15:15 H9

Density functional theory for transport through correlated systems — •Stefan Kurth — Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — Donostia International Physics Center DIPC, San Sebastian, Spain

A recently proposed density functional formalism to describe electronic transport through correlated systems in the steady state uses both the density on the junction and the steady current as basic variables. The corresponding Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias, which are universal functionals of the basic variables.

A recent parametrization of the xc potentials for the single-impurity Anderson model correctly incorporates both the Kondo and Coulomb blockade regimes. It allows for calculation of currents and differential conductances at arbitrary bias and temperature at negligible numerical cost but with the accuracy of sophisticated renormalization group methods. A time-local version of this functional is used to study the Anderson model under the influence of both DC and AC biases. We observe interaction-induced shifts of the photon-assisted conductance peaks, supression of the Kondo plateau at zero temperature and lifting of Coulomb blockade at finite temperature.

TT 45.3 Wed 15:30 H9

Exact factorization of the many-electron wave function — •Camilla Pellegrini[1], Antonio Sanna[1], and Eberhard K. U. Gross[1,2] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — [2]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

The exact factorization approach [1], originally developed for a system of electrons and nuclei, is extended to a system of electrons only. This allows for a two-particle Schroedinger equation, which uniquely defines the exact effective interaction between two electrons in the medium. This interaction differs from the effective interaction, W, used in many-body Green's function techniques. In particular, it is spin-dependent. We illustrate the formalism for the simplest case of exchange interactions only.

[1] A. Abedi, N.T. Maitra, E.K.U. Gross, PRL 105, 123002 (2010).

TT 45.4 Wed 15:45 H9

Many-body spectral functions from steady state density functional theory — •David Jacob[1,2] and Stefan Kurth[1,2,3] — [1]Dpto. de Física de Materiales, Universidad del País Vasco UPV/EHU, San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]DIPC, San Sebastián, Spain

We present a scheme to extract the true many-body spectral function of an interacting many-electron system from an equilibrium density functional theory (DFT) calculation [1]. To this end we devise an ideal STM-like setup and employ the recently proposed steady-state DFT formalism (i-DFT) which allows to calculate the steady current through a nanoscopic region coupled to two biased electrodes [2]. In our setup one of the electrodes serves as a probe ("STM tip"). In the ideal STM limit of vanishing coupling to the tip, the system to be probed is in quasi-equilibrium with the "substrate" and the normalized differential conductance yields the exact equilibrium many-body spectral function. Moreover, from the i-DFT equations we derive an exact relationship which expresses the interacting spectral function in terms of the Kohn-Sham one. Making use of i-DFT xc functionals that capture Coulomb blockade as well as Kondo physics, the method yields spectral functions for Anderson impurity models in good agreement with NRG calculations. It is thus possible to calculate spectral functions of interacting many-electron systems at the cost of an equilibrium DFT calculation.

References: [1] D. Jacob and S. Kurth, Nano Lett. **18**, 2086 (2018) [2] G. Stefanucci and S. Kurth, Nano Lett. **15**, 8020 (2015)

TT 45.5 Wed 16:00 H9

Magnetic phase transitions induced by pressure and magnetic field: the case of antiferromagnetic USb2 — •Leonid Sandratskii — Max Planck Institute of Microstructure Physics, Halle, Germany

Fascinating phenomena observed under applied pressure and magnetic field are currently attracting much research attention. Recent experiments have shown that application of the pressure or magnetic field to the USb2 compound induce the transformations of the ground-state antiferromagnetic (AFM) up-down-down-up structure to, respectively, ferromagnetic (FM) or ferrimagnetic configurations. Remarkably, the magnetic critical temperature of the FM state, induced by pressure, is more than two times smaller than the Neel temperature of the ground state. We performed density-functional theory (DFT) and DFT+U studies to reveal the origin of the unusual magnetic ground-state of the system and the driving mechanisms of the phase transitions. We investigate both the magnetic anisotropy properties and the parameters of the interatomic exchange interactions. To study pressure-induced effects we carry out calculations for reduced volume and demonstrate that the AFM-FM phase transformation indeed takes place but depends crucially on the peculiar features of the magnetic anisotropy. We also explain why the magnetic field that couples directly to the magnetic moments of atoms leads to the phase transition to the ferrimagnetic state whereas the pressure that does not couple directly to magnetic moments results in the FM structure.

TT 45.6 Wed 16:15 H9

Charge localization at a weakly coupled molecule-metal system studied by linear expansion Δ-self-consistent field density-functional theory (ΔSCF-DFT) — •Hadi H. Arefi[1,2], Daniel Corken[3], Reinhard Maurer[3], F. Stefan Tautz[1,2], and Christian Wagner[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology — [3]Department of Chemistry, University of Warwick, Coventry, United Kingdom

Predicting the charge arrangements at the interface between molecules and metals represents a formidable challenge for semi-local approximations to Density Functional Theory (DFT). This could become even more critical when molecules are only weakly coupled to the metal. Single-molecular devices based on such weak coupling have recently been created by molecular manipulation with a scanning probe microscope (SPM), where a single PTCDA (perylene-tetracarboxylic dianhydride) molecule was placed in a free-standing upright configuration either on a SPM tip [1] or on a pedestal of two adatoms on the Ag(111) surface [2]. There are indications that the mechanism stabilizing these unexpected configurations is linked to an integer charge transfer creating a singly occupied molecular orbital. We use the ΔSCF-DFT method [3] to confine charge on the LUMO of the PTCDA and study the consequences with vdW-corrected DFT.

[1] C. Wagner et al. Phys. Rev. Lett. 115, 026101 (2015) [2] T. Esat et al. Nature 558, 573 (2018) [3] R. J Maurer, K. Reuter, JCP 139, 014708 (2013)

TT 45.7 Wed 16:30 H9

Dispersion corrected density functional theory studies on PVDF/hydrated aluminium nitrate composite system — •Ranjini Sarkar and Tarun Kundu — Indian Institute of Technology, Kharagpur

Electro-active polymer Polyvinylidene fluoride (PVDF) based ferroelectric composites have gained significant technological importance over conventional ceramic ferroelectrics. This article provides quantum chemical description of PVDF/ hydrated aluminium nitrate salt composite system in the light of density functional theory. Four monomer units of pristine α and β-PVDF, pure Al(NO3)3.9H2O, and PVDF/ Al(NO3)3.9H2O structures are optimized using dispersion corrected exchange correlation functional B3LYP-D and 6-311+G(d,p) basis set. Similar to the experimental findings, the current theoretical investigation also suggests that hydrogen bond interaction between PVDF and the hydrated salt molecule plays the major role for the enhancement of ferroelectric properties in this composite system. Non-covalent interaction phenomenon is elucidated on the basis of natural bond orbital analysis, Bader's quantum theory of atoms in molecules and reduced density gradient analysis. Chemical Reactivity and charge transfer mechanisms are explained using atomic-dipole corrected Hirshfeld population analysis, molecular electrostatic potential plot and frontier molecular orbital analyses, respectively.

TT 45.8 Wed 16:45 H9

Band-structure effects in vertical layered material heterostructures — •Nicholas D. M. Hine[1], Gabriel C. Constantinescu[2], Nelson Yeung[1], Siow-Mean Loh[1], José María Escartín[2], Cuauhtemoc Salazar Gonzalez[1], and Neil R. Wilson[1] — [1]Department of Physics, University of Warwick, United Kingdom — [2]Cavendish Laboratory, University of Cambridge, 19 JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom

Controlling the properties of layered material heterostructures is crucial to the success of devices based on the novel capabilities of 2D

materials, yet theoretical insight has been limited by the large system sizes required to study rotated, incommensurate interfaces. We use linear-scaling DFT calculations with non-local vdW functionals to explore large-scale models of heterostructures of interest for device applications. Results will be presented for heterostructures including MoS2/MoSe2, MoSe2/WSe2, and other Transition Metal Dichalcogenide pairings, TMDCs with graphene and hBN substrates, and hBN/Phosphorene. Band-structure changes caused by stacking and rotation of the layers are obtained by unfolding the supercell spectral function into the primitive cells, incorporating spin-orbit coupling. Changes in spectral weight and band-structure between the monolayers and heterostructured interfaces show how lattice mismatch (MoS2/MoSe2) or spacer layers (Phosphorene/hBN/Phosphorene) can allow the component monolayers to retain more independence in heterostructures than in homo-stacks. Finally, applying electric fields allows the behaviour of gated structures to be predicted and explained.

TT 45.9 Wed 17:00 H9

Global Trends in Calcium-Silicate-Hydrate Phases Identified by Infrared Spectroscopy and Density Functional Theory — •Mohammadreza Izadifar, Franz Königer, Andreas Gerdes, Christof Wöll, and Peter Thissen — Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Building and construction industry are at the same time the backbone and the driving force of our modern society. Nearly all our today's technical infrastructure is based on cement-based materials. Detailed, spectroscopic investigations of model reactions on well-defined mineral substrates under UHV-conditions are largely lacking, thus prohibiting a validation of theoretical methods. Eight different Calcium-Silicate-Hydrate (CSH) phases, namely Tobermorite 14Å, Tobermorite 11Å, and Tobermorite 9Å, Wollastonite, Jaffeite, Jennite, γ-C2S, and α-C2SH, are calculated with the help of Density Functional Theory using the Vienna ab initio simulation package (VASP). First, we take care of the mechanical properties of the material. Our results revealed that Jaffeite, γ-C2S, and α-C2SH have a linear bulk modulus due to the monomer structure of silicate tetrahedra. Tobermorite 14Å and Jaffeite have the lowest and highest bulk modulus, respectively. In the second part, the optimized geometries allow for the precise calculations vibrational eigenmodes and frequencies by the force-constant (FC) approach. The proportions of C/S and H/C are major criteria for the classification of the calculated wavenumber of ν(Si-O) for all phases in our model system.

TT 45.10 Wed 17:15 H9

Origin of carbon 1s binding energy shifts in amorphous carbon materials — •Michael Walter[1,4,5], Filippo Mangolini[2], Robert W. Carpick[3], and Michael Moseler[4,5] — [1]FIT, University of Freiburg, Germany — [2]University of Texas at Austin, USA — [3]University of Pennsylvania, USA — [4]Fraunhofer IWM, Freiburg, Germany — [5]Physikalisches Institut, Universität Freiburg, Germany

The quantitative evaluation of the carbon hybridization state by X-ray photoelectron spectroscopy (XPS) has been a surface-analysis problem for the last three decades due to the challenges associated with the unambiguous identification of the characteristic binding energy values of sp^2- and sp^3-bonded carbon. Here, we compute the binding energy values for model structures of various carbon allotropes, including graphite, diamond, doped-diamond, and amorphous carbon (a-C), using density functional theory (DFT). The large band-gap of diamond allows defects to pin the Fermi level, which results in large variations of the C(1s) core electron energies for sp^3-bonded carbon, in agreement with the large spread of experimental C(1s) binding energy values for sp^3 carbon. In case of hydrogen-free a-C, the C(1s) core electron binding energy for sp^3 carbon atoms is approximately 1 eV higher than the binding energy for sp^2-hybridized carbon. However, the introduction of hydrogen hinders the unambiguous quantification of the carbon hybridization state on the basis of C(1s) XPS alone. This work can assist surface scientists in the use of XPS for the accurate characterization of carbon-based materials.

TT 45.11 Wed 17:30 H9

Mechanically tuned conductivity of graphene grain boundaries from first-principles calculations — Delwin Perera, •Jochen Rohrer, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Nanocrystalline graphene has recently been shown to have a strong piezoresistivity and strain gauge factors that are notably higher compared to single- or microcrystalline graphene [1]. The origin of the enhanced piezoresistivity in nanocrystalline graphene is still not fully understood, but several theoretical works suggest that grain boundaries are the main cause as these can evoke transport gaps.

In our work we test this assumption with density functional theory based transport calculations of graphene bicrystals. In particular, we extend our analysis of the interplay between grain boundary structure and transport properties [2] by including mechanical strain. We compute transmission functions and current-voltage curves and compare them with tight binding calculations. Our findings suggest that the strain-induced transport gap modulation can be fully described by the response of the bulk graphene band structure towards strain.

[1] Riaz *et al.*, Nanotechnology **26**, 325202 (2015)
[2] Perera *et al.*, Phys. Rev. B **98**, 155432 (2018)

TT 46: Quantum Dots, Quantum Wires, Point Contacts

Time: Wednesday 15:00–18:30 Location: H22

TT 46.1 Wed 15:00 H22

Spectral and transport properties of superconducting quantum dots — •Vladislav Pokorný[1] and Martin Žonda[2] — [1]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 18221 Praha, Czech Republic — [2]Institute of Physics, Albert Ludwig University of Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany

We study the effects of electron correlations on a system consisting of one or two single-level quantum dots attached to superconducting leads. We use the superconducting Anderson impurity model to study the system and solve it using the self-consistent, second-order perturbation theory method as well as the hybridization-expansion, continuous-time quantum Monte Carlo (CT-HYB) and the numerical renormalization group (NRG). We study the behavior of the Andreev subgap states, the Josephson current and the fate of the zero-pi (singlet-doublet) quantum phase transition and compare the results of different methods, setting the limits of their reliability in various regimes.

TT 46.2 Wed 15:15 H22

Enhancing entanglement by spin manipulation in Cooper pair splitters — •Ciprian Padurariu[1], Jami Rönkkö[2], Michael V. Moskalets[3], and Christian Flindt[2] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, 89069 Ulm, Germany — [2]Department of Applied Physics, Aalto University, 00076 Aalto, Finland — [3]Department of Metal and Semiconductor Physics, NTU Kharkiv Polytechnic Institute, 61002 Kharkiv, Ukraine

We study a Cooper pair splitter device consisting of two single level quantum dots fabricated in a strong spin-orbit coupling material (such as InAs or InSb) and coupled to a superconductor. The combined presence of spin-orbit coupling and Zeeman field gives rise to a finite probability of Cooper pair tunneling accompanied by spin flip, thereby involving the spin-triplet states of the doubly occupied dots.

We show that the population of triplet states leads to the spin blockade of Cooper pair tunneling. The blockade is advantageous for entanglement production if Cooper pair tunneling is resonant, when the blockaded electrons are in a fully entangled spin state. The entangled state is a superposition of singlet and triplet Bell states.

We propose two detection schemes, the first based on conventional transport spectroscopy and a second, based on charge detectors, [1] suitable for future devices capable of producing on-demand spin-entangled pairs.

[1] N. Walldorf, C. Padurariu, A.-P. Jauho, and C. Flindt, Phys. Rev. Lett. **120**, 087701 (2018).

TT 46.3 Wed 15:30 H22

Phase-dependent heat and charge transport through

superconductor-quantum dot hybrids. — •Mathias Kamp and Björn Sothmann — Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany

In the context of modern electronics, it becomes increasingly important to understand and control heat transport in nanostructures. So far, there has been a great activity on phase-coherent heat transport in superconducting tunnel junctions. Here, we consider heat transport through superconductor-quantum dot hybrids [1]. We evaluate heat and charge currents via a real-time diagrammatic technique which allows us to treat strong Coulomb interactions in a nonequilibrium system. We find a finite thermoelectric effect due to the proximity effect which surprisingly persist even at the particle-hole symmetric point. Furthermore the system can act as an efficient thermal diode.
[1] M. Kamp, B. Sothmann, arXiv 1809.09428 (2018)

TT 46.4 Wed 15:45 H22

Nonlocal heat transfer between resonators by splitting Cooper pairs — •Mattia Mantovani[1], Gianluca Rastelli[1,2], Wolfgang Belzig[1], and Robert Hussein[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Zukunftskolleg, Universität Konstanz, D-78457 Konstanz, Germany

Hybrid quantum dot-superconductor and quantum dot-oscillator systems have become attractive platforms to inspect quantum coherence effects and heat transport at the nanoscale [1,2]. Here, we investigate a Cooper-pair splitter setup [3] consisting of two quantum dots, each coupled capacitively to a local oscillator. The latter can be represented either by a microwave cavity or a nanomechanical resonator. Focusing on the subgap regime, we demonstrate that cross-Andreev reflection, through which Cooper pairs are split into both dots, generates nonlocal heat transfer between the two oscillators. The proposed scheme can then act as an efficient heat-pump device. Our findings have interesting potential applications for nanomechanical systems and energy harvesting with quantum dot systems [4].
[1] P. Stadler, *et al.*, Phys. Rev. Lett. **117**, 197202 (2016).
[2] R. Hussein, *et al.*, arXiv:1806.04569 (2018).
[3] R. Hussein, *et al.*, Phys. Rev. B **94**, 235134 (2016).
[4] B. Sothmann, *et al.*, Nanotechnology **26**, 032001 (2015).

TT 46.5 Wed 16:00 H22

Phase-coherent heat circulator based on multiterminal Josephson junctions — •Sun-Yong Hwang[1], Francesco Giazotto[2], and Björn Sothmann[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany — [2]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Piazza San Silvestro 12, 56127 Pisa, Italy

We propose a phase-coherent thermal circulator based on ballistic multiterminal Josephson junctions. The breaking of time-reversal symmetry by either a magnetic flux or a superconducting phase bias allows heat to flow preferentially in one direction from one terminal to the next while heat flow in the opposite direction is suppressed. We find that our device can achieve a high circulation efficiency over a wide range of parameters and that its performance is robust with respect to the presence of disorder. We provide estimates for the expected heat currents for realistic samples.

TT 46.6 Wed 16:15 H22

An integrable multi-channel sine-Gordon model with Josephson circuits — •Ananda Roy[1,2] and Hubert Saleur[1] — [1]Institut de Physique Theorique, CEA-Saclay — [2]Institute for Quatum Information, RWTH Aachen University

Integrable field theories have always fascinated physicists. In particular, those which describe quantum impurity problems have been of much interest to both theorists and experimentalists. A prominent example is the boundary sine-Gordon (bSG) field theory. The latter describes a Luttinger liquid in the presence of an impurity. In this work, we propose an experimentally realizable, multi-channel generalization of the bSG model. We establish the classical and quantum integrability of the model by constructing a corresponding integrable bulk theory. We provide the first nontrivial conserved current of the bulk theory. Subsequently, we postulate the factorized scattering matrix describing the bulk theory and verify it using Bethe Ansatz computation of the ground state energy. Subsequently, we provide the factorized scattering matrix of the boundary field theory. Thermodynamic properties of both the bulk and boundary model are computed using the Thermodynamic Bethe Ansatz. Finally, we propose an experimental realization of the model with superconducting circuits, making use of the robust, tunable and dispersive Josephson nonlinearity. Our proposal can be realized with state-of-the-art system parameters.

TT 46.7 Wed 16:30 H22

Manipulation of non-linear heat currents in the dissipative Anderson-Holstein model — •Bitan De[1] and Bhaskaran Muralidharan[2] — [1]Indian Institute of Technology, Bombay — [2]Indian Institute of Technology, Bombay

The anomalous behavior of electron induced phonon transport is investigated using an *Anderson-Holstein* based dissipative quantum dot setup under two relevant bias situations: (a) a voltage bias in the absence of an electronic temperature gradient and (b) an electronic temperature gradient at zero voltage. It is shown that the direction of phonon transport in the non-linear regime is different in the two cases since the first case facilitates the accumulation of phonons in the dot and the second case leads to the absorption of phonons in the dot. In the linear regime, both the phonon and electronic transport get decoupled and Onsager's symmetry is verified. We explain the observed cumulative effects of voltage and electronic temperature gradients on the non-linear phonon currents by introducing a new transport coefficient that we term as the electron-induced phonon thermal conductivity. It is demonstrated that under suitable operating conditions in Case (a) the dot can pump in phonons into the hotter phonon reservoirs and in Case (b) the dot can extract phonons out of the colder phonon reservoirs. Finally, we elaborate on how the non-linear electronic heat current can be stimulated and controlled by engineering the temperature of the phonon reservoirs even under vanishing effective electron flow.

15 min. break.

TT 46.8 Wed 17:00 H22

Resonant transport through interacting proximitized quantum dots — •Stephan Weiss and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

For a single level quantum dot that is resonantly coupled to a normal and a superconducting metal, we have calculated the current voltage characteristics. Numerically exact results are obtained within the iterative summation of path integrals (ISPI) [1] scheme. It builds upon the truncation of exponentially vanishing real-time correlations at finite temperature and/or bias voltage. Thereafter, the calculation of emerging partial spin traces along the Keldysh contour are performed in an iterative manner. Within the quantum regime, i.e. if there is no small parameter, ISPI calculations are performed to deduce the impact of Coulomb interactions, change of temperature, as well as gate voltage on the Andreev bound state spectrum for finite gap parameter Δ in a nonequilibrium situation.
[1] S. Weiss, et. al, Phys. Status Solidi B, **250** (11), 2298-2314 (2013).
[2] S. Weiss and J. König, in preparation (2018).

TT 46.9 Wed 17:15 H22

Resonant tunneling through interacting quantum-dot spin valves - ISPI results — •Simon Mundinar, Jürgen König, and Stephan Weiss — Theoretische Physik, Universität Duisburg-Essen and CENIDE, Lotharstr. 1, 47048 Duisburg

We study an interacting quantum dot coupled resonantly to ferromagnetic leads that induce spin-dependent tunneling. Starting with a real-time path integral approach expectation values of interest in the stationary limit are obtained from functional derivatives of the Keldysh partition function. Interactions are decoupled via a Hubbard-Stratonovich transformation which results in a discrete spin trace along the Keldysh contour. This trace is performed by means of iterative summation of path integrals (ISPI) [1], which is based on the truncation of lead-induced correlations after a characteristic memory time. Within this scheme we explore current-based observables and the density matrix for different system parameters, such as temperature, gate/bias voltage, polarization and Coulomb interaction strength. We tune parameters of interest beyond the perturbative regime. Especially in the low-temperature regime we find a strong impact of resonant tunneling processes on transport properties through quantum dot, leading to a rich structure in the tunnel magnetoresistance.
[1] S. Weiss, R. Hützen, D. Becker, J. Eckel, R. Egger, and M. Thorwart, Phys. Status Solidi B **250**, 2298-2314 (2013)
[2] S. Mundinar, J. König, S. Weiss *in preperation*

TT 46.10 Wed 17:30 H22

Interference effects in the cotunnelling transport regime — •Christoph Rohrmeier, Milena Grifoni, and Andrea Donarini — Institute of Theoretical Physics University of Regensburg, Regensburg, Germany

Interference, being intimately related to the superposition principle, plays a central role in quantum mechanics. I will report on interference effects in the transport characteristics of interacting systems in the cotunnelling regime. Particular emphasis will be given to quantum dot molecules exhibiting a quasi-degenerate spectrum. The method of choice for studying the transport characteristics is the Liouville approach. To this end, we systematically include coherences, essential to capture consistently interference effects and solve a generalized master equation for the reduced density matrix up to the fourth perturbative order in the coupling to the leads. Experimental fingerprints of such many-body quantum interference have been reported in semiconductor [1, 2] as well as in carbon nanotube based quantum dots [3]. These interacting systems certainly represents suitable candidates of experimental validation of our theory.

[1] C. Payette, et al., Phys. Rev. Lett. **102** , 026808 (2009);
[2] O. Karlström et al., Phys. Rev. B **83** , 205412 (2011);
[3] A. Donarini et al., arXiv:1804.02234, accepted for publication in Nat. Comm.

TT 46.11 Wed 17:45 H22

Feynman-Vernon approach to transport in interacting quantum dots beyond the weak tunneling regime — •Luca Magazzù and Milena Grifoni — Universität Regensburg, Regensburg, Germany

Quantum transport setups based on quantum dots display a rich variety of transport regimes, also involving exquisitely many-body phenomena (e.g. the Kondo effect), that arise by varying the relative magnitude of intra-dot interactions and tunnel coupling to the electronic reservoirs (leads). Despite the large variety of available approximation schemes, a unique framework enabling one to satisfactorily address this complexity is still missing.

In this work we discuss a path integral approach to transport where the trace over the leads degrees of freedom is performed exactly. As a result, formally exact expressions for the dot dynamics and the current are obtained, where the effect of the coupling to the leads is encapsulated in the Feynman-Vernon influence functional, a functional of the Grassmann-valued paths of the dot variables. In the presence of interactions, the path integral is not exactly solvable. Nevertheless, expansion of the influence functional in the number of tunneling events, in conjunction with a convenient parametrization of the paths allowed by properties of the Grassmann variables, provides a diagrammatic representation of the dynamics and offers an efficient means to systematically sum diagram classes. We propose a resummation which recovers results known from the nonperturbative resonant tunneling and second order von Neumann approximations and beyond.

TT 46.12 Wed 18:00 H22

Coherent long-range transfer of two-electron states in ac driven triple quantum dots — •Jordi Picó-Cortés[1,2], Fernando Gallego-Marcos[2], and Gloria Platero[2] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Instituto de Ciencia de Materiales de Madrid (CSIC), E-28049, Madrid, Spain

Since the proposal by Cirac and Zoller to use photons for quantum state transfer between atoms located at spatially-separated nodes of a quantum network [1], different works have explored how to transfer quantum states. In our work [2] we propose a protocol to prepare a state in the left and center quantum dots of a triple dot array and transfer it directly to the center and right dots. Initially the state in the left and center dots is prepared combining the exchange interaction and magnetic field gradients. Once in the desired state, ac gate voltages in the outer dots are switched on, allowing to select a given photoassisted long-range path and to transfer the prepared state directly from one edge to the other with high fidelity. We investigate the effect of charge noise on the protocol and propose a configuration in which the transfer can be performed with high fidelity. Our proposal can be experimentally implemented and is a promising avenue for transferring quantum states between two spatially separated two-level systems.

[1] J. I. Cirac, P. Zoller, H. J. Kimble, H. Mabuchi, Phys. Rev. Lett. 78, 3221 (1997)
[2] J. Picó-Cortés, F. Gallego-Marcos, G. Platero, arXiv:1810.06517 (2018)

TT 46.13 Wed 18:15 H22

Improved quantum transport calculations using the Numerical Renormalization Group — •Emma L. Minarelli and Andrew K. Mitchell — School of Physics, University College Dublin, Belfield, Dublin 4, Dublin, Ireland

Generalized quantum transport calculations, involving a mesoscopic interacting region coupled two or more leads, are essential to understand the properties and potential applications of the new generation of complex nanoelectronic devices, including semiconductor quantum dot systems and single-molecule transistors. Within linear response, the Numerical Renormalization Group (NRG) is arguably the numerical method of choice, when combined with standard techniques for quantum transport such as Kubo and Meir-Wingreen. However, these methods have practical limitations, as discussed in this talk. We describe some alternative formulations for charge and heat transport calculations within NRG, and demonstrate dramatically improved numerical accuracy over standard methods.

TT 47: Quantum Magnets, Molecular Magnets and Skyrmions

Time: Wednesday 15:00–18:45 Location: H23

TT 47.1 Wed 15:00 H23

Electric field control of magnonic heat flow — •Benjamin Köhler and Wolfram Brenig — Institut für Theoretische Physik, Technische Universität Braunschweig, Germany

Insulating quantum magnets allow for genuine spin transport phenomena without carrier dynamics. Here we study the thermal conductivity of a two dimensional square lattice spin-1/2 Heisenberg antiferromagnet in the presence of a spatially confined, external electric field. The latter is used to alter the Dzyaloshinskii-Moriya interaction and hence the spin canting which controls the heat flow.

Using linear spin wave theory and a Kubo approach we evaluate the thermal conductivity taking into account current relaxation via intrinsic magnon-phonon scattering for finite fields and temperature. Semi-quantitative estimates for attainable variations of the heat conductivity in realistic materials will be presented as a function of the temperature, the external fields, and the size of the region the field is applied to.

TT 47.2 Wed 15:15 H23

NMR of the two-dimensional $S = 1/2$ Heisenberg antiferromagnet CuPOF — •D. Dmytriieva[1,2], Z. T. Zhang[1], M. Uhlarz[1], C. P. Landee[3], J. Wosnitza[1,2], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Clark University, Worcester, Massachusetts, USA

The metal-organic compound $[Cu(pz)_2(2\text{-}OHpy)_2](PF_6)_2$ (CuPOF) is a molecular-based analog of the two-dimensional square-lattice quantum $S = \frac{1}{2}$ Heisenberg antiferromagnet with well-isolated Cu(pz) layers and a very low $k_B T_N/J = 0.21$ ratio ($J/k_B = 6.8$ K, $T_N = 1.38$ K). We present a focus study of the low-T phase transition to long-range order, performed via ^{1}H and ^{31}P nuclear magnetic resonance (NMR) and high-field magnetometry. The very good agreement between the measured high-field magnetization and QMC simulations indicates an exceptional two-dimensionality of CuPOF, with an estimated ratio of the intra- to inter-plane exchange energies of $J'/J \propto 10^{-4}$. Within the ordered state, a splitting of the ^{1}H NMR spectra reveals commensurate AF order, presumably of checkerboard type. A strong increase of T_N in applied magnetic fields furthermore manifests the low dimensionality of CuPOF. A detailed analysis of the uniform magnetization and the ^{31}P nuclear spin-lattice relaxation rate $1/T_1$ reveals an easy-plane anisotropy and a crossover from isotropic to XY behavior. Moreover,

approaching the phase transition, the ^{31}P relaxation rate indicates an exponential growth of the average inter-spin correlation length.

TT 47.3 Wed 15:30 H23

HF-EPR study on the exchange couplings in 3*d*-4*f* heterometallic complexes — •Changhyun Koo[1], Arne Bahr[1], Sebastian Schmidt[2], Yan Peng[2], Ahmed Naushad[3], Maheswaran Shanmugam[3], Annie K. Powell[2], and Rüdiger Klingeler[1,4] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Department of Chemistry, Indian Institute of Technology, Mumbai, India — [4]Center for Advanced Materials, Heidelberg University, Heidelberg, Germany

3*d*-4*f* heterometallic complexes are suggested to enhance the magnetic anisotropy barrier in metal-organic coordination complexes. Though magnetic exchange coupling between 3*d* and 4*f* ions is essential, its quantitative determination by conventional magnetometry remains challenging. Our high-frequency electron paramagnetic resonance (HF-EPR) studies enable to determine the precise values of 3*d*-4*f* exchange interaction (J_{3d-4f}) as well as anisotropy of the 3*d*-ions. The EPR data, analyzed in terms of a Hamiltonian involving the Ising-spin concept for Ln ions, enable to derive information on the ground state and J_{3d-4f} in the complexes. The results on several series of complexes, i.e., $[Fe_4^{III}Ln_2^{III}(Htea)_4(\mu\text{-}N_3)_4(N_3)_3(piv)_3]$, $[Ni_2^{II}Ln_2^{III}(CH_3CO_2)_3(HL)_4(H_2O)_2](NO_3)_3$ (Ln = Tb, Dy, Ho, Yb, and Gd), and $[Co_2^{II}Dy_2^{III}(L)_4(NO_3)_2X$ (X = $(MeOH)_2$ and $(DMF)_2$]) will be presented and general conclusions about magneto-structural correlations will be drawn which suggest routes to optimizing ferromagnetic J_{3d-4f}.

TT 47.4 Wed 15:45 H23

High-frequency EPR studies on 3*d*-4*f* heterometallic complexes — •Arne Bahr[1], Changhyun Koo[1], Ahmed Naushad[2], Maheswaran Shanmugam[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — [2]Department of Chemistry, Indian Institute of Technology Mumbai

In the single molecular magnets (SMMs) research field, 3*d*-4*f* heterometallic complexes are expected as a solution to enhance the anisotropy barrier with the strong exchange interaction between 3*d* and 4*f* ions. Recently synthesized $[Ni_2^{II}Ln_2^{III}(CH_3CO_2)_3(HL)_4(H_2O)_2](NO_3)_3$ (Ln = Tb, Dy, Ho, and Yb) complexes, and a NiGd complex are studied by means of high frequency electron parmagnetic resonance (HF-EPR) measurments. The overall behaviour in specra for the complexes is largely dependent on the Ni-Ln and relatively weak Ln-Ln interaction. The resonance branches within the EPR spectra provide information of the *g*-values as a slope and the zero field splitting. Based on the observed EPR data, the ground states and the magnetic coupling between 3*d* and 4*f* ions of complexes will be discussed.

TT 47.5 Wed 16:00 H23

Anisotropy in Mn_2- and Co-complexes studied by high-frequency EPR spectroscopy — •Lena Spillecke[1], Changhyun Koo[1], Sajedeh Shahbazi[1], Marcel Patrick Merkel[2], Sebastian Schmidt[2], Annie K. Powell[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — [2]Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany

We present high-frequency/high-field electron paramagnetic resonance (HF-EPR) and static magnetisation studies on a Mn-($[TBA]_2[Mn_2^{III}Mo_4^{VI}(\mu_2\text{-}O)_6(Ot)_8(HTea)_2]$) and a Co-$Cl_2$ metal-organic coordination complex. Magnetic susceptibility of the Mn_2-complex indicates weak ferromagnetic exchange interaction between the octahedrally coordinated Mn^{3+} ions, $S = 2$. A strong anisotropy is suggested by a zero-field splitting (ZFS) of about $\Delta = 300$ GHz observed in HF-EPR data. For the Co-monomer, our data imply high-spin Co^{2+} which is presumingly antiferromagnetically coupled to a radical in the ligand-shell, hence forming an $S = 1$ ground state. Based on the measured ZFS and *g*-factor as well as the temperature dependence of the linewidth, the potential of the Co-complex as single molecular magnets is discussed.

TT 47.6 Wed 16:15 H23

Coupled dynamics of long-range and internal spin cluster order in Cu_2OSeO_3 — •Rolf B. Versteeg[1], Jingyi Zhu[1], Christoph Boguschewski[1], Fumiya Sekiguchi[1], Anuja Sahasrabudhe[1], Kestutis Budzinauskas[1], Petra Becker[2], Daniel I. Khomskii[1], and Paul H.M. van Loosdrecht[1] — [1]University of Cologne, Institute of Physics 2, Zülpicher Straße 77, D-50937 Cologne — [2]University of Cologne, Institute of Geology and Mineralogy, Zülpicher Straße 49b, D-50674 Cologne

Quantum materials with multiple length scales for electronic interactions lead to the self-organization of long-range ordered "molecules" of charge, spin, and orbital nature. The order to disorder phase transition pathways in such quantum materials comprises disordering of both the order inside the individual molecules or "clusters", as well as the emerging long-range order.

Here, we reveal optically induced dual order parameter dynamics in the cluster magnet Cu_2OSeO_3 (Ref. [1,2,3]) using time-resolved spontaneous Raman spectroscopy. (Ref. [4]) Multiple ps-decade spin-lattice relaxation dynamics is observed, which evidences a separation of the magnetic order parameter dynamics into disordering of long-range and internal spin cluster order. Our study demonstrates the dual nature of long-range and internal cluster order dynamics in cluster magnets.

[1] S. Seki et al., Science **336**, 198 (2012)
[2] O. Janson et al., Nat. Commun. **5**, 5376 (2014)
[3] R. B. Versteeg et al., Phys. Rev. B **94**, 094409 (2016)
[4] R. B. Versteeg et al., Struct. Dyn. **5**, 044301 (2018)

TT 47.7 Wed 16:30 H23

Strong influence of 'bystanders' on the exchange in edge-shared Cu-O chain compounds — •Helge Rosner[1], Dijana Milosavljevic[1], Jan Tomczak[2], Stefan-Ludwig Drechsler[3], and Oleg Janson[3] — [1]MPI CPfS Dresden, Germany — [2]TU Wien, Austria — [3]IFW Dresden, Germany

The influence of the structural features like bond angles and distances on the exchange integrals in cuprate materials has been studied in detail for many years. One of the dominating structural features is the Cu-O-Cu bond angle in chain-like compounds. However, similarly strong influence on the exchange couplings by side groups was observed recently. As an example, we analyse the origin of the huge difference $\delta_{J1} \sim 200$ K for the nearest neighbour exchange in Li_2CuO_2 and $SiCuO_3$, which have structurally nearly identical CuO_2 chains. For closely related materials, we also demonstrate the strong influence of hydrogen positions in the crystal structure for O-H groups or crystal water on the leading exchange terms, changing from strongly antiferromagnetic to moderately ferromagnetic. We elucidate the underlying microscopic mechanisms based on detailed DFT studies and subsequently derived multi-band tight-binding models. The results widely improve our understanding of magneto-structural correlations in cuprate compounds.

15 min. break.

TT 47.8 Wed 17:00 H23

Quantum tunneling and large coercivity in Fe-doped Li_3N — Manuel Fix[1], Enrique del Barco[2], and •Anton Jesche[1] — [1]EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86135 Augsburg, Germany — [2]Department of Physics, University of Central Florida, Orlando, Florida 32816, USA

The basic magnetic unit in Fe-doped Li_3N is not a cluster or a domain but the magnetic moment of single, isolated Fe ions [1]. This novel model system shows large magnetic anisotropy and allows to study quantum tunneling of the magnetization in a rather simple, inorganic material at liquid helium temperatures.

For small concentrations of roughly 0.1 % Fe, we have found an extreme field-dependence of the magnetic tunneling [2]. Applied *longitudinal* fields lift the ground-state degeneracy and destroy the tunneling condition. The relaxation time increases from $\tau \sim 10^4$ by four orders of magnitude in applied fields of only a few milliTesla, which reveals exceptionally sharp tunneling resonances. In applied *transverse* magnetic fields, on the other hand, the spin-flip probability increases, which proves the resonant character of this tunneling process. Therefore, it is possible either to freeze the orientation or to promote the flip of a spin-state by tiny applied fields.

[1] A. Jesche *et al.*, Nat. Commun. **5**:3333 (2014)
[2] M. Fix, J. H. Atkinson, P. C. Canfield, E. del Barco, A. Jesche, Phys. Rev. Lett. **120**, 147202 (2018)

TT 47.9 Wed 17:15 H23

Spiral ordering in the edge sharing chain cuprate $CuSiO_3$ — •Dijana Milosavljevic[1], Andrei Gippius[2], Michael Baenitz[1],

Stefan-Ludwig Drechsler[3], Oleg Janson[3], Johannes Richter[4], and Helge Rosner[1] — [1]MPI Chemical Physics of Solids, Dresden — [2]Lomonosov Moscow State University — [3]IFW Dresden — [4]MPI Physics of Complex Systems, Dresden

$CuSiO_3$ is spin-1/2 cuprate system isostructural to the famous Spin-Peierls system $CuGeO_3$ [1]. Due to this similarity, the compound was described previously as a quasi one-dimensional $J_1 - J_2$ chain compound with strongly dominating J_2 [2]. Experimentally, the system orders antiferromagnetically at about 8 K with a propagation vector of (1/2 0 1/8) with the structural Cu-O chains running along c [3]. This spiral ordering is inconsistent with the previous parametrisation, motivating a re-investigation of the compound. Re-determining crystal structure and sample composition by synchrotron XRD and applying density functional calculations together with high temperature series expansion, we suggest a new parameter set of exchange couplings that is consistent with all experimental findings. The new magnetic model describes the compound in terms of strongly antiferromagnetically coupled $J_1 - J_2$ chains with a ferromagnetic J_1 of about 35 K and a frustration ratio $\alpha = |J_2/J_1| \sim 0.35$..

[1] H. H. Otto, M. Meibohm, Z. Kristallogr. **214**, 558 (1999)
[2] M. Baenitz et al., Phys. Rev. B **62**, 12201 (2002)
[3] H. Wolfram et al., Phys. Rev. B **69**, 144115 (2004)

TT 47.10 Wed 17:30 H23

Magnon spectrum of the noncollinear antiferromagnet Mn_3Ge — •Aleksandr S. Sukhanov[1,2], Ph. Bourges[3], H. C. Walker[4], M. S. Pavlovskii[5], K. Manna[1], C. Felser[1], and D. S. Inosov[2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [3]Laboratoire Léon Brillouin, CEA-CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette, France — [4]ISIS Facility, STFC, Rutherford Appleton Laboratory,Didcot, Oxfordshire OX11-0QX, United Kingdom — [5]Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia

We discuss the full spin-wave spectrum of the noncollinear antiferromagnet Mn_3Ge obtained using neutron time-of-flight and triple-axis spectroscopy. The sublattice of magnetic ions in hexagonal Mn_3Ge can be viewed as two adjacent kagome layers stacked along the crystallographic [001] axis. Below T_N of 370 K the Mn atoms form the coplanar triangular 120° antiferromagnetic (AFM) order. Our measurements revealed a magnon mode with a spin-wave gap of 5 meV and a very steep anisotropic dispersion. The obtained spectra allows one to build an effective model of magnetic interactions in the system. We found two coupled magnon-phonon excitations seen in the vicinity of the zone center on the energies of 14 meV and 17.5 meV. We argue that this mixed excitations represent a strong magneto-elastic coupling in Mn_3Ge.

TT 47.11 Wed 17:45 H23

Observation of two independent skyrmion phases in a chiral magnet material — •Alfonso Chacon[1], Lukas Heinen[2], Marco Halder[1], Andreas Bauer[1], Wolfgang Simeth[1], Sebastian Mühlbauer[3], Helmuth Berger[4], Markus Garst[5], Achim Rosch[2], and Christian Pfleiderer[1] — [1]Physik Department, Technische Universität München, Garching, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Köln, Germany — [3]Heinz Maier-Leibnitz (MLZ), Technische Universität München, Garching, Germany — [4]École Polytechnique Federale de Laussane, Laussane, Switzerland — [5]Institut für Theoretische Physik, Technische Universität Dresden, Dresden, Germany

Magnetic materials can host skyrmions, which are topologically nontrivial spin textures. In chiral magnets with cubic lattice symmetry, all previously observed skyrmion phases require thermal flucturations to become thermodynamically stable in bulk materials, and therefore exist only at relatively high temperature, close to the helimagnetic transition temperature. Here, we report the identification of a second skyrmion phase in Cu_2OSeO_3 at low temperature and in the presence of an applied magnetic field, from small angle neutron scattering and magnetization measurements. Theoretical modelling provides evidence that the stabilization mechanism is given by well-known cubic anisotropy terms, and accounts for an additional observation of metastable helices tilted away from the applied field. The generic character of the underlying mechanism suggests a new avenue for the discovery, design and manipulation of topological spin textures.

TT 47.12 Wed 18:00 H23

Interaction of Skyrmions and Pearl Vortices in Superconductor-Chiral Ferromagnet Heterostructures — •Samme M. Dahir, Anatoly F. Volkov, and Ilya M. Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

We investigate a hybrid heterostructure with magnetic skyrmions (Sk) inside a chiral ferromagnet interfaced by a thin superconducting film via an insulating barrier. The barrier prevents the electronic transport between the superconductor and the chiral magnet, such that the coupling can only occur through the magnetic fields generated by these materials. We find that Pearl vortices (PV) are generated spontaneously in the superconductor within the skyrmion radius, while anti-Pearl vortices ($\overline{\text{PV}}$) compensating the magnetic moment of the Pearl vortices are generated outside of the Sk radius, forming an energetically stable topological hybrid structure. Finally, we analyze the interplay of skyrmion and vortex lattices and their mutual feedback on each other. In particular, we argue that the size of the skyrmions will be greatly affected by the presence of the vortices offering another prospect of manipulating the skyrmionic size by the proximity to a superconductor.

TT 47.13 Wed 18:15 H23

Tracing domain wall conductivity in the skyrmion-host multiferroic GaV_4S_8 — •Somnath Ghara, Korbinian Geirhos, Peter Lunkenheimer, Vladimir Tsurkan, and István Kézsmárki — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

The lacunar spinel, GaV_4S_8, has attracted tremendous interests due to the presence of Néel-type magnetic skyrmion and its multiferroic properties. It crystallizes in a non-centrosymmetric cubic structure ($F\bar{4}3m$) at room temperature and undergoes a ferroelectric transition at 43 K, reducing the crystal symmetry to rhombohedral ($R3m$). In the rhombohedral state, the crystals usually consist of four types of polar domains, whose populations can be controlled by applying static electric fields while cooling the samples through the rhombohedral transition. To monitor the domain population, we performed pyro- and magnetoelectric polarization, resistivity and magnetization measurements. We found that the single-domain state with high resistance can be realized upon poling, while the resistance in the multi-domain state is several orders of magnitude lower, which imply the presence of highly conductive domain walls.

TT 47.14 Wed 18:30 H23

Winding up quantum spin helices: Avoided level crossing vs. topological protection — •Thore Posske and Michael Thorwart — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

A magnetic helix can be wound into a classical Heisenberg chain by fixing one end while rotating the other one. We show that in quantum Heisenberg chains, the magnetization slips back to the trivial state beyond a finite turning angle. Avoided level crossings thus undermine classical topolog- ical protection. Yet, for special values of the axial Heisenberg anisotropy, stable spin helices form again, which are nonlocally entangled. Away from these sweet spots, spin helices can be stabilized dynamically or by dissipation. For half-integer spin chains of odd length, a spin slippage state and its Kramers partner define a qubit with a non-trivial Berry connection.

TT 48: Focus Session: Direct-Write Nanofabrication and Applications II (Electron Beam Induced Processing) (joint session DS/TT)

Part II: New Approaches & Chemsitry

Organizers:
• Michael Huth, Physikalisches Institut, Goethe-Universität, Frankfurt, Germany
• Harald Plank, FELMI-ZFE, TU Graz, Austria
(Synopsis provided with part I of this session)

Time: Wednesday 15:00–18:00 Location: H32

Invited Talk TT 48.1 Wed 15:00 H32

Fabrication of functional nanostructures by electron and ion beams — •Milos Toth — University of Technology Sydney, Australia

Focused electron and ion beams can be used to restructure/mill materials and initiate surface reactions supplied by gas-phase precursor molecules. The chemical reactions give rise to processes that fall into two broad categories: direct-write lithography and emergent phenomena. The latter include topographic surface patterns defined by the crystal symmetry of the sample and chemical structure of a precursor gas, and self-assembly of complex 3D nanostructures. Here I will review the underlying mechanisms, and applications of the techniques to materials used in optoelectronics, plasmonics and quantum photonics. Specific applications include the fabrication and iterative editing/tuning of plasmonic nanostructures and dielectric optical cavities, site-selective electron beam induced fluorination of surfaces, fabrication of isolated colour centres that act as on-demand single-photon-emitters in 2D hBN, and dynamic SEM studies of the degradation of phosphorene in which an electron beam is used to simultaneously initiate chemical reactions and to image propagating reaction fronts. These applications demonstrate the benefits and shortcomings of ion beam and electron beam techniques in terms resolution, throughput and damage imparted to functional materials by beams comprised of electrons, and Ga, Xe, O and He ions.

TT 48.2 Wed 15:30 H32

Avoiding amorphization in silicon nano structures — •Gregor Hlawacek[1], Xiaomo Xu[1,2], Hans-Jürgen Engelmann[1], Karl-Heinz Heinig[1], Wolfhard Möller[1], Ahmed Gharbi[3], Raluca Tiron[3], Lothar Bischoff[1], Thomas Prüfer[1], Rene Hübner[1], Stefan Facsko[1], and Johannes von Borany[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Faculty of Physics, Technische Universität Dresden, Dresden, Germany — [3]CEA-Leti, Grenoble, France

The usage of ion beam irradiation on vertical nanopillar structures is a prerequisite for fabricating a vertical GAA-SET device. After room temperature irradiation (2×10^{16} ions/cm^2) of nanopillars (with a diameter of 35 nm-50 nm and a height of 70 nm) with either 50 keV broad beam Si^+ or 25 keV focused Ne^+ from a helium ion microscope (HIM), strong plastic deformation has been observed which hinders further device integration. This differs from predictions made by Monte-Carlo based simulations using the program TRI3DYN. To avoid this, ion irradiation at elevated temperatures (up to 672 K) has been performed and no plastic deformation was observed under these conditions. Additionally a pillar diameter reduction by 50% can ab achieved in this way without changing the shape of the pillar.

This work is supported by the European Union's H-2020 research project *IONS4SET* under Grant Agreement No. 688072.

TT 48.3 Wed 15:45 H32

Non-classical Liquid Metal Ion Sources for advanced FIB nano-patterning — •Paul Mazarov[1], Lothar Bischoff[2], Wolfgang Pilz[2], Nico Klingner[2], Achim Nadzeyka[1], Jorg Stodolka[1], and Jacques Gierak[3] — [1]Raith GmbH, Konrad-Adenauer-Allee 8, 44263 Dortmund, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — [3]LPN-CNRS, Route de Nozay, 91460 Marcoussis, France

Focused Ion Beam (FIB) processing has been developed into a well-established and still promising technique for direct patterning and proto-typing on the nm scale. Exploring the Liquid Metal Alloy Ion Sources (LMAIS) potential represents a promising alternative to expand the global FIB application fields. Especially, ion beam nanofabrication as direct, resistless and three-dimensional patterning enables a simultaneous in-situ process control by cross-sectioning and inspection. Thanks to this, nearly half of the elements of the periodic table are made available in the FIB technology as a result of continuous research in this area during the last forty years. Recent developments could make these sources to an alternative technology feasible for nanopatterning challenges. In this contribution the operation principle, the preparation and testing process as well as prospective domains for modern FIB applications will be presented. As an example we will introduce a Ga35Bi60Li5 LMAIS in detail. It enables high resolution imaging with light Li ions and sample modification with Ga or heavy polyatomic Bi clusters, all coming from one ion source.

TT 48.4 Wed 16:00 H32

Opening the Door to New Beam Induced Processing Applications: A Compact and Flexible Gas Injection System — •Andrew Jonathan Smith, Klaus Schock, Andreas Rummel, and Stephan Kleindiek — Kleindiek Nanotechnik, Aspenhaustr. 25, 72770 Reutlingen, Deutschland

A flexible GIS module that can be filled with precursor material by the user is introduced. This module is comprised of a small temperature controlled reservoir, a nozzle, and a motor that actuates a valve. Using a micromanipulator, it is possible to position the GIS nozzle precisely while being able to move it far away from the sample so that it is not an obstacle during other processing/imaging steps.

The reservoir can be loaded with solid or liquid precursor materials. It is also possible to feed gaseous precursors from a source outside of the microscope's vacuum chamber. The gas is then introduced using a precisely controllable needle valve.

This approach allows for a high degree of flexibility in choosing precursor materials. Switching precursors is as simple as exchanging the plug-in module on the MM3A-EM micromanipulator. Also, utilizing multiple GI-Systems for specialized tasks is made easy and cost effective.

Having a compact and flexible GIS that can be loaded with virtually any precursor ma- terial provides a multitude of possibilities for exploring novel solutions to existing problems as well as new applications for beam induced deposition processes.

TT 48.5 Wed 16:15 H32

FXBID - an X-ray based sibling to FEBIP — •Andreas Späth[1], Kim Thomann[1], Florian Vollnhals[1], Jörg Raabe[2], Kevin C. Prince[3], Robert Richter[3], Wolfgang Hieringer[4], Hubertus Marbach[1], and Rainer H. Fink[1] — [1]Physikalische Chemie II, FAU Erlangen-Nürnberg, Germany — [2]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — [3]Elettra Sincrotrone, Basovizza, Italy — [4]Theoretische Chemie, FAU Erlangen-Nürnberg, Germany

Focused X-ray beam induced deposition (FXBID) is a novel technique for the additive fabrication of metallic nanostructures by illuminating metal organic precursor molecules with focused soft X-rays in a Fresnel zone plate based scanning transmission X-ray microscope (STXM)[1,2]. An advantage of the technique is the possibility to optimize precursor fragmentation by proper selection of the incident photon energy. For a better understanding of basic X-ray induced fragmentation processes, we have performed photon energy dependent mass spectrometry and secondary electron spectroscopy studies for several metal organic precursors[3]. The results are correlated with TD-DFT calculations of the molecular orbitals relevant for soft X-ray absorption and have been transferred to advanced deposition experiments. We have started to explore the capabilities of in-situ cleaning procedures (reactive gases, annealing, etc.) to enhance the chemical purity of FXBID deposits. The project is funded by DFG grant SP 1775/1-1.

[1] A. Späth et al., RSC Advances, 2016, 6, 98344.
[2] F. Tu et al., J. Vac. Sci. Technol. B, 2017, 35(3), 031601.
[3] A. Späth et al., Microsc. Microanal. 2018, 24(S2), 114.

15 min. break

Invited Talk TT 48.6 Wed 16:45 H32

Fundamentals of low-energy electron induced dissociation of focused electron beam induced deposition precursors — •Oddur Ingólfsson — Science Institute and the Department of Chemistry, University of Iceland,, Dunhagi 3, 107 Reykjavík. Iceland.

When high-energy electron beams imping on a solid surface, as is the case in FEBID, backscattered and secondary electrons (SEs) are abundant. The energy distribution of the SEs typically peaks well below 10 eV, has a significant contribution close to 0 eV and a tail to higher energies. In this energy range, electron induced bond ruptures through Dissociative Ionization, Dissociative Electron Attachment and Neutral and Dipolar Dissociation can be very efficient. These processes have different energy dependence and the nature and thus the reactivity of the fragments formed is also distinctly different. The cross sections for these processes and the branching ratios for different dissociation paths depend critically on the respective molecular composition. This, in turn opens opportunities to tailor the sensitivity of potential FEBID precursors towards preferred paths to achieve better deposition efficiency and better composition control. In this contribution fundamental aspect of electron induced dissociation processes are discussed in context to their role in FEBID. Acknowledgement; This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 722149.

TT 48.7 Wed 17:15 H32

Which molecular structures in metal organic compounds are favourable for electron-induced decomposition? — Kai Ahlenhoff and •Petra Swiderek — University of Bremen, Institute for Applied and Physical Chemistry, Bremen, Germany

Electron beam induced processing calls for precursor molecules or materials that can be converted to a deposit with well-defined final composition. An approach to this problem is to use ligands which fragment to non-reactive and volatile products leaving behind only the desired material. This concept can guide the design of precursor materials. We have started to investigate this hypothesis by comparing the electron-induced decomposition of surface-grown copper-containing coordination materials that are constructed using different organic counterions, namely, copper(II)oxalate, copper(II)squarate, and HKUST-1 [1]. As a second class of compounds, silver carboxylates with different organic side chain have been considered. Using these examples, we discuss in this contribution a new concept for precursor design. [1] K. Ahlenhoff et al., Phys. Chem. Chem. Phys., submitted.

TT 48.8 Wed 17:30 H32

Cisplatin as potential Pt FEBID precursor: NH_3 ligands enhance the electron-induced removal of chlorine — •Markus Rohdenburg[1], Kai Ahlenhoff[1], Sascha Koch[2], Armin Gölzhäuser[2], and Petra Swiderek[1] — [1]Institute for Applied and Physical Chemistry, University of Bremen, Leobener Str. 5, 28359 Bremen, Germany — [2]Department of Physics, University of Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

As recently shown, electron beam exposure to crystals of cisplatin (cis-$Pt(NH_3)_2Cl_2$) leads to a violent reaction. The crystal literally boils with a deposit of pure Pt remaining behind [1]. We have proposed that this reaction is driven by the electron-induced fragmentation of the NH_3 ligands which supplies hydrogen that converts chlorine ligands into HCl. In contrast, the structurally similar cis-$Pt(CO)_2Cl_2$ rapidly loses CO upon irradiation but yields deposits with high chlorine contents that can only be removed by extensive electron exposure [2]. We therefore present new results that confirm the formation of HCl by use of electron-stimulated desorption (ESD) experiments. Furthermore, XPS data reveals that electron irradiation removes N and Cl from cisplatin on a similar time scale. The exposure required for quantitative removal of Cl is much smaller in the case of cisplatin than for cis-$Pt(CO)_2Cl_2$ underlining the favourable effect of the NH_3 ligands.

[1] J. Warneke et al., J. Phys. Chem. C 120 (2016) 4112.
[2] J.A. Spencer et al., J. Am. Chem. Soc. 138 (2016) 9172.

TT 48.9 Wed 17:45 H32

Amidinate and carboxylate coordination compounds for focused electron beam induced deposition (FEBID) — Katarzyna Madajska and •Iwona Szymańska — Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

Focused electron beam induced deposition (FEBID) is said to play a fundamental role for making sophisticated 2D and 3D nanostructures with an ultimate resolution of less than 1 nm. It is frequently so-called *3D nanoprinting*.[1] The choice of the precursor is crucial for the success of FEBID: its chemical nature and dissociation behavior determine the composition of the deposit.[2]

Research was focused on the copper(II), silver(I) and rhenium(III) complexes with an amidinate and/or carboxylate ligands, which seems to be promising for a FEBID process. Mass spectrometry (EI MS) exhibited in the gas phase following ions: [Cux(NH2(NH=)CR1)y(O2CR2)z]+, [Agx(NH(NH=)CR1)y(O2CR2)z]+, [Agz(NH(NH=)CR1)y]+, [Re2Clx(NH(NH=)CR1)y], where R1, R2 = perfluorinated aliphatic groups. Sublimation experiments and temperature-variable infrared spectroscopy were carried out to determine compounds volatility and decomposition mechanisms.

References [1] D. Belić, M. M. Shawrav, E. Bertagnolli, H. D. Wanzenboeck, Beilnstein J. Nanotechnol, 8 (2017) 2530*2543. [2] I. Utke, P. Hoffmann, J. Melngailis, J. Vac. Sci. Technol. B, 26 (2008) 1197*1276.

TT 49: Poster Session: Superconductivity

Time: Wednesday 15:00–18:30 Location: Poster D

TT 49.1 Wed 15:00 Poster D

High pressure study of hydrogen sulfide — •Takaki Muramatsu, Owen Moulding, Yan Zhou, Martin Kubal, and Sven Friedemann — HH Wills Laboratory, University of Bristol, UK

High T_c superconductivity (about 200K) of hydrogen sulfide (H_2S) was discovered by Drozdov *el al.* in 2015 and it was observed in its high-pressure metallic phase ($P > 100$ GPa). Several groups reported that new structural phase (H_3S) is synthesized in the high-pressure superconducting phase. The temperature must be kept below around 200 K while pressure is increased up to 100 GPa to form the high T_c superconducting phase. In this work we show our sample loading system capable of liquefying and pressurising H_2S in a diamond-anvil high-pressure cell to beyond 100 GPa. We show Raman spectroscopy and electrical transport measurements. For a pressurisation at room temperature, the Raman results show the dissociation of H_2S resulting in hydrogen and elemental sulphur. The latter is detected as a superconducting phase above 100 GPa with resistance measurements. Our studies highlight the sensitivity of the high-pressure synthesis of superconducting hydrogen sulphide.

TT 49.2 Wed 15:00 Poster D

High-Pressure Measurements of Upper and Lower critical fields in 2H-$NbSe_2$ — •Israel Osmond and Sven Freidemann — H.H Wills Physics Laboratory, University of Bristol

With superconductivity often found in the vicinity of ordered states such as charge density waves (CDW) and antiferromagnetism, the ability to tune materials through these states serves as a vital tool in exploring the interplay of these phases with superconductivity. For characterising a given superconductor, magnetic measurements provide a non-invasive method of studying vortex dynamics and measuring critical temperatures and fields.

Likewise, pressure measurements serve as a continuous tuning parameter across many of these phases. As such, the application of pressure provides a method to both access novel structures not available at ambient pressure, and to explore the competition between phases such as the CDW and superconducting order. This work develops current

pressure cell technology compatible with commercial SQUID magnetometers, with both piston cylinder and gemstone anvil type cells.

Previous research into 2H-$NbSe_2$ has shown multiband superconductivity, CDW ordering, and the existence of a quantum critical point beneath the superconducting state. Here, we use the aforementioned pressure cells for magnetic susceptibility measurements, mapping the behavior of both upper and lower critical fields in 2H-$NbSe_2$ with temperature and pressure.

TT 49.3 Wed 15:00 Poster D

Electrical properties of $[SnSe]_m[NbSe_2]_n$ ferecrystals with $m = 6, 9$ and $n = 1$ — •Klara Mihov[1], Olivio Chiatti[1], Martina Trahms[1], Corinna Grosse[1], Kyle Hite[2], Matty B. Alemayehu[2], Dave C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Solid State Chemistry, Inorganic Chemistry, Electrochemistry and Materials Science, University of Oregon, Eugene, OR 97403-1253, U.S.A.

In the last years, much attention has been paid to the electrical properties of layered superconducting thin films [1]. The ferecrystals provide a possible model systems for layered superconductors. In this work, the ferecrystals are composed of a superconducting transition metal dichalgonide ($NbSe_2$) stacked repeatedly with metal monochalgogenide (SnSe)[2]. Here, we examine ferecrystals with $m = 6, 9$ and $n = 1$ which show a superconducting phase below a critical temperature. The Ginzburg-Landau coherence lengths are determinded from the critical magnetic fields and give information about the coupling between the superconducting $NbSe_2$-layers[3]. In addition, the investigated ferecrystals provide a striking opportunity to investigate superconducting fluctuations above the critical temperature.

[1] C. Grosse *et al.*, Scientific Reports **6**, 33457, (2016).
[2] C. Grosse *et al.*, Crystal Research and technology **52**(10), (2017).
[3] M. Trahms *et al.*, Superconductor Science and Technology **31**(6), (2018).

TT 49.4 Wed 15:00 Poster D

Growth and characterization of high-quality $Tl_2Mo_6Se_6$ crystals and nanowires — •Yongjian Wang, Mengmeng Bai, Mahasweta Bagchi, Zhiwei Wang, and Yoichi Ando — Institute of Physics II, University of Cologne, D-50937 Cologne, Germany

Topological superconductor (TSC) has attracted extensive interest because of its potential application to topological quantum computation, which is based on Majorana fermion (MF). Recently, the long-existed quasi-one-dimensional superconductor, $Tl_2Mo_6Se_6$, was predicted to be a new TSC [1]. Here we report the growth and characterizations of high-quality superconducting $Tl_2Mo_6Se_6$ crystals and nanowires. Fiber-shaped crystals with typical size of $0.3\times0.3\times10$ mm^3 were grown by reacting the starting raw materials in a quartz tube. The highest critical temperature (T_c) was observed to be 6.7 K from both resistivity and magnetic susceptibility measurements. The highest shielding fraction was estimated to be 100%. The upper critical field (H_{c2}) behaviour shows an upturn with lowering temperature, which is similar to the results reported before [2], suggesting unconventional superconductivity. $Tl_2Mo_6Se_6$ nanowires with typical diameter of 100 nm were obtained by exfoliating $Tl_2Mo_6Se_6$ crystals, which were used for fabricating devices by e-beam lithography for transport measurements. Superconductivity with T_c up to 6 K was observed.

[1] S. M. Huang et al., Phys. Rev. B 97, 014510 (2018)
[2] R. Brusetti et al., Phys. Rev. B 49, 8931 (1994)

TT 49.5 Wed 15:00 Poster D

Mapping the nematic axis of $Cu_xBi_2Se_3$ at high doping — •Mahasweta Bagchi, Jens Brede, Jeison Fischer, Thomas Michely, and Yoichi Ando — Physics Institute II, University of Cologne, Germany

Recently, NMR Knight-shift measurements[1] and measurements of angular dependent specific heat in a magnetic field[2] show spontaneous symmetry breaking in the superconducting state of bulk samples of $Cu_xBi_2Se_3$. Both observations firmly establish an odd parity nematic superconducting state in $Cu_xBi_2Se_3$. More recently, STM experiments[3] demonstrated mapping of the elongation of the vortex core in the vortex state of $Cu_xBi_2Se_3$ under an applied magnetic field. The orientation of the vortex core with respect to the crystallographic axis of the sample, as inferred from atomic-resolution images, gives the orientation of the nematic axis.

Here, we study $Cu_xBi_2Se_3$ with varying x. In particular, we study samples near optimum doping (x=0.3) and at higher doping levels (x=0.6) with an STM operated at 350 mK and under applied magnetic field and determine the nematic axis as a function of x.

[1] K. Matano *et al.*, Nat. Phys. **12**(9) 852 (2016)
[2] S. Yonezawa *et al.*, Nat. Phys. **13**(2) 123 (2017)
[3] R. Tao *et al.*, Phys. Rev. X **8**(4) 041024 (2018)

TT 49.6 Wed 15:00 Poster D

Toward the theory of the higher harmonic in superconducting gap dispersion of hole- and electron-doped cuprates — •Mikhail Malakhov[1,2], Mikhail Eremin[2], and Daniil Kochergin[2] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, Universitätsstraße 150, DE-44801 Bochum, Germany — [2]Institute of Physics, Kazan Federal University, Kazan, 420008 Russia

Numerical solutions of the Bardeen-Cooper-Schrieffer equation are obtained, taking into account superexchange, three site correlation term, spin-fluctuation, plasmon, and phonon mediated mechanisms. Expression for charge and spin susceptibilities derived beyond RPA approximation. For both e- and h- doped cuprates at carrier concentrations close to optimal the energy gap dispersions where approximated by expression $\Delta_{\mathbf{k}} = \Delta_0(B\cos(2\phi) + (1-B)\cos(6\phi))$, where the angle is measured from the antinodal direction in the Brillouin zone. In agreement with ARPES data we have got $(1-B) > 0$ for h- doped cuprates and $(1-B) < 0$ for e-doped one and right value of Δ_0. In $Bi_2Sr_2CaCu_2O_8$ we found that the amplitude before $\cos(6\phi)$ is determined by spin-fluctuation and phonon mediated mechanisms. In case $Pr_{0.89}LaCe_{0.11}CuO_4$ the higher-harmonic is originated from spin-fluctuation and plasmon (Coulomb) pairing mechanisms. Numerically and analytically shown that role of three site correlations is weakening superexchange interaction.

TT 49.7 Wed 15:00 Poster D

Superconductivity in doped tungsten oxide: a first principles description — •Antonio Sanna[1], Camilla Pellegrini[1], and Henning Glawe[2] — [1]Max Planck Institute of microstructure physics, Halle (Saale), Germany — [2]Max Planck Institute for the structure and dynamics of matter, Hamburg, Germany

Tungsten Oxide (WO_3), its bronzes (M_xWO_3), oxygen vacant (WO_{3-x}) and fluorine doped ($WO_{3-x}F_x$) are a family of crystals showing a large variety of electronic properties, including superconductivity. Most measurements report a consistent scenario of low T_c, although there have been some reports on possible high-T_c low dimensional and metastable superconductivity in sodium doped surfaces, at the W/WO_3 interface and upon H doping. We attempt a characterization of superconductivity in doped WO_3 by *ab initio* methods, focusing on the two key questions:

- Are the stable low temperature superconducting phases driven by conventional electron phonon pairing? or, like in $BaBiO_3$, conventional approaches fail and the correct pairing mechanism is still an open problem.
- Can electron phonon coupling, in any geometry and doping regime, provide enough coupling strength to lead to high-T_c?

TT 49.8 Wed 15:00 Poster D

Effects of self-consistency in mean-field theories of disordered systems: Superconductor Insulator Transition — •Matthias Stosiek and Ferdinand Evers — Institute of Theoretical Physics, University of Regensburg, Germany

Our general interest is in aspects of self-consistency with respect to disorder in the mean-field treatment of disordered interacting systems. The example we here consider is the Superconductor Insulator Transition (SIT), where the superconducting gap is calculated in the presence of short-range disorder. Our focus is on disordered films with conventional s-wave pairing that we study numerically employing the negative-U Hubbard model within the standard Bogoliubov-deGennes approximation. The general question that we would like to address concerns the auto-correlation function of the pairing amplitude: Does it qualitatively change if full self-consistency is accounted for? Our research might have significant impact on the understanding of the SIT, if extra correlations appear due to the self-consistency condition that turn out sufficiently long-ranged. Such correlation effects are ignored in major analytical theories. To study the long-range behavior of the order parameter correlations, the treatment of large system sizes is necessary. Due to the self-consistency requirement, the relevant sizes (e.g. 10^6 sites) are numerically very expensive to achieve. For this reason, we have developed a parallelized code based on the Kernel Polynomial Method. We present data that indicates the existence of

very long ranged (power-law) correlations that may indeed change the critical behavior in a significant way.

TT 49.9 Wed 15:00 Poster D

Dynamics of nanostructured superconductors in curl-free vectorpotentials — •Björn Niedzielski and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg, Insitut für Physik, Germany

In the theory of macroscopic quantum materials, like superconductors, the electromagnetic vectorpotential plays a crucial role. We show for nanoscopically structured superconductors how vectorpotentials with zero curl can be used to manipulate the state of such a system. It is demonstrated how a relation between flux quantization and the Aharonov-Bohm effect can be used to drive and control superconducting tunneling devices in a non-invasive way.

TT 49.10 Wed 15:00 Poster D

Spin effects in a superconductor in proximity to an antiferromagnetic insulator — Akashdeep Kamra[1], •Ali Rezaei[2], and Wolfgang Belzig[2] — [1]Center for Quantum Spintronics, Department of Physics, NTNU, Norway — [2]Department of Physics, University of Konstanz, Germany

Inspired by recent feats in exchange coupling antiferromagnets to an adjacent material, we demonstrate the possibility of employing them for inducing spin-splitting in a superconductor, thereby avoiding the parasitic effects of ferromagnets employed to this end. We derive the Gor'kov equation for the matrix Green's function in the superconducting layer, considering a microscopic model for its disordered interface with a two-sublattice magnetic insulator. We find that an antiferromagnetic insulator with effectively uncompensated interface induces a large, disorder-resistant spin-splitting in the adjacent superconductor, thereby addressing the feasibility of a wide range of devices involving spin-split superconductors. In addition, we find contributions to the self-energy stemming from the interfacial disorder. Within our model, these mimic impurity and spin-flip scattering, while another breaks the symmetries in particle-hole and spin spaces. The latter contribution, however, vanishes in the quasi-classical approximation and thus, does not significantly affect the superconducting state. Our results illustrate the potential of antiferromagnets for superconducting spintronics avoiding stray fields usually accompanying ferromagnets.
[1] Akashdeep Kamra, Ali Rezaei, Wolfgang Belzig, arXiv:1806.10356 (2018); accepted in PRL

TT 49.11 Wed 15:00 Poster D

Phonon anomalies in FeS — •Leander Peis[1,2], Andreas Baum[1,2], Ana Milosavljević[3], Nenad Lazarević[3], Miloš M. Radonjić[3], Božidar Nikolić[4], Merlin Mitscheck[1,2], Zahra Inanloo Maranloo[1], Maja Šćepanović[3], Mirjana Grujić-Brojčin[3], Nenad Stojilović[3,5], Matthias Opel[1], Aifeng Wang[6], Cedomir Petrovic[6], Zoran V. Popović[3,7], and Rudi Hackl[1] — [1]Walther-Meissner-Institut, 85748 Garching, Germany — [2]Fakultät für Physik, Technische Universität München, 85748 Garching, Germany — [3]Institute of Physics Belgrade, 11080 Belgrade, Serbia — [4]Faculty of Physics, University of Belgrade, Belgrade, Serbia — [5]Department of Physics and Astronomy, University of Wisconsin Oshkosh, Oshkosh, WI 54901, USA — [6]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, USA — [7]Serbian Academy of Sciences and Arts, 11000 Belgrade, Serbia

Tetragonal FeS is studied using Raman spectroscopy. We identify the A_{1g} and B_{1g} phonon modes, a second order scattering process, and contributions from potentially defect-induced scattering. The temperature dependence between 300 and 20 K of all observed phonon energies is governed by the lattice contraction. The increase in energy of all modes below 20 K may indicate short range magnetic order. Lattice-dynamical simulations and a symmetry analysis for potential overtones are in good agreement with the experiments. The two-phonon excitation observed in a gap between the optical branches presumably becomes observable due to significant electron-phonon interaction.

TT 49.12 Wed 15:00 Poster D

Microscopic phase diagram of LaFeAsO single crystals under pressure: A Mössbauer study — •Philipp Materne[1], Wenli Bi[2,1], Jiyong Zhao[1], Michael Yu Hu[1], Rhea Kappenberger[3,4], Sabine Wurmehl[3,4], Saicharan Aswartham[3], Bernd Büchner[3,4], and Esen Ercan Alp[1] — [1]Argonne National Laboratory, Lemont, IL 60439, USA — [2]Department of Geology, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA — [3]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, D-01069, Germany — [4]Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany

We investigated a LaFeAsO single crystal by means of synchrotron Mössbauer spectroscopy under pressure up to 7.5 GPa and down to 13 K and provide a microscopic phase diagram. A continuous suppression of the magnetic hyperfine field with increasing pressure was found and it completely vanishes at $\sim$ 7.5 GPa which is in contrast to the behaviour in polycrystalline samples where the magnetic order vanishes at $\sim$ 20 GPa. We discuss the sample dependence of the magnetic order among different single and polycrystalline samples and its relationship to the structural parameters.
[1] P. Materne *et al.*, Phys. Rev. B. **98**, 174510 (2018)

TT 49.13 Wed 15:00 Poster D

Observation of a highly ordered vortex lattice in LiFeAs — •Sven Hoffmann[1], Christian Salazar[1], Pavlo Khanenko[1], Danny Baumann[1], Ronny Schlegel[1], Saicharan Aswartham[1], I. Morozov[2], Bernd Büchner[1], and Christian Hess[1] — [1]IFW Dresden, Helmholtzstraße 20, D-01069 Dresden — [2]MSU, Leninskiye Gory 1, R-119991 Moscow

Unlike other Fe-based superconductors, LiFeAs is a stoichiometric superconductor, showing no trace of nematic order, charge ordering or magnetic ordering and no Fermi surface nesting, while still maintaining a fairly high transition temperature. To gain additional information about the order parameter in this material we performed low temperature scanning tunneling microscopy and spectroscopy measurements. Differential conductance maps revealed a highly ordered vortex lattice, even at high magnetic fields. These findings contradict previous reports, where substantially disordered vortex lattices were observed at a broad range of magnetic fields, indicative of a strong pinning effect and small coherence length in LiFeAs. Our data therefore suggest weaker pinning and a substantially larger coherence length for this sample as compared to previous reports.

TT 49.14 Wed 15:00 Poster D

The nematic phase of $LaFe_{1-x}Co_xAsO$ single crystals probed by thermodynamic methods — •Francesco Scaravaggi[1,2], Sven Sauerland[3], Rhea Kappenberger[1,2], Liran Wang[3], Saicharan Aswartham[1], Sabine Wurmehl[1], Rüdiger Klingeler[3], Anja U. B. Wolter[1], and Bernd Büchner[1,2] — [1]Leibniz-Institute for Solid State and Materials Research, IFW Dresden, Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, Dresden, Germany — [3]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany

The phase diagram of electron doped LaFeAsO has been extensively studied on polycrystalline samples, showing significant differences when compared with other members of the FeAs family. The electronic nematic phase present in the parent compound, gradually suppressed by doping, appears to be separated from the emerging superconducting phase by a fairly abrupt transition. The interplay between these two phases in Iron-based superconductors as well as the origin of the nematic order are still under debate. By measuring single crystalline samples [1], we report the study of the evolution of the nematic phase in LaFeAsO as a function of Co doping by magnetization, specific heat and thermal expansion measurements. Macroscopic faceted single crystals allow us to effectively trace the structural order parameter (δ) as a function of temperature and doping by high resolution dilatometry.
[1] R. Kappenberger et al., J. Cryst. Growth 483, 9 (2018)

TT 49.15 Wed 15:00 Poster D

Elastotransport and Nernst effect in 122- and 1111-Fe-based superconductors: Evidence for superconductivity driven by nematic fluctuations — •Christoph Wuttke[1], Federico Caglieris[1], Xiaochen Hong[1], Steffen Sykora[1], Frank Steckel[1], Seunghyun Kim[1], Rhea Kappenberger[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Sheng Ran[2], Paul C. Canfield[2], Bernd Büchner[1,3], and Christian Hess[1] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — [3]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany

The role of nematic fluctuations in the appearance of high temperature superconductivity is still controversial. In this work we investigate the

phase diagrams of $BaFe_2As_2$ and LaFeAsO as a function of electron-doping through elastotransport and Nernst effect measurements. We obtain an anomalously large Nernst coefficient in the tetragonal phase, upon doping its magnitude strikingly mimicking the superconducting dome. Similar but slightly different non-monotonic behavior is found for the elastoresistivity. Using a minimal orbital model for iron-based superconductors we show that the Nernst coefficient couples directly to the nematic fluctuations. We explain the difference between elastoresistivity and Nernst effect by incorporating the coupling to a soft phonon mode in our theory. Thus, our experimental results provide supportive evidence that nematic fluctuations are crucial for the formation of the superconducting state in iron-based superconductors.

TT 49.16 Wed 15:00 Poster D

NMR investigations of the iron-pnictide superconductor KFe_2As_2 near the upper critical field — •Sh. Yamamoto[1], S. Molatta[1], F. Hardy[2], R. Lortz[3], J. Wosnitza[1], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Department of Physics, The Hong Kong University of Science and Technology, Kowloon, Hong Kong

Recent measurements by thermodynamic probes provided evidence for a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state in the iron-pnictide superconductor KFe_2As_2 beyond the Pauli limit for in-plane applied fields. We report two aspects of the ^{75}As nuclear magnetic resonance in KFe_2As_2 near the upper critical field (H_{c2}). First, according to the angular and temperature dependence of spin-echo measurements, no observable line broadening above the Pauli limit was observed for a high-quality single crystal. The result gives a spectroscopic viewpoint on the proposed FFLO state. Second, we observed an angle-independent line broadening of the central and the satellite peak below 500 mK near H_{c2}. Furthermore, two distinct nuclear spin-lattice relaxation times were observed at low temperatures. These results are compatible with the existence of charge order or charge fluctuations that has been, so far, only observed under pressure (KFe_2As_2) or in zero field ($RbFe_2As_2$) in strongly hole-doped 122 iron-based superconductors.

TT 49.17 Wed 15:00 Poster D

Fermi-surface topology of (Rb,Cs)Fe_2As_2 — •Tobias Förster[1], Johannes Klotz[1], Seunghyun Khim[2], Saicharan Aswartham[3], Helge Rosner[2], Ilya Sheikin[4], and Jochen Wosnitza[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research (IFW), Dresden Germany — [4]Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL), Grenoble, France

The unique Fermi-surface topology of many iron-pnictide superconductors stimulates a number of theories on the nature of the pairing interactions in these materials. In the case of (K,Rb,Cs)Fe_2As_2, there is an ongoing discussion whether a Lifshitz transition is connected to the superconducting properties of these 122 iron arsenides. Studies of the pressure dependence of H_{c2} did not find evidence for that kind of transition [1]. In contrast, high-resolution band-structure calculations show a van Hove singularity close to the Fermi energy, favoring a Lifshitz transition. In order to investigate the possible impact of this feature, a precise knowledge of the electronic structure is eminent. We, therefore, calculated the Fermi surface in (Rb,Cs)Fe_2As_2 and investigated the de Haas-van Alphen effect of (Rb,Cs)Fe_2As_2 in static fields up to 38 T. In our contribution, we show the results of our torque-magnetometry measurements and use them to refine band-structure calculations.

[1] F. F. Tafti et al., Phys. Rev. B. **89**, 134502 (2014).

TT 49.18 Wed 15:00 Poster D

Design of a 30 mK STM for spin-polarized measurements — •Sebastian Schimmel, Danny Baumann, Alexander Horst, Ralf Voigtländer, Dirk Lindackers, Saicharan Aswartham, Sabine Wurmehl, Bernd Büchner, and Christian Hess — IFW-Dresden; Helmholtzstraße 20; 01069 Dresden

We present a scanning tunneling microscope (STM) system which is especially designed to perform investigations with spin-polarization and very high resolution in energy as well as in real space. Using a ^{3}He/^{4}He Dilution refrigerator allows to cool the tip and sample to a measurement temperature of 30 mK which improves the energy resolution to the micro-eV-scale and enables to study all classes of unconventional superconductors, also including heavy fermion compounds. Long-term measurements at base temperature can be performed for up to 7 days. A UHV system will be employed to prepare tips and samples for spin-polarized STM measurements. Furthermore, a 9-4 T vector magnet allows the systematic in-situ manipulation of the spin-polarization axis. The whole apparatus is suspended on a sophisticated two-stage passive/ active damping system. Therefore, this instrument constitutes a novel approach to reveal the ubiquitous interplay of superconductivity, magnetism and electronic order in unconventional superconductors.

TT 49.19 Wed 15:00 Poster D

Out-of-plane electronic contributions in Bi-cuprates studied by resonant photoelectron spectroscopy at the Cu 2p edge — •Christoph Janowitz[1] and Dieter Schmeisser[2] — [1]Humboldt Universität, Institut für Physik — [2]Brandenburgisch Technische Universität Cottbus-Senftenberg

In high-temperature superconductors with a layered crystal structure out-of-plane contributions are often neglected, while the copper-oxygen planes are commonly considered to dominate the electronic properties around the Fermi energy. Here we report on a resonant photoemission study of (Pb,Bi)2201 and (Pb,Bi)2212 single crystals to unravel the resonant decay mechanisms at the Cu 2p absorption edge. We demonstrate a pronounced polarization dependence caused by two different Auger processes for in-plane and out-of-plane orientations. We deduce that the lowest energy valence state being involved in the two Auger processes, consists of three-dimensional contributions by admixed out-of-plane Sr, Bi, and O 2p states. It also suggests that the doping-induced charge density is dynamic, fluctuating within the Cu-O plane, and spills out perpendicular to it.

[1] C. Janowitz and D. Schmeißer, Supercond. Sci. Technol. 31, 045006 (2018)

TT 49.20 Wed 15:00 Poster D

Lifetime of the magnetic resonance mode in high-temperature superconductors — •Davide Valentinis[1], Toshinao Loew[2], and Joerg Schmalian[1] — [1]Institute for Theoretical Condensed Matter physics, Karlsruhe Institute of Technology, Wolfgang-Gaede Straße 1, 76131 Karlsruhe (DE) — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart (DE)

The spin-resonance collective mode emerges in the electronic spectrum of high-temperature superconductors as a consequence of the sign-changing pairing symmetry of the superconducting gap [1], as measured by inelastic neutron scattering. A detailed study of the spectral lineshape for the spin resonance thus yields valuable insight on the microscopic interactions which promote or compete with pairing [2]. In this work, we analyze new neutron inelastic scattering measurements on $YBa_2Co_3O_{6.55}$ in terms of the spin-fermion model near the antiferromagnetic instability in 2 dimensions [3], where self-energy corrections from disorder are treated in Born approximation. We compare quantitatively the calculated temperature dependence of resonance energy and linewidth with experiments, thus inferring characteristic energy scales for pairing and disorder strength.

[1] P. Hlobil, B. Narozhny and J. Schmalian, Phys. Rev. B **88**, 205104 (2013)
[2] M. Eschrig, Adv. Phys. **55**, 47 (2006)
[3] A. Abanov, A. V. Chubukov and J. Schmalian, Adv. Phys. **52**, 119 (2003)

TT 49.21 Wed 15:00 Poster D

Triplet superconducting correlations: Magnet-superconductor hybrid structures in nonequilibrium — •Kevin Marc Seja[1], Oleksii Shevtsov[2], and Tomas Löfwander[1] — [1]Chalmers University of Technology, Göteborg, Sweden — [2]Northwestern University, Evanston (IL), United States

We examine a superconductor that is in contact with a normal metal via a spin-active interface. Using quasiclassical theory of superconductivity, we study the system in equilibrium as well as in nonequilibrium induced by a voltage bias. Earlier investigations have shown that in equilibrium the interface gives rise to Andreev bound states that induce a spin magnetization in the supercon- ductor. It was found that this equilibrium magnetization is related to non- trivial triplet superconducting correlations, a key feature of unconventional superconductivity. Out of equilibrium there is an additional contribution to spin imbalance related to spin-filtering and spin-mixing mechanisms. [1,2] However, in non-equilibrium the possible connection between magneti-

zation and superconducting triplet correlations is not yet understood. We examine this relation, the change in distribution as well as the structure and spatial behavior of these correlations in non-equilibrium configurations.

[1] Shevtsov O and Löfwander T, J. Phys Conf. Ser. 568, 2 (2014)
[2] Shevtsov O and Löfwander T, Phys. Rev. B 90, 085432 (2014)

TT 49.22 Wed 15:00 Poster D

Single-Channel Josephson Effect in a High-Transmission Atomic Contact — Jacob Senkpiel[1], •Simon Dambach[2], Markus Etzkorn[1], Robert Drost[1], Ciprian Padurariu[2], Björn Kubala[2], Wolfgang Belzig[3], Alfredo Levy Yeyati[4], Juan Carlos Cuevas[4], Joachim Ankerhold[2], Christian R. Ast[1], and Klaus Kern[1,5] — [1]Max-Planck-Institut für Festkörperforschung, Germany — [2]Institut für komplexe Quantensysteme, Universität Ulm, Germany — [3]Fachbereich Physik, Universität Konstanz, Germany — [4]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain — [5]Institut de Physique, École Polytechnique Fédérale de Lausanne, Switzerland

The Josephson effect in scanning tunneling microscopy is an excellent tool to probe the properties of the superconducting order parameter on a local scale through the Ambegaokar-Baratoff (AB) relation. Using single atomic contacts created by means of atom manipulation, we demonstrate that in the extreme case of a single transport channel through the atomic junction, modifications of the current-phase relation lead to significant deviations from the linear AB formula. Using the full current-phase relation for arbitrary transmission, we model the Josephson effect in the dynamical–Coulomb-blockade regime because the charging energy of the junction capacitance cannot be neglected. We find excellent agreement with the experimental data. Projecting the current-phase relation onto the charge-transfer operator shows that at high transmission multi–Cooper-pair tunneling processes may occur.

[1] J. Senkpiel et al., arXiv:1810.10609.

TT 49.23 Wed 15:00 Poster D

Development of RF-Power Dividers for the Josephson Arbitrary Waveform Synthesizer — •Hao Tian, Oliver Kieler, Ralf Behr, Rüdiger Wendisch, Rolf-Werner Gerdau, Karsten Kuhlmann, and Johannes Kohlmann — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

The JAWS, based on pulse-driven series arrays of SNS Josephson Junctions (JJs) at 4 K, enables spectrally pure AC voltages to be synthesized from DC up to MHz. To make the experimental set-up less complex and to increase the JJs operated by a single PPG channel, we designed two types of on-chip power dividers. One type is a serial-parallel power divider, the second type is a Wilkinson power divider. Each output of the power divider is equipped with a DC-block capacitor. Different designs were simulated, integrated to JJs arrays and fabricated. The results showed that the test chips containing a 2-stage serial-parallel power divider and 2000 JJs are operational up to a maximal clock frequency of 8 GHz. However, the operation margins are rather small and spectrally pure sinusoidal waveforms could be synthesized with sigma-delta code amplitudes $< 30\%$. The 1-stage Wilkinson power divider with 1000 JJs is operating up to a clock frequency of 15 GHz. We successfully synthesized spectrally pure output voltages of 11.7 mV (RMS). The operation margins are much larger than for the previous design.

This work was partly supported by the EMPIR programme co-financed by the Participating States and from the EU H2020 programme (JRP 15SIB04 QuADC) and by the German BMWi (project ZF4104104AB7).

TT 49.24 Wed 15:00 Poster D

Driving optomechanics with quantum microwaves from inelastic Cooper pair tunneling — •Surangana Sengupta, Björn Kubala, Ciprian Padurariu, and Joachim Ankerhold — Institute for Complex Quantum Systems and IQST, Ulm University, 89069 Ulm, Germany

In cavity optomechanics the radiation-pressure forces of optical-light or microwave excitations of a resonator have been harnessed for a wide variety of purposes [1]: from cooling and the observation of quintessential quantum-mechanical effects, to archetypal nonlinear-dynamics phenomena, and the quantum-classical crossover between these regimes. On the other hand, inelastic Cooper-pair tunneling across a dc-biased junction can create diverse quantum states of microwave light in a cavity connected in series with the junction; owing to the inherent nonlinearity of the Josephson coupling [2].

Here, we theoretically investigate, how such states may be exploited to drive a mechanical degree of freedom to supplement or substitute classical or squeezed drives explored previously. Various possible coupling scenarios and first results of a semiclassical analysis will be discussed.

[1] Markus Aspelmeyer, Tobias J. Kippenberg, and Florian Marquardt, Rev. Mod. Phys. **86**, 1391 (2014).
[2] M. Westig, B. Kubala, O. Parlavecchio, Y. Mukharsky, C. Altimiras, P. Joyez, D. Vion, P. Roche, M. Hofheinz, D. Esteve, M. Trif, P. Simon, J. Ankerhold, and F. Portier, Phys. Rev. Lett. **119**, 137001 (2017).

TT 49.25 Wed 15:00 Poster D

Proximity-induced superconductivity in Pd/$(Bi_{1-x}Sb_x)_2Te_3$ heterostructures — •Mengmeng Bai[1], Fan Yang[1], Andrea Bliesener[1], Gertjan Lippertz[1], Martina Luysberg[2], Alexey Taskin[1], Joachim Mayer[2], and Yoichi Ando[1] — [1]Physics Institute II, University of Cologne, 50937 Cologne, Germany — [2]Forschungszentrum Jülich GmbH, Ernst Ruska-Centrum, 52425 Jülich, Germany

Josephson junctions (JJs) based on topological insulators (TIs) are interesting because of the possibility to generate Majorana fermions. Previous reports on TI–based JJs have employed deposited superconducting films such as Al and Nb for proximitization, which inevitably faces the challenge of the interface quality. In fact, the transparency of the JJs reported so far has been limited. Here we report that simply sputtering Pd on MBE–grown $(Bi_{1-x}Sb_x)_2Te_3$ (BST) thin films naturally gives us a superconducting layer due to an epitaxial alloy formation at the interface. This superconducting layer allows us to fabricate JJ devices which show dissipationless supercurrents below a critical temperature of 0.9 K, confirming a strong proximity effect on the TI surface.

TT 49.26 Wed 15:00 Poster D

Phase separation and proximity effects in itinerant ferromagnet/ superconductor heterostructures — •Christian Martens[1], Andreas Bill[2], and Götz Seibold[1] — [1]Institut für Physik, BTU Cottbus-Senftenberg, Postfach 101344, 03013 Cottbus, Germany — [2]Department of Physics and Astronomy, California State University, Long Beach, California 90840, USA

Heterostructures made of itinerant ferromagnets and superconductors are studied. In contrast to most previous models, ferromagnetism is not enforced by an effective Zeeman field but induced in a correlated single-band model (CSBM) that displays itinerant ferromagnetism as a mean-field ground state. In this model superconductivity and magnetism are both calculated self-consistently. We calculate the magnitude of the magnetization, the superconducting correlations, and variations of the charge density self-consistently for a superconductingmagnetic bilayer by solving the Bogoliubov-de Gennes equations on a two-dimensional lattice. We determine all three quantities as a function of the Coulomb repulsion U and the ferromagnetic exchange interaction J. The CSBM displays a variety of features not present in the Zeeman exchange model-for example, the occurrence of electronic phase separation and the competition of magnetic and superconducting orders far away from the interface.

TT 49.27 Wed 15:00 Poster D

Coulomb blockade experiments beyond orthodox theory — •Laura Sobral Rey, Susanne Sprenger, and Elke Scheer — Universität Konstanz, 78467 Konstanz, Deutschland

A single electron transistor (SET) can be built by connecting a island with two tunnel junctions to their respective leads and a gate electrode. Previous works were focused on studying all superconducting SET (SSS) [1] or a normal island with superconducting leads (SNS)[2]. The contributions to the current through these devices (related to Coulomb blockade (CB)) are quantitatively covered by the orthodox theory in this weak-coupling regime. The strong-coupling regime can be studied by replacing one tunnel junction by a mechanically controlled break junction (MCBJ) [3]. In this regime, in a SSS SET, new effects not covered by the orthodox theory appear, like for instance multiple Andreev reflection (MAR).

To further investigate the non-orthodox Josephson quasiparticle cycle we design a SSN SET to suppress the Josephson coupling of the island to one of the leads. This should be done by using Cu lead connected to the island by a CuO_x barrier. All the coupling regimes can be addressed by opening or closing the MCBJ: MAR is expected when it's closed and tunnelling transport when it's broken.

[1] R. J. Fitzgerald, Phys. Rev. B 57, R11073(R) (1997)
[2] J.M. Hergenrother, Phys. Rev. Lett. 72, 1742 (1994)
[3] T. Lorenz, J. Low Temp. Phys. 191, 301 (2017)

TT 49.28 Wed 15:00 Poster D

Multi-level Rabi transitions in driven swept-bias Josephson junctions — •Harald Losert[1], Karl Vogel[1], and Wolfgang P. Schleich[1,2] — [1]Institut für Quantenphysik and Center for Integrated Quantum Science and Technology (IQ^{ST}), Universität Ulm, D-89069 Ulm — [2]Institute for Quantum Science and Engineering (IQSE), Department of Physics and Astronomy, Texas A&M University, College Station, TX 77843

Josephson junctions are a well-known model system for the observation of quantum tunneling. The phase difference in a current-biased junction behaves like the position of a particle in a tilted washboard potential.
The escape of this phase-particle from the potential can be explained by quantum tunneling from the ground state, or an excited state. However, it has been shown [1][2], that in the presence of a periodic driving field even a classical theory reproduces the experimental data for quantum mechanical key features, e.g. energy level quantization.
Resuming this discussion, we theoretically investigate the multi-peak structures observed in the switching current distributions of swept-bias experiments. We identify these resonances as (higher order) Rabi oscillations between various energy levels of the washboard potential and suspect that this phenomenon cannot be explained by a classical model.
[1] Marchese *et al.*, Eur. Phys. J. Special Topics **147**, 333 (2007)
[2] Blackburn *et al.*, Phys. Rev. B **85**, 104501 (2012)

TT 49.29 Wed 15:00 Poster D

Gate-tunable supercurrent in epitaxial Al-InAs-based Josephson junctions — •Christian Baumgartner[1], Nicola Paradiso[1], Geoffrey C. Gardner[2], Michael J. Manfra[2,3], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Station Q Purdue, Purdue University, West Lafayette, Indiana 47907, USA — [3]Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907, USA

Coupling an s-wave superconductor to a two-dimensional semiconductor with strong spin-orbit interaction (SOI) offers new technological and research opportunities. Carriers in proximitized semiconductors acquire superconducting correlations while maintaining the charge tunability and the long mean free path typical of high mobility semiconductors. In the presence of strong SOI and an external magnetic field, several exotic phenomena are expected to emerge as, e.g., anisotropic supercurrent and φ_0-Josephson junctions.

We study SNS Josephson junctions where the SC is epitaxial Al and the weak link in between the banks is an InGaAs/InAs 2D electron gas. A challenge in the fabrication of such devices is the etching of the superconductor, which must preserve the high mobility of the 2DEG underneath. We demonstrate several working quantum point contacts and SNS junctions, whose supercurrent can be controlled by gating. A regular Fraunhofer pattern is observed, indicating a good homogeneity of the junction. These results constitute essential building block towards the implementation of more complex topological devices.

TT 49.30 Wed 15:00 Poster D

Josephson current switches on topological insulators — •Oleksii Maistrenko[1], Benedikt Scharf[2], Ewelina Hankiewicz[2], and Dirk Manske[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Institut für theoretische Physik (TP4), Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Magnetic Josephson junctions based on triplet-superconductors, such as Sr_2RuO_4, offer promising possibilities for building several types of Josephson current switches [1]. In topological insulator/superconductor heterostructures, triplet pairing correlations are induced in the Dirac surface states, offering a potential alternative to native triplet-superconductors. Introducing magnetization to the system via an external magnetic field or a nearby ferromagnet changes the spin structure of the anomalous Green's function and hence the superconducting d-vector. We study how this affects charge and spin transport properties of the Josephson junction. We calculate the current phase relation analytically using the Green's function technique and numerically with a tight-binding model. Our model addresses both quantum spin Hall edge states as well as surface states of three-dimensional topological insulators.
[1] B. Kastening, D. K. Morr, D. Manske, K. Bennemann, Phys. Rev. Lett. **96**, 47009 (2006)

TT 49.31 Wed 15:00 Poster D

A superconducting detector that counts microwave photons up to two — •Andrii Sokolov[1,2] and Frank Wilhelm-Mauch[1] — [1]Saarland University, Saarbrücken, Germany — [2]Institute of Physics of the National Academy of Sciences, Kyiv, Ukraine

In the last decade, there has been a substantial interest in Josephson junction based detectors. The detectors that have been demonstrated [1, 4] provide no information besides the presence or absence of photons. However, a number resolving photon detector may be of use for optimal discrimination of coherent states [2], qubit readout [3], and various quantum optics experiments in the microwave domain.

To resolve one- and two-photon inputs, we propose to use a two-photon transition. First, at least two photons are necessary to deliver a click. Then, if the detector does not fire, one can quickly tune it such that a single photon is enough to give a click. Using this method, the vacuum state, single-photon state, and states with two and more photons can be distinguished. We present a theory of our detector and evaluate its performance.
[1] Y.-F. Chen et al., Phys. Rev. Lett. 107, 217401, (2011)
[2] Ch. Wittmann et al., Phys. Rev. A 81, 062338 (2010)
[3] A. Sokolov, Phys. Rev. A 93, 032323 (2016)
[4] A. Opremcak et al., Science 361, 1239 (2018)

TT 49.32 Wed 15:00 Poster D

Chip-based magnetic traps for superconducting levitation of μm-sized particles — •Martí Gutierrez Latorre, David Niepce, Matthias Rudolph, and Witlef Wieczorek — Quantum Technology Laboratory, Chalmers University of Technology, Gothenburg, Sweden

Levitated mechanical resonators are a unique platform capable of reaching unrivaled performance in sensing and, potentially, in realizing macroscopic superposition states. This is based on their expected ultra-low coupling to the environment resulting in unprecedented high mechanical quality factors. As a first step, we develop chip-based magnetomechanical devices for superconducting magnetic levitation. We present FEM simulations of integrated trap architectures for levitation of μm-sized particles. The force on the levitated particle and its potential energy are calculated, showing that trapping frequencies of a few hundreds of kHz are readily achievable. Additionally, we demonstrate the fabrication of integrated magnetic traps and particles made of Nb films on Si substrates via conventional micro-fabrication techniques. Our results pave the way to observing superconducting levitation of μm sized particles at 4K.

TT 49.33 Wed 15:00 Poster D

Nb SQUIDs for the detection of the motion of macroscopic mechanical oscillators — •K. Uhl[1], M. Rudolph[1], J. Hofer[2], J. Slater[2], M. Aspelmeyer[2], C. Schneider[3], M. L. Juan[3], D. Zoepfl[3], G. Kirchmair[3], O. F. Kieler[4], T. Weimann[4], R. Kleiner[1], and D. Koelle[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Vienna Center for Quantum Science and Technology, University of Vienna, Austria — [3]Institute for Experimental Physics, University of Innsbruck, Austria — [4]Fachbereich Quantenelektronik, Physikalisch-Technische Bundesanstalt (PTB) Braunschweig, Germany

Macroscopic mechanical oscillators can be used to investigate fundamental questions in macroscopic quantum physics and for quantum sensing applications. Such systems, however, suffer from decoherence effects, e.g. due to parasitic coupling to the environment or light absorption. Levitating solid-state objects, like a superconducting particle in a magnetic trap or a cantilever with a superconducting strip, offer a unique approach to the realization of nano- or even micro-sized quantum systems with potentially minimal decoherence. In combination with cryogenic temperatures, the coherence times in the quantum mechanical ground state can be increased significantly. To gain information on position and oscillatory behavior, a dc SQUID is employed. To optimize magnetic coupling between oscillator and SQUID, we performed numerical simulations based on London equations and evaluated various SQUID designs The results of the numerical simulations and experimentally determined SQUID performance will be presented.

TT 49.34 Wed 15:00 Poster D

YBCO nanoSQUIDs on bi-crystal MgO — •Jianxin Lin,

Benedikt Mueller, Julian Linek, Max Karrer, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut and Center for Quantum Science (CQ) in LISA+, Universität Tübingen, Germany

We report on the fabrication and characterization of nanopatterned YBa2Cu3O7 (YBCO) dc SQUIDs based on grain boundary Josephson junctions (GBJJs). The nanoSQUIDs are fabricated by epitaxial growth of YBCO films via pulsed laser deposition on MgO bicrystal substrates with 24* misorientation angle. Nanopatterning is performed by Ga focused ion beam (FIB) milling. Due to its much lower dielectric permittivity , as compared to SrTiO3 (STO), the use of MgO substrates avoids a significant stray capacitance of the GBJJs and hence provides nonhysteretic current-voltage characteristics (IVCs) at low temperature (4.2 K), even without a resistively shunting Au layer on top of YBCO. Hence, our approach of using MgO instead of STO offers the potential of achieving a much larger characteristic voltage and therfore a significantly improved noise performance of unshunted YBCO nanoSQUIDs.

On the other hand, the role of Au on top of YBCO as a protection layer during FIB milling has not been clarified yet. Here, we present experimental results on electric trans*port and noise properties of our YBCO nanoSQUDs on MgO that have been fabricated with different Au shunt layer thicknesses or even with*out Au on top of YBCO, and we discuss promising routes to further improve the performance of such YBCO nanoSQUDs.

TT 49.35 Wed 15:00 Poster D

Spectral properties of a SQUID-terminated tunable coplanar resonator at high microwave frequencies — •Sergey Lotkhov — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig Germany

An integrated superconducting circuit including a shunted Josephson junction as an irradiation source and a single-electron transistor as a photon detector (see, e.g., Ref. [1] for a similar setup), was implemented for an $in-situ$ study at $T = 15$ mK and up to $f \sim 100$ GHz of the transmission spectrum of a tunable high-frequency resonator. The resonator was composed of a sub-mm-long coplanar waveguide connected to a magnetic-flux-tunable Josephson interferometer (SQUID). All basic components were made of Aluminum in the same shadow-deposition cycle. The transistor was operated as a threshold-type detector utilizing photon-activated sequences of Cooper pair – Electron cotunneling cycles to produce the current signal. Varying the applied flux $\Phi_{\rm ext}$ over multiple flux quanta Φ_0 demonstrated significant signal suppression within limited, frequency-dependent ranges centered around the frustration points $\Phi_{\rm ext} = \Phi_0(n + 1/2)$. Sharp and almost flux independent geometric resonances were observed outside of the suppression ranges. The reported deep modulation of the transmitted signal is promising for application in fast frequency-selective propagation switches and microwave routing on-chip. The developed chip-scale spectrometric circuit provides an invaluable microwave tool for the point-of-use study of microscopic objects.

[1] B. Jalali-Jafari *etal.*, Appl. Sci. **6**, 35 (2016).

TT 49.36 Wed 15:00 Poster D

Experimental characterization of a wideband Josephson traveling-wave parametric amplifier — •Christoph Kissling, Marat Khabipov, Ralf Dolata, and Alexander B. Zorin — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

A Josephson traveling-wave parametric amplifier was developed and experimentally characterized. The amplifier consists of an array of N=1000-1500 RF-SQUIDs embedded in a coplanar transmission line. With a magnetic field bias, an optimal operation point ensuring a large quadratic and zero cubic nonlinearity in the current-phase relation of the SQUID can be set. Thus, the amplifier operates in a three-wave mixing regime, featuring large separation of pump and signal frequency, high bandwidth at a decent gain, and promisingly quantum-limited noise. The amplifier was realized in Niobium tri-layer technology with different circuit designs. The experimental results will be presented.

TT 49.37 Wed 15:00 Poster D

Dc-SQUID readout with high dynamic range and intrinsic frequency-domain multiplexing capability — •Daniel Richter, Andreas Fleischmann, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Dc superconducting quantum interference devices (dc-SQUIDs) are periodic flux-to-voltage converters whose linear flux range is rather small. For this reason, a flux locked loop (FLL) circuit is typically used to linearize the output signal. At the same time, FLL operation significantly increases the dynamic range if a linear relation between the input and output signal is crucial. However, the measurement of large signals while maintaining the excellent noise performance of SQUIDs sets high demands on the digitizer sampling the SQUID signal in terms of voltage resolution. Furthermore, FLL operation often sets a practical limit for the realization of massive multi-channel SQUID systems since feedback wires have to be routed to every SQUID.

In this contribution, we discuss a SQUID readout approach which relaxes the hardware requirements of a SQUID system while maintaining a linearized output signal and a large dynamic range. At the same time, it allows for reducing the number of wires within multi-channel SQUID systems due to its intrinsic frequency-domain multiplexing (FDM) capability. We introduce the basic concept of our readout approach and demonstrate that it yields a very high dynamic range. Furthermore, we demonstrate its intrinsic FDM-capability using a custom-made four channel multiplexer device.

TT 49.38 Wed 15:00 Poster D

Implementation of coherent cross junctions for superconducting quantum circuits — •Alexander Stehli[1], Hannes Rotzinger[1], Jan Brehm[1], Alexey V. Ustinov[1,2], and Martin Weides[1,3] — [1]Karlsruher Institut für Technologie, Karlsruhe, Deutschland — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia — [3]University of Glasgow, Glasgow, United Kingdom

Josephson tunnel junctions are the centerpiece of almost any superconducting quantum circuit. By harnessing their nonlinear current-phase relation it is possible to engineer various devices with quantum properties, including superconducting qubits. Typically, the Josephson tunnel junctions for these qubits are fabricated using shadow evaporation techniques. However, lately cross and overlap junctions have gained more and more attention. Compared to shadow mask techniques, neither an angle dependent metal deposition nor free-standing bridges or overlaps are needed. This comes at the cost of breaking the vacuum during fabrication, but simplifies their integration in multi-layered circuits, and on larger substrates. Their implementation in coherent quantum circuits has been demonstrated in a recent work [1]. In this work, we implement cross junctions with superconducting transmon qubits and evaluate qubit coherence properties.

[1] Wu *et al.*, Appl. Phys. Lett. **111**, 032602 (2017)

TT 49.39 Wed 15:00 Poster D

Design of a granular aluminium fluxonium qubit with phonon traps — •Alexandru Ionita[1], Martin Spiecker[1], Lukas Grünhaupt[1], Daria Gusenkova[1], and Ioan Pop[1,2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

Fluxonium qubits employing the high kinetic inductance of granular aluminum (grAl) have recently been implemented, demonstrating state of the art coherence. One of the main sources of decoherence can be attributed to non-equilibrium quasiparticles (QPs) inside the grAl superinductance of the qubit. The generation of QPs can be partially traced back to bursts of phonons in the sapphire substrate, of yet unknown origin, which are followed by a slow QP population decay on a characteristic time-scale of 1 second. We present a grAl fluxonium design in a 2D-environment with phonon traps filling the entire waver, potentially decreasing the number of quasiparticle bursts.

TT 49.40 Wed 15:00 Poster D

Cryogenic microwave attenuators — •Julian Ferrero[1], Fabio Henriques[1], Lukas Grünhaupt[1], and Ioan Pop[1,2] — [1]Physikalisches Institut, Karlsruhe Institue of Technology, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institue of Technology, 76344 Eggenstein-Leopoldshafen, Germany

Qubits in cavities show an effective temperature higher than the base temperature of the cryostat due to RF heating from the input line. Usually control and input pulses are thermalized using multiple wideband resistive attenuators fixed at the different cryostat stages.

The dissipated power causes heating in the attenuators. Since the qubit-cavity system is directly connected to the attenuator fixed at the 20 mK stage, any self-heating of the device will have a strong impact on the qubit performance.

In order to adress this problem, we develop fast thermalizing cryogenic attenuators. We present finite element simulations of the thermal and electromagnetic characteristics of the devices based on a low temperature heat transport model.

TT 49.41 Wed 15:00 Poster D

Josephson vortices in a high kinetic inductive environment — •Lukas Powalla[1], Micha Wildermuth[1], Jan Nicolas Voss[1], Yannick Schön[1], Hannes Rotzinger[1], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

The dynamics of Josephson vortices in long Josephson junctions is a well-known example of solitons in physics and allows to study highly nonlinear effects on a mesoscopic scale. A possible path to approach a quantum limit of soliton propagation is to study the Josephson vortices in an environment with high kinetic inductance. We experimentally study long Josephson junctions with electrodes having a large fraction of high kinetic inductance. The kinetic inductance of the electrodes is expected to strongly reduce the Josephson penetration depth and leads to nonlocal electrodynamics of vortices in the junction.
We will present transport measurements of long Josephson junctions with electrodes made from disordered oxidized aluminium and evaluate the influence of high kinetic inductance on the vortex properties.

TT 49.42 Wed 15:00 Poster D

Vortex dynamics in nanoscale Josephson junction parallel arrays — •Micha Wildermuth[1], Amadeus Dieter[1], Lukas Powalla[1], Jan Nicolas Voss[1], Yannick Schön[1], Hannes Rotzinger[1], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow 119049, Russia

A periodic arrangement of Josephson junctions is a toy model to experimentally study topological excitations in spatially modulated systems, e.g., dislocations in crystals, domain walls in various condensed matter systems, and dynamics of nonlinear lattices. Quantum limit for such lattices can be achieved by using ultra-small junctions, with their charging energy being on the order of Josephson energy. Using both ultra-small Josephson tunnel junctions and additional kinetic inductances in the array loops, we approach the quantum regime for both plasma oscillations and Josephson vortices and accompanied the interplay of charges and fluxoids in the array. Here, charge and magnetic flux become quantum-mechanical conjugated variables, wherefore the dynamics of spatially localized fluxoids entail local phase slips and concomitant charge quantum transfer across the junctions.
We present transport measurement of discrete parallel arrays of nanoscale Josephson junctions, observe appealing novel features in the current-voltage characteristics and compare them with the theoretical models.

TT 49.43 Wed 15:00 Poster D

Time resolved quantum sensing of microwave frequencies and fields with transmons — •Maximilian Kristen[1], Andre Schneider[1], Alexander Stehli[1], Tim Wolz[1], Alexey V. Ustinov[1,2], and Martin Weides[1,3] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia — [3]University of Glasgow, Glasgow, UK

Within the last years, quantum sensing has become a steadily growing field of research leading to numerous new technologies. For instance, it was recently demonstrated that off-resonant anharmonic quantum systems, e.g., transmon qubits, work as sensors for extremely weak microwave signals which are usually not measurable with conventional room-temperature electronics due to thermal background noise. However, these spectroscopic proof of principle experiments offered limited precision for reasonable data acquisition times [1]. In this work, we explore the opportunities provided by time resolved measurements. Using Ramsey fringes, we determine the shift of the first and second qubit transition induced by the applied microwave signal. This allows us to infer amplitude and frequency of this signal with a precision of a few MHz. From numerical simulations of the system we find that perturbative treatment of the transmon Hamiltonian yields insufficient results for the sensing scheme at this level of precision. Finally, we discuss the implementation of a phase estimation algorithm, enabling us to further increase the sensitivity and speed of our sensor.
[1] A.Schneider et al., Phys. Rev. A 97, 062334 (2018)

TT 49.44 Wed 15:00 Poster D

Implementing an inductively shunted transmon qubit with tunable transverse and longitudinal coupling — •Daria Gusenkova[1], Nataliya Maleeva[1], Sebastian T. Skacel[1,2], Martin Spiecker[1], Lukas Grünhaupt[1], Susanne Richer[3], David DiVincenzo[3], and Ioan M. Pop[1,2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [3]JARA Institute for Quantum Information, RWTH Aachen University, Germany

The longitudinal qubit-resonator coupling is a prospective alternative to the commonly used transverse coupling scheme. The longitudinal interaction does not lead to the entanglement of qubit and resonator states. In addition to the advantage of a purely QND readout, it allows to build a scalable architecture with strictly local interactions.

We present first results towards the implementation of an inductively shunted transmon qubit with tunable transverse and longitudinal coupling to an embedded harmonic mode. The inductive shunt acts as a coupler and it combines Josephson junction arrays with compact, linear, low-loss inductances, making use of the high kinetic inductance of granular aluminum.

Besides overcoming fabrication challenges, originating from strict requirements on the circuit parameters, the main goal is to suppress phase slips in the JJ array, which prevent tuning to the pure longitudinal coupling regime.

TT 49.45 Wed 15:00 Poster D

Quantization of non-reciprocal, singular superconducting circuits — •Martin Rymarz[1,2] and David DiVincenzo[1,2] — [1]Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany — [2]Peter Grünberg Institut: Theoretical Nanoelectronics, Research Center Jülich, D-52425 Jülich, Germany

Non-reciprocal circuit elements play an essential role for the practical realization of a solid-state quantum computer, independent of the chosen implementation. For that matter, non-reciprocal circuit elements often constitute the interface between the quantum and classical description of an electrical network.

In electrical network theory, the gyrator proposed by Tellegen in 1948 is considered to be the most fundamental non-reciprocal circuit element. The miniaturization of the actual device allows for the description of the gyrator within the lumped element model.

We propose a possible incorporation of the gyrator into circuit Quantum Electrodynamics using node fluxes. In theory effective descriptions of circuits involving gyrators can easily result in singular Lagrangians, which cannot be transformed to the corresponding Hamiltonian using the Legendre transformation since they describe constrained systems. For this reason, a generalization to the quantization of non-reciprocal, singular circuits will be presented, giving rise to physically as well as mathematically interesting models such as the Hofstadter Hamiltonian promising an implementation of the GKP code.

TT 49.46 Wed 15:00 Poster D

Gauge dependence of the two-level approximation in circuit QED — •Marco Roth[1,2], David DiVincenzo[1,2], and Fabian Hassler[1] — [1]Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany — [2]JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, 52428 Jülich, Germany

The Rabi model describes a qubit coupled to a single bosonic degree of freedom. In circuit QED, the qubit is usually obtained by projecting an anharmonic oscillator onto its two lowest eigenstates. This two-level approximation breaks the gauge invariance of the full-system Hamiltonian and results in gauge dependent Rabi models. Although the gauge invariance can be restored by block-diagonalizing the full Hamiltonian prior to the projection, this approach yields a strongly dressed model which lacks the physical interpretability of the Rabi model. We thus perform the block diagonalization perturbatively and investigate the gauge-related effects on different qubits. We find that in many cases, one can find a gauge that requires only a small number of perturbative terms to achieve good agreement between approximated and full Hamiltonian.

TT 49.47 Wed 15:00 Poster D

Calibrating the Individual Properties in Coupled Nonlinear Resonators — •Qi-Ming Chen[1,2], Michael Fischer[1,2,3], Frank Deppe[1,2,3], Michael Renger[1,2], Stefan Pogorzalek[1,2], Edwar Xie[1,2,3], Kirill G. Fedorov[1,2], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der

Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

Precise and effective control of the properties of the individual items in a coupled system is crucial to the study of quantum information and quantum simulation. In a system composed of coupled nonlinear resonators, the tunability of resonance frequency and nonlinearity attracts most interests since it leads to different regimes with significantly different physics. Here we report the local control of two capacitively coupled nonlinear microwave resonators in the driven-dissipative regime. Following calibration, both the frequency and the nonlinearity of the individual resonators can be controlled effectively. The ability to control the local properties of coupled nonlinear resonators paves the way for applications in quantum information and quantum simulation in the future.

We acknowledge support by the German Research Foundation through FE 1564/1-1 and the Excellence Cluster MCQST, the Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (Grant No 820505).

TT 49.48 Wed 15:00 Poster D

Helimagnons meet circuit quantum electrodynamics — •Mohammad T. Amawi[1,2], Philip Schmidt[1,2,3], Aisha Aqeel[2], Christian Back[2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Germany — [2]Physik-Departement, Technische Universität München, Garching, Germany — [3]Nanosystems Initiative Munich, München, Germany

A wealth of hybrid quantum systems is discussed in the context of converting quantum information between various frequency domains, such as from microwave to optical frequencies. Besides conversion concepts based on opto-mechanics or electromechanics, the strong coupling regime of spin excitations interacting with microwave resonators offers an alternative pathway to this goal.

We present a hybrid system consisting of tunable resonators and a helimagnonic mode . The tunable resonator is a superconducting coplanar microwave resonator shunted to ground via a dc-SQUID. Thus the resonator is frequency tunable using a magnetic field bias. At low temperatures and close to zero magnetic field helimagnetic modes form in Cu_2OSeO_3 (CSO) crystals, as the system orders magnetically in a helical spin structure. We investigate the magnetization dynamics of the CSO as millikelvin temperatures using broadband techniques and present initial results regarding the coupling of CSO to flux-tunable microwave resonators.

TT 49.49 Wed 15:00 Poster D

Comparison of superconducting microwave resonators for electron paramagnetic resonance at low tempertures — •Andreas Faltermeier[1,2], Stefan Weichselbaumer[1,2], Matthias Althammer[1,2], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Nanosystems Inititative Munich, München, Germany

Superconducting coplanar microwave resonators are used for various applications, ranging from sensitive radiation detectors to photon storage units required for quantum information processing. All applications rely on a careful tailoring of the resonator. We investigate superconducting microwave resonators made from niobium nitride and niobium grown by ultra-high vacuum sputter deposition with the aim of pursuing electron paramagnetic resonance (EPR) spectroscopy. The geometric layout of our resonator is based on coplanar lumped element design, which guaranatees small mode volumes and large filling factors. Moreover, these resonators have typically ultra-high quality factors. Together, this results in an improved spin sensitivity compared to conventional EPR resonators. We quantitatively compare the performance of the resonator properties for Nb and NbN including the impact of the kinetic inductance. Furthermore, we compare between experimental results with numerical simulations.

TT 49.50 Wed 15:00 Poster D

Entropic measures in propagating quantum microwaves — •Robert Neagu[1,2], Kirill G. Fedorov[1,2], Stefan Pogorzalek[1,2], Qi-Ming Chen[1,2], Michael Fischer[1,2,3], Michael Renger[1,2], Edwar Xie[1,2,3], Achim Marx[1], Frank Deppe[1,2,3], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

Classical information theory is a useful tool to describe the communication, storage, and processing of classical information by exploiting the Shannon entropy. In quantum information theory, similar tasks can be achieved for quantum system by utilizing the von Neumann entropy. Furthermore, quantum correlations lead to additional intriguing effects which can be utilized in various protocols. We experimentally investigate two-mode squeezed (TMS) microwave states as a source of such nonclassical correlations and characterize the latter in terms of different entropic measures. Additionally, we realize a fundamental quantum communication protocol by employing the TMS states and a feedforward. Finally, we relate this quantum communication protocol to an extension of the one-time pad to the quantum regime and investigate the security of the protocol using entropic measures.

We acknowledge support by the German Research Foundation through FE 1564/1-1 and the Excellence Cluster MCQST, the Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (Grant No 820505).

TT 50: Poster Session: Correlated Electrons 2

Time: Wednesday 15:00–18:30 Location: Poster D

TT 50.1 Wed 15:00 Poster D

Competing magnetic orders and spin liquids in three-dimensional quantum magnets — •Finn Lasse Buessen and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Quantum magnetism and the formation of quantum spin liquids remains one of the most intriguing aspects of contemporary solid-state physics, which is corroborated by the high research activity of experimentalists and theorists alike. Candidate materials to host spin-liquid behavior include a variety of two-dimensional compounds, but they also comprise three-dimensional structures. Only recently, interest was sparked by the discovery of spin liquid signatures in $NiRh_2O_4$, a three-dimensional material that realizes spin-1 moments on the diamond lattice with additional frustration mediated by next-nearest neighbor interactions. To complement experimental findings with appropriate theoretical understanding, an efficient methodological framework is vital that is capable of capturing quantum magnetism in three dimensions – a challenging regime, which is inaccessible to many conventional (both numerical and analytical) methods.

In this work, we report on recent methodological advances of the pseudofermion functional renormalization group (pf-FRG), which is suited to describe three-dimensional frustrated quantum magnetism even at finite temperatures, and leverage the method to model the interplay of magnetic order, quantum order-by-disorder, and spin liquids in $NiRh_2O_4$ as well as in other materials.

TT 50.2 Wed 15:00 Poster D

Interaction effects on surface flat bands in 3D Kitaev spin liquids — •Christoph Berke and Simon Trebst — Institut für theoretische Physik, Universität zu Köln

Frustrated quantum magnets can give rise to unconventional spin-liquid ground states. Paradigmatic examples are two- and three-dimensional Kitaev systems that exhibit gapless spin liquids which are best described as Majorana metals that, depending on the underlying lattice structure, exhibit Fermi surfaces, nodal lines or Weyl nodes. Here we will discuss the physics of nodal-line Kitaev spin liquids, which are protected by the particle-hole symmetry inherent to Majorana fermions. Our interest is particularly on the flat-band surface states that accompany these bulk nodal lines. We investigate instabilities of these highly degenerated bands arising from additional spin exchange terms which introduce interactions between the Majorana fermions.

TT 50.3 Wed 15:00 Poster D

Chiral spin liquid phase in a generalized Kitaev model — •Tim Eschmann, Vatsal Dwivedi, Ciarán Hickey, and Simon Trebst — Institute for Theoretical Physics, University of Cologne, Germany

In the field of frustrated magnets, chiral spin liquids are of particular interest for their realization of fractional quantum Hall physics in quantum lattice systems. In this poster, we will discuss the formation of a chiral spin liquid in a generalized Kitaev model on the Shastry-Sutherland lattice. Similar to the original solution for the Kitaev honeycomb model, this five-coordinated lattice allows for an exact solution where the original spin degrees of freedom fractionalize into Majorana fermions and a $\mathbb{Z}_2$ gauge field. Varying the coupling strengths one finds a variety of spin liquid phases, the most interesting one being a spin analog of a second-order topological insulator. Using large-scale sign-problem free quantum Monte Carlo simulations, we identify the thermodynamic signatures of these phases and show that the ordering of the $\mathbb{Z}_2$ gauge field occurs at a particularly high transition temperature.

TT 50.4 Wed 15:00 Poster D

One and two particle excitations in the Kitaev-Heisenberg bilayer — •Erik Wagner and Wolfram Brenig — Institute for Theoretical Physics, Technical UniversityBraunschweig, Braunschweig, Germany

We study the magnetism of a honeycomb Kitaev spin-model with (an-)isotropic intralayer exchange $J_{x,y,z}$, coupled by additional interlayer Heisenberg exchange J to form a bilayer. Starting from the limit of decoupled dimers we use a perturbative continuous unitary transformation (pCUT), based on the flow equation method, to perform series expansion to analyze the spectrum. In particular we consider the groundstate energy and one particle dispersion up to 9th order in $J_{x,y,z}$ as well as the two particle interactions and spectrum up to 6th order. Results for (anti-)bound states will be presented versus anisotropy and for various bilayer-stackings. Known results for the condensation of single particle states [1] will be contrasted to findings from the two particle sector.

[1] U.F.P. Seifert, J. Gritsch, E. Wagner, D.G. Joshi, W. Brenig, M. Vojta, K.P. Schmidt, Phys. Rev. B **98**, 155101 (2018)

TT 50.5 Wed 15:00 Poster D

Thermal transport in the anisotropic two-dimensional Kitaev spin liquid — •Angelo Pidatella[1], Alexandros Metavitsiadis[2], and Wolfram Brenig[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden — [2]Institut für Theoretische Physik, Technische Universität Braunschweig

We investigate the longitudinal thermal transport of the two-dimensional Kitaev spin model on the honeycomb lattice, focusing on the role of anisotropic exchange to cover either gapless or gapped phases of the model. Combining exact diagonalization on small systems with an average gauge configuration approach for up to $\sim O(10^4)$ spinful sites, we report our findings for the thermodynamic properties, the dynamical energy current auto-correlation function, as well as the static dc heat conductivity, over a wide range of temperatures and exchange anisotropies. We find that, despite a thermal gauge-disorder induced pseudogap in the correlation spectra on finite systems, and regardless of the anisotropy, both phases feature normal dissipative transport in the thermodynamic limit, with a low-temperature dependence crossing over from power law to exponentially activated behavior upon entering the gapped phase.

TT 50.6 Wed 15:00 Poster D

Magnetic properties of the Breathing Kagome Lattice $S = 1/2$ XY Model with Four-Site Ring Exchange — •Niklas Casper and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We study the magnetic properties of the breathing kagome lattice $S = 1/2$ XY model with four-site ring exchange. In this trimerized variation, spins which belong to upward or downward facing triangles have different coupling strengths. This model may be of relevance to synthesized vanadium oxyfluoride compound $[NH_4]_2[C_7H_{14}N][V_7O_6F_{18}]$ (DQVOF). Even though it is a frustrated quantum spin model, it does not suffer from the infamous sign problem and can be treated by Quantum Monte Carlo (QMC). In particular, we use the stochastic series expansion (SSE) method which is extended by including a four-site ring exchange term that flips spins on a square plaquette using an update procedure proposed by [1]. Results for thermodynamic properties as well as the structure factor will be presented.

[1] R. G. Melko and A. W. Sandvik, Phys. Rev. E **72**, 026702

TT 50.7 Wed 15:00 Poster D

RIXS on $Ba_3CeIr_2O_9$: an inelastic incarnation of Young's double-slit experiment — •Alessandro Revelli[1], Marco Moretti Sala[2], Giulio Monaco[3], Petra Becker[4], Maria Hermanns[5], Philipp Warzanowski[1], Paul van Loosdrecht[1], Daniel Khomskii[1], Jeroen van den Brink[6], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]ESRF, Grenoble, France — [3]Universita di Trento, Italy — [4]Abt. Kristallographie, Institut fur Geologie und Mineralogie, Universitat zu Köln, Germany — [5]Stockholm University, Sweden — [6]IFW Dresden

Young's archetypal double-slit experiment forms the basis for modern diffraction techniques. We report on an inelastic incarnation of Young's experiment and demonstrate that resonant inelastic x-ray scattering (RIXS) measures interference patterns which reveal the symmetry and character of electronic excited states in the same way as elastic scattering does for the ground state. A prototypical example is provided by the quasi-molecular electronic structure of insulating $Ba_3CeIr_2O_9$ with face-sharing IrO_6 octahedra forming structural Ir dimers. The double 'slits' in this resonant experiment are the highly localized core levels of the two Ir atoms within a dimer. The clear double-slit-type sinusoidal interference patterns that we observe allow us to characterize the electronic excitations. The physics is well described by quasi-molecular orbitals. The ground state shows a spin-orbit-entangled $j = 0$ singlet predominantly built from $j = 1/2$ moments with the corresponding triplet excitation lying at an extraordinarily large energy of 1.2 eV.

[1] A. Revelli *et al.*, Science Advances, in press (2018).

TT 50.8 Wed 15:00 Poster D

j=1/2 moments on the fcc lattice in Ba_2CeIrO_6 — Alessandro Revelli[1], •Chin Chyi Loo[1], Marco Moretti Sala[2], Giulio Monaco[3], Tobias Fröhlich[1], Thomas Lorenz[1], Petra Becker[4], Ladislav Bohatý[4], Dominik Kiese[5], Finn Lasse Büssen[5], Jan Attig[5], Sergey Streltsov[6], Arun Paramekanti[7], Markus Braden[1], Simon Trebst[5], Paul van Loosdrecht[1], and Markus Grüninger[1] — [1]II. Physics Institute, University of Cologne — [2]ESRF, Grenoble, France — [3]Universita di Trento, Italy — [4]Sect. Crystallography, Institute of Geology and Mineralogy, University of Cologne — [5]Institute for Theoretical Physics, University of Cologne — [6]Russian Academy of Sciences, Ekaterinburg, Russia — [7]Department of Physics, University of Toronto, Canada

Spin-orbit-entangled j=1/2 iridates were predicted to host exotic quantum states, e.g. a Kitaev spin liquid. In real materials, deviations from cubic symmetry mix j=1/2 and 3/2 states, which may strongly affect the properties. We establish the double perovskite Ba_2CeIrO_6 as a nearly ideal model system for j=1/2 on an fcc lattice combining geometrical and exchange frustration. XRD finds an average cubic structure, while RIXS reveals the smallest crystal-field splitting observed thus far in $5d^5$ iridates, showing that the ground state has 98.4% j=1/2 character. Significant exchange interactions are supported by the large Curie-Weiss temperature, the dispersion of the j=3/2 states, and DFT results. We estimate the ratio of Kitaev to Heisenberg coupling as K/J=0.1-0.2. Magnetic order sets in at 14 K, while a theoretical study of the J_1-J_2-K model suggests that Ba_2CeIrO_6 is close to a spin liquid.

TT 50.9 Wed 15:00 Poster D

Crystal growth and magnetic characterization of novel kagome-type materials — •Christian Klein[1], Mahmoud Abdel-Hafiez[1,2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt am Main, Max-von-Laue-Straße 1, D-60438 Frankfurt am Main — [2]Department of Physics, Harvard University, 17 Oxford Street, Cambridge, MA 02138

Kagome-lattices are promising materials to investigate frustrated quantum spin systems with a possible quantum spin liquid (QSL) ground state [1].

We report on synthesis and characterization of the spin-1/2 antiferromagnet material Barlowite ($Cu_4(OH)_6BrF$) and the isostructural Cl-analogue Claringbullite ($Cu_4(OH)_6ClF$). The kagome-layers are build up by copper ions and separated from each other through a transition-metal cation, so that a quasi-two-dimensional system is created [2]. Substitution with a non-magnetic ion on the interlayer position leads to a magnetic decoupling between the kagome layers. The synthesis was carried out under hydrothermal conditions [3]. Single Crystals of Claringbullite were obtained as well as polycrystalline samples of the Zn-doped Barlowite. Characterization of the samples was done by

x-ray diffraction, energy dispersive x-ray analysis and thermodynamic measurements for determining the magnetic ground state of these samples and its dependence on the respective substitution level.
[1] P. A. Lee, Science 321, 1306 (2008)
[2] H. Jeschke et al., PRB 92, 094417, (2015)
[3] R. Smaha et al., J. Solid State Chem. 268, 123 (2018)

TT 50.10 Wed 15:00 Poster D

Kagome quantum spin systems in the atacamite family — Pascal Puphal[1], •Katharina M. Zoch[1], Joy Désor[1], Michael Bolte[2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Institut für Organische Chemie der Universität Frankfurt, 60439 Frankfurt am Main, Germany

The atacamite family of compounds presents a rich field of different substitution possibilities based on the three basic polymorphs of $Cu_2(OH)_3Cl$: atacamite, clinoatacamite and botallackite, allowing substitutions both on the Cu and Cl place. We present the hydrothermal synthesis, as well as structural and chemical analysis, of single crystals of $EuCu_3(OH)_6Cl_3$, $Zn_xCu_{4-x}(OH)_6(NO_3)_2$ and haydeeite, and $MgCu_3(OH)_6Cl_2$ compounds, all arising from the atacamite family [1]. Magnetic and specific-heat measurements down to 1.8 K are carried out for these systems. $EuCu_3(OH)_6Cl_3$ has a frustrated antiferromagnetic Cu^{2+} ground state with order at 15 K, and a strong anisotropy and increased magnetization from Van Vleck paramagnetic Eu^{3+} contributions. $ZnCu_3(OH)_6(NO_3)_2$ reveals antiferromagnetic order at 9 K and measurements on haydeeite single crystals confirm the ferromagnetic order at 4.2 K with the easy axis within the kagome plane.
[1] P. Puphal et. al., Phys. Rev. Materials 2, 063402

TT 50.11 Wed 15:00 Poster D

Crystal growth and characterization of the frustrated spin systems $Cs_{2-x}Rb_xCuCl_4$ — •Sarah Krebber, Christian Klein, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt am Main, Max-von-Laue-Straße 1, D-60438 Frankfurt am Main-

Crystals of the antiferromagnetic insulator Cs_2CuCl_4 and the substitution series $(Cs_{2-x}Rb_x)CuCl_4$ (x = 0.1, 0.2) were grown by vertical Bridgman method. The controlled substitution of cesium atoms with the smaller rubidium, causes chemical pressure on the crystal lattice [1]. The essential magnetic units in these systems are Jahn-Teller distorted ($CuCl_4$) tetrahedra, which are arranged in layers separated by the alkali atoms. These layers form a triangular lattice of localized Cu^{2+} spins, where the spins interact through exchange couplings. The resulting geometric frustration leads to quantum spin-liquid properties at low temperatures [2].

In addition to the growth and characterization of $(Cs_{2-x}Rb_x)CuCl_4$, we discuss the structural changes in the lattice parameters and the magnetic behavior of the substituted system in comparison to the well understood parent compound Cs_2CuCl_4.
[1] H. T. Witteveen, D. L. Jongejan and V. Brandwijk, Mater. Res. Bull. 9, 345 (1974)
[2] O. A. Starykh, H. Katsura, and L. Balents, Phys. Rev. B 82, 014421 (2010)

TT 50.12 Wed 15:00 Poster D

Thermal expansion studies on the quantum-spin-liquid candidate $Ca_{10}Cr_7O_{28}$ — •C. Thurn[1], S. Thallapaka[1], U. Tutsch[1], C. Balz[2,3,4], B. Lake[3,4], and M. Lang[1] — [1]PI, Goethe Uni, Frankfurt/M., SFB/TR49, Germany — [2]Oak Ridge National Laboratory, USA — [3]HZ Berlin, Germany — [4]TU Berlin, Germany

In a quantum spin liquid (QSL) strong zero-point fluctuations prevent long-range magnetic order down to lowest temperatures [1]. A common approach for a realization of a QSL is via the help of magnetic frustration of geometric origin. In $Ca_{10}Cr_7O_{28}$ magnetic $S = 1/2$ Cr^{5+}-ions are arranged in distorted kagome bilayers formed by two inequivalent planes of corner-sharing equilateral triangles: an upper triangle coupled ferromagnetically (FM) and a lower triangle coupled antiferromagnetically (AFM) with the FM coupling being dominant. A weak FM inter-plane interaction prevents each plane from reaching its ground state leading to frustration. Previous studies fail to detect any hints of long-range magnetic order down to 19 mK and found persistent spin dynamics down to lowest temperatures [2,3]. Here we present studies of the thermal expansion α and the specific heat C from 1.7 K down to 50 mK for various magnetic fields. For both quantities we find a kink-like anomaly around 0.5 K, indicative of a crossover rather than a phase transition. Measurements of α in low fields reveal a broadening of this feature accompanied by a shift to higher temperatures upon increasing the field, suggesting that FM correlations are at the origin of this feature.
[1] Balents, Nature **464**, 199-208 (2010)
[2] Balz *et al.*, Nat. Phys. **12**, 942-949 (2016)
[3] Balz *et al.*, PRB **95**, 174414 (2017)

TT 50.13 Wed 15:00 Poster D

Anisotropy and spin dynamics in new kagome compound Fe4Si2Sn7O16 — •S. Dengre[1], R. Sarkar[1], J.-C. Orian[2], C. Baines[2], L. Opherden[3], M. Uhlarz[3], T. Herrmannsdörfer[3], T. Söhnel[4], C. D. Ling[5], M. Allision[5], J. Gardner[6], and H.-H. Klauss[1] — [1]Institute of Solid State and Materials Physics, Technical University of Dresden, 01062 Dresden, Germany — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland — [3]Institute of Resource Ecology and Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Germany — [4]School of Chemical Sciences, University of Auckland, Auckland 1142, New Zealand — [5]School of Chemistry, The University of Sydney, Sydney 2006, Australia — [6]Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organization, Menai 2234, Australia

$Fe_4Si_2Sn_7O_{16}$ is a new Fe-based (S=2) kagome compound and a classical analogue of Herbertsmithite. In this work, we analyse $Fe_4Si_2Sn_7O_{16}$ using ^{119,117}Sn NMR, bulk AC - DC susceptibility and μSR. NMR reveals the planar anisotropic nature of the system . Moreover, with AC - DC susceptibility, we identify the presence 2 energy scales, i.e. a spin glass-like state at $\sim$ 3 K and a possible spin liquid state below 500 mK. Eventually, μSR results show a persistent spin dynamics down to 20 mK. In conclusion, we describe a compound characterised by the simultaneous presence of static and dynamic spins, which can serve as a model for further theoretical investigations.

TT 50.14 Wed 15:00 Poster D

Effect of silicon substitution in the spin-ice material $Dy_2Ge_{2-x}Si_xO_7$ — •T. Stöter[1,2,3], M. Antlauf[3,4], L. Opherden[1,2], T. Gottschall[2], J. Hornung[1,2], J. Gronemann[1,2], T. Herrmannsdörfer[2], S. Granovsky[1,3,5], M. Schwarz[3,4], M. Doerr[1,3], H.-H. Klauss[1,3], E. Kroke[3,4], and J. Wosnitza[1,2,3] — [1]Institut für Festkörper- und Materialphysik, TU Dresden — [2]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR — [3]SFB 1143 — [4]Institut für Anorganische Chemie, TU Bergakademie Freiberg — [5]Faculty of Physics, M. V. Lomonossov Moscow State University, Russia

The pyrochlores $R_2X_2O_7$ (R = Ho, Dy, X = Sn, Ti, Ge) have attracted interest for their geometrical frustration from which the spin-ice state emerges. The main parameter of the spin-ice physics is the effective nearest-neighbor interaction resulting from the competition of dipolar and exchange interaction. The strength of these competing interactions strongly depends on the interatomic distances. The germanate pyrochlore $Dy_2Ge_2O_7$ possesses one of the smallest known lattice constants ($a = 9.929$ Å), requiring high pressures over 5 GPa for its synthesis. Here we present results of pyrochlores with even smaller lattice parameter by partially substituting silicon for germanium for which pressures of more than 10 GPa are necessary during preparation. We established via magnetization, ac susceptibility and specific-heat measurements that these new compounds are spin-ices with reduced effective interaction,

TT 50.15 Wed 15:00 Poster D

Low-temperature ^{23}Na NMR on the spin liquid candidate $NaYbO_2$ — •D. Dmytriieva[1,2], K. M. Ranjith[3], S. Khim[3], H. Yasuoka[3], J. Wosnitza[1,2], M. Baenitz[3], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Max Plank Insitute for Chemical Physics of Solids, Dresden, Germany

The planar $J_{\text{eff}} = 1/2$ triangular-lattice magnet $NaYbO_2$ is a rare-earth chalcogenide with delafossite structure of the $R\bar{3}m$ space group. The antiferromagnetically coupled Yb^{3+} ions form perfect triangular layers, well-separated along the c-axis, designating $NaYbO_2$ as a promising quantum spin-liquid candidate. The combination of strong spin-orbit coupling and crystal electric field results in an effective magnetic moment $J_{\text{eff}} = 1/2$ at low temperatures. We present a study of the low-temperature field-induced phase transition to long-range order, probed by ^{23}Na nuclear magnetic resonance (NMR) spec-

troscopy and spin-lattice relaxation-rate measurements on a polycrystalline $NaYbO_2$ sample. In contrast to the related spin-liquid candidate $YbMgGaO_4$, exchange disorder is absent, which is further manifested by the narrow electron-spin resonance lines. A sharp maximum of the ^{23}Na spin-lattice relaxation rate, as well as a minimum of the related stretching exponent, indicates the phase transition to long-range order in applied finite fields ($\mu_0 H > 1$ T).

TT 50.16 Wed 15:00 Poster D

High-field ESR studies of the honeycomb-lattice material α-$RuCl_3$ — •A. Ponomaryov[1], E. Schulze[1,2], J. Wosnitza[1,2], P. Lampen-Kelley[3,4], A. Banerjee[5], J.-Q. Yan[4], C.A. Bridges[6], D.G. Mandrus[3], S.E. Nagler[5], and S.A. Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, USA — [4]Department of Materials Science and Engineering, University of Tennessee, Knoxville, USA — [5]Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, USA — [6]Chemical Science Division, Oak Ridge National Laboratory, Oak Ridge, USA

We present results of high-field high-frequency electron spin resonance (ESR) studies of the honeycomb-lattice magnet α-$RuCl_3$ for two principle magnetic-field orientations up to 16 T. For both orientations,$H \parallel [100]$ and $H \parallel [110]$, the polarization dependences are studied. It was found that in contrast to $H \parallel [100]$, the gap at $H \sim 7$ T remains open for $H \parallel [110]$. Peculiarities of the spin dynamics in α-$RuCl_3$ are discussed.

This work was supported by DFG (project ZV 6/2-2 and SFB 1143).

TT 50.17 Wed 15:00 Poster D

Multipolar ordered magnetic ground state of the triangular Ising antiferromagnet $TmMgGaO_4$ — •A. Hauspurg[1,2], L. Opherden[1], S. Chattopadhyay[1], M. Uhlarz[1], T. Herrmannsdörfer[1], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany

$TmMgGaO_4$ is a quasi-two-dimensional triangular spin system with Ising anisotropy. As a sister compound of $YbMgGaO_4$, which recently was identified as a spin liquid material, it turned out to show a different magnetic ground state at low temperatures. In terms of an almost absent zero-point entropy and distinct anomalies in ac susceptibility a variety of exotic magnetically ordered multipolar phases is observed at very low temperatures. In our work, we present latest results of ac-susceptibility and vector-magnetometry experiments performed on single-crystalline $TmMgGaO_4$ at lowest temperatures and up to high magnetic fields.

TT 50.18 Wed 15:00 Poster D

Exploring the magnetism of the new frustrated $S = 1$ isolated spin-triangle system BHAP-Ni_3 — •S. Chattopadhyay[1], B. Lenz[2], S. Kanungo[3], S. K. Panda[2], S. Biermann[2,5], W. Schnelle[6], K. Manna[6], M. Uhlarz[1], Y. Skourski[1], T. Herrmannsdorfer[1], R. Patra[4], and J. Wosnitza[1,7] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, Germany — [2]Centre de Physique Théorique, Ecole Polytechnique, France — [3]School of Physical Sciences, IIT Goa, India — [4]Department of Chemistry and Centre for Advanced Studies in Chemistry, Panjab University, India — [5]Collège de France, Paris, France — [6]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [7]Institut für Festkörper- und Materialphysik, TU Dresden, Germany

We report a combined experimental and theoretical study on the new frustrated quantum-magnet BHAP-Ni_3 synthesized in single-crystalline form. BHAP-Ni_3 provides an ideal opportunity to study the magnetism of a frustrated spin-triangle unit as it is comprised of spin-1 triangles where each triangle is essentially magnetically isolated. Our pulsed-field magnetometry reveals the presence of an exotic state that stabilizes a pronounced 2/3 magnetization plateau between 7 and 20 T. AC-susceptibility measurements performed down to 60 mK show the absence of magnetic order or a glassy state in this material. The magnetic ground state is found to be disordered and specific-heat measurements show a gapped nature of spin excitations. Our theoretical modeling suggests that the 2/3 plateau originates from the interplay between Heisenberg and biquadratic spin-spin interactions.

TT 50.19 Wed 15:00 Poster D

Phase diagram of the natural mineral green dioptase $Cu_6[Si_6O_{18}]\cdot 6H_2O$ — •Erik Schulze[1,2], Alexey N. Ponomaryov[1], Denis I. Gorbunov[1], Toshihiro Nomura[1], Sergei Zherlitsyn[1], Jochen Wosnitza[1,2], Andrey Podlesnyak[3], and Sergei A. Zvyagin[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Dresden, Germany — [3]Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

We present combined high-field ultrasound, magnetization, and electron spin resonance studies of the natural mineral green dioptase ($Cu_6[Si_6O_{18}]\cdot 6H_2O$). This material orders antiferromagnetically below $T_N = 14.5$ K, forming a spiral chain structure with a propagation vector along the c axis. Although a ferromagnetic interaction in the ab plane couples the system into a three-dimensional framework, the material shows clear signatures of large quantum fluctuations, suggesting the low-dimensional nature of the spin correlations. The obtained phase diagram, studied in magnetic fields up to 80 T, reveals several magnetic phases, whose peculiarities are discussed.

This work was supported by Deutsche Forschungsgemeinschaft (project ZV 6/2-2).

TT 50.20 Wed 15:00 Poster D

Magnetic and ultrasound investigation of the frustrated magnet $Nd_2Zr_2O_7$ at low temperatures. — •Y. Gritsenko[1,2,3], M. Ciomaga Hatnean[4], O. A. Petrenko[4], G. Balakrishnan[4], S. Zherlitsyn[3], and J. Wosnitza[1,2,3] — [1]SFB 1143, Dresden — [2]Institut für Festkörper- und Materialphysik, TU Dresden — [3]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Germany — [4]Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom

We report ultrasound and magnetic property studies of large high-quality single crystals of the frustrated magnet $Nd_2Zr_2O_7$, with pyrochlore structure. The temperature dependence of the magnetic susceptibility and the acoustic properties show no magnetic ordering down to 0.5 K. Fits to the magnetic-susceptibility data using a Curie-Weiss law reveal a ferromagnetic coupling between the Nd moments. Magnetization versus field measurements show a local Ising anisotropy along the <111> axes of the Nd^{3+} ions in the ground state. We performed ultrasound measurements for c_{44} acoustic mode (with wave vector parallel to [110], and polarization along [001]), with magnetic field applied along the [110] direction. We observed distinct anomalies below 1 K. A sharp minimum at about 0.25 T suggests a field-induced phase transition.

TT 50.21 Wed 15:00 Poster D

Investigation of the magnetic interactions in the tripod-Kagome compound $Mg_2Gd_3Sb_3O_{14}$ by electron spin resonance experiments — •Christoph Wellm[1,2], Julian Zeisner[1,2], Mihai Sturza[1], Gaël Bastien[1,2], Sebastian Gass[1], Anja U.B. Wolter[1], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 — [2]Institut für Festkörper-und Materialphysik, TU Dresden, D-01062

As an example of a class of geometrically frustrated magnetic systems, the so-called tripod Kagome materials have been suggested as an interesting target of experimental investigation due to the frustrated nature and the question of dimensionality of the magnetic interactions. In our work we performed high-field electron spin resonance measurements on a powder sample of $Mg_2Gd_3Sb_3O_{14}$, a representative of a quasiclassical Heisenberg magnet, where the effect of spin-orbit coupling of Gd^{3+} ions vanishes to first order. Measurements were conducted over a frequency range of 70-420 GHz and temperatures ranging from 3-50 K. The Gaussian lineshape is consistent with a model of dominant dipolar spin-spin interactions, while the growing asymmetry of the lineshape upon decrease of temperature signifies an increase of an effective internal field, an indication of increasing short-range spin-spin-correlations. Such a behavior is typical for frustrated systems, making our studies one of the first to reveal such significant features in this family of materials. Furthermore, temperature dependent critical broadening of the linewidth and increase of the internal field strength provide insights into the dimensionality of the spin-spin correlations.

TT 50.22 Wed 15:00 Poster D

Unveiling the QSL ground state: An optical study on $Cu_5V_2O_{10}(CsCl)$ — •Tobias Biesner[1], Andrej Pustogow[1,2], Hong Zheng[3], John F. Mitchell[3], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]UCLA Physics and Astronomy, USA — [3]Materials Science Division, Argonne

National Laboratory, USA

The copper oxide Averievite $Cu_5V_2O_{10}(CsCl)$ hosts highly frustrated $S = 1/2$ kagome planes connected in 3D by a honeycomb sublattice. Due to the large intra- and interlayer coupling of the magnetic copper ions, the material possesses an antiferromagnetic ground state ($T_N = 24$ K). By replacing Cu ions within the honeycomb lattice by Zn, the kagome planes decouple and the long-range magnetic order is suppressed, glancing at the celebrated quantum spin liquid.

We present a comprehensive optical study on $Cu_{5-x}Zn_xV_2O_{10}(CsCl)$ for various Zn substitutions $x \leq 1.25$ in a broad range of frequencies from the THz region to the visible range and down to $T = 10$ K. Comparing our experimental results with the recent band structure calculations, we elaborate the rich electronic structure and the possible low-energy excitations.

TT 50.23 Wed 15:00 Poster D

The complex magnetic phase diagram of clinoatacamite — •Jannis Willwater[1], Jan Lennart Winter[1], Leonie Heinze[1], Dirk Menzel[1], Stefan Süllow[1], Manfred Reehuis[2], Fabiano Yokaichiya[2], Ralf Feyerherm[2], Harald O. Jeschke[3,4], and Roser Valentí[4] — [1]IPKM, TU Braunschweig, Braunschweig, Germany — [2]HZB, Berlin, Germany — [3]Okayama University, Okayama, Japan — [4]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Frankfurt, Germany

The natural mineral clinoatacamite ($Cu_2Cl(OH)_3$) has been discussed as geometrically frustrated magnet. The Cu^{2+} ions form a system of kagome layers with an antiferromagnetic in-plane coupling. This 2-dimensional geometrical frustration may lead to exotic quantum states at low temperatures.

Here, we present an extensive study using different experimental methods that reveal a complex magnetic phase diagram of the material at low temperatures. The measurements of the specific heat, magnetic susceptibility and magnetization as well as neutron scattering experiments indicate the existence of three phase transitions. Neutron scattering, specific heat and magnetization suggest a canted ferromagnetic order beneath the first transition at 6.4 K. A second transition seen by specific heat is close by in zero field at 6.6 K, but strongly field dependent. By specific heat and susceptibility a third transition at 18.2 K is identified. The nature of the latter two transitions are unknown yet and require further investigations.

TT 50.24 Wed 15:00 Poster D

Ground-state phase diagram of the frustrated spin-$\frac{1}{2}$ two-leg honeycomb ladder — Qiang Luo[1], Shijie Hu[2], Jize Zhao[3], •Alexandros Metavitsiadis[4], Sebastian Eggert[2], and Xiaoqun Wang[5,6] — [1]Department of Physics, Renmin University of China, Beijing 100872, China — [2]Department of Physics and Research Center Optimas, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — [3]Center for Interdisciplinary Studies, Lanzhou University, Lanzhou 730000, China — [4]Institute for Theoretical Physics, Technical University Braunschweig, 38106 Braunschweig, Germany — [5]Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), School of Physics and Astronomy, Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai 200240, China — [6]Collaborative Innovation Center for Advanced Microstructures, Nanjing 210093, China

We investigate a spin-1/2 two-leg honeycomb ladder with frustrating next-nearest-neighbor (NNN) coupling along the legs, which is equivalent to two J_1-J_2 spin chains coupled with $J_\perp$ at odd rungs. The full parameter region of the model is systematically studied using conventional and infinite density-matrix renormalization group as well as bosonization. We find a rich phase diagram consisting of five distinct phases. In addition, we fully analyze the universalities of the critical phase transitions.

TT 50.25 Wed 15:00 Poster D

Bose condensation of squeezed light — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics-UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

Light with an effective chemical potential and no mass is shown to possess a general phase-transition curve to Bose-Einstein condensation. This limiting density and temperature range is found by the diverging in-medium potential range of effective interaction. While usually the absorption and emission with Dye molecules is considered, here it is proposed that squeezing can create also such an effective chemical potential. The equivalence of squeezed light with a complex Bogoliubov transformation of interacting Bose system with finite lifetime is established with the help of which an effective gap is deduced. This gap phase creates a finite condensate in agreement with the general limiting density and temperature range. The phase diagram for condensation is presented due to squeezing and the appearance of two gaps is discussed.

[1] arXiv:1809.09525

TT 50.26 Wed 15:00 Poster D

Laser Control of Topological Polaritons — •Damian Hofmann and Michael Sentef — Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany

Polaritons are quasiparticles consisting of a superposition of photons and excitons. We study a semiconductor microcavity system in which multiple semiconductor layers are coupled to a single photonic mode. A momentum-dependent complex phase in the exciton-photon coupling gives rise to non-trivial topological properties of the polariton bands. In particular, the system possesses chiral edge modes which can be excited by optical pumping near the sample boundary.

We simulate the dynamics of the driven system in the semi-classical approximation using a Gross-Pitaevskii-type equation. This allows us to study topologically protected chiral transport along the edges of a finite sample. We further discuss the dynamics of a lattice version of the topological polariton model, from which we obtain time-resolved spectral information and demonstrate the selective excitation of the edge modes.

TT 51: Focus Session: Broken Time Reversal Symmetry in Multiband Superconductors

A broken time-reversal symmetry (BTRS) superconducting state is observed for several unconventional superconductors (SC) such as Sr_2RuO_4, SrPtAs, and UPt_3. This state can be described as a coherent chiral state of degenerate order parameter symmetries such as p_x +/- i p_y or $d_{x^2-y^2}$ +/- d_{xy} which form since they avoid the formation of node lines on the Fermi surface. The main experimental evidence for BTRS SC comes from the observation of a polar Kerr effect and the appearance of small static internal magnetic fields in muon spin relaxations measurements at zero external field below T_c. However, a clear experimental proof for a specific order parameter symmetry is difficult. Recently, a new strategy has been developed to identify these states in Sr_2RuO_4 by applying uniaxial strain which triggered many new experimental studies in this field. For multi-band iron-based superconductors a new route to chiral sc order parameters based on the frustrated competition of different sc phases has been proposed. This state is now found in the hole-doped $B_{1-x}K_xFe_2As_2$ system.

Organized by: Hans-Henning Klauss (TU Dresden), Ilya Eremin (RU Bochum), Dimitry V. Efremov (IFW Dresden)

Time: Thursday 9:30–13:00 Location: H2

Invited Talk TT 51.1 Thu 9:30 H2 **Evaluation of chiral superconductivity in Sr_2RuO_4** —

•Clifford Hicks — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Sr_2RuO_4 is among the very few superconductors that may have a chiral order parameter. Evidence for chirality comes from Kerr effect, muon spin rotation, and junction critical current measurements. One fundamental consequence of a chiral order parameter is that uniaxial stress, by lifting the tetragonal symmetry of the unpressurised lattice, should lift the degeneracy of the x and y components of the chiral order, resulting in a split transition. In this talk, I will discuss results of a set of measurements performed on uniaxially pressurised Sr_2RuO_4: scanning SQUID microscopy, heat capacity, and muon spin rotation. I will present an evaluation of chiral superconductivity in Sr_2RuO_4 taking these new results into account.

Invited Talk TT 51.2 Thu 10:00 H2

Magnetic excitations and their possible role in the superconducting pairing in Sr_2RuO_4 — •Markus Braden[1], Stefan Kunkemöller[1], Kevin Jenni[1], Paul Steffens[1,2], Yvan Sidis[3], Zhiqiang Q. Mao[4], Yoshiteru Maeno[5], and Igor Mazin[6] — [1]University of Cologne, Germany — [2]Institut Laue Langevin, France — [3]Laboratoire Léon Brillouin, France — [4]Tulane University, USA — [5]Kyoto University, Japan — [6]Naval Research Laboratory, USA

The mechanism of the unconventional superconductivity in Sr_2RuO_4 is subject of ongoing debate opposing the impact of antiferromagnetic (AFM) and ferromagnetic (FM) fluctuations. Indirect evidence for FM fluctuations can be deduced from the metallic FM $SrRuO_3$, while isovalent Ca_2RuO_4 is an AFM Mott insulator [1]. With the recent progress in inelastic neutron scattering, we could follow the AFM signal associated with quasi-one-dimensional bands across the superconducting transition down to very low energies. Even well below twice the superconducting gap, there is no change in the magnetic response in Sr_2RuO_4 [2], which seems incompatible with the picture of a large gap on these Fermi-surface sheets. The quantitative analysis of FM fluctuations in Sr_2RuO_4 was performed with polarized neutron scattering yielding good agreement with reports of specific heat, magnetic susceptibility and NMR. Incorporating this ferromagnetic response into the BCS gap equation, however, does not stabilize a triplet pairing [3].

[1] S. Kunkemöller et al., Phys. Rev. Lett. 115, 247201 (2015)
[2] S. Kunkemöller et al., Phys. Rev. Lett. 118, 147002 (2017)
[3] P. Steffens et al., arXiv1808.05855

Invited Talk TT 51.3 Thu 10:30 H2

Topologically protected Bogoliubov Fermi surfaces — •Daniel Agterberg[1], Philip Brydon[2], Henri Menke[2], and Carsten Timm[3] — [1]Department of Physics, University of Wisconsin - Milwaukee — [2]Department of Physics and MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Otago — [3]Institute of Theoretical Physics, Technische Universität Dresden

It is commonly believed that, in the absence of disorder or an external magnetic field, there are two possible types of nodal superconducting excitation gaps: the gap has point nodes or it has line nodes. Here, we show that, for an even-parity nodal superconducting state which spontaneously breaks time-reversal symmetry, the low-energy excitation spectrum generally does not belong to either of these categories; instead, it has extended Bogoliubov Fermi surfaces. These Fermi surfaces are topologically protected from being gapped by a non-trivial Z_2 invariant. In this talk, I will discuss the physical origin, topological protection, and energetic stability of these Bogoliubov Fermi surfaces, using chiral superconductivity in $j = 3/2$ fermions as a representative example.

15 min. break.

Invited Talk TT 51.4 Thu 11:15 H2

Time-reversal symmetry breaking in Fe-based superconductors — •Andrey Chubukov — University of Minnesota, Minneapolis, MN USA

I will discuss different scenario for time-reversal symmetry breaking in the superconducting state of Fe-based high Tc superconductors. I will review earlier works on s+id and s+is states and discuss recent theoretical and experimental results suggesting possible realization of time-reversal symmetry breaking nematic superconducting state in FeSe.

Invited Talk TT 51.5 Thu 11:45 H2

Emerging superconductivity with broken time reversal symmetry inside a superconducting s-wave state — •Vadim Grinenko[1,2], Rajib Sarkar[1], Philipp Materne[1], Kunihiro Kihou[3], Chul-Ho Lee[3], Saicharan Aswartham[2], Igor Morozov[2,4], Bernd Buechner[2], Ruben Huehne[2], Nielsch Kornelius[2], Konstantin Nenkov[2], Dmitriy Efremov[2], Stefan-Ludwig Drechsler[2], Paul Chekhonin[1], Werner Skrotzki[1], Vasiliy Vadimov[5], Mihail Silaev[6], Pavel Volkov[7], Ilya Eremin[7], Hubertus Luetkens[8], and Hans-Henning Klauss[1] — [1]TU Dresden, Germany — [2]IFW Dresden, Germany — [3]AIST, Tsukuba, Japan — [4]Lomonosov Moscow State University, Russia — [5]Institute for Physics of Microstructures, Russia — [6]University of Jyvaskyla, Finland — [7]Ruhr-Universitat Bochum, Germany — [8]PSI, Switzerland

In general, magnetism and superconductivity are antagonistic to each other. However, there are several families of superconductors, in which superconductivity may coexist with magnetism, and only a few examples are known, when superconductivity itself induces a magnetism. Here, we report the finding of a narrow dome of a novel $s + is'$ superconducting (SC) phase with broken time-reversal symmetry (BTRS) inside the broad s-wave SC region of the centrosymmetric multiband superconductor $Ba_{1-x}K_xFe_2As_2$ ($0.7 \lesssim x \lesssim 0.8$). The BTRS dome appears very close to a Lifshitz transition. With this, we experimentally demonstrate the emergence of a novel quantum state at topological changes of the electronic system [1].

[1] Phys. Rev. B 95, 214511 (2017); arXiv: 1809.03610 (2018)

TT 51.6 Thu 12:15 H2

Muon spin relaxation studies of Sr_2RuO_4 under uniaxial stress — •Shreenanda Ghosh[1], Rajib Sarkar[1], Vadim Grinenko[1], Jean-Christophe Orain[2], Felix Brückner[1], Artem Nikitin[2], Joonbum Park[3], Mark Barber[3], Dmitry Sokolov[3], Naoki Kikugawa[4], Jake Bobowski[5], Yoshiteru Maeno[6], Hubertus Luetkens[2], Andrew Mackenzie[3], Clifford Hicks[3], and Hans-Henning Klauss[1] — [1]Institute for Solid state and Materials Physics, TU Dresden, Gerrmany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Villigen, Switzerland — [3]Physics of Quantum Materials, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]National Institute for Materials Science, Tsukuba, Japan — [5]University of British Columbia, Canada — [6]Kyoto University, Japan

To probe its superconducting order parameter, we have performed muon spin relaxation(μSR) measurements on samples of Sr_2RuO_4 placed under uniaxial stress. Previous studies on unstressed Sr_2RuO_4 have revealed enhanced relaxation in the superconducting state, which is interpreted as evidence for a chiral $p_x \pm ip_y$ order parameter. With this order parameter, uniaxial stress is expected to induce a splitting between T_c and the onset of chirality. μSR requires large samples, so to perform these measurements. We have developed piezoelectric-based apparatus [1] capable of applying forces of up to ~ 700 N and using it we have increased T_c from 1.4 K up to 2.1 K. First set of results will be presented, from μSR experiments under different strain.

[1] C. Hicks et al., JPS Conf. Proc. **21**, 011040 (2018)

TT 51.7 Thu 12:30 H2

Unconventional pairing states based on first-principles — •Balazs Ujfalussy[1], Gabor Csire[1,2], and James Annett[2] — [1]Wigner Research Centre for Physics, Budapest, Hungary — [2]University of Bristol, Bristol, United Kingdom

We have combined the relativistic spin-polarized version of Korringa-Kohn-Rostoker method for the solution of the Dirac-Bogoliubov-de Gennes equations with a semiphenomenological parametrization of the pairing interaction. We employ this method to both $LaNiGa_2$ and its non-centrosymmetric relative $LaNiC_2$ which show spontaneous magnetism in the superconducting state. Based on symmetry considerations it was already shown that the breaking of time-reversal symmetry is only compatible with non-unitary triplet pairing states in these crystals. Our method allows to study different on-site triplet equal-spin pairing models involving the first-principle band structure. We compare our predictions for the temperature dependence of the specific heat and it is found that it can be described by an interorbital equal-spin pairing on the nickel which breaks the time-reversal symmetry. It is shown that this pairing induces nodeless, two-gapped quasiparticle spectrum and finite magnetisation due to the redistribution of Cooper pairs in spin space. The method is also applied for Nb/Au/Fe system where we show that the existence of spin-polarized quantum well states can lead to FFLO-like oscillations of the order parameter in the normal metal.

TT 51.8 Thu 12:45 H2

Anomalous Nonlocal Conductance in Superconductor/Ferromagnets Hybrids with Chiral p-wave pairing symmetry — •Satoshi Ikegaya and Dirk Manske — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

Finding a smoking-gun signature of chiral Majorana edge states is an urgent issue in physics of Sr_2RuO_4, which is a promising candidate material of intrinsic chiral p-wave superconductors. Thus far, the zero-bias conductance peak in the tunneling transport has been experimentally observed. However, the zero-bias conductance peak is not a conclusive evidence for the chiral Majorana edge states because it can be induced by any type of topologically protected edge states.

In this work, we demonstrate that the chiral nature of Majorana edge states is drastically manifested in nonlocal conductance in a junction consisting of a chiral p-wave superconductor and two ferromagnetic leads. The nonlocal conductance in the present junction is insensitive to the distance between the two leads and is sensitive to the chirality of the pair potential. These two drastic features enable us to identify the moving direction of the chiral Majorana edge states in the single experimental setup only by changing the lead wire to which the bias voltage is applied. We propose a smoking-gun experiment for detecting the chiral Majorana edge states in the chiral p-wave superconductor.

TT 52: Quantum Impurities and Kondo Physics

Time: Thursday 9:30–12:45 Location: H7

TT 52.1 Thu 9:30 H7

Drag of quantum impurities — •Falko Pientka[1,2], Ovidiu Cotlet[3], Richard Schmidt[2,4], Gergely Zarand[5], Eugene Demler[2], and Atac Imamoglu[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Physics, Harvard University, Cambridge, Massachusetts, USA — [3]Institute of Quantum Electronics, ETH Zurich, Zurich, Switzerland — [4]Max Planck Institute of Quantum Optics, Garching, Germany — [5]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Hungary

I will discuss transport of a mobile quantum impurity immersed in a moving bath. At strong interactions, the polaronic dressing of the impurity leads to a novel drag force exerted on the impurity by the bath. This drag force is absent for classical impurities and originates from coherent scattering events.

I will highlight experimental consequences of this effect for exciton polaritons in semiconductors, where the drag force allows for the control of photons by dc electric and magnetic fields as if they were charge carriers. Finally, I will mention an experiment which has recently demonstrated polariton drag in dc electric fields.

TT 52.2 Thu 9:45 H7

Conventional and ferromagnetic Kondo regimes in frustrated quantum dot trimers coupled to ferromagnetic lead — •Krzysztof Wójcik[1] and Ireneusz Weymann[2] — [1]Institute of Molecular Physics, Polish Academy of Sciences, 60-179 Poznań, Poland — [2]Faculty of Physics, Adam Mickiewicz University, 61-614 Poznań, Poland

Quantum dot trimers coupled to the metallic lead through one of the quantum dots are known to exhibit the quantum phase transition between the conventional anti-ferromagnetic Kondo regime and the ferromagnetic Kondo regime [1,2]. For geometrically symmetric case, the transition is protected by the symmetry arising from frustration in the nanostructure and has a level-crossing nature. On the contrary, for asymmetric trimers the level crossing may be avoided and the transition becomes of Kosterlitz-Thoules type [2,3]. In our contribution we examine the fate of this transition in the presence of ferromagnetic lead. We show that in the particle-hole symmetry (PHS) case the results remain qualitatively the same as in the non-magnetic case, and focus on presenting the consequences of the exchange field arising in the frustrated nanostructure outside the PHS point.

[1] A. K. Mitchell, T. F. Jarrold, D. E. Logan, Phys. Rev. B **79**, 085124 (2009).
[2] A. K. Mitchell, T. F. Jarrold, M. R. Galpin, D. E. Logan, J. Phys. Chem. B **117**, 12777 (2013).
[3] P. P. Baruselli, R. Requist, M. Fabrizio, E. Tosatti, Phys. Rev. Lett. **111**, 047201 (2013).

TT 52.3 Thu 10:00 H7

Conductance of a molecular double-quantum dot in the Kondo regime: Effects of the Dzyaloshinskii-Moryia interaction — •Peter Zalom, Richard Korytár, and Tomáš Novotný — Charles University, Prague, Czech Republic

Motivated by a recent experiment in a molecular junction [1], we investigate a double-dot singlet-triplet model in the Coulomb blockade by the means of a numerical renormalization group. We confirm that the magnetic-field induced degeneracy leads to a Kondo effect [2], which is perturbatively stable when Dzyaloshinskii-Moryia interaction (DMI) is included. Strong DMI suppresses the Kondo resonance in the differential conductance and leads to a non-trivial temperature dependence.

[1] M. Koole, J. C. Hummelen, H. S. van der Zant, Phys. Rev. B 94, 165414 (2016)
[2] M. Pustilnik, L. Glazman, Phys. Rev. B 64, 045328 (2001)

TT 52.4 Thu 10:15 H7

Heat and charge transport in a charge 2-channel Kondo setup — •Lars Fritz[1], Gerwin van Dalum[1], and Andrew Mitchell[2] — [1]Institute for Theoretical Physics and Center for Extreme Matter and Emergent Phenomena, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands — [2]School of Physics, University College Dublin, Dublin 4, Ireland

In this talk we describe charge and heat transport in a charge 2-channel Kondo setup. Charge transport in such a device has been measured recently and is theoretically well understood. We extend this work to study heat transport at the 2-channel non-Fermi liquid fixed point and find that the Wiedemann-Franz law is obeyed. We furthermore describe the Fermi liquid crossover towards the Kondo screened fixed point at which Wiedemann-Franz is violated. We end by connecting our findings at the non-Fermi-liquid fixed point to the Majorana character of the effective description of the critical point and argue that heat transport gives access to their central charge.

TT 52.5 Thu 10:30 H7

Exploring Kondo lattices with inequivalent Ce-sites — Jiří Pospíšil, Jiří Prchal, and •Jeroen Custers — Dept. of Condensed Matter Physics, Charles University, Ke Karlovu, 5, 121 16 Praha, Czech Republic

Strongly correlated electron systems with competing interactions provide a fertile ground for discovering exotic states of matter. As a particularly interesting setting we study heavy fermion (HF) systems with two crystallographically inequivalent local moment sites. These may lead to the formation of two Kondo sublattices with largely different Kondo temperatures. We expect such systems to show better tunability towards various kinds of quantum phase transitions than single-site Kondo systems, and to form novel phases. Here we present recent results on selected compounds, like Ce_3Al_{11} [1], Ce_3PtIn_{11} [2,3] and other. Ce_3PtIn_{11} is highly interesting as it shows coexistence of antiferromagnetism ($T_N = 2$ K) and superconductivity ($T_c = 0.32$ K). From entropy analysis it has been speculated that in this compound the Ce_I (2 ions) remains paramagnetic and at lower T evokes superconductivity while the Ce_{II} site is responsible for the magnetic ordering. Furthermore we will discuss several pressing questions: Do the two Kondo scales compete or cooperate? Can the interplay lead to Kondo breakdown, partially screened phases, or even fractionalized Fermi liquids?

[1] A. Berton *et al.*, J. Magn. Magn. Mat. **15-18,** 379 (1980)
[2] M. Kratochvílová *et al.*, J. Cryst. Growth **387**, 47 (2014)
[3] J. Prokleška *et al.*, Phys. Rev. B **92,** 161114(R) (2015)

TT 52.6 Thu 10:45 H7

Quantum Monte Carlo study of the SU(N) Kondo Lattice Model — •Marcin Raczkowski and Fakher Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The two-dimensional half-filled Kondo lattice model with exchange J features a quantum phase transition which stems from the competition between the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction and the Kondo screening. Quantum Monte Carlo (QMC) simulations predict that below the magnetic energy scale T_{RKKY}, the single-particle gap scales as J. This contrasts with an exponentially small gap in paramagnetic large-N and dynamical mean-field theories which omit spatial fluctuations. Here, we perform zero-temperature QMC simulations of the SU(N) symmetric Kondo lattice model and elucidate necessary conditions for recovering the large-N limit.

TT 52.7 Thu 11:00 H7

Heavy quasiparticle bands in the underscreened quasiquartet Kondo lattice — •Alireza Akbari[1] and Peter Thalmeier[2] — [1]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Korea — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

We study the quasiparticle spectrum in an underscreened Kondo-lattice (KL) model that involves a single spin degenerate conduction band and two crystalline-electric-field (CEF) split Kramers doublets coupled by both orbital-diagonal and non-diagonal exchange interactions. We find the three quasiparticle bands of the model using a constrained fermionic mean field approach. While two bands are similar to the one-orbital model a new genuinely heavy band inside the main hybridization gap appears in the quasiquartet model. Its dispersion is due to effective hybridization with conduction states but the bandwidth is controled by the size of the CEF splitting. Furthermore several new indirect and direct hybridztion gaps may be identified. By solving the selfconsistency equation we calculate the CEF-splitting and exchange dependence of effective Kondo low energy scale, hybridization gaps and band widths. We also derive the quasiparticle spectral densities and their partial orbital contributions. We suggest that the two-orbital KL model can exhibit mixed CEF/Kondo excitonic magnetism.

[1] Phys. Rev. B 98, 155121 (2018)

15 min. break.

TT 52.8 Thu 11:30 H7

Many-body approach to Luttinger's theorem of the Kondo lattice — •Steffen Sykora[1] and Klaus W. Becker[2] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Institut für Theoretische Physik, TU Dresden, 01062 Dresden, Germany

A numerical verification of Luttinger's theorem, based on a recently developed many-body approach, is given for the Kondo-lattice model. For a two-dimensional lattice the completely localized spins ($S = 1/2$) are found to contribute to the Fermi sea volume as if they were electrons, which is in agreement with Oshikawa's topological proof of Luttinger's theorem. Underpinning this result we show results of the momentum-resolved one-particle spectral function where nearly dispersionless excitations appear clearly below the Fermi level for different values of the conduction electron filling. Numerical integration over momentum and energy always leads to the correct particle number of the localized spins according to the well-accepted picture of a large Fermi surface. To our knowledge, the present study is the first many-body approach, which is able to reproduce the correct value of Luttinger's theorem for this model.

TT 52.9 Thu 11:45 H7

Mutual information in a frustrated Kondo lattice model — •Toshihiro Sato, Francesco Parisen Toldin, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

A key notion in heavy fermion systems is the entanglement between conduction electrons and localized spin degrees of freedom. To study these systems from this point of view, we investigate the mutual information in a half-filled Kondo lattice model with geometrical frustration. In addition to the conventional Kondo insulating and antiferromagnetic phases, frustration leads to a so called partial Kondo screened phase [T. Sato, F. F. Assaad, T. Grover, Phys. Rev. Lett. 120, 107201 (2018)]. Using a negative-sign-free auxiliary field quantum Monte Carlo approach, we demonstrate that the area law coefficient of the mutual information shows sharp crossovers (on our finite lattices) at quantum phase transitions. Furthermore, and deep in the respective phases, it can be understood in terms of a product wave function [1].

[1] F. Parisen Toldin, T. Sato, F. F. Assaad, arXiv:1811.11194 (2018)

TT 52.10 Thu 12:00 H7

M-edge RIXS as a probe of coherent dynamics in strongly hybridized Kondo systems — •Marein Rahn[1], Eric Bauer[1], Jon Lawrence[2], Filip Ronning[1], and Marc Janoschek[3] — [1]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [2]Department of Physics and Astronomy, University of California, Irvine, CA 92697, USA — [3]Laboratory for Neutron Scattering, ETH Zürich and Paul Scherrer Institute, CH-5232 Villigen, Switzerland

In rare earth intermetallics with a Kondo energy scale that is much larger than magnetic interactions or crystal field splittings, the screening of local moments leads to a non-magnetic Fermi liquid ground state. The corresponding electronic fluctuations between magnetic and non-magnetic valence configurations renormalize the charge and spin excitations. Due to recent instrumental advances in high-resolution soft resonant inelastic x-ray scattering (RIXS), Kondo phenomena on the order of 30 meV have become accessible to this new spectroscopic technique. The observation of a pronounced momentum-space dependence of the corresponding f-f inter-band transitions points to the fact that, at low temperature, the lattice character of the dense Kondo system is imprinted onto the local screening process. This aspect goes beyond traditional impurity-based theoretical approaches, and would instead require a computation of the RIXS response on the basis of a strongly hybridized electronic band structure (as achieved by LDA+DMFT). With the interest to work towards a universal quantitative model of these three spectroscopies, we present our recent insights from RIXS, photoemission and inelastic neutron scattering.

TT 52.11 Thu 12:15 H7

Residual Conduction in Kondo Insulators — •Emanuele Maggio, Matthias Pickem, and Jan Tomczak — Institute of Solid State Physics, TU Wien, A-1040 Vienna, Austria

Correlated narrow-gap semiconductors [1] display a pronounced tendency towards resistivity saturation at low temperatures. Especially in heavy-fermion Kondo insulators, the persistence of residual conduction is a long-standing puzzle. Theories of conventional semi-conductors hint at extrinsic impurity-states. Complementarily, it has recently been suggested that certain Kondo insulators may harbour surface states that are protected by topological properties of their bulk electronic structure [2]. Experimentally, there is contrasting evidence (e.g., [3]), insinuating that the nature of conducting states in Kondo insulators may be non-universal. In this contribution, we put forward a new interpretation: we attribute the deviation from activated behaviour in the resistivity to short-comings of the relaxation-time approximation in the calculation of transport properties for correlated materials. Based on a dynamical mean-field theory description and a new linear-response transport scheme, we investigate Ce-based Kondo insulators*such as the prototypical $Ce_3Bi_4Pt_3$. Finding overall good agreement with experiment, we characterise the resistivity in terms of a crossover temperature T* marking the onset of saturation. Studying its control parameters, we delineate the applicability of our scenario to other systems.

[1] J. M. Tomczak, J. Phys.: Condens Mat 30, 183001 (2018)
[2] M. Dzero et al., Phys. Rev. Lett. 104, 106408 (2010)
[3] N. Wakeham et al., Phys. Rev. B 94, 035127 (2016)

TT 52.12 Thu 12:30 H7

Possible topological effects seen by ESR in the Kondo insulator SmB_6 doped by Gd. — Jean Carlo Souza[1,2], P.F.S. Rosa[3], •Jörg Sichelschmidt[1], S. Wirth[1], Z. Fisk[4], and P.G. Pagliuso[1] — [1]MPI for Chemical Physics of Solids, Dresden — [2]Instituto de Física "Gleb Wataghin", UNICAMP, Campinas, SP, Brazil — [3]Los Alamos National Laboratory, New Mexico 87545, USA — [4]Department of Physics and Astronomy, University of California, Irvine, USA

We utilized Electron spin resonance (ESR) as a microscopic technique to explore the spin dynamics of Gd^{3+} substituted in the Kondo insulator SmB_6. For Gd concentrations larger than 400 ppm the ESR spectra at $T < 30$ K acquire a typical metallic line shape while the resistivity shows a Kondo-insulating bulk material. This demonstrates that the hybridization gap is closing locally around the Gd-site. For highly diluted Gd (200 ppm) the spectral shapes are affected by the diffusive transport of spins near the surface. The dependence on temperature, magnetic field, and microwave power provides a link between this diffusive ESR line shape to the presence of topological surface states. A similar result was reported for anomalous diffusive ESR effects for Nd^{3+} in the semimetal YBiPt [1]. Moreover, the temperature dependence of these diffusive ESR effects is similarly seen in the surface

response of scanning tunneling spectroscopy [2].
[1] G. G. Lesseux et al., J. Phys. Condens. Matter 28, 125601 (2016)
[2] L. Jiao et al., Nat. Commun. 7, 13762 (2016)

TT 53: Frustrated Magnets - Strong Spin-Orbit Coupling (joint session TT/MA)

Time: Thursday 9:30–13:00 Location: Theater

TT 53.1 Thu 9:30 Theater

Dimerization of the honeycomb iridate α-Li_2IrO_3 under pressure — •Jihaan Ebad-Allah[1,2], V. Hermann[1], M. Altmeyer[3], F. Freund[1], A. Jesche[1], A. A. Tsirlin[1], M. Hanfland[4], P. Gegenwart[1], I. I. Mazin[5], D. I. Khomskii[6], R. Valenti[3], and C. A. Kuntscher[1] — [1]Universität Augsburg, 86159 Augsburg, Germany — [2]University of Tanta, 31527 Tanta, Egypt — [3]Goethe- Universität Frankfurt, 60438 Frankfurt am Main, Germany — [4]European Synchrotron Radiation Facility, BP 220, 38043 Grenoble, France — [5]Code 6393, Naval Research Laboratory, Washington DC 20375, USA — [6]Universität zu Köln, 50937 Köln, Germany

The honeycomb iridates A_2IrO_3 (A= Na, Li) show novel behavior and phases arising from the competition between spin-orbit coupling, magnetization, and dimerization. Here, we show the results of x-ray diffraction and optical spectroscopy measurements under pressure on α-Li_2IrO_3 and Na_2IrO_3 single crystals. In α-Li_2IrO_3, a pressure-induced dimerization of Ir-Ir bonds is observed at P_c=3.8 GPa, concomitant with anomalies in the optical response, while in Na_2IrO_3 this transition is expected at a much higher pressure [1]. The results are discussed in terms of the effect of Ir-Ir bonds on the magnetic and electronic properties and compared to other honeycomb materials.
[1] V. Hermann et al., Phys. Rev. B **97**, 020104(R) (2018)

TT 53.2 Thu 9:45 Theater

Fingerprints of Kitaev physics in RIXS on Na_2IrO_3 and α-Li_2IrO_3 — •Alessandro Revelli[1], Marco Moretti Sala[2], Giulio Monaco[3], Maria Hermanns[4], Petra Becker[5], Ladislav Bohatý[5], Friedrich Freund[6], Anton Jesche[6], Philipp Gegenwart[6], Paul van Loosdrecht[1], Jeroen van den Brink[7], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]ESRF, Grenoble, France — [3]Universitá di Trento, Italy — [4]Stockholm University, Sweden — [5]Abt. Kristallographie, Institut fur Geologie und Mineralogie, Universität zu Köln, Germany — [6]Experimentalphysik VI, Universität Augsburg, Germany — [7]IFW Dresden, Germany

The honeycomb iridates Na_2IrO_3 and α-Li_2IrO_3 are discussed as candidate materials for hosting Kitaev physics. We study the magnetic excitations in these compounds by resonant inelastic x-ray scattering (RIXS) at the Ir L_3 edge, searching for experimental fingerprints of Kitaev physics. In both compounds, we find a broad continuum of excitations centered at q=0. This continuum survives up to 300 K, roughly 20 times the magnetic ordering temperature. The dynamical structure factor shows that spin-spin correlations are restricted to nearest neighbors, a characteristic property of the Kitaev model. Also the polarisation dependence agrees with an interpretation in terms of bond-directional Kitaev exchange interactions.

TT 53.3 Thu 10:00 Theater

Thermodynamic evidence for proximity to the Kitaev QSL in A_2IrO_3 (A = Na, Li) — •Kavita Mehlawat[1,2], A Thamizhavel[3], and Yogesh Singh[1] — [1]Department of Physical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Knowledge City, Sector 81, Mohali 140306, India. — [2]Leibniz Institute for Solid State and Materials Research IFW Dresden, 01069 Dresden, Germany — [3]Department of Condensed Matter Physics and Material Sciences, Tata Institute of Fundamental Research, Mumbai 400005, India

The honeycomb lattice iridates A_2IrO_3 (A = Na, Li) are candidates for the realization of the Kitaev-Heisenberg model although their proximity to Kitaev's quantum Spin-Liquid (QSL) is still debated. We report on heat capacity C and entropy S_{mag} for A_2IrO_3 (A = Na, Li) in the temperature range 0.075 K $\leq T \leq$ 155 K [1]. We find a two-peak structure for the magnetic heat capacity C_{mag} for both materials and S_{mag} shows a plateau between the peaks with a value close to $\frac{1}{2}$Rln2. These features signal the fractionalization of spins into Majorana Fermions close to Kitaev's QSL as predicted recently [2, 3]. These results provide the first thermodynamic evidence for the proximity of A_2IrO_3 to the Kitaev QSL [1].

Financial support: Hallwachs-Röntgen Postdoc Program, UGC-CSIR India.
[1] K. Mehlawat, A. Thamizhavel, and Y. Singh, Phy. Rev. B 95, 144406 (2017)
[2] J. Nasu, M. Udagawa, and Y. Motome, Phys. Rev. B 92 115122 (2015)
[3] Y. Yamaji, T. Suzuki, T. Yamada, S. I. Suga, N. Kawashima, and M. Imada, Phys. Rev. B 93, 174425 (2016)

TT 53.4 Thu 10:15 Theater

Copper and zinc iridates - new derivatives of the β-Li_2IrO_3 structure — •Alexander O. Zubtsovskii and Alexander A. Tsirlin — EP VI, EKM, University of Augsburg, Germany

Lithium and sodium iridates (A_2IrO_3 where A = Li, Na) form a narrow group of real-world material prototypes of the Kitaev model on the honeycomb and 3D honeycomb-like lattices. Tuning their properties by suitable chemical substituions remains a challenging problem, because only a few A_2IrO_3 iridates can be obtained by high-temperature solid synthesis. Here, we report two new compounds based on the β-Li_2IrO_3 structure and obtained by low-temperature ionic exchange of the Li^+-ions for the nonmagnetic (Zn^{2+}) and magnetic (Cu^{2+}) ions. Crystal structures refined using synchrotron X-ray diffraction data suggest the same motif of IrO_6 octaedra as in the parent compound, but with different positions of Cu^{2+} and Zn^{2+} compared to Li^+. We further report magnetic susceptibility data and discuss the nature of magnetism in these new compounds.

TT 53.5 Thu 10:30 Theater

Microscopic study of the Kitaev material β-Li_2IrO_3 under pressure and magnetic field — •Mayukh Majumder[1], Markus Pritz-Zwick[2], Tushar Kanti Dey[1], Rudra Sekhar Manna[1], Gediminas Simutis[3], Jean-Christophe Orain[3], Friedrich Freund[1], Rustem Khasanov[3], Pabitra Kumar Biswas[4], Norbert Büttgen[2], Aleaxander Tsirlin[1], and Philipp Gegenwart[1] — [1]EP VI, University of Augsburg — [2]EP V, University of Augsburg — [3]PSI, Switzerland — [4]ISIS Pulsed Neutron and Muon Source, UK

β-Li_2IrO_3 with Ir^{4+} moments on a three-dimensional hyperhoneycomb lattice belongs to the class of much-discussed Kitaev materials [1]. At zero-field and ambient pressure, it displays a phase transition at 38 K to an incommensurate non-coplanar and counter-rotating spiral magnetic state [2]. Application of magnetic fields exceeding 2.8 T along the easy *b*-axis transforms the ground state into a partially polarized quantum paramagnet, which we characterize by thermodynamic as well as ^{7}Li NMR experiments. Furthermore, long-range order (at zero-field) can also be suppressed by the application of hydrostatic pressure. We also discuss our comparative study of bulk and μSR experiments under pressure, which reveal a first-order transition at 1.4 GPa giving way to a new ground state with the coexistence of dynamically correlated and frozen spins [3]. No accompanying structural transition was found and further characterization by ^{7}Li NMR experiments under pressure is intended.

Work supported by DFG through TRR 80.
[1] Phys. Rev. Lett. 114, 077202 (2015)
[2] Phys. Rev. B 90, 205116 (2014)
[3] Phys. Rev. Lett. 120 237202 (2018)

TT 53.6 Thu 10:45 Theater

Structural and magnetic properties of antifluorite $(NH_4)_2IrCl_6$: Candidate J_{eff}=1/2 Mott insulator — •Nazir Khan, Anton Jesche, and Alexander A. Tsirlin — EP VI, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Ammonium hexachloroiridate, $(NH_4)_2IrCl_6$, possesses a face centered cubic (fcc) lattice of the antifluorite K_2PtCl_6-type with isolated and regular $IrCl_6$ octahedra at high temperatures. The lattice symmetry and the 5d magnetic ion (Ir^{4+}) render realization of ideal J_{eff}=1/2 moment on the frustrated fcc lattice that has been predicted to host rich magnetic phases driven by Heisenberg and Kitaev exchanges. Using synchrotron X-ray powder diffraction and dilatometry, we inves-

tigate structural effects in $(NH_4)_2IrCl_6$ at low temperatures and in applied magnetic fields. Magnetization measurements indicate long-range antiferromagnetic ordering sets in below T_N=2.2 K. The field dependence of magnetization suggests a field induced magnetic phase transition at a critical field which depends on the crystallographic directions. The estimated effective magnetic moment seems consistent with the J_{eff}=1/2 picture. However, dilatometry shows a sharp drop in the length change along the <111> direction just below T_N. This indicates a possible lattice distortion at low temperature which may result in a deviation from the ideal J_{eff}=1/2 ground state. Magnetostriction measurements show that the field induced magnetization in the compound is strongly coupled to its lattice.

TT 53.7 Thu 11:00 Theater

Syntheses and magnetic properties of two sodium ruthenates: Na_3RuO_4 and Na_2RuO_3 — •Vera P. Bader, Alexander Tsirlin, Anton Jesche, and Philipp Gegenwart — EP VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Ruthenates show a diversity of magnetic phenomena, e.g. due to strong Ru-O covalency in the case of Ru^{5+} [1] and due to the non-magnetic $J = 0$ state potentially leading to Van Vleck excitons in Ru^{4+} [2]. Additionally, geometrical frustration may affect the magnetic properties. We focus on two ruthenates with the Ru-ions in the oxidation state 5+ and 4+, respectively. In Na_3RuO_4 the $Ru^{5+}O_6$ octahedra condense into tetramers which are composed of two equilateral triangles. In Na_2RuO_3 the Ru^{4+} ions form honeycomb layers. We prepare powder samples of Na_3RuO_4 via solid state reaction in a controlled atmosphere. The measurement of the magnetic susceptibility shows an antiferromagnetic transition at 30 K and suggests suppression of the magnetic order. Specific heat measurements reveal two consecutive phase transitions at 25 K and 28 K. Na_2RuO_3 powder is synthesized by thermal decomposition of a precursor in argon. Due to the layered structure the compound is prone to stacking faults. To improve the quality of the sample different synthesis routes have been compared.

[1] A. Hariki *et al.*, PRB 96, 155135 (2017)
[2] G. Khaliullin, PRL 111, 197201 (2013)

15 min. break.

TT 53.8 Thu 11:30 Theater

Bilayer Kitaev models: Phase diagrams and novel phases — •Urban F. P. Seifert[1], Julian Gritsch[2], Erik Wagner[3], Darshan G. Joshi[4], Wolfram Brenig[3,1], Matthias Vojta[1], and Kai P. Schmidt[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [2]Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Germany — [3]Institut für Theoretische Physik, Technische Universität Braunschweig, Germany — [4]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

We study the fate of $\mathbb{Z}_2$ spin liquid phases in differently stacked bilayer versions of Kitaev's honeycomb model. Increasing the inter-layer Heisenberg coupling $J_\perp$ (at fixed Kitaev couplings $K^{x,y,z}$) eventually destroys the topological spin liquid in favor of a paramagnetic dimer phase. We establish phase diagrams as a function of $J_\perp/K$ and Kitaev coupling anisotropies using Majorana-fermion mean-field theory, and employ different expansion techniques in the limits of small and large $J_\perp/K$. For strong anisotropies, we use effective models for the different layer stackings to discuss the quantum phase transition out of the Kitaev phase. The phase diagrams depend sensitively on the nature of the stacking and anisotropy strength. In some stackings and at strong anisotropies we find a single transition between the Kitaev and dimer phases. Importantly, for other stackings we prove the existence of two novel macro-spin phases which can be understood in terms of Ising chains which can be either coupled ferromagnetically, or remain degenerate, thus realizing a classical spin liquid. We also suggest the existence of a flux phase with spontaneous inter-layer coherence.

TT 53.9 Thu 11:45 Theater

Magnetic Frustration in Cd-substituted $HoInCu_4$ — Maximilian Wolf[1], Christina Baumeister[1], Sebastian Bachus[1], Jens-Uwe Hoffmann[2], Oliver Stockert[3], and •Veronika Fritsch[1] — [1]EP 6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

$HoInCu_4$ is one of the rare examples of a partially frustrated magnetic metal [1, 2], due to the Ho ions forming an fcc lattice, with alternating antiferromagnetic planes along [100], which are separated by frustrated planes. The substitution of In with Cd in $HoInCu_4$ yields a breakdown of magnetic frustration, resulting for $HoCdCu_4$ in a fully ordered magnetic structure of ferromagnetic planes, stacked antiferromagnetically along the [111] direction [3, 4]. We have investigated the evolution of magnetic order and magnetic frustration in $HoIn_{1-x}Cd_xCu_4$ with thermodynamic and transport measurements at low temperatures. Our data indicate the presence of a bicritical point between the frustrated and the unfrustrated phase. Furthermore we present neutron-diffraction data on single crystals of $HoInCu_4$ showing enhanced diffuse scattering as a consequence of magnetic frustration.

[1] V. Fritsch *et al.* PRB **71**, 132401 (2005)
[2] O. Stockert *et al.* unpublished
[3] V. Fritsch *et al.* PRB **73**, 094413 (2006)
[4] O. Stockert *et al.*, Experimental Report, MLZ Garching (2017)

TT 53.10 Thu 12:00 Theater

Discovery of kagome spin ice with crystallized magnetic monopoles in intermetallic compound HoAgGe — •Kan Zhao and Philipp Gegenwart — Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Spin ices are exotic phases of matter characterized by frustrated spins obeying local ice rules that minimize the number of spatially isolated magnetic monopoles, in analogy with the electric dipoles in water ice. In two dimension (2D), one can similarly define ice rules for in-plane Ising-like spins arranged on a kagome lattice, which require each triangle plaquette to have a single monopole, and can lead to a variety of unique orders and excitations at different temperatures.

By integral experimental and theoretical approaches including single crystal synthesis, magnetometry, thermodynamic measurements, neutron scattering and Monte Carlo simulations, we establish the intermetallic compound HoAgGe as the first example of crystalline (i.e. non-artificial) kagome spin ice[1]. It features a variety of partial and fully ordered states and sequence of field-induced phases at low temperatures, all consistent with the kagome ice rule. The multi-stage ordering behavior characteristic of kagome ice are further confirmed by specific heat and magnetic entropy data. Our discovery provides unique possibilities for the study of two-dimensional spin-ice physics.

[1] Zhao, K. et al. submitted (2018)

TT 53.11 Thu 12:15 Theater

Field-induced phases in extended Kitaev models: Insights from hidden symmetries and relevance for real materials — •David Kaib, Stephen Winter, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt

At zero magnetic field, Kitaev's honeycomb model hosts a Z_2 spin liquid with itinerant Majorana fermions. We study a field-induced intermediate phase (IP) in the antiferromagnetic (AFM) Kitaev model, which has been discussed in terms of a gapless $U(1)$ spin liquid [1-3].

In order to characterize the IP, we consider various dynamical correlations, calculated via exact diagonalization (ED). By analyzing hidden symmetries of the model, we discuss which general nonuniform fields retain the IP, and introduce nonuniform fields that relate the field-response of the AFM model to the FM model. Within ED resolution, we find that the IP could represent a line of critical points within the parameter space of such fields.

At last, we turn to models with extended interactions, in order to relate to real materials. Since the candidate materials are thought to realize ferromagnetic (FM) coupling, we identify an extended model with FM Kitaev coupling, that is dual to the pure AFM Kitaev model, and study its vicinity to Hamiltonians of real materials.

[1] C. Hickey et al., arXiv:1805.05953
[2] H.-C. Jiang et al., arXiv:1809.08247
[3] L. Zou et al., arXiv:1809.09091

TT 53.12 Thu 12:30 Theater

Excitations in the high magnetic field phase of the putative Kitaev material $RuCl_3$ — •Anuja Sahasrabudhe[1], Raphael German[1], Thomas C. Keothe[1], Jonathan Buhot[2], Vladimir Tsurkan[3], Alois Loidl[3], Petra Becker[1], Markus Grüninger[1], and Paul H.M. van Loosdrecht[1] — [1]Universität zu Köln, II. Physikalisches Institut. — [2]Radboud University Nijmegen, HMFL. — [3]Universität Augsburg, Institut für Physik.

$RuCl_3$ is discussed as one of the closest realizations of a J=1/2 Kitaev system on a hexagonal lattice. Yet it shows antiferromagnetic (AF) ordering at low temperature signaling the presence of important inter-

actions in addition to the anisotropic Kitaev interactions. AF order can be suppressed by an external magnetic field. The phase diagram and the behavior in high fields are vividly discussed. Here, we probe the magnetic excitation spectrum of $RuCl_3$ with Raman spectroscopy in high magnetic fields. The observed high field excitation spectra yield a detailed insight into the nature of the high field phase.

TT 53.13 Thu 12:45 Theater

Heat transport in the putative Kitaev-Heisenberg spin liquid α-$RuCl_3$ under high magnetic fields — •Matthias Gillig[1], Xiaochen Hong[1], Richard Hentrich[1], Federico Caglieris[1], Maryam Shahrokhvand[2], Uli Zeitler[2], Maria Roslova[3], Anna Isaeva[3], Thomas Doert[3], Bernd Büchner[1], and Christian Hess[1] — [1]Leibniz Institute for Solid State and Material Research Dresden, Germany — [2]HFML, Radboud University, Nijmegen, Netherlands — [3]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany

α-$RuCl_3$ is due to the honeycomb structure of its Ru-sites and the exchange frustration a prime candidate to realize the Kitaev model in a material. The model bears interesting physics with a quantum spin liquid (QSL) ground state and exotic excitations. Although α-$RuCl_3$ orders antiferromagnetically (AFM) below 7 K, indications of a QSL were found experimentally.

We have performed heat transport measurements on α-$RuCl_3$ down to $T = 0.4$ K and up to $B = 33$ T. Below $T = 4$ K thermal conductivity κ is raised in low magnetic fields up to 5 T before it decreases again to a minimum at 8 T. This decline coincides with the suppression of the AFM phase. For $B > 8$ T, κ is strongly enhanced for all temperatures and no sign of saturation is observed. The increase of thermal conductivity can be assigned to a field-induced phase featuring a field-dependent excitation spectrum. More specifically the data suggest the opening of a spin excitation gap which reduces the phononic scattering rate. For the whole T- and B-range investigated the data are consistent with a pure phononic heat transport mechanism.

TT 54: Correlated Electrons: Complex Oxides and Other Materials

Time: Thursday 9:30–13:00 Location: H22

TT 54.1 Thu 9:30 H22

Study of the correlation effects in single-crystal $TbFeO_3$ — •Alexander Engelhardt[1], Georg Benka[1], Christian Oberleitner[1], Andreas Bauer[1], Johanna Jochum[2], Andreas Erb[3] und Christian Pfleiderer[1] — [1]Physik Department E51, Technische Universität München, D-85748 Garching, Germany — [2]Technische Universität München, Heinz Maier-Leibnitz Zentrum, Lichtenbergstraße 1, 85748 Garching, Germany — [3]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meißner-Str. 8, D-85748 Garching, Germany

Single crystals of the multiferroic rare earth orthoferrite $TbFeO_3$ have been grown by means of the optical floating zone method. Using measurements of the magnetization, ac susceptibility and specific heat we have studied the complex, anisotropic magnetic phase diagram of $TbFeO_3$ for magnetic fields up to 9 T applied along all three major crystallographic axes. In particular, our findings may help to shed light on the nature and origin of the various magnetic phase transition and crossovers observed as a function of magnetic field and temperature.

TT 54.2 Thu 9:45 H22

Fluctuation regime based on dimer correlations in a novel $s = 1/2$ spin chain compound with $(IO_3)^-$ as stereochemically active lone pair group — Eleni Mitoudi-Vagourdi[1], Vladimir Gnezdilov[2,3], Dirk Wulferding[2,4], •Peter Lemmens[2,4], Karina V. Lamonova[5], Yurii Pashkevich[5], Reinhard Kremer[6], and Mats Johnsson[1] — [1]Dept. of Chem., Stockholm Univ., Stockholm, Sweden — [2]IPKM, TU-BS, Braunschweig, Germany — [3]ILTPE, Kharkov, Ukraine — [4]LENA, TU-BS, Braunschweig, Germany — [5]Galkin DonFTI, Kyiv, Ukraine — [6]MPI-FKF, Stuttgart, Germany

The novel iodate $KCu(IO_3)_3$ contains spin chains formed by $[CuO_6]$ octahedra, corner sharing with $[IO_3]$ groups. This leads to an oxygen plane around each Cu ion and two apical oxygens with larger Cu-O distances along chains. The resulting Cu binding potential is rather soft and allows pronounced fluctuations. Based on thermodynamic and Raman scattering data we give evidence for Cu dimer fluctuations, their commensurate lock-in, and long range ordering with a sequence of characteristic temperatures, $T_N = 1.3\text{K} < T_{JT} = 175\text{K} < T^* = 200\text{K}$.

Work supported by QUANOMET NL-4, DFG LE967/16-1, and NTH Contacs in Nanosystems.

TT 54.3 Thu 10:00 H22

Percolation of frustrated polarons in the doped perovskite cobaltite $La_{1-x}Sr_xCoO_{3-\delta}$ — •Peter P. Orth[1], Daniel Phelan[2], Chris Leighton[3], and Rafael Fernandes[3] — [1]Iowa State University, USA — [2]Argonne National Laboratory, USA — [3]University of Minnesota, USA

Due to fascinating phenomena such as magneto-electronic phase separation and Co ion spin-state transitions, the archetypal cobaltite $La_{1-x}Sr_xCoO_{3-\delta}$ (LSCO) remains of high interest. Chemical substitution of La by Sr introduces both holes and magnetic moments into the diamagnetic parent compound. The tendency of Co to undergo spin-state transitions leads to the formation of 7-site spin polarons. Further doping results in a glassy magnetic state that transforms at x=0.18 into a ferromagnetic metal. As simple statistical considerations predict a percolation of polarons at much smaller values of x=0.05, this raises the question what suppresses the formation of ferromagnetism. Here, we address this question within a microscopic model capturing both competing magnetic interactions between the Co moments in different spin states as well the spatial inhomogeneity introduced by disorder. Large-scale parallel tempering classical Monte-Carlo simulations reveal that the origin of the delayed percolation transition lies in the frustration of ferromagnetic polarons via competing (anti-)ferromagnetic interactions. Our simulations explicitly show how frustrated polarons act as seeds of the observed magneto-electronic phase separated glassy state at intermediate doping $0.05 < x < 0.18$, providing a consistent microscopic understanding across the full doping range.

TT 54.4 Thu 10:15 H22

Tuning the electronic structure of $LaNiO_3$ heterostructures — •Jasmin Jandke[1], Muntaser Naamneh[1], Marco Caputo[1,2], Eduardo B. Guedes[1,2], Anna Zhakarova[1], Cinthia Piamonteze[1], Nicholas C. Plumb[1], Ming Shi[1], and Milan Radovic[1] — [1]Photon Science Department, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland — [2]Institute of Condensed Matter Physics, Ecole Polytechnique Fédrale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Since many years rare earth nickelates ($RNiO_3$) attract researchers interests due to their wide variety of fascinating physical properties which are tunable by the interplay of electron correlations and crystal structure [1]. It was suggested that the tunability of electron correlations could be used to induce a cupratelike Fermi surface in $RNiO_3$ thin films. Motivated by this, we are investigating the evolution of the electronic structure of $LaNiO_3$ (LNO) thin films in proximity to manganite layers (strontium and calcium doped lanthanum manganite - LSMO and LCMO) grown on STO and NGO substrates. The films were grown by pulsed laser deposition (PLD). The combined study of angle resolved photoemission spectroscopy (ARPES), transport properties and X-ray magnetic circular dichroism (XMCD) reveal an anomalies around T=50K and T=150K as well as a strong dependence on the substrate. Understanding these properties could be crucial for tuning the nickelates towards superconductivity.

[1] J. Chaloupka et al., Phys. Rev. Lett. 100, 016404 (2008)

TT 54.5 Thu 10:30 H22

High-pressure floating-zone growth of $LaNiO_3$ single crystals — •Kaustav Dey, Mahmoud M.Abdel-Hafiez, and Rüdiger Klingeler — Kirchhoff Institute for Physics, Heidelberg University, Germany

$LaNiO_3$ is known to be a correlated metal in the vicinity of a bandwidth controlled metal-insulator transition. A variety of experimental studies on polycrystalline $LaNiO_3$ have indicated it to be a Pauli paramagnetic metal. Recently, the successful growth of $LaNiO_3$ single crystals was published [1,2]. Suprisingly, Guo *et. al.* have reported

that $LaNiO_3$ has an antiferromagnetic metallic ground state [2]. We discuss the successful growth and characterization of centimeter-sized single crystals of $LaNiO_3$ by means of the floating zone technique at oxygen pressures of up to 80 bar. Indeed, magnetisation and specific heat data on several $LaNiO_3$ single crystals grown at 40 bar show the presence of a anomaly in the range 150-160 K similar to what is reported in Ref. [2]. In contrast, no anomaly was observed in the crystals grown at 80 bar in agreement with Ref. [1]. We infer that higher pressure leads to better crystal quality in terms of phase purity and that the anomaly associated with antiferromagnetism reported in $LaNiO_3$ single crystals may not be of intrinsic nature.

[1] J. Zhang et al., Cryst. Growth Des. 17, 2730 (2017)
[2] H. Guo et al., Nat. Comm. 9:43 (2018).

TT 54.6 Thu 10:45 H22

Bond and magnetic order in rare-earth nickelates simultaniously probed by resonant inelastic x-ray scattering — •Katrin Fürsich[1], Yi Lu[1,2], Davide Betto[1], Georg Christiani[1], Eva Benckiser[1], Giniyat Khaliullin[1], Matteo Minola[1], and Bernhard Keimer[1] — [1]Max Planck Insitutte for Solid State Research, Stuttgart — [2]University of Heildelberg

We used high-resolution resonant inelastic x-ray scattering (RIXS) at the Ni L_3 edge to simultaneously investigate bond and magnetic order in the rare-earth nickelates $RNiO_3$. With the support of calculations based on a double-cluster model, we quantify bond order (BO) amplitudes for different thin films and heterostructures, and discriminate short-range BO type fluctuations from long-range static order. Moreover we investigate the magnetic order in spatially confined nickelate layers following the method described in Ref. 1. While our study reveals a robust non-collinear spin spiral magnetic order, which is essentially unperturbed by bond order modulations and spatial confinement, we find a dramatically reduced magnon energy in systems with collinear magnetic order. These results give valuable insight into the interplay of different collective ordering phenomena in a prototypical 3d transition metal oxide and establish RIXS as tool of choice to quantitatively study several order parameters within one experiment.

[1] Lu, Betto, KF *et al.*, Phys. Rev. X **8**, 031014 (2018)

15 min. break.

TT 54.7 Thu 11:15 H22

Raman spectroscopy study of the lattice and spin dynamics in CrAs — •Yi Yao[1], Matthieu Le Tacon[1], Kaushik Sen[1], Michaela Souliou[1], Amir-Abbas Haghighirad[1], Michael Merz[1], Christoph Meingast[1], Frederic Hardy[1], Anahita Omoumi[2], Measson Marie-Aude[3], and Pawbake Amit[3] — [1]Karlsruhe Institute of Technology, Institute for Solid State Physics — [2]University Paris Sud — [3]Institut Néel, Magnetic and superconductivity group

We performed Raman measurements to probe the lattice and spin dynamics of high quality single crystals of CrAs, an antiferromagnetic (AFM) double-helical system that becomes superconducting under pressure[1]. The samples were grown using a flux method, and characterized using XRD and magnetic susceptibility measurements. At the AFM ordering temperature $T_N = 265$ K, below which helical AFM order sets in, the sample exhibits a strong first order structural transition, upon which the lattice parameter b expands by $\approx 3.39\%$. In the Raman experiments, four Raman active modes with A_g symmetry were observed, as predicted from group theory. All these modes exhibit pronounced anomalies in their frequencies and linewidths across T_N. In addition, we found a signature of magnon scattering, and signatures of spin-phonon coupling are discussed. Finally, our high-pressure Raman experiments show the suppression of T_N under hydrostatic compression, in agreement with previous studies[1,2].

[1] W. Wei. et al., Nature Comm. 5 (2014)
[2] Y. Shen. et al., Phys. Rev. B 93 (2016)

TT 54.8 Thu 11:30 H22

Structural and magnetic properties of vanadium trihalides VX_3 (X = Cl, Br) — •Neetika Neetika[1], Reinhard K Kremer[1], and Christina Drahten[2] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569, Stuttgart, Germany — [2]ESRF - the European Synchrotron, 71, Avenue des Martyrs, 38000 Grenoble, France

We have examined the structural and magnetic properties of the layered vanadium trihalides, VX_3 (X = Cl, Br). For both systems, specific heat measurements indicate two anomalies at $\sim$ 25K and $\sim$ 100K. Magnetization measurements prove antiferromagnetic ordering below $\sim$ 25K and negative Weiss temperatures indicating predominant antiferromagnetic interactions. Laboratory-based and synchrotron x-ray diffraction measurements show that anomaly at $\sim$ 100K is associated to a structural phase transition from the rhombohedral BiI_3 structure-type ($R\bar{3}$) at high temperature to either a monoclinic (C2/c) or triclinic ($P\bar{1}$) crystal structure at low temperature. First-principle calculations also indicate that the structural phase transition from rhombohedral to either monoclinic or triclinic is energetically favorable.

TT 54.9 Thu 11:45 H22

New insights into doped Sr_2IrO_4 — •Benjamin Lenz[1], Cyril Martins[2], and Silke Biermann[1,3] — [1]CPHT, Ecole Polytechnique, Palaiseau, France — [2]LCPQ, Université Paul Sabatier, Toulouse, France — [3]Collège de France, Paris, France

The spin-orbit system Sr_2IrO_4 has been in the spotlight in recent years due to its striking similarity to isostructural high-T_c superconducting copper oxides. Here, we present new insights into the spectral properties of Sr_2IrO_4 using a combination of ab-initio density functional theory and quantum cluster techniques. We find good agreement with available angular-resolved photoemission spectra in the antiferromagnetic low-temperature and high-temperature paramagnetic phases of pure Sr_2IrO_4, as well as for electron- and hole-doped compounds. Furthermore, we discuss an intriguing k-dependence in the composition of the spin-orbit entangled $j_{\text{eff}} = 1/2$ states.

TT 54.10 Thu 12:00 H22

Propagation of a single hole in Ca_2RuO_4 — •Adam Kłosiński[1], Jeroen van den Brink[2], Dmitri V. Efremov[2], and Krzysztof Wohlfeld[1] — [1]Faculty of Physics, University of Warsaw, Warsaw, Poland — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany

In recent years there has been a growing interest in the understanding of the correlated physics of Ca_2RuO_4, fuelled by the fundamental importance of the spin-orbit interaction in this compound on the one hand and by its close resemblance to the well-studied copper oxides on the other. In order to understand the latter, we focus here on the propagation of a single hole introduced into the Mott insulating ground state of Ca_2RuO_4 and verify its quantitative as well as qualitative differences w.r.t. the cuprates. To this end we introduce an effective multiorbital t-J-like model which we then solve using the linear spin wave theory and self-consistent Born approximation. We obtain the spectral function for fermionic spinless holes whose most striking feauture is its quasi-1D character.

TT 54.11 Thu 12:15 H22

Near-field optical probes of the current- and temperature-driven insulator-to-metal transition in the Mott insulator Ca_2RuO_4 — •Desislava Daskalova[1,2], Parmida Shabestari[1,2], Hao Chu[1,2], Maximilian Krautloher[1], Joel Bertinshaw[1], Bernhard Keimer[1], and Stefan Kaiser[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]4th Physics Institute, Stuttgart University, Germany

Many-body effects in correlated materials give rise to exciting quantum phenomena and phases of matter. Here we study calcium ruthenate (Ca_2RuO_4), a Mott insulator at room temperature, because it exhibits interesting magnetic, transport and structural properties. The delicate balance in its ground state is easily perturbed by temperature, pressure and small electric field (40 V/cm) which all induce an insulator-to-metal transition (IMT). However, distinctly different metallic phases in a temperature- or current-driven case are being stabilized. One goal is to distinguish the different mechanisms driving the transition, especially to understand the current-driven IMT which remains to be fully explained.

To this end we probe the changes in the optical properties of Ca_2RuO_4 during the current- and temperature-driven IMT using far-field infrared spectroscopy and scattering-type scanning near-field optical microscopy. Probing the nanoscale optical response throughout the transition allows us to identify the Mott insulating and metallic phases. We image the two different phases of Ca_2RuO_4 coexisting and evolving in a manner, characteristic to the driving mechanism.

TT 54.12 Thu 12:30 H22

Magnetic order and short-range correlations in γ_{II}-Li_2FeSiO_4 — •Martin Jonak[1], Christoph Neef[1], Waldemar Hergett[1], Sven Spachmann[1], Mahmoud Abdel-Hafiez[1,2], Jo-

hannes Werner[1], Changhyun Koo[1], Sven Sauerland[1], Clemens Ritter[3], Sergei Zvyagin[4], Alexey Ponomaryov[4], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany — [2]Physikalisches Institut, Goethe-Universität, Frankfurt am Main, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Multi-faceted magnetic characterisation of γ_{II}-Li_2FeSiO_4 single crystals (space group *Pmnb*) is presented. The system exhibits tetrahedrally coordinated Fe^{2+} ions in a high-spin $e_g^3t_{2g}^3$ (i.e., $S = 2$) configuration. While static magnetic susceptibility shows a maximum at $T \approx 28$ K, long-range AFM order is found to evolve at $T_N = 17.0(5)$ K. Elastic neutron scattering on a powder sample reveals commensurate two-sublattice AFM order with a propagation vector (1/2, 0, 1/2). At $T = 4$ K, high-frequency electron-spin resonance (HF ESR) observes zero-field splitting of $\Delta = 700(20)$ GHz, and the closing of the AFM gap at $B = 16.2(2)$ T which is separated from a spin-flop-like phase emerging at $B = 18.0(5)$ T. Both transitions are confirmed by pulsed-field magnetisation. At high temperatures, magnetic anisotropy beyond the g-factor anisotropy extends up to $T \gtrsim 150$ K. The presence of short-range magnetic correlations at least up to $T \approx 110$ K is detected by specific heat and magnetostriction, as well as by HF ESR.

TT 54.13 Thu 12:45 H22

Multiferroicity in $Fe_4Ta_2O_9$ — Soumendra Panja[1], Jitender Kumar[1], Luminita Harnagea[1], Arun Nigam[2], Ramesh Nath[3], P . K Mukharjee[3], and •Sunil Nair[1] — [1]IISER Pune, India — [2]TIFR Mumbai, India — [3]IISER Tvm, India

We report on the observation of multiple coupled magnetic and ferroelectric states in the $Fe_4Ta_2O_9$ system, which appears to be the only genuine multiferroic in its material class. We suggest that the observed properties arise as a consequence of an effective reduction in the dimensionality of the magnetic lattice, with the magnetically active Fe^{2+} ions preferentially occupying a quasi 2D buckled honeycomb structure. A rich variety of coupled magnetic and ferroelectric states are seen which is similar to that observed in the distorted Kagome systems.

TT 55: Superconductivity: Tunneling and Josephson Junctions

Time: Thursday 9:30–13:00 Location: H23

TT 55.1 Thu 9:30 H23

Design of an on-Chip Sideband Separating (2SB) SIS Balanced Mixer for 400 to 500 GHz on a Silicon Membrane — •Sina Widdig, Karl Jacobs, Michael Schultz, Matthias Justen, Nadine Wehres, Netty Honingh, and Jürgen Stutzki — I. Physikalisches Institut, Universität zu Köln, Cologne, Germany

Superconductor-Insulator-Superconductor (SIS) tunnel junctions are currently used as heterodyne mixers with quantum limited sensitivity for receivers in astronomy. Well-engineered technology offers the opportunity to replace the single-ended double-sideband (DSB) mixers by balanced or sideband separating (2SB) mixers. 2SB mixers are used to prevent the increase of system noise due atmospheric noise in the image sideband. They are usually made in waveguide technology, using an assembly of separate pre-tested units. The large size of these mixers makes it difficult to build multi-pixel-array receivers where the footprint of each pixel must be reduced (10mm x 10mm e.g. for CHAI receiver).

We are developing the RF part of an on-chip 2SB balanced SIS mixer between 400 and 500 GHz, in the same technology as the existing balanced mixer. The total size of the complete RF part is 2.3mm x 1.7mm, including 3 hybrids, 4 SIS junctions, a LO-power divider and a RF load. The mixer reduces the LO AM noise due to the balanced mixers. For testing the RF performance of the chip we designed a prototype block with 4 separate SIS mixer IF-outputs. In addition THz spectrometer measurements are planned show the sideband suppression with detection of rotational lines of CH_3CN.

TT 55.2 Thu 9:45 H23

Fabrication and characterization of cross-type Nb/Al-AlO_x/Nb Josephson junctions — •Fabienne Bauer, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Josephson tunnel junctions are the basic element of numerous superconducting electronic devices such as SQUIDs or qubits. The performance and sensitivity of many of those devices depend on and particularly improve with decreasing junction capacitance. The latter depends on the material and the thickness of the tunnel barrier, the junction area as well as the overlap of different wiring layers adding parasitic capacitance. Therefore, the junction capacitance can be reduced by avoiding parasitic overlaps as well as by optimizing the oxidation parameters and the junction area.

Within this context, we present an anodization-free fabrication process for cross-type Nb/Al-AlO_x/Nb Josephson junctions. They are built by the overlap of two perpendicular superconducting stripes with the tunnel barrier in between eliminating any parasitic capacitance and making a reduced junction area easily possible. As a further advantage, restrictions in alignment accuracy do not limit the junction size. We will show that our cross-type tunnel junctions have a smaller capacitance compared to our window-type junctions and that they exhibit a reproducible high quality. In addition, we discuss the performance of dc-SQUIDs based on cross-type junctions to demonstrate the profit resulting from this new fabrication process.

TT 55.3 Thu 10:00 H23

Hysteresis in current-voltage characteristics of sub-micron Nb-HfTi-Nb SNS-type Josephson junctions — •Julian Linek[1], Benedikt Müller[1], Viacheslav Morosh[2], Thomas Weinmann[2], Oliver Kieler[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Fachbereich Quantenelektronik, PTB Braunschweig, Germany

SNS-type Josephson junctions (JJs) based on superconducting (S) Nb thin films with a normal metal (N) HfTi barrier offer high critical current densities up to 1 MA/cm^2 with usually non-hysteretic current-voltage characteristics (IVCs) at temperature $T = 4.2$ K. By patterning a Nb-HfTi-Nb trilayer with e-beam lithography, highly sensitive dc SQUIDs with sub-μm lateral dimensions can be fabricated. Such nanoSQUIDs are suited for the investigation of magnetism at the nano scale. Unfavorably, hysteresis in the IVCs appears upon increasing the critical current; this prevents SQUID operation at the optimum working point and thus leads to a degradation in sensitivity. Main features of IVCs measured at variable T resemble those of constriction type JJs with thermaly induced hysteresis. We performed numerical simulations of IVCs and compared those to measurements on our SNS-JJs from 0.3 to 9 K. RSJ-based simulations include the balance of Joule heating and 1-dim. thermal heat flow to describe the increase of T in the barrier layer. Despite the simplicity of our model, major properties of the experimentally determined IVCs, such as the saturation of the return current $I_r(T)$ at low T, can be reproduced by our simulations.

TT 55.4 Thu 10:15 H23

$YBa_2Cu_3O_7$ Josephson junctions and SQUIDs defined by focused He ion beam irradiation — •Max Karrer, Benedikt Müller, Fabienne Limberger, Jianxin Lin, Christian Vöhringer, Malena Höhn, Edward Goldobin, Reinhold Kleiner, and Dieter Koelle — Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany

The invention of the He ion microscope (HIM) with sub-nm spatial resolution offers exciting perspectives, not only for high-resolution imaging of surfaces, but also for their nanoscale modification. For epitaxially grown thin films of the high-T_c cuprate superconductor $YBa_2Cu_3O_7$ (YBCO), He focused ion beam (He-FIB) irradiation can be used to directly write Josephson junction (JJ) barriers into the material by driving locally the material into the insulating state [1]. In addition to the fabrication of such beam-induced barrier junctions (bJJs), He-FIB irradiation can also be used to pattern YBCO films on the nanoscale, without removing material [2]. This may provide an alternative way to define insulating areas for nanoSQUID fabrication. Here, we will present our recent progress in the fabrication of

He-FIB-induced bJJs and SQUIDs as well as the analysis of their electric transport and noise properties, in particular with respect to the possible control of the critical current density of bJJs by variation of the He-FIB dose.
[1] S. Cybart *et al.*, Nature Nanotechnol. **10**, 598–602 (2015)
[2] E. Y. Cho *et al.*, Appl. Phys. Lett. **113**, 022604 (2018)

TT 55.5 Thu 10:30 H23

Scanning tunneling spectroscopy of superconducting Granular Aluminium — •Tim Storbeck, Fang Yang, Ioan Pop, and Wulf Wulfhekel — Karlsruhe Institut of Technology

Granular Al films are of high interest for quantum superconducting circuit design due to their large kinetic inductance and low intrinsic dissipation. Interestingly, it has been known for several decades that T_c can be increased by a factor more than 2 in granular Al compared to bulk Al. The enhancement of T_c has been attributed to microscopic mechanisms involving electron quantization and Kubo spins, however, the exact mechanisms are still debated. We report the measurement of scanning tunneling spectroscopy of granular Al films on Nb-doped $SrTiO_3$ in ultra-high vacuum at 30mK. We observed both superconducting and insulating grains in the same samples. The local single electron tunneling between the tip and the Al grains show rich features at energy scales from 1 eV down to 0.1 meV. The size of the gap in superconducting grains, in the range of 0.28-0.32 meV, agrees with previously reported values for similar films. We also observed signatures of in-gap states, hinting at unpaired electrons on the grains.

TT 55.6 Thu 10:45 H23

Electrical and mechanical behavior of Al/AlO_x nanobridges — •Patrick Haiber, Susanne Sprenger, Laura Sobral-Rey, and Elke Scheer — Universität Konstanz, Germany

Mesoscopic transport through single atom contacts is an intensively studied topic. Especially aluminum in a mechanically controllable break junction design (MCBJ) has received great attention for its superconducting properties [1,2]. Histograms show a pronounced peak at 0.8 G_0 signalling the single atom contact. These contacts have proven to be of high mechanical stability over several hours in cryogenic vacuum, enabling comprehensive investigation of the same atomic contact configuration. On the other hand Al/AlO_x/Al junctions are very popular realizations for studying mesoscopic transport in the superconducting state. Aluminium MCBJ in series with an Al/AlO_x junction have been used to build a tunable all superconducting SET [3]. In those experiments it has been shown that not only contacts with conductance close to 0.8 G_0 but also contacts of higher resistance can be mechanically stabilized over several hours.

Here we study the role of the AlO_x layer on the contact formation. The oxide layer is formed on top of the Al MCBJ via plasma or thermal oxidation. We systematically compare oxidized Al MCBJ with non-oxidized MCBJ regarding their preferred conductance values and stretching behavior.
[1] Agraït et al., 2003 , PR 377 81-279
[2] Scheer et al., 1997, PRL 78 3535
[3] Lorenz et al., 2018, JLTP 191 301-315

TT 55.7 Thu 11:00 H23

Quantum properties of a strongly driven Josephson junction — Jennifer Gosner, •Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems and IQST, University of Ulm, 89069 Ulm, Germany

A Josephson junction embedded in a dissipative circuit can be externally driven to induce nonlinear dynamics of its phase. Classically, under sufficiently strong driving and weak damping, dynamic multistability emerges associated with dynamical bifurcations so that the often used modeling as a Duffing oscillator, which can exhibit bi-stability at the most, is insufficient. Here, corresponding quantum properties in this regime are analyzed by mapping the problem onto a highly-nonlinear quasi-energy operator in a rotating frame. This allows us to identify in detail parameter regions where simplifications such as the Duffing one are valid, to explore classical-quantum correspondences and to study how quantum fluctuations impact the effective junction parameters as well as the dynamics around higher amplitude classical fixed points.

15 min. break.

TT 55.8 Thu 11:30 H23

Particle-conserving theory for transport through interacting Josephson junctions — •Jordi Picó-Cortés[1,2], Andrea Donarini[1], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Instituto de Ciencia de Materiales de Madrid (CSIC), E-28049, Madrid, Spain

When two superconductors are coupled together through a weak link, tunneling of Cooper pairs gives rise to a supercurrent through the junction, as predicted by Josephson [1]. Usually, transport through mesoscopic Josephson junctions (JJ) is described using the mean field theory of superconductivity. This approach has the obvious limitation of treating an inherently many-body effect through an effective single-particle theory which violates particle's conservation. We investigate charge transport and the Josephson effect through an interacting quantum dot coupled to two superconductors within a particle-conserving theory of superconductivity. Within a reduced density matrix approach to transport [2], we can account for the many-body aspects of superconductivity and interactions in the dot on the same footing.
[1] B. D. Josephson, Phys. Lett. 1 , 251253 (1962)
[2] S. Koller, M. Leijnse, M. R. Wegewijs, and M. Grifoni Phys. Rev. B 82, 235307 (2010)

TT 55.9 Thu 11:45 H23

Local density of states in clean 2D SNS heterostructures — •Danilo Nikolic[1], Juan Carlos Cuevas[2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain

The advent of 2D materials like graphene have reignited the interest in the study of the proximity effect in clean hybrid superconducting structures. Motivated by the recent experimental results [1] we present a systematic theoretical analysis of the local density of states in a clean 2D normal metal sandwiched between two standard s-wave superconductors. By solving the Eilenberger equation in the framework of quasiclassical Green's function theory we are able to describe the Andreev bound state spectrum in presence of, among others, a finite transparency of the junction or a weak magnetic field with different geometries of the junction. We analytically obtain a relation between the supercurrent and the global density of states.
[1] L. Bretheau, J.I.J. Wang, R. Pisoni, K. Watanabe, T. Taniguchi, P. Jarillo-Herrero, Nature Physics, doi:10.1038/nphys4110 (2017)

TT 55.10 Thu 12:00 H23

Phase-controlled triplet correlations and thermoelectric effects in a hybrid superconductor-ferromagnet device — •Ali Rezaei[1], Robert Hussein[1], Akashdeep Kamra[2], and Wolfgang Belzig[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Center for Quantum Spintronics, Department of Physics, NTNU, Norway

We study charge and heat transport in superconductor-ferromagnet (S/FM) hybrid structures. Firstly, we analyse a bilayer tunnel junction consisting of a spin-split superconductor connected to a spin-polarized ferromagnet and find that spin-flip scattering strongly enhances the thermoelectric response of the system at low temperature and spin-splitting [1]. A large spin-splitting is also obtainable by employing an antiferromagnetic insulator (AFMI) adjacent to a superconductor in an S|AFMI device [2]. The advantage of using AFMs is the minimization of stray magnetic fields which normally accompany ferromagnets. Finally, we investigate the effects of spin-polarized quasiparticles and spin-mixing on the thermoelectric transport properties of a four-terminal hybrid device incorporating two superconductors which are connected to two ferromagnetic leads via a common central normal node. This geometry allows us to induce phase- and voltage-controlled triplet correlations, and to change the direction of the spin-currents.
[1] A. Rezaei, A. Kamra, P. Machon, and W. Belzig, New J. Phys. **20**, 073034 (2018)
[2] Akashdeep Kamra, Ali Rezaei, Wolfgang Belzig, arXiv:1806.10356 (2018); accepted in PRL

TT 55.11 Thu 12:15 H23

Tunneling Anomalous Hall (TAH) Effect in Ferromagnet/Superconductor Junctions — •Andreas Costa[1], Alex Matos-Abiague[2], and Jaroslav Fabian[1] — [1]University of Regensburg, Germany — [2]Wayne State University Detroit, USA

The competition of two antagonistic interactions, spin-singlet superconducting pairing and ferromagnetic exchange, in one heterojunction

leads to extraordinary phenomena. Owing to the additionally broken inversion symmetry in such systems, not only the interplay of superconductivity and ferromagnetism, but also the induced strong spin-orbit fields (SOFs) offer interesting subjects for experimental and theoretical investigations; several studies unraveled an intriguing impact of interfacial SOFs on transport already in normal-conducting systems, e.g., TAMR [1] and TAH [2] effects. Our theoretical work focuses on ferromagnet/superconductor junctions, demonstrating the existence of a superconducting TAH effect. While the effect's fundamental characteristics are comparable to the normal-conducting analog [2], our numerical simulations predict a much larger tunability of the TAH conductance in the superconducting scenario. Together with the prediction of a simultaneously generated transverse supercurrent response in the superconductor, these findings might offer an interesting future perspective for experimentalists.

This work was supported by ENB IDK Topological Insulators and by DFG SFB No. 1277 (project B07).

[1] Phys. Rev. Lett. **99**, 056601 (2007)
[2] Phys. Rev. Lett. **115**, 056602 (2015)

TT 55.12 Thu 12:30 H23

Microwave spectroscopy reveals the quantum geometric tensor of topological Josephson matter — •Raffael L. Klees[1], Gianluca Rastelli[1], Juan Carlos Cuevas[2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Concepts like Chern numbers and their relation to physical phenomena have become very familiar, but actually, key quantities like the quantum geometric tensor [1], which provides a much deeper information about quantum states, remain experimentally difficult to access. Recently it has been shown that multiterminal superconducting junctions constitute an ideal playground to mimic topological systems in a controlled manner [2]. We study the spectrum of Andreev bound states in topological Josephson matter and demonstrate that the quantum geometric tensor of the ground state manifold can be extracted with the help of microwave spectroscopy [3]. We develop the concept of artificially polarized microwaves, which can be used to obtain both the quantum metric tensor and the Berry curvature. The quantized integrated absorption provides a direct evidence of topological quantum properties of the Andreev states.

[1] M. Kolodrubetz *et al.*, Phys. Rep. **697**, 1 (2017)
[2] R.-P. Riwar *et al.*, Nat. Commun. **7**, 11167 (2016);
J. S. Meyer and M. Houzet, Phys. Rev. Lett. **119**, 136807 (2017);
H.-Y. Xie *et al.*, Phys. Rev. B **96**, 161406 (2017);
Phys. Rev. B **97**, 035443 (2018). [3] R. L. Klees *et al.*, arXiv:1810.11277

TT 55.13 Thu 12:45 H23

Manipulation of Cooper pair entanglement in hybrid topological Josephson junctions — Gianmichele Blasi, Fabio Taddei, Vittorio Giovannetti, and •Alessandro Braggio — NEST, Scuola Normale Superiore and Istituto Nanoscienze-CNR, I-56126 Pisa, Italy

We investigated the supercurrent in a hybrid topological Josephson junction consisting of two planes of topological insulator (TI), which allows both local (LAR) and crossed (CAR) Andreev processes at the interfaces with two conventional s-wave superconductors. We describe the effects of local Rashba-like and Zeeman-like fields applied to the edge states. In particular, we demonstrate that the Rashba-like field, as induced by local gating, allows the manipulation of the entaglement symmetry of non-local Cooper pairs associated to the CAR process. We establish a connection between the Josephson current-phase relationship of the system and the action of the two local fields, finding that they selectively modify the LAR or the CAR contributions. Remarkably, we find that the critical current of the junction takes a very simple form which reflects the change in the symmetry occurred to the entangled state and allows to determine the microscopic parameters of the junction.

[1] G. Blasi, F. Taddei, V. Giovannetti, A. Braggio, arxiv:1808.09709

TT 56: Topological Semimetals - Experiment (joint session TT/MA)

Time: Thursday 15:00–17:45 Location: H2

TT 56.1 Thu 15:00 H2

Electronic structure of Weyl semimetal TaAs under pressure — •Zuzana Medvecka, Marcel Naumann, Markus Schmidt, Vicky Süss und Michael Nicklas — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Weyl semimetals are topological materials with linear band dispersion around pair of nodes with fixed opposite chirality. The quasiparticles from such nodes are predicted to induce novel quantum mechanical phenomena, such as Fermi arcs. However, to observe them in transport experiments, the Weyl nodes have to be sufficiently close to the Fermi level. Tantalum arsenide is a Weyl semimetal with a well-studied electronic structure, where the Weyl nodes lie 6 meV from Fermi level [1].

Here, we study how hydrostatic pressure impacts the Fermi level and electronic structure of TaAs. Quantum oscillations in resistivity of single-crystal TaAs samples are investigated in a piston type pressure cell. Pressure dependence of the electronic structure in TaAs is then obtained from the evolution of quantum oscillation frequencies.

[1] F. Arnold, M. Naumann, S.-C. Wu, Y. Sun, M. Schmidt, H. Borrmann, C. Felser, B. Yan and E. Hassinger, PRL 117, 146401 (2016)

TT 56.2 Thu 15:15 H2

Absence of the chiral anomaly - the longitudinal magnetoresistance in TaAs-type Weyl metals — •Marcel Naumann[1,2], Frank Arnold[1], Maja Bachmann[1], Kimberley Modic[1], Vicky Süss[1], Marcus Schmidt[1], Philip Moll[1], Brad Ramshaw[3], and Elena Hassinger[1,2] — [1]MPI CPfS, Dresden, Germany — [2]Technische Universität München, Garching, Germany — [3]Cornell University, Ithaca, NY, USA

The discovery of materials with 3D linear band-crossing points close to the Fermi level, such as Dirac and Weyl semimetals, has offered the possibility to study relativistic fermions in solid state systems. One manifestation, the 'chiral anomaly', should appear as a reduction of the longitudinal magnetoresistance (LMR), as was quickly observed in TaAs [1]. Subsequent studies found that current inhomogeneities ('current jetting') often induce an apparent negative LMR in semimetals, and that the true LMR is still unknown [2,3].

In this study, we determine the intrinsic LMR in the TaAs family (TaAs, TaP, NbAs, NbP) of Weyl semimetals. We reduced current jetting effects by trying to achieve a homogeneous current injection and by increasing the aspect ratio of our samples. The results show an *absence* of the negative LMR in chiral materials and a *presence* of a negative LMR in non-chiral materials. This suggests a chirality independent effect, which we believe to be weak-localisation physics.

[1] Huang et at., PRX 5, 031023 (2015)
[2] Arnold et al., Nat. Com. 7, 11615 (2016)
[3] dos Reis et al., New J. Phys. 18, 085006 (2016)

TT 56.3 Thu 15:30 H2

Magneto-optical response of the Weyl semimetal TaP — •Sascha Polatkan[1], Milan Orlita[2], Artur Slobodeniuk[2], Mark O. Goerbig[3], Chandra Shekhar[4], Claudia Felser[4], Martin Dressel[1], and Artem V. Pronin[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]LNCMI, CNRS-UGA-UPS-INSA-EMFL, 38042 Grenoble, France — [3]LPS, Univ. Paris-Sud, Univ. Paris-Saclay, CNRS UMR 8502, 91405 Orsay, France — [4]MPI für Chemische Physik fester Stoffe, 01187 Dresden, Germany

Theory predicts that TaP, being structurally akin to TaAs, hosts two distinct Weyl-type band crossings. Optical (infrared) spectroscopy in magnetic fields offers crucial information about the band structure by means of analyzing the inter-Landau-level transitions. We investigated the magneto-optical response of TaP up to $B = 33$ T in the infrared regime ($5-200$ meV). The reflection spectra are rich of features, many of which show a $\sqrt{B}$-dependence, hinting at the massless nature of the involved (presumably Weyl) bands. Moreover, we observe a peculiar fan-shaped subset of the transitions. In this subset, the energies

of some of the transitions increase, while the energies of other transitions decrease with field. We discuss how the topological nature of the involved bands might be connected to this peculiar behavior.

TT 56.4 Thu 15:45 H2

Dirac semimetal $PtBi_2$: polymorphism and challenges in crystal growth — •Grigory Shipunov, Boy Roman Piening, Saicharan Aswartham, and Bernd Büchner — IFW-Dresden, Dresden, Germany

$PtBi_2$ is showing rich polymorphism, with at least 3 different crystal structures corresponding to this composition are reported. At least two of this structures, pyrite-type cubic (space group $Pa\bar{3}$) and hexagonal (space group $P31m$), are showing linearly dispersive Dirac states and anomalous transport properties, such as extremly large linear magnetoresistance.

Here, we present our results on targeted crystal growth of cubic or hexagonal modification. Cubic and hexagonal modifications were grown via self-flux method, with growth parameteres such as Pt:Bi ratio and temperature profile chosen based on thermodynamical phase diagram data. High quality of the crystals is confirmed by powder and single crystal x-ray diffraction and scanning electron microscopy with energy dispersive x-ray spectroscopy techniques. Optimization of the growth parameters for the metastable trigonal polymorph is also discussed.

TT 56.5 Thu 16:00 H2

Chemical-pressure effect on the optical conductivity of topological nodal-line semimetals ZrSiS type — •Markus Krottenmüller[1], Jihaan Ebad-Allah[1,2], Juan Fernandez Afonso[3], Zhiqiang Mao[4], Jan Kunes[3,5], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Department of Physics, Tanta University, 31527 Tanta, Egypt — [3]Institute of Solid State Physics, TU Wien, 1020 Vienna, Austria — [4]Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70118, USA — [5]Institute of Physics, The Czeck Academy of Sciences, 18221 Praha, Czech Republic

ZrSiS is a prototype nodal-line semimetal, whose electronic band structure contains a diamond-shaped nodal line. We studied the optical conductivity of ZrSiS and other members of the compound family ZrXY with X=Si, Ge and Y =S, Se, Te by reflectivity measurements over a broad frequeny range. The optical conductivity spectrum of ZrSiS has a distinct U-shape, ending at a sharp high-energy peak. Other ZrXY compounds have a very similar profile of the optical conductivity, except ZrSiTe. We will discuss our findings in terms of the theoretical optical conductivity obtained by density functional theory calculations.

TT 56.6 Thu 16:15 H2

ZrP_2 family of materials as topological semimetal candidates — Jörn Bannies[1,2], Elia Razzoli[2], Matteo Michiardi[1,2], •Ilya Elfimov[2], Andrea Damascelli[2], and Claudia Felser[1] — [1]Max Planck Instistute for Chemical Physics of Solids, Dresden, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver, Canada

In recent years transition metal pnictides including dipnictides have attracted much research interest in the context of topological semimetals. These include type-I and type-II Weyl semimetals, triple-point fermions and weak topological insulators. Here we propose group IV dipnictides as potential nodal line semimetals, a class with only a few verified members to date.

We have successfully grown crystals of ZrP_2 and $ZrAs_2$ and, for the first time, investigated their transport properties. These materials are isostructural and crystallize in the non-symmorphic space group *Pnma*. For ZrP_2 an unsaturated magnetoresistance of $1.5{\cdot}10^4$ % at 2 K and 9 T with nearly quadratic field dependence is observed. This is accompanied by a resistivity plateau up to 20 K in high magnetic fields. Similar behavior in other topological semimetals suggests a topological origin. Indeed, ZrX_2 (X = P, As) compounds were recently identified as topological materials. Our DFT band structure calculations show a Dirac like band crossing close to the Fermi level as well as a nodal line in the k_x=0 plane. We discuss the role of non-symmorphic symmetry in stabilizing these features.

15 min. break.

TT 56.7 Thu 16:45 H2

Effect of inversion symmetry on the excitations in WP_2 — •Dirk Wulferding[1,2], Peter Lemmens[1,2], Yurii Pashkevich[1,3], Tanya Shevtsova[3], Claudia Felser[4], and Chandra Shekhar[4] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]Galkin DonFTI, Kyiv, Ukraine — [4]MPI CPfS, Dresden, Germany

The two structural modifications of WP_2, one with and one without a center of inversion, allow to probe the effect of global symmetry on a Weyl semimetal. In our report we uncover phonon anomalies as well as electronic fluctuation of both phases using Raman scattering and compare their impact on anomalous charge transport [1,2,3].

Work supported by QUANOMET NL-4 and DFG LE967/16-1.

[1] Kumar et al., Nat. Commun. 8, 1642 (2017)
[2] Gooth el al., arXiv:1706.05925 (2017)
[3] Du et al., PRB 97, 245101 (2018)

TT 56.8 Thu 17:00 H2

Magnetotransport in microribbons of the magnetic Weyl semimetal $Co_3Sn_2S_2$ — •Kevin Geishendorf[1], Richard Schlitz[2], Praveen Vir[3], Chandra Shekhar[3], Claudia Felser[3], Kornelius Nielsch[1], Sebastian T.B. Goennenwein[2], and Andy Thomas[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Institute for Metallic Materials — [2]Institut für Festkörper- und Materialphysik — [3]Max Planck Institute for Chemical Physics of Solids, Dresden

Magnetic Weyl semimetals exhibit intriguing phenomena due to their non-trivial band structure. Recent experiments in bulk crystals have shown that shandite-type $Co_3Sn_2S_2$ is a magnetic Weyl semimetal [1,2]. To access the length scales relevant for electrical transport, it is mandatory to fabricate microstructures of this fascinating compound. We therefore have cut microribbons (typical size 0.3 x 3 x 50 μm^3) from $Co_3Sn_2S_2$ single crystals using a focused beam of Ga^{2+}-ions (FIB) and investigated the impact of the sample dimensions and possible surface doping on the magnetotransport properties. The large intrinsic anomalous Hall effect observed in the microribbons is quantitatively consistent with the one in bulk samples [1]. It is evident from our results that FIB cutting can be used for patterning single crystalline $Co_3Sn_2S_2$, enabling future transport experiments in complex microstructures of this compound.

[1] E. Liu et al., Nat. Phys. **14**, 1125-1131 (2018)
[2] Q. Wang et al., Nat. Commun. **9**, 3681 (2018)

TT 56.9 Thu 17:15 H2

Comparative analysis of the effects of pressure on Bi, NbP and Cd_3As_2 — •Aleksandar Vasiljković[1], Filip Orbanić[2], Mario Novak[2], Malte Grosche[1], and Ivan Kokanović[2,1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [2]Department of Physics, Faculty of Science, University of Zagreb, 10002 Zagreb, Croatia

Bismuth is a non-topological low carrier density semimetal, which has been investigated for a long time [1]. Cd_3As_2 is a symmetry-protected three dimensional Dirac semimetal with high carrier mobility [2]. Shubnikov-de Haas oscillations have previously been reported with frequencies of around 55 T, corresponding to tiny Fermi surface pockets in a semimetallic band structure [3]. NbP is a Weyl semimetal with large magnetoresistance and very high mobility[4]. We present a comparative analysis of the Shubnikov-de Haas oscillations of these three materials under pressure.

[1] L. Shubnikov, W. Y. de Haas, Comm. Phys. Lab. Univ. Leiden, 207a, 207c, 207d, 210a (1930)
[2] Z.Wang, et al., Phys. Rev. B 88, 125427 (2013)
[3] A. Pariari et al., Phys. Rev. B 91, 155139 (2015)
[4] C. Shekhar et al, Nat. Phys. 11, 724 (2015)

TT 56.10 Thu 17:30 H2

Spin-orbital texture in $MoTe_2$ and its response to the phase transition — •Andrew Patton Weber[1,2,3], Philipp Rüssmann[4], Nan Xu[2,3], Stefan Muff[2,3], Mauro Fanciulli[2,3], Arnaud Magrez[2], Philippe Bugnon[2], Helmuth Berger[2], Nicholas C. Plumb[3], Ming Shi[3], Stefan Blügel[4], Phivos Mavropoulos[4], and J. Hugo Dil[2,3] — [1]Donostia International Physics Center, 20018 Donostia, Gipuzkoa, Spain — [2]Institute of Physics, École Polytechnique Fédérale de Lausanne, CH-1015, Lausanne, Switzerland — [3]Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — [4]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Ger-

many

The basis of exotic electromagnetic phenomena in $MoTe_2$ lies not only in the electronic band structure, but also in the crystal-momentum-dependence of spin-orbit-entangled wave functions. Here we discuss the challenges involved in obtaining this information directly from experiments and report the angular distribution of photoelectron spin-polarization and intensity dichroism in $MoTe_2$. A novel spin-orbital texture is uncovered in the bulk Fermi surface that is consistent with first-principles calculations. The spin-texture is three-dimensional and is not completely suppressed above the centrosymmetry-breaking transition temperature of the bulk crystal. The results indicate that a new form of polar instability exists near the surface when the bulk is largely in a centrosymmetric phase.

TT 57: Superconductivity: Properties and Electronic Structure

Time: Thursday 15:00–18:00 Location: H7

TT 57.1 Thu 15:00 H7

Phase slip lines in few-layer $NbSe_2$ superconducting devices — •Nicola Paradiso, Anh-Tuan Nguyen, Karl Enzo Kloss, and Christoph Strunk — University of Regensburg

The advent of van der Waals superconductors made it possible to study 2D superconductivity in a fascinating clean regime, so far rarely studied in conventional films. In this work we show that, owing to their low level of disorder and atomically sharp edges, few-layer monocrystalline $NbSe_2$ flakes do not switch directly to the normal phase under large current bias. Instead, a sequential nucleation of phase slip lines (PSLs) is observed in all the samples under study. We investigate the dynamic of PSL nucleation in a Au-$NbSe_2$ point contact, where the temperature and bias dependence of the PSL-induced conductance step is quantitatively described by the simple model of Skocpol, Beasley and Tinkham. In plain devices, the PSL pattern is sample dependent. However, we demonstrate that it is possible to induce an artificial PSL nucleation site by mechanically stressing a flake across its whole width.

TT 57.2 Thu 15:15 H7

High-pressure transport studies in the superconducting and charge density wave material $NbSe_2$ — •Owen Moulding[1], Takaki Muramatsu[1], Charles Sayers[2], Enrico Da Como[2], and Sven Friedemann[1] — [1]University of Bristol, Bristol, UK — [2]University of Bath, Bath, UK

The transition metal dichalcogenide 2H-$NbSe_2$ has a well-documented charge density wave (CDW) and superconducting transition at 33K and 7K at ambient pressure. The CDW transition is suppressed under high pressure and is absent beyond its quantum critical point (QCP). The effect of this QCP on superconductivity is of great interest and stimulates discussions on the relation between superconductivity and the CDW order. So far, resistivity, magnetic susceptibility, and X-ray measurements have explored the vicinity of this QCP and they indicate a weak relation between superconductivity and the CDW: either a weak competition between CDW order and superconductivity or a weak promotion of superconductivity by fluctuations at the CDW QCP.

Here, we present high-pressure Hall effect measurements as a clear probe of the CDW order and trace the CDW transition to higher pressures than previously measured with transport methods. Further, the sign-change in the Hall coefficient observed at ambient pressure is suppressed and ultimately saturates to hole-like beyond the CDW QCP. We also observe a peak in the superconducting temperature about the QCP of the CDW of 4.7GPa, which indicates an enhancement of the electron-phonon coupling at the QCP.

TT 57.3 Thu 15:30 H7

Three-dimensional collective charge excitations in electron-doped copper oxide superconductors — •Matthias Hepting[1,9], Laura Chaix[1], Edwin W. Huang[1,2], Roberto Fumagalli[3], Ying Y. Peng[3], Brian Moritz[1], Kurt Kummer[4], Nicholas B. Brookes[4], Wei Cheng Lee[5], Makoto Hashimoto[6], Tarapada Sarkar[7], Jun-Feng He[1], Costel R. Rotundu[1], Young S. Lee[1], Richard L. Greene[7], Lucio Braicovich[3,4], Giacomo Ghiringhelli[3,8], Zhi Xun Shen[1], Thomas P. Devereaux[1], and Wei Sheng Lee[1] — [1]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory and Stanford University, USA — [2]Department of Physics, Stanford University, USA — [3]Dipartimento di Fisica, Politecnico di Milano, Italy — [4]European Synchrotron Radiation Facility (ESRF), France — [5]Department of Physics, Binghamton University, USA — [6]Stanford Synchrotron Radiation Lightsource, SLAC, USA — [7]Center for Nanophysics and Advanced Materials, University of Maryland, USA — [8]CNR-SPIN, Politecnico di Milano, Italy — [9]Max-Planck-Institute for Solid State Research, Germany

We report on three-dimensional charge collective modes observed in electron-doped copper oxides by resonant inelastic X-ray scattering (RIXS) [1]. The modes are reminiscent of acoustic plasmons predicted for layered copper oxides and suggested to play a substantial role in mediating high-temperature superconductivity.

[1] M. Hepting et al., Nature 563, 374-378 (2018)

TT 57.4 Thu 15:45 H7

Superconducting Higgs mode in cuprates — •Min-Jae Kim[1,4], Hao Chu[1,4], Kota Katsumi[2], Sergey Kovalev[3], Robert David Dawson[1], Lukas Schwarz[1], Naotaka Yoshikawa[2], Gideok Kim[1], Daniel Putzky[1], Georg Cristiani[1], Gennady Logvenov[1], Andreas Schnyder[1], Dirk Manske[1], Michael Gensch[3], Zhe Wang[3], Ryo Shimano[2], and Stefan Kaiser[1,4] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Tokyo, Japan — [3]Helmholtz-Zentrum Dresden- Rossendorf, Germany — [4]4th Physics Institute, University of Stuttgart, Germany

The complex phase diagram of cuprate high-Tc superconductor is due to an intriguing interplay of different orders such as the pseudogap, or charge order. Despite intensive spectroscopic measurements of these ordered states, yet the microscopic mechanism behind high-Tc superconductivity is still lacking. In particular the collective dynamics of the superconducting order parameter, the Higgs mode, was not accessible so far. Here we report on *Higgs spectroscopy* in cuprate superconductors that we accomplished by using a high-field multicycle THz pulse, which nonlinearly couples to the superconducting condensate and leads to characteristic third harmonic generation. We identify the driven Higgs amplitude response of the superconducting order parameter in three archetypal families of cuprate thin films and we report on a novel collective mode universally exhibited by optimally doped samples. In addition, we find a finite Higgs-like response above Tc that might be interpreted as finite pairing amplitude even above Tc.

TT 57.5 Thu 16:00 H7

Optical second-harmonic generation spectroscopy of superconducting $YBa_2Cu_3O_y$ — •M.C. Weber[1], Th. Lottermoser[1], T. Loew[2], J.P. Porras[2], D. Hsieh[3], B. Keimer[2], and M. Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Max-Planck Institute, Stuttgart — [3]California Institute of Technology, Pasadena

The cuprate-family – famous for their high-T_c superconductivity – is characterized by a complex phase diagram. The understanding of competition or coexistence of the different phases represents one of the intriguing questions in the field. An important milestone in order to scrutinize these questions is the understanding of the symmetry properties of the different phases. Recently, using optical second-harmonic generation (SHG) a new study on $YBa_2Cu_3O_y$ revealed a monoclinic symmetry at RT followed by an inversion-symmetry breaking upon entering the pseudo-gap phase [1]. The introduction of this symmetry-sensitive technique into the realm of superconductivity opens new doors for the investigation of the rich phase diagram of $YBa_2Cu_3O_y$-compounds. In particular, spectroscopic SHG-studies allow for a deeper insight into the microscopic nature and electronic origin of the optical nonlinearities. In the present work, we report a thorough SHG-spectroscopy investigation on $YBa_2Cu_3O_y$-compounds. We find a strong spectral dependence of the optical non-linear response. Tracing the evolution of this spectral dependence across phase transitions, we aim to enlarge the understanding of the complex phase diagram of the cuprate-family.

[1] Zhao et al., Nat. Phys. **13**, 250 (2017)

TT 57.6 Thu 16:15 H7

Dramatic asymmetry of magnetic moment reversal in superconductor-ferromagnet thin film elements — •Manuel Bihler[1], Julian Simmendinger[1], and Joachim Albrecht[2] — [1]Max Plank Institute for Intelligent Systems, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Research Institute for Innovative Surfaces FINO, Beethovenstr. 1, 73430 Aalen, Germany

Loss-free electric currents in superconductors create persistent magnetic moments. In case of thin-film elements, this can result in two distinct states depending on the orientation of the circulating supercurrents. The reversal of such magnetic moments can be addressed by the application of external magnetic fields. The reversal process is locally investigated in small bilayers of high-temperature superconducting $YBa_2Cu_3O_7$-$Ba_2Y(Nb,Ta)O_6$ (YBCO:BYNTO) nanocomposite and soft-magnetic permalloy using magnetic scanning x-ray microscopy at low temperatures. In case of micron-sized elements, creation and reversal by external fields becomes largely asymmetric. Already small external magnetic fields allow the preparation of a defined magnetization state. The required field to reverse the magnetic moment by inverting the supercurrent orientation is substantially increased. This effect might be used for the development of a non-volatile magnetic memory device at low temperatures.

15 min. break.

TT 57.7 Thu 16:45 H7

Pressure tuning of $CeRhIn_5$ microstructures — •Janas K. John[1], Maja D. Bachmann[1], Filip Ronning[3], Eric D. Bauer[3], Joe D. Thompson[3], Philip J. W. Moll[1,2], and Michael Nicklas[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Laboratory of Quantum Materials, EPFL, Lausanne, Switzerland — [3]Los Alamos National Laboratory, MPA-CMMS, USA

$CeRhIn_5$ orders antiferromagnetically below $T_N = 3.8$K at ambient pressure. External pressure suppresses the antiferromagnetic state and induces an unconventional superconducting state. Motivated by the study of M. Bachmann *et.al.* on $CeIrIn_5$ microstructures we revisited the pressure-temperature ($p-T$) phase diagram of its relative $CeRhIn_5$ utilizing microstructures to probe the electrical resistivity for well-defined crystalline directions, along the crystallographic a- and c-axes. The obtained $p-T$ phase diagram resembles the general results in literature. Once the antiferromagnetic state is suppressed, superconductivity appears. We noted slightly different superconducting transition temperatures T_c along both crystallographic directions, which might be attributed to strain inhomogeneities. The superconducting transition is first rather broad, but sharpens upon increasing pressure and approaching the maximum in $T_c(p)$. To our surprise the temperature dependence as well as the $I-V$ curves for in-plane measurements along the a-axis follows the predictions of the Berezinskii-Kosterlitz-Thouless theory. This might hint at two-dimensional superconductivity.

[1] M. D. Bachmann *et al.*, arxiv:1807.05079.

TT 57.8 Thu 17:00 H7

Spatial modulation of the superconducting order parameter: A microscopic study of the FFLO state in an all-organic superconductor — •Sebastian Molatta[1,2], H. H. Wang[3], G. Koutroulakis[3], J. A. Schlueter[4], J. Wosnitza[1,2], S. E. Brown[3], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Dresden, Germany — [2]Institut für Festkörper und Materialphysik, TU Dresden, Germany — [3]Department of Physics and Astronomy, UCLA, Los Angeles, USA — [4]Division of Materials Research, National Science Foundation, Arlington, USA

The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state was theoretically predicted in 1964. A hallmark of this state is the spatial modulation of the superconducting order parameter, caused by a strong spinpopulation imbalance of a Fermi liquid. So far, experimental signatures of this superconducting state were found in only very few materials. Recently, microscopic evidence for spatially modulated superconductivity was found by nuclear magnetic resonance (NMR) spectroscopy. We report on our latest results of a comprehensive NMR study of the all-organic superconductor β''-$(ET)_2SF_5CH_2CF_2SO_3$, focused on the spectroscopic investigation of the spatial inhomogeneous distribution of the local spin susceptibility in the FFLO phase, with related signatures in the nuclear spin-lattice relaxation rate. The inhomogeneous broadening of the ^{13}C-NMR spectra, as well as the frequencydependent distribution of spin-lattice relaxation times is consistent with a one-dimensional sinusoidally modulated superconducting order parameter in the FFLO state.

TT 57.9 Thu 17:15 H7

Unconventional Magnetic Properties of Nitrogen-doped Diamond: Coexistence of superconductivity and superparamagnetism — •Jose Luis Barzola Quiquia[1], Markus Stiller[1], Pablo Esquinazi[1], Axel Molle[1], Ralf Wunderlich[1], Sebastian Pessagna[1], Jan Meijer[1], Wilhelm Kossack[2], and Sergei Buga[3] — [1]Felix-Bloch Institute for Solid State Physics, University of Leipzig, 04103 Leipzig, Germany — [2]Peter-Debye Institute for Soft Matter Physics, University of Leipzig, 04103 Leipzig, Germany — [3]Technological Institute for Superhard and Novel Carbon Materials, 7a Centralnaya street, Troitsk, Moscow, 108840 Russia

We report on the magnetization of nitrogen-doped single crystalline diamond bulk samples. We found unconventional field and temperature hysteresis loops in the magnetization at T $<$ 25 K. The results indicate the superposition of superparamagnetism and superconductivity in eight measured samples with different nitrogen concentration ($<$ 200 ppm). At temperatures above 25 K, the samples show diamagnetic behavior similar to undoped diamond. The coexistence of superparamagnetism and superconductivity is attributed to the nitrogen doping and the existence of defective regions. To support our results and interpretation we investigated the magnetic properties of ferromagnetic/high-temperature superconducting oxide bilayers. The results obtained from those bilayers show remarkable similarities to the ones in nitrogen-doped diamond. Using a simple model based on the superposition of a superparamagnetic, a superconducting and a diamagnetic contribution, we can describe very well all results.

TT 57.10 Thu 17:30 H7

Interfaces in Graphite: A Path to Room Temperature Superconductivity — •Pablo D. Esquinazi — Division of Superconductivity and Magnetism, University of Leipzig, Leipzig, Germany

Galvanomagnetic, Magnetization and Magnetic Force Microscopy studies in different graphite samples, from twisted graphene bilayers to bulk graphite samples, indicate that interfaces (e.g., between twisted Bernal or twisted rhombohedral crystalline regions or between Bernal and rhombohedral stacking) are the reason for the superconducting and metallic-like properties of graphite. In this contribution we emphasize and discuss the similarities in the superconducting-like signals obtained in twisted graphene bilayers [1] with critical temperature $T_c \sim 1$ K, in TEM lamella [2] and in bulk graphite samples [3] with 3 K $\lesssim T_c \lesssim$ 350 K. Experimental as well as theoretical work indicate that the origin of the observed superconductivity is related to the existence of flat bands at certain interfaces.

[1] Y. Cao et al., Nature **556**, 1476 (2018)
[2] A. Ballestar et al., New Journal of Physics **15**, 023024 (2013)
[3] C. Precker et al., New Journal of Physics **18**, 113041 (2016)

TT 57.11 Thu 17:45 H7

Local Magnetic Measurements of Trapped Flux Through a Permanent Current Path in Graphite — •Markus Stiller, José Barzola-Quiquia, Pablo D. Esquinazi, and Christian E. Precker — Felix-Bloch Institute for Solid-state Physics, Universität Leipzig, Linnestr. 5, D-04103, Germany

Measurements of the electrical resistance of different natural graphite samples suggest the existence of superconductivity at room temperature in some regions of the samples. To verify whether dissipationless electrical currents are responsible for the trapped magnetic flux, we localized them using magnetic force microscopy on a natural graphite sample in remanent state after applying a magnetic field. The results indicate that at room temperature a permanent current flows at the border of the trapped flux region. The current path vanishes at the same transition temperature $T_c = 370$ K as the one obtained from electrical resistance measurements on the same sample. Magnetic coupling is excluded as origin of the observed phase signal. Time-dependent measurements of the signal show the typical behavior of flux creep of a permanent current flowing in a superconductor. The overall results support the existence of room-temperature superconductivity at certain regions in the graphite structure.

TT 58: Superconductivity: Qubits 2

Time: Thursday 15:00–18:30 Location: Theater

TT 58.1 Thu 15:00 Theater

Observation and stabilization of photonic Fock states in a hot radio-frequency resonator — Mario F. Gely[1], •Christian Dickel[1], Marios Kounalakis[1], Jacob Dalle[1], Remy Vatre[1], Brian Baker[2], Mark D. Jenkins[1], and Gary A. Steele[1] — [1]Kavli Institut of Nanoscience, Delft University of Technology, The Netherlands — [2]Department of Physics and Astronomy, Northwestern University, United States of America

Detecting weak radio-frequency electromagnetic fields plays a crucial role in a wide range of fields, from radio astronomy to nuclear magnetic resonance imaging. In quantum mechanics, the ultimate limit of a weak field is a single-photon. Detecting and manipulating single-photons at megahertz frequencies present a challenge as, even at millikelvin temperatures, thermal fluctuations are significant. Here, we use a superconducting transmon qubit to directly observe photon-number splitting of the transition frequency due to a megahertz electrical resonator. Using the qubit, we achieve quantum control over thermal photons, sideband cooling the system and stabilizing photonic Fock states. Releasing the resonator from our control, we directly observe its re-thermalization with nanosecond resolution. Extending circuit quantum electrodynamics to a new regime, we enable the exploration of thermodynamics with photon-number resolution and allow interfacing quantum circuits with megahertz systems, for example, electromechanical oscillators.

TT 58.2 Thu 15:15 Theater

Al based microwave resonators in the clean and dirty limit — •Karthik Bharadwaj[1,2], Farshad Foroughi[1,2], Remy Dassonneville[1,2], Luca Planat[1,2], Sebastien Leger[1,2], Jovian Delaforce[1,2], Valdmir Milchakov[1,2], Cecile Naud[1], Olivier Buisson[1], Nicolas Roch[1], and Wiebke Hasch-Guichard[1,2] — [1]Univ. Grenoble Alpes, F-38000 Grenoble France — [2]Institut Neel, CNRS, F-38000 Grenoble France

Resonators have become a very important part superconducting Circuit QED. And they are an excellent candidate to understand the dissipation sources in qubit systems. We present a comparative experimental study of the internal quality factor of Al based microwave resonators. Microwave resonators with a typical frequency of 4GHz have been fabricated with different film thicknesses. We have developed a new fabrication technique to fabricate microwave resonators having a film thickness of around 6microns. For these film thicknesses Al turns into a clean type 1 superconductor. The behavior of the internal quality factor as a function of applied microwave power is discussed as well as the limiting dissipation mechanism of each resonator.

TT 58.3 Thu 15:30 Theater

Quantum-correlated photons generated by non-local electron transport — •Felicitas Hellbach[1], Wolfgang Belzig[1], Fabian Pauly[2,1], and Gianluca Rastelli[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz — [2]OIST Graduate University, Onna-son, Okinawa 904-0395, Japan

Since the realization of high-quality superconducting microwave cavities, one can envisage the possibility to investigate the coherent interaction of light and matter [1]. We study a parallel double quantum dot device operating as single-electron splitter interferometer, with each dot coupled to a local photon cavity. We explore how quantum correlation and entanglement between the two cavities is generated by the coherent transport of a single electron passing simultaneous through the two different dots. We calculate the covariance of the cavity occupations by use of a diagrammatic perturbative expansion (Keldysh Green's functions) to the fourth order in the dot-cavity interaction strength, taking into account vertex diagrams. In this way, we demonstrate the creation of entanglement by showing that the Cauchy-Schwarz inequality can be violated.

[1] A. Stockklauser et. al., Phys. Rev. X **7**, 011030 (2017),
X. Mi et al., Science **355**, 156-158 (2017),
J. J. Viennot et. al., Science **349**, 408-411 (2015)

TT 58.4 Thu 15:45 Theater

Thermal Engineering for Superconducting Microwave Circuits — •Matti Partanen[1,2], Jan Goetz[1], Kuan Yen Tan[1], Shumpei Masuda[1], Russell E. Lake[1,3], Joonas Govenius[1], Matti Silveri[1,4], Máté Jenei[1], Kassius Kohvakka[1], Vasilii Sevriuk[1], Roope Kokkoniemi[1], Joni Ikonen[1], Dibyendu Hazra[1], Eric Hyyppä[1], Leif Grönberg[5], Juha Hassel[5], Slawomir Simbierowicz[5], Visa Vesterinen[1,5], Jani Tuorila[1,4,6], Tapio Ala-Nissila[6,7,8], and Mikko Möttönen[1] — [1]QCD Labs, Aalto University, Finland — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Germany — [3]National Institute of Standards and Technology, Boulder, Colorado, USA — [4]Research Unit of Nano and Molecular Systems, University of Oulu, Finland — [5]VTT Technical Research Centre of Finland Ltd, Finland — [6]MSP group, Aalto University, Finland — [7]Departments of Mathematical Sciences and Physics, Loughborough University, United Kingdom — [8]Department of Physics, Brown University, Providence, Rhode Island, USA

Circuit quantum electrodynamics is a versatile architecture for various experiments in fundamental physics, as well as for different applications. Since excess heat is a substantial source of errors in cryogenic devices, it is of vital importance to evacuate heat. Here, we present our experimental results on optimized energy transfer between two resonators, and discuss photon absorption and emission techniques. We utilize photon-assisted electron tunneling through hybrid tunnel junctions coupled to resonators, and a heat sink based on a resistor in a flux-tunable resonator.

TT 58.5 Thu 16:00 Theater

Observation of dissipation driven geometric phase in superconducting microwave resonators — •Vasilii Sevriuk[1], Kuan Tan[1], Shumpei Masuda[1,2], Arto Viitanen[1], Mate Jenei[1], Matti Partanen[1], Matti Silveri[1,3], Jan Goetz[1], Eric Hyyppä[1], Leif Grönberg[4], and Mikko Möttönen[1] — [1]QCD Labs, Department of Applied Physics, Aalto University, Espoo, Finland — [2]Collage of Liberal Arts and Sciences, Tokyo Medical and Dental University, Ichikawa, Japan — [3]Research Unit of Nano and Molecular Systems, University of Oulu, Finland — [4]VTT Technical Research Centre of Finland, QFT Center of Excellence, Espoo, Finland

We recently introduced quantum-circuit refrigerator (QCR) [1] which gives possibility to tune dissipation of superconducting circuits. In this work we present an experiment in which coplanar waveguide resonator is capacitively coupled to a QCR on the one end, and to the transmission line on the other end. Coupled to the microwave resonator, QCR creates topologically nontrivial parameter space for the transmission line input-output relationship. In this work we utilize this feature to create a dynamical geometrical phase in a probe signal reflected from the superconducting resonator. Here we present our observation of this effect in a form of an additional tone, created by a frequency shift of the probe signal.

[1] K. Y. Tan, et al., Nat. Commun. 8, 15189 (2017)

TT 58.6 Thu 16:15 Theater

Metallic, superconducting and insulating low-temperature transport properties of disordered nanowires — •Jan Nicolas Voss[1], Yannick Schön[1], Micha Wildermuth[1], Lukas Powalla[1], Hannes Rotzinger[1], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow 119049, Russia

Lithographically fabricated nanowires are a promising alternative to Josephson tunnel junctions as a nonlinear element in superconducting quantum circuits. They potentially offer low intrinsic loss, high impedance, and low fabrication requirements. In the superconducting regime, a key requirement is a high kinetic inductance stemming from a low normal state conductance. Our nanowire material of choice is disordered oxidized aluminum, which, depending on the implanted oxygen impurities, allows for implementing a wide range of resistivities. Microscopically the material forms a natural, disordered network of nanometer-sized aluminum grains that are separated by thin aluminum-oxide barriers. Given this nanoscale morphology, the transport at very low temperatures ranges from insulating to superconducting depending on the resistance of the wires. We will present experimental results on nanowires with a length ranging from 50 nm up to 1000 nm and a width of about 20 nm and compare the measured data with theoretical predictions.

TT 58.7 Thu 16:30 Theater

Rabi-oscillations in disordered superconducting nanowire qubit — •Yannick Schön[1], Jan Nicolas Voss[1], Micha Wildermuth[1], Andre Schneider[1], Martin Weides[1], Hannes Rotzinger[1], and Alexey V. Ustinov[1,2] — [1]Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow 119049, Russia

At feature sizes of nanometer scale, superconducting wires made from a material with high normal state resistance show a pronounced nonlinear microwave response.

Our material of choice, granular aluminum oxide, is a new material for superconducting quantum circuits which features not only a very high kinetic inductance but also microwave resonators with high quality factors. Microscopically, it can be described as a disordered network of nano-scale aluminum grains, coupled via the Josephson effect.

We demonstrate a new type of superconducting quantum circuit, using capacitively shunted granular aluminum nanowires embedded as nonlinear circuit element. We present circuit characterization in microwave response measurements featuring Rabi-oscillations and measure state life times in the μs range.

15 min. break.

TT 58.8 Thu 17:00 Theater

Investigating a Superconducting Quantum Metamaterial in a Waveguide — •Jan David Brehm[1], Tim Wolz[1], Alexander Stehli[1], Hannes Rotzinger[1], and Alexey V. Ustinov[1,2] — [1]Karlsruhe Institute of Technology, Institute of Physics, Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

Quantum metamaterials extend the idea of classical metamaterials to a regime where the quantum coherence of the meta-atoms exceeds the typical time of a wave propagation through the medium. In recent works, it was proposed that this regime gives rise to various collective light-matter interaction effects such as self-induced transparency, quasi-superradiant phase transitions and lasing. Here, we investigate a one-dimensional quantum material which consists of an array of 80 transmon qubits coupled to a continuum of light modes of a coplanar waveguide. Since specific frequency control of the individual qubits is at the current stage of technology not feasible, we rely on strong qubit-waveguide coupling and optimizing the parameter spread by improving the circuit fabrication techniques, to reduce disorder in the metamaterial. Our qubit-based material exhibits a broad engineered bandgap, which is significantly larger than a single qubit linewidth. Beside detailed spectroscopic characterization we will present first experimental results on the time-resolved transmission of short microwave pulses through the metamterial.

TT 58.9 Thu 17:15 Theater

Phonon traps to reduce the quasiparticle density in superconducting circuits — •Francesco Valenti[1,2], Fabio Henriques[1], Maria Martinez[3,4], Lukas Grünhaupt[1], Daria Gusenkova[1], Julian Ferrero[1], Sebastian T. Skacel[5], Nataliya Maleeva[1], Alexey V. Ustinov[1,6], and Ioan M. Pop[1,5] — [1]Physikalisches Institut, Karlsruhe Institue of Technology, 76131 Karlsruhe, Germany — [2]Institute for Data Processing and Electronics, Karlsruhe Institue of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [3]Laboratorio de Física Nuclear y Astropartículas, Universidad de Zaragoza, C/ Pedro Cerbuna 12, 50009 Zaragoza, Spain — [4]Fundacíon ARAID, Av. de Ranillas 1D, 50018 Zaragoza, Spain — [5]Institute of Nanotechnology, Karlsruhe Institue of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [6]Russian Quantum Center, National University of Science and Technology MISIS, 119049 Moscow, Russia

Out of equilibrium quasiparticles (QPs) are a main source of dissipation and noise in superconducting circuits, and pinpointing their origin and decreasing their density remain outstanding tasks. The generation-recombination processes of QPs link their dynamics to the phonon dynamics of the circuit + substrate ensemble. We demonstrate that surrounding granular aluminum resonators with lower gapped aluminum islands increases the internal quality factors of the resonators in the single photon regime, suppresses the noise, and reduces the rate of observed QP generation events. The aluminum islands are positioned far enough from the resonators to be electromagnetically decoupled, and we attribute the decrease in dissipation and noise to phonon trapping.

TT 58.10 Thu 17:30 Theater

Efficient quasiparticle traps with low dissipation through gap engineering — •Roman-Pascal Riwar and Gianluigi Catelani — JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, Germany

Quasiparticles represent an intrinsic source of perturbation for superconducting qubits, leading to both dissipation of the qubit energy and dephasing. Recently, it has been shown that normal-metal traps may efficiently reduce the quasiparticle population and improve the qubit lifetime, provided the trap surpasses a certain characteristic size. Moreover, while the trap itself introduces new relaxation mechanisms, these perturbations should not hamper with state-of-the-art transmon qubits – under the condition that the traps are not placed too close to extremal positions where electric fields are high. Here, we study a different type of trap, realized through gap engineering. We find that the gap-engineered traps relax the remaining constraints imposed by normal metal traps. Firstly, the characteristic trap size, above which the trap is efficient, is reduced with respect to normal metal traps, such that here, strong traps are possible in smaller devices. Secondly, the relaxation caused by the trap is now greatly reduced, providing more flexibility in trap placement. The latter point is of particular importance, since for efficient protection from quasiparticles, the traps ideally should be placed close to the active parts of the qubit device, where electric fields are typically high.

TT 58.11 Thu 17:45 Theater

Single-spin relaxation in Si quantum dots induced by spin-valley coupling — •Amin Hosseinkhani and Guido Burkard — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

The spin of isolated electrons in Silicon quantum dot heterostructures is a promising candidate for quantum information processing. While silicon offers weak spin-orbit coupling and nuclear-spin free isotopes, the valley degree of freedom in silicon couples to spin and therefore can degrade the qubit performance by opening a relaxation channel. We have developed the theory of qubit relaxation induced by spin-valley coupling. In this talk, we will discuss the results of our theory for single qubit relaxation in an applied magnetic field and compare our results with experimental findings.

TT 58.12 Thu 18:00 Theater

Towards single-shot readout of NV centers in diamond by low-temperature spin-to-charge conversion — •Dominik M. Irber[1], Michael Kieschnick[2], Jan Meijer[2], and Friedemann Reinhard[1] — [1]TU München, Walter Schottky Institut und Physik-Department, Am Coulombwall 4, 85748 München — [2]Felix-Bloch-Institut für Festkörperphysik Abteilung Nukleare Festkörperphysik, Linnéstraße 5, 04103 Leipzig

We present our recent progress in implementing an improved readout scheme for the nitrogen-vacancy (NV) center's spin-state combining resonant excitation at low temperature with spin-to-charge conversion. Resonant excitation exploits that the optical excitation spectrum at low temperature has sufficiently narrow linewidths to selectively address the spin-sublevels. In combination with a second laser pulse, a spin-to-charge conversion protocol can be implemented, where the NV center is spin-selectively excited and converted to different charge-states. These are more stable than the initial spin-state and can currently be read-out with near single-shot fidelity.

Compared to the state-of-the-art readout, this work promises to accelerate readout by a factor of up to 100. Besides, laser power in the optical regime can be reduced by orders of magnitude. This reduces the risk of photodamage for future sensing experiments with biological samples.

TT 58.13 Thu 18:15 Theater

Topological Frequency Pump with a Decohering Qubit — •Matthias Droth and David Carpentier — École Normale Supérieure de Lyon, 69007 Lyon, France

The underlying topological order of a physical device can lead to very robust phenomena. The most prominent example is the quantum Hall effect where measurement of the quantized transverse conductance σ_{xy} yields the conductance quantum e^2/h with high accuracy [1,2]. We study topological protection in a system with a driven quantum bit that features a topological phase in frequency space. A recent theoretical work proposed to realize an analog of the half Bernevig-Hughes-Zhang (BHZ) model – which realizes a quantum Hall effect – in the

frequency domain by driving periodically a quantum spin, leading to an effective time dependent Hamiltonian [3,4].

It is known that for such a realization of the half-BHZ model, the power transfer rate between the frequency drives, $P_{1\to2}$, takes the role of σ_{xy} as the quantized and topologically protected quantity [4]. Here, we investigate the robustness of this quantization in a realistic setup that involves a decohering qubit.

[1] K. v. Klitzing *et al.*, Phys. Rev. Lett. **45**, 494 (1980)
[2] M. H. Freedman *et al.*, Bull. Amer. Math. Soc. **40**, 31 (2003) Ch. Nayak *et al.*, Rev. Mod. Phys. **80**, 1083 (2008)
[3] B. A. Bernevig *et al.*, Science **314**, 1757 (2006).
[4] I. Martin *et al.*, Phys. Rev. X **7**, 041008 (2017).

TT 59: Complex Oxides Interfaces and Charge Order

Time: Thursday 15:00–18:00 Location: H22

TT 59.1 Thu 15:00 H22

Anisotropic transport properties in LAO/STO nanostructures — •Mithun S Prasad[1] and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120 Halle, Germany — [2]. Interdisziplinäres Zentrum für Meterialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Straße 4, D-06120 Halle, Germany

The high-mobility two-dimensional electron gas (2DEG) confined at the interface of two insulating complex oxides, LaAlO3 (LAO) and SrTiO3 (STO) provides new opportunities to explore nano electronic devices. In our group we have developed an industry compatible nano patterning technique [1] for the LAO/STO interface. Recent studies on this interface have revealed that at low temperature the current is confined to filaments which are linked to structural domain walls in the STO [2] with drastic consequences for example for the temperature dependence of local transport properties [3]. We have investigated magneto transport in nanostructures of different orientation with respect to the lattice. Our experiments show that not only the resistance but also the magnetoresistance varies with orientation. The magnetoresistance can even change sign strongly supporting the model of filamentary charge transport.

[1] M. Z. Minhas et al. , AIP Advances 6, 035002 (2016)

TT 59.2 Thu 15:15 H22

Tuning the superconducting transition of the $SrTiO_3$/$LaAlO_3$-interface with light — •Daniel Arnold, Dirk Fuchs, Karsten Wolff, and Roland Schäfer — Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

The conductance of the $SrTiO_3/LaAlO_3$ interface is sensitive to illumination by visible light [1,2]. We can tune the low temperature conductance of a sample in Hall bar geometry by up to a factor of 5 while we illuminate the sample at low temperatures in a controlled manner. Simultaneously the superconducting transition temperature shifts. The change in electrical conductance as well as the change in transition temperature persist even at low temperatures when the light is turned off. However, the initial state of the sample can be reestablished by increasing the temperature.
We present temperature and magnetic field dependent transport measurements and discuss the U/I characteristics regarding the inhomogeneous nature of the superconducting state.

[1] M. Huijben et al., Nat. Mater. 5 (2006)
[2] M. Yazdi-Rizi, PRB 95 (2017)

TT 59.3 Thu 15:30 H22

Comparative study of the two-dimensional electron gas at the $EuTiO_3$(001) and $SrTiO_3$(001) surfaces — •manish verma[1], m. salluzzo[2,3], m. radovic[3], j.h. dil[4], and rossitza pentcheva[5] — [1]Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany — [2]Dipartimento di Fisica, Università di Napoli Federico II, Italy — [3]CNR-SPIN, Italy — [4]Swiss Light Source and SwissFel, PSI, Switzerland — [5]Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Since the discovery of the two-dimensional electron gas (2-DEG) at the interface between the two band insulators $LaAlO_3$ and $SrTiO_3$ or at the $SrTiO_3$(001) surface, rich and intriguing physics has been uncovered at oxide interfaces. A significant effort concentrates on finding further possibly magnetic 2DEG oxide systems. $EuTiO_3$ serves as a suitable candidate in this direction, as it exhibits an antiferromagnetic ground state below 5.5K switchable to a ferromagnetic one by doping or lattice strain. In a combined density functional theory+U calculations with a Hubbard U on Eu $4f$ and Ti $3d$ states and angle resolved photoemission spectroscopy we explore the properties of the 2DEG at $EuTiO_3$(001) surface and compare to the much studied $SrTiO_3$(001) surface. In particular we focus on the effect of spin-orbit coupling on the 2DEGs at the two surfaces.

Funding by the DFG, CRC/TRR80 project G3 and computational time at magnitUDE supercomputer at University of Duisburg-Essen are acknowledged.

TT 59.4 Thu 15:45 H22

Magnetism and pseudo gap physics in $SrVO_3$ | $SrTiO_3$ heterostructures — •Matthias Pickem, Jan M. Tomczak, and Karsten Held — Institute of Solid State Physics, TU Wien, Austria

Modern atomic layer-by-layer deposition techniques allow for the study of materials in restricted geometries. Resulting effects of quantum confinement, e.g., in ultra-thin films are expected to be particularly pronounced for systems with strong electronic correlations. Indeed, the conventional Fermi-liquid state of bulk $SrVO_3$ was recently discovered to be destroyed in films below a critical thickness.

On the basis of these result we perform state-of-the-art density functional theory (DFT) + dynamical mean-field theory (DMFT) calculations. We first compute susceptibilities within DMFT and find antiferromagnetic ordering in the undoped cases and evidence of competing phases when doping, opening perspectives for oxide-based spin-tronic devices.

In order to properly describe possible non-local correlation effects stemming from the reduced dimensionality and the (potential) proximity of long-range ordered phases, we additionally apply the dynamical vertex approximation — a promising method beyond DMFT — that was recently extended to realistic materials calculations. Preliminary results suggest the presence of pseudo-gap physics, vaguely reminiscent of cuprate superconductors. The encountered large self-energy corrections to the local (DMFT) descriptors advocate for further studies of thin films and heterostructure in both theory and experiment.

TT 59.5 Thu 16:00 H22

Coupled charge density wave and magnetism in $TbTe_3$ — •Shravani Chillal[1], Enrico Schierle[1], Eugen Weschke[1], Jens Uwe Hoffmann[1], Fabiano Yokaichiya[1], Alexandre Vassiliev[2], Olga Volkova[2], Pierre Monceau[3], and Bella Lake[1,4] — [1]Helmholtz-Zentrum-Berlin für Materialien und Energie, Germany — [2]M.V. Lomonosov Moscow State University, Russia — [3]Université Grenoble Alpes, CNRS, Grenoble INP, Institut NEEL, France — [4]Technische Universität Berlin, Germany

$TbTe_3$ is a quasi-two dimensional system displaying a rich combination of quantum cooperative phenomenon including two charge density wave orders, complex incommensurate and commensurate magnetic orders as well as unconventional superconductivity under pressure. Hence, a delicate interplay of the three collective states is expected similar to the copper-oxide high-T_c superconductors leading to a novel phase diagram. Here, we present the interaction of the CDW and magnetic orders in $TbTe_3$ as a function of temperature and magnetic field. We find that these two collective states coexist at all the temperatures below the magnetic transition and that the magnetic order is coupled to the CDW state such that the magnetic wave vector can be described in terms of the CDW wave vector. Furthermore, we find an additional field induced phase where the magnetic wave vector locks-in to the CDW wave vector. Therefore, $TbTe_3$ can be considered as an ideal system to study the competition and coexistence of magnetism and CDW orders.

TT 59.6 Thu 16:15 H22

High-harmonic spectroscopy of the charge-density wave transition in 1T-$TiSe_2$ — •Tobias Heinrich[1], Sergey Zayko[1], Mu-

RAT SIVIS[1], KAI ROSSNAGEL[2], OFER KFIR[1], and CLAUS ROPERS[1] — [1]4th Physical Institute - Solids and Nanostructures, University of Göttingen, Germany — [2]Institute for Experimental and Applied Physics, University of Kiel, Germany

Correlated materials exhibit a wide variety of intriguing ordering phenomena, such as the charge-density wave (CDW) state in layered transition-metal dichalcogenides. The charge-density at the transition metal site and the CDW-induced band structure changes can be probed by photoemission spectroscopy [1,2]. However, also near-edge optical and x-ray spectroscopy of core-levels should provide valuable time-resolved information.

Here, we employ an extreme-ultraviolet pump-probe setup to study the CDW-to-normal phase transition in 1T-$TiSe_2$. Our setup features femtosecond infrared pump and high-harmonic ($25-50$eV) probe pulses, suitable to access CDW-features near the Ti M-edge. In our experiments, we find characteristic spectral changes upon thermally inducing the phase transition near 202 K, which are indicative of a splitting of the Ti-M edge into nonequivalent Ti sites. In ongoing experiments, we investigate the temporal evolution of the spectral signatures with a temporal resolution below 40 fs, complementing ultrafast photoemission spectroscopy studies.

[1] Timm Rohwer *et al.*, Nature **471**, 490-493 (2011)
[2] S. Hellmann *et al.*, PRL **105**, 187401 (2010)

15 min. break.

TT 59.7 Thu 16:45 H22

Photo-induced rearrangement of orbitally ordered layers in thin 1T-TaS_2 — •QUIRIN STAHL[1], TOBIAS RITSCHEL[1,2], MAXIMILIAN KUSCH[1], FLORIAN HEINSCH[1,3], GASTON GARBARINO[4], NORMAN KRETZSCHMAR[4], and JOCHEN GECK[1] — [1]TU Dresden, Germany — [2]UBC, Vancouver, Canada — [3]HZDR, Germany — [4]ESRF, Grenoble, France

The ultra-fast semiconductor-to-metal transition in nano-thick 1T-TaS_2 crystals induced by femtosecond laser pulses currently attracts a lot of interest [1,2]. In particular, since it is believed that such laser pulses stabilize so-called hidden states, which cannot be reached from thermal equilibrium and which exhibit unique electronic properties. We present a detailed XRD study of nano-thick 1T-TaS_2 single crystals. In a first experiment we studied the charge density wave order in the supercooled state, which has been observed earlier in resistivity measurements [3]. This phase is then compared to the charge density wave order created by a femtosecond laser pulse. Our measurements reveal the existence of commensurate domains separated by discommensurations in both phases, implying that the hidden state of 1T-TaS_2 stands in close relation to the nearly commensurate state. The electronic characteristics are discussed in terms of switching between orbital configurations, caused by the rearrangement of orbitally ordered layers.

[1] L. Stojchevska et al., Science 334, 177 (2014)
[2] I. Vaskivskyi et al., Science Advances 1, 6 (2015)
[3] M. Yoshida et al., Scientific Reports 4, 7302 (2014)

TT 59.8 Thu 17:00 H22

Scanning tunneling microscopy on an excitonic insulator Ta_2NiSe_5 — QINGYU HE[1], XINGLU QUE[1], ALEXANDER YARESKO[1], •ANDREAS ROST[1], MASAHIKO ISOBE[1], TOMOHIRO TAKAYAMA[1], LIHUI ZHOU[1], and HIDENORI TAKAGI[1,2] — [1]Max Planck Institute for solid state research, Stuttgart, Germany — [2]University of Tokyo, Tokyo, Japan

Ta_2NiSe_5 is the strongest candidate for the long conjectured excitonic insulator state. It is a direct zero gap semiconductor at high temperature, and undergoes at $T_c = 326$ K a semiconductor-insulator transition simultaneous with an orthorhombic-monoclinic q = 0 structure transition. Our low temperature STM evidences its layered structure with rippling atomic chains. The local spectroscopy reveals the opening of the excitonic insulator gap and the spectral weight shift with decreasing temperature. High resolution STM topography shows a local distortion associated with the structure transition. This distortion may play an important role in the formation of the excitonic state, as also supported by our band structure calculations.

TT 59.9 Thu 17:15 H22

LDA+U and LDA+DMFT study on structurally-triggered metal insulator transition in $CaCu_3Fe_4O_{12}$ — •ATSUSHI HARIKI, MATHIAS WINDER, and JAN KUNEŠ — Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

We study structurally-triggered metal-insulator transition of $CaCu_3Fe_4O_{12}$ by means of local density approximation (LDA) +U and LDA+dynamical mean-field theory (DMFT). We show from the LDA+U calculations that the metal-insulator transition is induced by the breathing distortion of Fe-O bonds, that is structurally triggered by rotation of FeO_6 octahedra. Based on the LDA+DMFT calculations, taking all Cu 3d, Fe 3d and O 2p bands into account explicitly, we discuss electronic coupling of Fe (formally tetravalent) 3d and O 2p states under the breathing distortion as well as origin of the experimental ferrimagnetic ordering.

TT 59.10 Thu 17:30 H22

Correlation between charge- and oxygen-ordering in 214-type hole-doped $Pr_{2-x}Sr_xNiO_{4+d}$ systems — •AVISHEK MAITY[1,2], RAJESH DUTTA[2], LAURA GUASCO[3], ALEXIE BOSSAK[4], MONICA CERETTI[3], and WERNER PAULUS[3] — [1]Georg-August-Universität-Goettingen, Göttingen, 37077 Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, 85747 Germany — [3]Université de Montpellier, Montpellier, 34095 France — [4]The European Synchrotron-ESRF, Grenoble, 38000 France

The research on charge-ordered (CO) stripes in 214-type cobaltates/nickelates has become a fertile territory of research in the last two decades after they were experimentally evidenced in homologous superconducting cuprates $La_{2-x}Sr_xCuO_{4+d}$[1]. Although contentious, fluctuation of such organized quantum mater e.g. stripe is believed to be responsible for high-Tc superconductivity [2]. What still remains poorly discussed, is the influence of nonstoichiometric interstitial oxygen (Oint) on the organization of holes in a line shape. We have investigated CO state in $Pr_{2-x}Sr_xNiO_{4+d}$ by several synchrotron and neutron diffraction measurements. $Pr_{2-x}Sr_xNiO_{4+d}$ being a potential O-ion conductor, the high mobility of Oint gives rise to a complex long-range O-ordering even at RT. Investigating different doping level, we have found that the spacing in between the stripes is defined by the Oint-ordered supercell. I will present the relation between O-order and CO and the effect on CO correlation.

[1] J. M.Tranquada et al., Nature 375, 561-563 (1995)
[2] J. Zaanen, Nature 471, 314-316 (2011)

TT 59.11 Thu 17:45 H22

Spin, charge and orbital order in $Pr_{1-x}Ca_xMnO_3$ — •MICHAEL TEN BRINK[1,2], SANGEETA RAJPUROHIT[2], MOHSEN SOTOUDEH[2], CHRISTIAN JOOSS[3], and PETER E. BLÖCHL[1,2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [2]Institut für Theoretische Physik, Technische Universität Clausthal — [3]Institut für Materialphysik, Georg-August-Universität Göttingen

The strong coupling of electron, phonon and spin degrees of freedom in manganites leads to a rich phase diagram with several competing ordering principles. We investigate the ground state phases for the whole doping range of $Pr_{1-x}Ca_xMnO_3$ using two theoretical methods: 1. density functional calculations (DFT) with local hybrid functionals, which allows us to compare to experimental spectra (EELS, XPS and optical absorption), 2. from the DFT calculations we determine the parameters of a tight-binding model, which captures the interactions between the relevant electron, spin and phonon degrees of freedom. This model allows us to study a variety of defect structures in larger systems and the spin, charge and orbital order in a unified framework.

TT 60: Quantum-Critical Phenomena (joint session TT/DY)

Time: Thursday 15:00–18:00 Location: H23

TT 60.1 Thu 15:00 H23

Superconductivity from the Condensation of Topological Defects in a Quantum Spin-Hall Insulator — Yuhai Liu[1], Zhenjiu Wang[2], Toshihiro Sato[2], Martin Hohenadler[2], Chong Wang[3], Wenan Guo[1], and •Fakher F. Assaad[2] — [1]Department of Physics, Beijing Normal University, Beijing 100875, China — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada N2L 2Y5

The discovery that spin-orbit coupling can generate a new state of matter in the form of quantum spin-Hall (QSH) insulators has brought topology to the forefront of condensed matter physics. While QSH states from spin-orbit coupling can be fully understood in terms of band theory, fascinating many-body effects are expected if the state instead results from interaction-generated symmetry breaking. In particular, topological defects of the corresponding order parameter provide a route to exotic quantum phase transitions. Here, we introduce a model in which the condensation of skyrmion defects in an interaction-generated QSH insulator produces a superconducting (SC) phase. Because vortex excitations of the latter carry a spin-1/2 degree of freedom numbers, the SC order may be understood as emerging from a gapless spin liquid normal state. The QSH-SC transition is an example of a deconfined quantum critical point (DQCP), for which we provide an improved model with only a single length scale that is accessible to large-scale quantum Monte Carlo simulations.

TT 60.2 Thu 15:15 H23

Studies of Deconfined Quantum Criticality in a Half-filled Laudau Level — •Zhenjiu Wang[1], Matteo Matteo Ippoliti[2], Roger S. K Mong[3], and Michael P Zaletel[2,4] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, Princeton University, Princeton, NJ 08544, USA — [3]Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA — [4]Department of Physics, University of California, Berkeley, CA 94720, USA

We perform Quantum Monte Carlo studies of deconfined quantum criticality (DQC) based on models of interacting fermions. As opposed to previous studies, this suggests an emergent SO(5) symmetry at criticality, our model has an exact SO(5) symmetry at the Hamiltonian level. This relies on the fact that our model is defined in the continuum. As opposed to lattice regularization, that would break the SO(5) symmetry, we follow a suggestion by [1], where the ultra-violet cutoff is realized by a magnetic field. Our model corresponds to 4 flavors of fermions with Hilbert space restricted to the zeroth Landau level (ZLL) of 8 component Dirac fermions as realized in Graphene, which maps to a nonlinear sigma model containing only bosonic degrees of freedom is studied, with the competition between the stiffness and an SO(5) Wess-Zumino-Witten topological term. AFQMC studies are free of the negative sign problem due to the existence of two anti-unitary particle-hole transformations that leaves the propagator invariant for each MC configuration.
[1] Ippoliti et al., arXiv:1810.00009 (2018)

TT 60.3 Thu 15:30 H23

Deconfined criticality from the QED3-Gross-Neveu model — •Lukas Janssen[1], Bernhard Ihrig[2], Luminita N. Mihaila[3], and Michael M. Scherer[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Germany — [3]Institut für Theoretische Physik, Universität Heidelberg, Germany

The QED$_3$-Gross-Neveu model is a (2+1)-dimensional U(1) gauge field theory involving Dirac fermions and a critical real scalar field. It has been argued that this theory represents a dual description of the deconfined quantum critical point between Néel and valence bond solid orders in frustrated quantum magnets. I will present evidence for a novel scaling relation that implies emergent SO(5) symmetry at criticality.

TT 60.4 Thu 15:45 H23

Deconfined quantum criticality in the two-dimensional Su-Schrieffer-Heeger model — •Stefan Beyl, Martin Hohenadler, Florian Goth, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland

The Su-Schrieffer-Heeger model is one of the most basic models for electron-phonon coupling. It captures the effects of fluctuating bond lengths—as described by quantum mechanical bond phonons—on the electronic hopping. While much work has been devoted to the one-dimensional case, systematic results in two dimensions are not available. Here, we present results from sign-free hybrid quantum Monte Carlo simulations at half-filling that support a deconfined quantum critical point between a valence bond solid and an antiferromagnet, as well as remarkable connections to an Ising lattice gauge theory with topologically ordered metallic and insulating phases.

TT 60.5 Thu 16:00 H23

Quantum Criticality near the Mott Transition — •Heike Eisenlohr[1], Seung-Sup B. Lee[2], Andreas Weichselbaum[2], and Matthias Vojta[1,3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstraße 37, 80333 München, Germany — [3]Center for Transport and Devices of Emergent Materials, Technische Universität Dresden, 01062 Dresden, Germany

The Mott metal-insulator transition is known to be a first order transition, with the transition line terminating in a classical critical end point at finite temperature Tc. Recent numerical studies of the half-filled Hubbard model, which employed dynamical mean-field theory and a quantum Monte Carlo impurity solver, and experiments in 2d organic salts have concordantly observed apparent quantum critical scaling of the resistivity in the regime T>Tc [1,2]. Although this conventionally indicates a nearby quantum critical point at T=0, the studied system shows only a classical first order transition at T=0. So far no theoretical explanation was able to identify the degrees of freedom which behave as if they were quantum critical, and why. To understand this unexpected scaling regime, we study the system with dynamical mean-field theory in combination with the numerical renormalization group.

TT 60.6 Thu 16:15 H23

Quantum critical behaviour in 2D Fermi systems with quadratic band touching — •Shouryya Ray, Matthias Vojta, and Lukas Janssen — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We consider two-dimensional Fermi systems with quadratic band touching and C_3 symmetry, as realizable in Bernal-stacked honeycomb bilayers. Within a renormalization-group analysis, we demonstrate the existence of a quantum critical point at a finite value of the density-density interactions, separating a semimetallic disordered phase at weak coupling from a gapped ordered phase at strong coupling. The latter may be characterized by, for instance, antiferromagnetic, quantum anomalous Hall, or charge density wave order. In the semimetallic phase, each point of quadratic band touching splits into four Dirac cones as a consequence of the nontrivial interaction-induced self-energy correction, which we compute to the two-loop order. We show that the quantum critical point is in the $(2 + 1)$-dimensional Gross-Neveu universality class, characterized by emergent Lorentz invariance and a dynamic critical exponent $z = 1$. At finite temperatures, $T > 0$, we hence conjecture a crossover between $z = 2$ at intermediate T and $z = 1$ at low T, and construct the resulting nontrivial phase diagram as function of coupling strength and temperature.

15 min. break.

TT 60.7 Thu 16:45 H23

Quantum Criticality of an Ising-like Spin-1/2 Antiferromagnetic Chain in a Transverse Magnetic Field — •Zhe Wang[1], Thomas Lorenz[2], Denis Gorbunov[1], Pham Thanh Cong[1], Yoshimitsu Kohama[3], Sandra Niesen[2], Olivier Breunig[2], Johannes Engelmayer[2], Alexander Herman[2], Jianda Wu[4], Koichi Kindo[3], Joachim Wosnitza[1], Sergei Zherlitsyn[1], and Alois Loidl[5] — [1]Helmholtz Zentrum Dresden Rossendorf, Dresden, Germany — [2]University of Cologne, Cologne, Germany — [3]University of Tokyo, Kashiwa, Japan — [4]Tsung-Dao Lee Institute, Shanghai —

[5]University of Augsburg, Germany

We report on magnetization, sound velocity, and magnetocaloric-effect measurements of the Ising-like spin-1/2 antiferromagnetic chain system $BaCo_2V_2O_8$ as a function of temperature down to 1.3 K and applied transverse magnetic field up to 60 T [1]. At $B_\perp^c = 40$ T, the $T(B)$ curve shows a broad minimum, accompanied by a broad minimum in the sound velocity and a saturation-like magnetization. These features signal a quantum phase transition which is further characterized by the divergent behavior of the Grüneisen parameter $\Gamma_B \propto (B - B_\perp^c)^{-1}$. By contrast, around the critical field, the Grüneisen parameter converges as temperature decreases, pointing to a quantum critical point of the one-dimensional transverse-field Ising model [2].

[1] Zhe Wang et al., Phys. Rev. Lett. 120, 207205 (2018)
[2] Jianda Wu et al., Phys. Rev. B 97, 245127 (2018)

TT 60.8 Thu 17:00 H23

Phase diagram of SU(N) Dirac fermions on the π-flux lattice with a bond-bond interaction — •Johannes S Hofmann, Martin Hohenadler, and Fakher F Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We use auxiliary-field quantum Monte Carlo simulations to study the phase diagram of SU(N) Dirac fermions with a bond-bond interaction V similar to Ref. [1] and an associated O($2N$) symmetry. In contrast to previous work, we consider a π-flux rather than a honeycomb lattice. The different coordination number is expected to favor antiferromagnetic (AFM) over valence bond solid (VBS) order. Accordingly, whereas AFM order is absent from the N-V phase diagram for $N > 2$ in Ref. [1], we find an AFM phase up to $N = 3$. Our results are consistent with Gross-Neveu semimetal-VBS transitions for $N > 1$ and deconfined VBS-AFM quantum critical points for $N = 2$ and $N = 3$.

[1] Z.-X. Li, Y.-F. Jiang, S.-K. Jian, and H. Yao, Nature Communications 8, 314 (2017)

TT 60.9 Thu 17:15 H23

Quantum criticality on a chiral ladder: a model study — Philipp Schmoll[1,2], •Andreas Haller[1,2], Matteo Rizzi[1], and Román Orús[1,3,4] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany — [3]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain — [4]Ikerbasque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain

In our work we focus on exotic SU(2) invariant three-spin interactions which are exploited to engineer non-trivial helical phases in quasi one-dimensional ladder setups, also dubbed as wire deconstructionism. Such interactions are typically treated as a perturbation of the famous spin-1/2 Heisenberg model. Here, we extend the existing literature and tackle the non-perturbative low-energy regime by means of exact diagonalization, blockspin renormalization and bosonization. Our Luttinger Liquid (LL) analysis predicts a subtle gapping mechanism between two of the four helical modes in the ladder, which yields a critical model with central charge c=1. We support our analysis by numerical data obtained from an SU(2) symmetric implementation of the infinite Density Matrix Renormalization Group (iDMRG) algorithm.

TT 60.10 Thu 17:30 H23

Quantum criticality on a chiral ladder: an $SU(2)$ iDMRG study — •Philipp Schmoll[1,2], Andreas Haller[1,2], Matteo Rizzi[1], and Román Orús[1,3,4] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany — [3]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain — [4]Ikerbasque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain

We study the ground state properties of a ladder Hamiltonian with chiral $SU(2)$-invariant three-spin interactions, a possible first step towards the construction of truly two dimensional non-trivial systems with chiral properties starting from quasi-one dimensional ones. Extending our analysis by means of blockspin renormalization and bosonization we use a recent implementation of $SU(2)$ symmetry in the infinite Density Matrix Renormalization Group (iDMRG) algorithm. The numerical findings agree very well with the theoretical prediction of a gapless phase. In particular, the scaling of the entanglement entropy as well as finite-entanglement scaling data show that the ground state properties match those of the universality class of a $c = 1$ conformal field theory (CFT) in $(1 + 1)$ dimensions.

TT 60.11 Thu 17:45 H23

Statistically induced quantum phase-transitions in the extended Anyon-Hubbard model — •Martin Bonkhoff, Kevin Jägering, Shijie Hu, Imke Schneider, Axel Pelster, and Sebastian Eggert — Departement of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany

Recently it has been shown that one-dimensional abelian anyons can be realized via density dependent Peierls-phases in bosonic models [1]. Furthermore extended interactions as well as a particle number constraint in bosonic Hubbard models can lead to a Symmetry-Protected-Topological (SPT) Haldane insulator phase [2]. We study the fate of SPT-order under statistical transmutation, and additionally observe a new gapped dimerized phase for attractive on-site interaction. By the technique of bosonization, we establish a unified low-energy field theory characterizing phases and relevant quantum phase transitions in the whole parameter region. We analyze the mechanism behind statistically induced phase transitions in combination with large-scale numerical simulations by the density-matrix renormalization group method.

[1] T. Keilmann, S. Lanzmich, I. McCulloch, and M. Roncaglia, Nat. Comm. 2, 361 (2011)
[2] E. Berg, E. G. D. Torre, T. Giamarchi, and E. Altman, Phys. Rev. B 77, 245119 (2008)

TT 61: Topology and Symmetry-Protected Materials (joint session O/MA/TT)

Time: Thursday 15:00–17:45 Location: H24

TT 61.1 Thu 15:00 H24

Structural and electronic characterization of thin Fe(Se,Te) films on the quaternary (Bi,Sb)Se_xTe_{1-x} 3D topological insulator — •Philipp Kagerer, Thiago R. F. Peixoto, Celso Fornari, Hendrik Bentmann, and Friedrich Reinert — Experimental Physics VII, Julius Maximilian University of Würzburg

The combination of an s-wave superconductor iron-chalcogenide and a 3D-topological insulator (TI) has become a vivid research topic in condensed matter physics due to the proposed emergence of bound Majorana zero modes at the interface under the presence of a time-reversal-breaking magnetic field [1]. Owing to its simple cubic structure and good growth properties, thin FeSeTe layers on (Bi,Sb)Se_xTe_{1-x} pose a promising platform to test this prediction.

Here we report on the epitaxial growth and characterization of thin layers of Fe(Se,Te) on a quaternary (Bi,Sb)(Se,Te) TI single-crystal. LEED and XPS experiments as well as STM and STS scans confirm the formation of a few monolayers of Fe(Se,Te) on top of the TI substrate. Using ARPES we show the arising of the FeSeTe valence bands near the Fermi level, along with the heavily n-doped band structure of the underlying TI. In addition, photon-energy-dependent and resonant measurements using synchrotron radiation allow a distinction between substrate and overlayer bands, and show indications for strong electron correlation and a Hubbard-gap in the material [2].

[1] L.Fu, C.L. Kane, Phys. Rev. Lett. 100, 096407 (2008)
[2] M.D.Watson et al., Phys. Rev. B 95, 081106(R) (2017)

TT 61.2 Thu 15:15 H24

Magnetic and Electronic Structure of the proposed Antiferromagnetic Topological Insulator $MnBi_2Te_4$ — •Raphael Crespo Vidal[1], Hendrik Bentmann[1], Thiago Peixoto[1], Alexander Zeugner[2], Anna Isaeva[2], Anja Wolter[3], Bernd Büchner[3], Mikhail Otrokov[4], Evgueni Chulkov[4], and Friedrich Reinert[1] — [1]Chair for Experimental Physics VII, Universität Würzburg, Germany — [2]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Germany — [3]Leibniz-Institute for Solid State and Materials Research, Dresden, Germany — [4]Centro de Fisica de Materials, Centro Mixto, Spain

The interplay auf magnetism and topology gives rise to new topological quantum phases with broken time-reversal symmetry like the quantum anomalous Hall state.
Here we will present single-crystal measurements on the magnetic and electronic structure of $MnBi_2Te_4$ [1], a van der Waals bonded system composed of septuple layers stacked along its [0001]-axis. The layered structure results in a high accessibility for surface science methods, while its stochiometric nature leads to intrinsic magnetism without the need of free parameters like dopand concentration. By X-Ray magnetic circular dichroism, linear dichroism and bulk magnetization measurements we determine an out of plane A-type antiferromagnetic ordering below $T_N = 24\,K$. Angle-resolved photoemission spectroscopy shows a massive Dirac-like state with an energy gap of $\sim$100 meV.

[1] M. Otrokov et al., ArXiv., 1809.07389 (2018)

TT 61.3 Thu 15:30 H24

XAS/XMCD study of magnetically doped $(Bi,Sb)_2Te_3$ — •Abdul-Vakhab Tcakaev, Volodymyr Zabolotnyy, Steffen Schreyeck, Karl Brunner, Charles Gould, and Vladimir Hinkov — University Würzburg, Am Hubland, 97074 Würzburg

The magnetic topological insulators $Cr:(BiSb)_2Te_3$ and $V:(BiSb)_2Te_3$ have been extensively studied as realizations of the quantum anomalous Hall (QAH) effect. While the QAH state in V-doped films is found to be significantly superior, the differences in the electronic structure and in the mechanisms of magnetic ordering for V- and Cr-doping remain under intensive debate. Here we combine x-ray absorption(XAS) and x-ray magnetic circular dichroism (XMCD) to trace element-specific contributions to the electronic and magnetic properties of these systems. We use *ab initio* density functional theory (DFT) based multiplet ligand field theory calculations (MLFT) at Cr and V $L_{2,3}$ edges for understanding and interpreting experimental results and determine local electronic and magnetic properties of these topological insulators.

TT 61.4 Thu 15:45 H24

Laser-based ARPES and pressure dependent magneto-transport studies of BiSbTe3 topological insulator — •Shiv Kumar[1], Vinod Kumar Gangwar[2], Yufeng Zhang[3,4], Prashant Shahi[5], Hitoshi Takita[1], Swapnil Patil[2], Eike Fabian Schwier[1], Kenya Shimada[1], Yoshiya Uwatoko[4], and Sandip Chatterjee[2] — [1]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima City, 739-0046, Japan — [2]Dept. of Physics, Indian Institute of Technology (BHU) Varanasi 221005, India — [3]School of Physics and Key Laboratory of MEMS of the Ministry of Education, Southeast University, Nanjing 211189, China — [4]ISSP, University of Tokyo, Kashiwa, Chiba 277-8581, Japan — [5]Dept. of Physics, D.D.U. Gorakhpur University, Gorakhpur 273009, India

In recent years, 3D topological insulators (TIs), have drawn significant attention in condensed matter physics. Many TIs are known as good thermoelectric (TE) materials. We have grown single-crystal BiSbTe3 3D TI sample and studied structural, TE as well as pressure dependent magnetotransport properties. Large positive Seebeck coefficient confirmed the p-type nature of BiSbTe3, which is consistent with Hall measurement. We have also studied the electronic band structure using Laser-based ARPES, which revealed the existence of a Dirac-cone like metallic surface state in BiSbTe3 with a Dirac Point situated exactly at the Fermi level. The large Seebeck coefficient and good TE performance at room-temperature attract great attention for the application in TE devices. Additionally, superconductivity emerges under pressure of 8 GPa with a critical temperature of ~2.5 K.

Invited Talk TT 61.5 Thu 16:00 H24

Luttinger liquid in a box: electrons confined within MoS_2 mirror twin boundaries — •Wouter Jolie[1,2], Clifford Murray[1], Philipp Weiss[3], Joshua Hall[1], Fabian Portner[3], Nicolae Atodiresei[4], Arkady Krasheninnikov[5,6], Carsten Busse[1,2,7], Hannu-Pekka Komsa[6], Achim Rosch[3], and Thomas Michely[1] — [1]II. Physikalisches Institut, University of Cologne, Germany — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany — [3]Institute for Theoretical Physics, University of Cologne, Germany — [4]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [5]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [6]Department of Applied Physics, Aalto University, Finland — [7]Department Physik, Universität Siegen, Germany

Two- or three-dimensional metals are usually well described by weakly interacting, fermionic quasiparticles. This concept breaks down in one dimension due to strong Coulomb interactions. There, low-energy excitations are expected to be collective bosonic modes, which fractionalize into independent spin and charge density waves.

In this talk I will present how we construct a well-isolated, one-dimensional metal of finite length using mirror twin boundaries in molybdenum disulfide (MoS_2). We demonstrate how scanning tunneling spectroscopy can identify the unique fingerprints of confined, strongly interacting states, thereby providing a direct and local experimental tool to investigate spin-charge separation in real space.

TT 61.6 Thu 16:30 H24

Structure and electronic properties of antimonene layers on Bi2Se3 interfaces — •Kris Holtgrewe[1], Conor Hogan[2], and Simone Sanna[1] — [1]University of Giessen, Germany — [2]CNR-ISM, Rome, Italy

Topological insulators (TI) exhibit unconventional physical effects that have attracted the interest of the scientific community, especially when coupled to trivial insulators. A topologically insulating Bi_2Se_3 substrate covered by the trivial insulator antimonene, is an ideal testbed to study the interfacial phenomena [1], and is furthermore interesting for applications such as topological pn-junctions [2].

Much research effort has been dedicated to surface preparation [3], recording of STM and ARPES images, as well as band structure calculations. However, the Sb-coverage dependent spin texture (e. g. position of Dirac states, Rashba splitting) is still not fully understood. Our work is dedicated to the theoretical investigation of the relationships between structural motifs, band structures and STM pattern. Thereby we show that including both spin-orbit coupling and van-der-Waals interaction in our density functional theory based approach is crucial for the correct modelling of the system.

[1] K. Jin et al, Phys Rev B **93**, 075308 (2016)
[2] S. Kim et al., ACS Nano **11**, 9671 (2017)
[3] R. Flammini, S. Colonna, C. Hogan, S. K. Mahatha, M. Papagno, A. Barla, P. M. Sheverdyaeva, P. Moras, Z. S. Aliev, M. B. Babanly, E. V. Chulkov, C. Carbone, and F. Ronci, Nanotechnology **29**, 065704 (2018)

Invited Talk TT 61.7 Thu 16:45 H24

Quasiparticle interferences on Type I and Type II Weyl semimetal surfaces — •Hao Zheng — School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China

A Weyl semimetal is a new topological phase of matter that extends the topological classification beyond insulators, exhibits quantum anomalies, possess exotic surface Fermi arc electron states and provides the first ever realization of Weyl fermions in physics. In a Weyl semimetal, the chirality of the Weyl nodes give rise to topological charges, which can be understood as monopoles and anti-monopoles of Berry flux in momentum space. They are separated in momentum space and are connected only through the crystal boundary by an unusual topological surface state, a Fermi arc. The surface of a Weyl semimetal has been predicted to exhibit interesting tunneling and transport properties, leading to potential electronic and spintronic applications.

We employed scanning tunneling microscopy/spectroscopy to directly visualize the coherent quasiparticle interferences on both type-I and type-II Weyl semimetal surfaces. On NbP (type-I Weyl) surface, we reveal that the surface interference channels are restricted by their surface spin and/or orbit textures and discover the existence of surface Dirac cones. On $Mo_xW_{1-x}Te_2$ (type-II Weyl), the topological Fermi arc derived quantum interference is clearly discerned. Our results may pave a new way towards the future research on a Weyl fermion related surface transport phenomena and devices.

TT 61.8 Thu 17:15 H24

Bulk and Surface Electronic Structure of the Weyl-Semimetals TaP and TaAs — •Tim Figgemeier[1], Chul-Hee Min[1], Phillip Eck[2], Jennifer Neu[3], Maximilian Uenzelmann[1], Domenico Di Sante[2], Theo M. Siegrist[3,4], Giorgio Sangiovanni[2], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universitaet Wuerzburg — [2]Theoretische Physik I, Universitaet Wuerzburg — [3]National High Magnetic Field Laboratory, Tallahassee, Florida — [4]College of Engineering, FAMU-FSU, Tallahassee, Florida

Tantalum Arsenide (TaAs) and Tantalum Phosphide (TaP) are prototypical Weyl-Semimetals. We examine the electronic band structure using Angle-Resolved Photoemission Spectroscopy over a broad range of excitation energies from the VUV to the Soft X-Ray regime. With

this high flexibility in photon energies, we are able to analyse the entire complex band structure of TaP in detail. In particular the surface states and the bulk band structure are identified at different photon energies and compared to first principles DFT calculations. By use of linear polarized light, we disentangle the orbital character of the Fermi arcs and other electronic states in the Fermi surface along with their connection to the bulk band structure [1].

[1] Min et al., "Orbital Fingerprint of Topological Fermi Arcs in a Weyl Semimetal", arXiv:1803.03977 (2018)

TT 61.9 Thu 17:30 H24

Exploring the spin-orbital texture in a Dirac heavy metal by spin-resolving momentum microscopy — •Ying-Jiun Chen[1,2], Christian Tusche[1,2], Markus Hoffmann[3], Bernd Zimmermann[3], Gustav Bihlmayer[3], Stefan Blügel[3], and Claus Michael Schneider[1,2] — [1]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Entanglement of spin and orbital degrees of freedom in strongly spin-orbit coupled materials creates exotic spin/orbital textures in momentum space such as Rashba and topological protected surface states. Dichroism in spin-polarized photoemission plays a crucial role in understanding the influence of spin-orbit coupling on the electronic wave functions. By virtue of the recent invention of the spin-resolving Momentum Microscope, the spin-detection efficiency and momentum resolution has been improved tremendously. This development makes it now possible to probe the photoelectron spin polarization as well as linear and circular dichroism in the angular distribution over the whole Brillouin zone. In addition to the d-electron-drived Dirac-type helical spin texture, we directly characterize the momentum-dependent spin-orbital entangled states on W(110) throughout the entire surface Brillouin zone by using differently polarized light. Comparison between theory and experiment provides insights into the large anisotropy of spin relaxation in the prototype Dirac heavy metal.

TT 62: Direct-Write Nanofabrication and Applications III (Electron Beam Induced Processing) (joint session DS/TT)

Part III: Material Properties & Applications

Organizers:

- Michael Huth, Physikalisches Institut, Goethe-Universität, Frankfurt, Germany
- Harald Plank, FELMI-ZFE, TU Graz, Austria

(Synopsis provided with part I of this session)

Time: Thursday 15:00–17:45 Location: H32

Invited Talk TT 62.1 Thu 15:00 H32

Artificial nano-granular heterostructures: fundamentals and applications — •Oleg Udalov[1,2] and Igor Beloborodov[1] — [1]California State University, Northridge, USA — [2]Institute for Physics of Microstructures RAS, Nizhny Novgorod, Russia

Granular composites are a large class of artificial materials in which nanograins are embedded into a hosting matrix. Combining different types of grains and matrix one can obtain composites with desirable functionalities. Fabrication of granular materials is scalable and is much cheaper than, for example, the thin film preparation techniques. Such an advantage makes these materials very attractive for various applications, including medical, photonic, radiofrequency, mechanical, etc. Properties of granular materials are defined by the interplay of disorder, dimensionality, surface and size effects, superconductivity, magnetic interactions, strain, the Coulomb blockade, etc. Therefore, studying of these materials is a complicated challenge promising unexpected novel properties. Nanograins ensembles are often used as a prototype of systems with competitive interactions and strong many-body effects. This makes granular materials of a great fundamental interest. In this talk we will focus on recent developments in solid granular materials. First, we discuss different types of granular media and their applications. In particular, we will consider granular metals, ferromagnets, superconductors and semiconductors. Next, we will discuss granular multiferroics where two order parameters are combined: 1) magnetization and 2) polarization. We will consider theoretical and experimental works on magneto-electric coupling in these materials.

TT 62.2 Thu 15:30 H32

Ac conductivity of nano-granular metals prepared via FEBID — •Marc Hanefeld[1], Michael Huth[1], Joshua Gies[2], and Martin Kind[2] — [1]Physikalisches Institut, Goethe Universität, Max-von-Laue-Str. 1 — [2]Institut für Anorg. und Analyt. Chemie, Goethe Universität, Max-von-Laue-Str. 7, 60438 Frankfurt a. M., Germany

Focused Electron Beam Induced Deposition (FEBID) is a versatile technique to create nano-granular metals with tunable electronic transport properties [1]. In granular metals metallic nanoparticles are surrounded by a dielectric matrix which leads to a transport mechanism based on thermally assisted tunnelling. This opens up promising possibilities for sensing applications [1] and has triggered ongoing research concerning their response to a time-dependant ac stimulus [2].

Current research focuses mainly on two different material properties, namely an apparent universal power law and a temperature-independent scaling behaviour in the real part of the complex ac conductivity, both present in many disordered solids and recently reported in granular metals of palladium in zirconia [2].

We present recent results on the ac conductance response of nano-granular Pt(C)-FEBID deposits and show the capabilities of FEBID to create an ideal model environment for an in depth analysis of the ac conduction characteristics of granular metals. Possible applications of these results in dielectric sensors combining nano-granular Pt(C) with metal-organic frameworks will be discussed.

[1] Huth, et al., Microelect. Eng. 2017. doi:10.1016/j.mee.2017.10.012.
[2] Bakkali, et al., Sci. Rep. 2016;6:29676. doi:10.1038/srep29676.

TT 62.3 Thu 15:45 H32

Post-growth electron beam irradiation of co-deposited PtC-FeCo FEBID nanostructures — •Roland Sachser and Michael Huth — Physikalisches Institut, Goethe-University, Frankfurt am Main, Germany

FEBID using the precursor $(CH_3)_3CH_3C_5H_4Pt$ leads to low conductive, nanogranular samples. The resistivity is determined by the coupling of Pt nanocrystals by the carbonaceous matrix. This matrix, and thus the conductivity, can be strongly influenced by post-growth electron beam irradiation. On the other hand, deposits prepared employing the precursor $HFeCo_3(CO)_{12}$ feature high metal contents and metallic resistivity behavior. These samples are ferromagnetic but the tunability of their transport properties by post-growth treatments is limited. By co-deposition using both precursors under well-controlled mixing ratios it is possible to obtain a highly tunable granular ferromagnet. Granular ferromagnetic systems are known to show an enhanced anomalous Hall effect, which can also be observed in our deposits that are treated by post-growth electron beam irradiation under in situ conductance monitoring. The conductance can be tuned over a wide range, which is also prominently reflected in the magneto-transport properties that can be directly monitored in situ in the low field regime at room temperature. Complementary low temperature magneto-transport measurements reveal the optimal post-growth irradiation dose to obtain the largest anomalous Hall effect.

TT 62.4 Thu 16:00 H32

Micro-Hall Magnetometry of FEBID-fabricated 3D magnetic nano-architectures — •Jens Müller[1], Mohanad Al Mamoori[1], Lukas Keller[1], Michael Huth[1], and Christian Schröder[2] —

[1]Institute of Physics, Goethe University Frankfurt — [2]Institute for Applied Materials Research, Bielefeld University of Applied Sciences

Whereas most of the previous studies of nanoscale magnetic structures – owing to the fabrication by means of lithographic processes – have focused on one- or two-dimensional (1D/2D) nanomagnets, thanks to advances in fabrication and sensing techniques it is now possible to investigate free-standing magnetic 3D structures individually, in small arrays, or in complex connected lattice architectures. Here we report on the combination of focused electron beam induced deposition (FEBID) and micro-Hall magnetometry, as fabrication and high-resolution sensing tools, respectively. Free-form structures with minimal feature size of a few tens of nm of the metallic ferromagnets Fe, Co and Fe-Co are deposited directly on a semiconductor Hall sensor which serves as the substrate and allows to detect the magnetic stray field as a function of the external magnetic field and temperature. In the talk, we will discuss the measured and simulated magnetization reversal of small arrays of Fe-Co nanotrees and -cubes [1,2]. Furthermore, we will give an outlook on future possibilities of fabricating magnetic structures with geometrical frustration (towards 3D artificial spin ice) and studying dynamical processes by means of magnetic flux noise spectroscopy.

[1] L. Keller et al., *Sci. Rep.* **8**, 6160 (2018).
[2] M. Al Mamoori et al., *Materials* **11**, 289 (2018).

15 min. break

Invited Talk TT 62.5 Thu 16:30 H32

3D nanomagnetism and superconductivity: Current status and potential for future work — •Oleksandr Dobrovolskiy and Michael Huth — Goethe University, Frankfurt am Main

Extending 2D structures into the third dimension has become a general trend in various areas, including photonics, plasmonics and magnetics. This approach provides a means to modify conventional and to launch novel functionalities by tailoring vector potentials inducing anisotropic and chiral effects. Recently, there has been significant progress in the fabrication of free-standing ferromagnetic and superconducting nanostructures by focused particle direct-write techniques which is in part reviewed in [1]. In this respect, 3D shell structures such as framed tubes, spheres, Swiss rolls and helices are especially interesting as they offer unprecedented prospects for nanomagnetism and superconductivity because of topology and geometry-controlled effects. Namely, in magnetism, curvilinear geometry brings about two exchange driven interactions - effective anisotropy and antisymmetric vector exchange, i.e. an effective Dzyaloshinskii-Moriya interaction. In addition, another magneto-chiral contribution emerges due to the dipole-dipole interaction. In the case of superconducting nanostructures, the combination of low-dimensionality with a curvilinear geometry allows in principle for the observation of topology-driven effects, such as unconventional phase slips, reversible and irreversible switching, fractional flux-flow instabilities, and the Berezinskii-Kosterlitz-Thouless transition. [1] M. Huth, F. Porrati, O. V. Dobrovolskiy, FEBID meets materials science, Microelectron. Engineering, 185-186, 9-28 (2018).

TT 62.6 Thu 17:00 H32

3D Nano-Printing via FEBID: Complex 3D Nano-Structures — •Lukas Keller and Michael Huth — Institute of Physics, Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

[3]: https://youtu.be/v8s24WvGj9E
Fabrication of three-dimensional (3D) nano-architectures by focused electron beam induced deposition (FEBID) has matured to a level that highly complex and functional deposits are becoming available for nanomagnetics [1] and plasmonics. The main issue of generating a desired 3D nano-structure is to navigate the electron beam in the x-y-plane.
Here we present our pattern file generator program [2]. It considers several issues caused by limited precursor replenishment dynamics, which is important for the successful fabrication of 3D nano-structures. The target geometry can be defined by hand or using powerful 3D software tools like "blender" [3]. Several examples of 3D nano- and microstructures using different precursors are presented.

[1]: Scientific Reports 8, 6160 (2018)
[2]: Beilstein J. Nanotechnol., 9, 2581-2598 (2018)
[3]: https://youtu.be/v8s24WvGj9E

TT 62.7 Thu 17:15 H32

Crystalline NbC superconducting nanowires by direct-writing — •Fabrizio Porrati[1], Sven Barth[2], Roland Sachser[1], Oleksandr Dobrovolskiy[1], Anja Seybert[3], Achilleas Frangakis[3], and Michael Huth[1] — [1]Goethe-University, Institut of Physics, Frankfurt a. M. — [2]TU Wien, Institute of Materials Chemistry — [3]Goethe-University, Buchmann Institute

We present a comparative study of planar nanowires and 3D free-standing nanowires grown by focused electron- / ion (Ga+)-beam induced deposition (FEBID/FIBID) using the novel precursor $Nb(NMe_2)_3(N\text{-}t\text{-}Bu)$. FEBID planar nanowires contain 67at%C, 22at%N and 11at%Nb; FIBID planar nanowires 42.9at%C, 12.9at%N, 15.5at%Ga and 28.7at%Nb. TEM analysis shows that FEBID samples are amorphous, while FIBID samples are made of fcc NbC polycrystals, with grains of 15-20nm diameter and lattice constant 4.47Å. The RT electrical resistivity is $\approx 10^4$ $\mu\Omega$cm and 550 $\mu\Omega$cm for FEBID and FIBID samples. Conductivity vs. temperature measurements show that the FEBID nanowires are insulating, following a variable-range-hopping behavior. FIBID nanowires, with RRR=0.87, become superconducting at T_C=5.0 K. T_C can be slightly tuned either by an electron irradiation treatment (T_C=5.4, for 20nC/*m^2) or by changing the width of the nanowires (T_C=4.3-6.4, for w=50-1000 nm). 3D free-standing nanowires were grown by FIBID. TEM experiments confirm a fcc NbC microstructure. The electrical measurements of these nanowires, with RRR=1.02, show a superconducting transition with T_C 11K, a value close to the value of bulk NbC.

TT 62.8 Thu 17:30 H32

Effective protection of few-layer black phosphorus from reactive species generated by in-situ focused electron beam irradiation. — •Lobo Charlene and Elbadawi Christopher — School of Mathematical and Physical Sciences, University of Technology Sydney, Ultimo NSW 2007

Recent studies have shown that exposure of few-layer black phosphorus (FLBP) to reactive oxygen species (ROS) via photoactivated oxidation induces an immediate and permanent reduction in the electron and hole mobility of FLBP. Electron-beam irradiation in H2O vapour is known to generate ROS (such as *O2-, *OH and OH-) that are responsible for the degradation of FLBP in ambient environment, but FLBP stability has not been assessed during prolonged exposure to other gaseous environments.

Here, we study the stability of FLBP in H2O, O2, NF3 and NH3 environments using environmental scanning electron microscopy (ESEM) and in situ electrical conductance measurements. The electron beam is used both for ESEM imaging, and also to generate reactive species such as *O, *OH, *F and *H that can drive spatially-localized chemical reactions at the sample surface. Using this approach, we demonstrate two promising methods of protecting FLBP and other moisture-sensitive two-dimensional materials from degradation by ROS. Encapsulation of FLBP with ionic liquids dramatically slows the rate of degradation in ROS environments. FLBP degradation can also be prevented by maintaining the temperature in the range ~125-300 *C during ROS exposure, without requiring any protective coating.

TT 63: Poster Session: Cryogenic Particle Detectors and Cryotechnique

Time: Thursday 15:00–18:30 Location: Poster D

TT 63.1 Thu 15:00 Poster D

Metallic Magnetic Calorimeters for high resolution X-ray Spectroscopy — •S. Allgeier[1], M. Friedrich[1], J. Geist[1], D. Hengstler[1], C. Schötz[1], S. Kempf[1], L. Gastaldo[1], A. Fleischmann[1], C. Enss[1], S. Trotsenko[4], T. Morgenroth[4], M.O. Herdrich[2], G. Weber[2,4], G. Märtin[2,4], Th. Stöhlker[2,3,4], G.A. Kazakov[5], S.P. Stellmer[5], and T. Schumm[5] — [1]KIP, Heidelberg University — [2]Helmholtz-Institute Jena — [3]GSI Darmstadt — [4]IOQ, Jena University — [5]Vienna University of Technology

Metallic magnetic calorimeters are energy dispersive particle detectors which provide a high energy resolution over a wide range of energies as well as an excellent linearity. They are operated at millikelvin temperatures and convert the energy of a single absorbed particle into a temperature rise, which leads to a magnetization change in an attached paramagnetic sensor read out by a SQUID. Presently we are adopting our 64-pixel MMC series of maXs-20,-30,-200 and polarmaXs to measurements at CRYRING (GSI/FAIR, Darmstadt) for next generation QED test on hydrogen-like Uranium. We present the newly developed sidearm with a 32-channel-read-out-chain including the cryogenic SQUID-amplifier-modules. In addition we present the micro-fabricated detector array maXs-30 which is optimized for high resolution X-ray spectroscopy at energies up to 30 keV and the detector array polarmaXs for polarization sensitive high resolution X-ray spectroscopy and discuss their performances.

TT 63.2 Thu 15:00 Poster D

Development of the First Prototype of an MMC-Based Detector for Light Dark Matter Direct Detection — •Arnulf Barth[1], Klaus Eitel[2], Christian Enss[1], Andreas Fleischmann[1], Loredana Gastaldo[1], Sebastian Kempf[1], Bernhard Siebenborn[2], and Marc Weber[2] — [1]Kirchhoff Institute for Physics, Heidelberg University. — [2]Institute for Nuclear Physics, Karlsruhe Institute of Technology.

The use of low temperature detectors in the search for the direct interaction of dark matter (DM) particles in a suitable target has opened the possibility to reach high sensitivities even at masses well below $1\,\mathrm{GeV}/c^2$. We present the design for a low-threshold detector optimized for the search of light DM particles based on metallic magnetic calorimeters (MMCs) with a germanium (Ge) crystal as a scattering target. The interaction of a DM particle in the Ge crystal would create two different kinds of excitations: phonons and electron-hole pairs. We discuss the design of a 3-fold MMC system for the measurement of the temperature increase of the Ge crystal, and how the temperature signal can be amplified via the Neganov-Trofimov-Luke effect to ensure a high sensitivity. A first detector prototype has already been developed. We describe the fabrication steps and a first characterization of the performance.

TT 63.3 Thu 15:00 Poster D

Development of MMC based combined photon and phonon detector for rare event searches — •Freerik Forndran[1], Felix Ahrens[1], Christian Enss[1], Andreas Fleischmann[1], Loredana Gastaldo[1], Sebastian Kempf[1], Yong-Hamb Kim[2], Daniel Unger[1], and Clemens Velte[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]IBS Center for Underground Physics, Daejeon, Rep. of Korea.

In the search for rare events, a simultaneous measurement of photons and phonons produced after an event in a scintillating crystal operated at mK temperatures enables an efficient background rejection. This is due to the fact that the light yield depends on the mass, allowing for particle discrimination. This approach can be used for an investigation of the neutrinoless double beta decay as well as for a direct detection of dark matter. We present the design of a combined photon and phonon detector based on metallic magnetic calorimeters (MMCs). Simulations predict an energy resolution of $\Delta E_{\mathrm{FWHM}} < 10\,\mathrm{eV}$, a signal rise time of $\tau_0 < 50\,\mu\mathrm{s}$ and a signal decay time of $\tau_1 < 10\,\mathrm{ms}$ for the photon detector and $\Delta E_{\mathrm{FWHM}} < 100\,\mathrm{eV}$, $\tau_0 < 200\,\mu\mathrm{s}$ and $\tau_1 < 10\,\mathrm{ms}$ for the phonon detectors. The combined photon and phonon detector design will be described with emphasis on the tower design of the detector setup able to host several crystals. The challenges of the fabrication steps will be discussed. In conclusion we will present the characterization of first prototypes of photon and phonon detectors.

TT 63.4 Thu 15:00 Poster D

Low Temperature MMC Detector Arrays for the IAXO — •Daniel Unger, Christian Enss, Andreas Fleischmann, Lisa Gamer, Loredana Gastaldo, Daniel Hengstler, Sebastian Kempf, and Dennis Schulz for the iaxo collaboration — Kirchhoff Institute for Physics, Heidelberg University

The International Axion Observatory (IAXO) is searching for axions or axion-like particles generated in the Sun. A large magnetic field is used to convert solar axions to photons via the Primakoff effect. The major part of the expected spectrum considering only axion-photon coupling covers an energy range up to 10 keV with its maximum at about 3 keV. X-ray detectors with high efficiency in this energy range and low intrinsic background are required. Low temperature metallic magnetic calorimeters (MMCs) fulfil these requirements and can reach very low thresholds below 100 eV.

We present the design of a new detector system for the IAXO experiment with the possibility to operate two different kinds of two-dimensional MMC arrays. The setup is designed to host a large MMC array with moderate energy resolution aiming to discover events related to axions. If axions were discovered the focus would move to study the spectral shape. In this case a smaller MMC array featuring a higher energy resolution would replace the initial array using the same setup.

We show the current status of the platform and discuss methods to recognize background events based on pulse shape analysis and event coincidence in several pixels.

TT 63.5 Thu 15:00 Poster D

CryoGenX - A High-resolution Spectrometer for Advanced Nuclide Analysis — •Kevin Phelan[1,4], Andreas Fleischmann[1], Matthias Bühler[2], Theo Hertrich[2], and Michael Huber[3] — [1]Kirchhoff Institut für Physik, Universität Heidelberg — [2]Low Temperature Solutions UG — [3]PAYR Engineering GmbH — [4]Kaon GmbH

The EuroStars CryoGenX project is developing a complete, cryogenic detector system for x- and gamma-rays up to 200 keV. Target markets are non-destructive analysis for nuclear forensics, materials analysis and nuclear metrology for medical applications.

Cryogenic detectors can resolve energies where nuclear forensics communities have difficulty identifying the content and origin of nuclear active materials. A commercially available system could prove to be very useful for nuclear metrology, non-proliferation inspection and medical radiology.

There are currently two approaches for quantifying radioactive samples. Mass spectrometry with wet-chemistry is accurate but costly and complicated. Semiconductor detectors are easy but inaccurate. CryoGenX combines the advantages of both, ensuring fast, accurate results without destroying the samples, and with no radioactive waste.

The cryogenics is based on a very small ADR. The detectors are based on the MMC / MPT concept and will be tailored for a combination of energies and working temperatures. The SQUID read-out, cryostat automation and extensive data analysis including spectral information, peak identification and high-level analytics and file handling are all highly integrated.

TT 63.6 Thu 15:00 Poster D

MOCCA: a 4k-pixel molecule camera for the position and energy resolved detection of neutral molecule fragments — •Dennis Schulz[1], Steffen Allgeier[1], Christian Enss[1], Andreas Fleischmann[1], Lisa Gamer[1], Loredana Gastaldo[1], Julia Hauer[1], Sebastian Kempf[1], Sebastian Spaniol[2], Oldřich Novotný[2], and Andreas Wolf[2] — [1]Heidelberg University — [2]Max Planck Institute for Nuclear Physics, Heidelberg

The MOCCA detector is a 4k-pixel high-resolution molecule camera based on metallic magnetic calorimeters and read out with SQUIDs that is able to detect low-energy neutral molecule fragments. It will be deployed at the Cryogenic Storage Ring CSR at the Max Planck Institute for Nuclear Physics in Heidelberg, a storage ring built to prepare and store molecular ions in their rotational and vibrational ground states, enabling studies on electron-ion interactions. To reconstruct the reaction kinematics, MOCCA measures the energy and position of incident particles on the detector, even with multiple particles hitting the detector simultaneously. Using different read-out techniques,

MOCCAs 4096 pixel can be read out by using only 32 SQUID channels in total.

We present the most recent data from measurements of the MOCCA detector at 10 mK with a 6 keV photon source, demonstrating low crosstalk between rows and columns of the detector, the read-out principle and the energy resolution measured to be below 200 eV.

TT 63.7 Thu 15:00 Poster D

Measurement of low energy electron capture spectra to test the impact of high order processes — •Tobias Schmitt[1] and Martin Brass for the ECHo-Collaboration[2] — [1]Kirchhoff-Institute of Physics, Heidelberg University, Germany — [2]Institute of Theoretical Physics, Heidelberg University, Germany.

The neutrino mass can be determined by analyzing the shape of the endpoint region of electron capture spectra. The best candidate for this investigation is ^{163}Ho due to its low Q-value. Recent measurements of high statistic ^{163}Ho spectra, performed by the ECHo collaboration, showed that available theories can not describe the spectral shape. The deviations are on the order of 5 percent of the total spectrum. Nowadays, the best description of the ^{163}Ho spectrum is obtained using ab-initio calculations for the capturing process of the electron. To be able to better understand the excitations in which a ^{163}Dy atom can be left after an EC-process occurred in ^{163}Ho, we decided to study the calorimetrically measured EC spectrum of ^{193}Pt. With its low Q-value of 56 keV, which means ^{193}Pt can not undergo 1s-capture and the large atomic number it shares two important properties with ^{163}Ho. The larger energy interval will also provide more spectral lines for comparison with theories. At the same time it will provide a check that the theoretical description is not just fitted to the ^{163}Ho spectrum but indeed well understood. We will give a status report on the detector design, ^{193}Pt enclosure, and the completed experimental platform we developed with the goal to measure a ^{193}Pt electron capture spectrum.

TT 63.8 Thu 15:00 Poster D

Superconducting GHz Resonators for Microwave SQUID Multiplexing of Metallic Magnetic Calorimeters — •Felix Ahrens, Mathias Wegner, Patrick Paluch, Andreas Fleischmann, Christian Enss, and Sebastian Kempf — Kirchhoff Institute for Physics, Heidelberg University, Germany

Microwave SQUID multiplexing is the most promising way to read out large metallic magnetic calorimeter (MMC) detector arrays. Here, high quality superconducting GHz resonators are used for frequency encoding. The resonators are designed to have a bandwidth of ∼1 MHz to maintain the very fast signal rise time of MMCs. The frequency spacing between two neighbouring channels is set to ∼10 MHz to yield a crosstalk level below 10^{-4}. The bandwidth of the resonators is adjusted by tuning the coupling capacitor for each resonator based on simulations of the couplers' electromagnetic properties.

We investigate quarter-wave CPW transmission line (TLR) and lumped element resonators (LER) formed by a meander shaped inductor and an interdigital capacitor (IDC). The resonance frequency f_r of TLRs is set by adjusting the physical length of the resonator, whereas for LERs the number of IDC fingers is adjusted. Moreover, LERs allow to perform a post-production fine-tuning of the resonance frequency using a tile-and-trim process. We will present different aspects related to the fabrication, characterisation and optimisation of superconducting resonators to be used in a microwave SQUID multiplexer as well as our present tile-and trim process.

TT 63.9 Thu 15:00 Poster D

Effect of different host material for implantation of Ho-163 in metallic magnetic calorimeters — Martin Neidig, Benjamin Raach, Christian Enss, Andreas Fleischmann, •Loredana Gastaldo, Sebastian Velte, Federica Mantegazzini, and Clemens Velte — Kirchhoff Institute for Physics, Heidelberg University

The ECHo experiment has been designed for determining the value of the effective electron neutrino mass by the analysis of the endpoint region of the Ho-163 spectrum. The measurement of the Ho-163 spectrum is performed using low temperature metallic magnetic calorimeters (MMCs) with Ho-163 enclosed in the absorber. To achieve high sensitivity, detector performance as energy and time resolution are fundamental. In the process of optimizing MMCs for ECHo we have tested different materials for hosting Ho-163: gold, silver and aluminum. For that, high purity 163Ho has been implanted at Mainz University in three different MMC arrays having different implantation layers. We discuss the signal shape obtained with the different detectors as function of temperature as well as the energy resolution at the operating temperature of about 20 mK. In addition, we have also investigated if different host material could influence the decay mode for the electron capture in Ho-163. We present the comparison of Ho-163 spectra acquired with the different detectors and discuss the results at the light of available theories.

TT 63.10 Thu 15:00 Poster D

Specific Heat of Dilute Alloys of Holmium in Noble Metals at Low Temperatures — •Matthew Herbst, Clemens Velte, Andreas Reifenberger, Federica Mantegazzini, Andreas Fleischmann, Loredana Gastaldo, Andreas Reiser, Sebastian Kempf, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, D-69120 Heidelberg

We investigate dilute alloys of holmium in gold and silver in order to determine the impact of their specific heat on the performance of the microcalorimeters in the neutrino mass experiment ECHo. In particular, we focus on alloys with atomic concentrations of $x_{Ho} = 10^{-2} - 10^{-4}$ at temperatures between 10 mK and 800 mK. Due to the large total angular momentum $J = 8$ and nuclear spin $I = 7/2$ of holmium, the specific heat of Ag:Ho and Au:Ho depends on the detailed interplay of various interactions. This makes it unfeasible to accurately determine the specific heat of these materials numerically. Instead, we acquire the desired information through experiment, using three different experimental set-ups. The results from measurements on five holmium alloys show that the specific heat of these materials is dominated by a large Schottky anomaly with its maximum at $T \approx 250$ mK, which we attribute to hyperfine splitting and crystal field interactions. RKKY and dipole-dipole interactions between the holmium atoms cause additional, concentration-dependent effects. We find no significant difference between Ag:Ho and Au:Ho, and conclude that alloys with $x_{Ho} \approx 1\%$ are suitable for the ECHo project at $T \leq 30$ mK.

TT 63.11 Thu 15:00 Poster D

A versatile demagnetization refrigerator — •Alexander Regnat[1,2], Jan Spallek[1,2], Christopher Duvinage[1], Klaus Eibensteiner[1], Nico Huber[1], Carolina Burger[1], Anh Tong[1] und Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, Germany — [2]kiutra GmbH, München, Germany

Cooling devices providing temperatures well below 1 K are a key prerequisite for modern research and development, e.g., in materials science, quantum applications and the cooling of sensors and detectors. Here we present a versatile and compact demagnetization refrigerator for the cryogen-free, continuous generation of sub-Kelvin temperatures.

TT 63.12 Thu 15:00 Poster D

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

Among the family of regenerative cryocoolers, Pulse Tube Coolers (PTCs) distinguish themselves from Gifford-McMahon- or Stirling coolers by the absence of cold moving parts. This features a long live operation with low vibration of the PTC and less maintenance compared to conventional cryocoolers - making them attractive for low noise applications. Since their invention, 4 K PTCs [1] have become an excellent alternative for "dry" cooling of cryogenic experiments without liquid helium ("wet cooling") even below 4 K. Besides their advantages, PTCs – like all other regenerative cryocoolers – suffer from two intrinsic effects due to the periodic compression and expanding cycles in the cold head: a periodic elastic deformation ("breathing") of the thin walled pulse- and regenerator-tubes, which leads to residual vibrations and a periodic variation in temperature. Here we present unique applications of double-staged 4 K PTC based cryostats. By adapting the cooling power to the requirement of the experiment[2], the intrinsic effects of the PTC are minimized. Further decoupling and damping of the mechanical and thermal variations provide an excellent environment even for cooling of sensitive devices.

[1] G. Thummes et al., Cryogenics 38 (1998)
[2] B. Schmidt et al., Cryogenics 88 (2017)

TT 63.13 Thu 15:00 Poster D

Design of a scanning confocal microscope for fluorescence spectroscopy of single-photon sources at mK temperatures — •Marcel Schrodin[1], Philip Schneider[1], Christoph Sürgers[1],

and Wolfgang Wernsdorfer[1,2,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institut Néel, CNRS and Université Joseph Fourier, Grenoble, France — [3]Institute for Nanotechnology, Karlsruhe Institute of Technology

In recent years, different kinds of single-photon sources such as color centers in diamond, single molecules, and quantum dots became the focus of attention in the wide filed of quantum technology. Many experiments already exploit the single emitter characteristics in ambient conditions. However, a comprehensive investigation of single-photon sources and an integration in quantum devices still requires cryogenic temperatures.

We want to present the design of a scanning confocal microscope for fluorescence spectroscopy of single-photon sources at mK temperatures and will show first proof-of-principle results. The optical design is based on a high-NA objective and an optical fiber which guides both the excitation and response of the sample. On-axis scanning of the sample is provided by an xyz-positioning setup. For cryogenic operation, these parts are put into a home-built table-top dilution refrigerator with 20 mK base temperature. Special care has been taken to minimize the vibrations present in the proximity of the sample.

TT 64: Poster Session: Transport

Time: Thursday 15:00–18:30 Location: Poster D

TT 64.1 Thu 15:00 Poster D

Spin effects in resonant transport through interacting quantum dots — •Simon Mundinar, Jürgen König, and Stephan Weiss — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

We report on numerically exact iterative path-integral calculations (ISPI) for spin-dependent transport through small interacting quantum dots [1-3]. Our ISPI method builds upon the truncation of exponentially vanishing real-time correlations at finite temperature and/or bias voltage. In particular, we study two distinct systems (i) a spin-valve, where ferromagnetic leads induce spin-dependent tunnel couplings between leads and dot [2] and (ii) a hybrid structure, where the quantum dot is coupled to a normal and a superconducting lead [3]. For the spin-valve setup, the observable of interest is the tunneling magnetoresistance through the quantum dot, which is investigated for various system parameters. We find that, especially at low temperatures, resonant tunneling effects are dominant and the sequential picture does not apply. The role of Coulomb interactions together with changing the temperature of the system is explored. Within the hybrid system, a finite gap parameter Δ induces anomalous self energies in the Keldysh partition function. ISPI calculations are performed to deduce, e.g. the impact of Coulomb interactions on the Andreev bound state spectrum in a nonequilibrium situation.

[1] S. Weiss, et. al, Phys. Status Solidi B, **250** (11), 2298-2314 (2013).
[2] S. Mundinar, J. König, and S. Weiss, in preparation (2018).
[3] S. Weiss and J. König, in preparation (2018).

TT 64.2 Thu 15:00 Poster D

Synchronization of coherent charge oscillations of two coupled double quantum dots — •Eric Kleinherbers, Philipp Stegmann, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, Lotharstr. 1, 47048 Duisburg

In a double-dot system, charge oscillates coherently between two tunnel-coupled quantum dots. These oscillations have a distinct impact on the electron transport through the system and can be detected by means of the finite-frequency noise or the waiting-time distribution [1].

Here, we discuss how the oscillations of two distinct double-dot systems influence each other by means of electrostatic coupling. The electron transport is modeled by a generalized master equation obtained from a real-time diagrammatic approach [2]. By calculating the waiting-time distribution and performing a spectral analysis, synchronization effects are revealed.

[1] T. Brandes, Ann. Phys. **17**, 477 (2008)
[2] B. Wunsch, M. Braun, J. König, and D. Pfannkuche, Phys. Rev. B **72**, 205319 (2005)

TT 64.3 Thu 15:00 Poster D

Superconducting proximity effect and conductance quantization in bilayer graphene quantum wires — •Vanessa Gall[1,2] and Igor Gornyi[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute for Condensed Matter Theory, Karlsruhe Institute of Technology, Karlsruhe, Germany

Quantum wires or Quantum Point Contacts (QPCs) built from two dimensional material, like bilayer graphene (BLG), might pave the way towards quantum circuits. We consider a gate defined BLG based quantum wire with a perpendicular magnetic field and both superconducting and non superconducting leads. In the superconducting regime we study the magnetic interference pattern in rectangular junctions by means of a semi-classical model. A similar study was recently conducted on BLG QPCs, where it could be shown, that a variation in the gate potentials leads to a tailoring of the supercurrent. Here we find a dependence on the aspect ratio, where scattering off the side edges is of high importance in narrow junctions, but not in wide ones. In the normal conducting regime, we investigate the quantized conductance due to finite size effects and the emergence of Landau levels. We find an accidential degeneracy for wide channels and large gaps. The experimental confirmation in the case of BLG QPCs was recently given. The conduction plateaus of height $4\frac{e^2}{h}$ are clearly visible and the first step has a height of $8\frac{e^2}{h}$ for certain values of the splitgate. The conditions for this accidential degeneracy can be expressed analytically by means of the effective two band hamiltonian.

TT 64.4 Thu 15:00 Poster D

Fluctuation relations in interacting quantum pumps — •Roman-Pascal Riwar[1] and Janine Splettstoesser[2] — [1]JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, Germany — [2]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Sweden

The understanding of out-of-equilibrium fluctuation relations in small open quantum systems has been a focal point of research in recent years. Here, we consider symmetries and fluctuation relations of the charge and energy current statistics in time-dependently driven, interacting quantum systems, such as quantum dot pumps. In particular, we study slowly driven pumps, where we systematically expand the full-counting statistics in orders of the driving parameter. We find that while in zeroth (instantaneous) order, it suffices to consider the charge current cumulants separately to formulate fluctuation relations, for the first order, this is no longer possible. The energy displacement currents necessarily appear as extra terms, as a consequence of the highly geometric nature of the pumping current statistics. Surprisingly, there is one exception: when the Coulomb interactions disappear in the dot, so does this correction. We therefore find that it is possible to recover the standard equilibrium fluctuation-dissipation theorem, notably in presence of a non-equilibrium pump, as long as the system is noninteracting.

TT 64.5 Thu 15:00 Poster D

Control of the critical temperature of Nb by spin-helix reorientation in the chiral magnet MnSi — •Julius Grefe, Bastian Rubrecht, Nico Steinki, David Schroeter, Stefan Süllow, and Dirk Menzel — Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig

Theory has predicted the possibility to control the critical temperature T_C of a superconductor via a proximity effect with a non-collinear magnet. The chiral magnet MnSi as a representative of the cubic B20 structure shows such a magnetic behavior below $T_N = 29.5$ K and $B_{C1} = 100$ mT. To examine this prediction, Nb ($T_C = 9.2$ K) thin films have been deposited by molecular beam epitaxy on (111)-oriented MnSi monocrystalline substrates grown by the Chochralski process. The dependence of the critical temperature of Nb on the orientation of the spin helices in MnSi switched by an external magnetic field has been investigated. The critical temperature of the superconducting Nb films has been determined by four-point resistance and SQUID susceptibility measurements. For comparison, diamagnetic CoSi substrates have been used as reference samples. This proximity effect can be used for switching a superconducting spin valve consisting only of a single

magnetic layer.

TT 64.6 Thu 15:00 Poster D

Low temperature MCBJ measurements of C_{60} Fullerenes — •Alexander Strobel[1,2], Filip Kilibarda[1,2], Elke Scheer[2], and Artur Erbe[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]University of Konstanz, Faculty of sciences, 78457 Konstanz, Germany

Current industrial semiconductor scaling processes are reaching limits. We see not only diminished returns with further scaling attempts, but also physical limitations that come more and more into play. In our research we offer a novel approach, where we try to drop altogether the concept of 3D scaling of electronic components and go to practically 1D molecular systems. This approach offers not only reduction in power consumption and costs, but also a deeper understanding of the electron transport behavior of molecules. Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junction (MCBJ) technique.

The Poster shows the investigation of the conductance of C_{60} Fullerene molecules using a unique mechanical controllable break junction (MCBJ) setup. The C_{60} molecule with its high stability and symmetry is convenient to investigate the Bonding between electrodes (Au) and molecule. The MCBJ setup enables to evaporate in situ and measure under high vacuum conditions. Furthermore low temperatures measurements down to 10 K are possible. From conductance histograms preferred conductance values of single C_{60} molecules are deduced. I-V and dI-dV curves give rise to a deeper understanding of electron transport mechanisms in C_{60} molecules.

TT 64.7 Thu 15:00 Poster D

Thermoelectric transport in nanosystems: A hierarchical quantum master equation approach — •Jakob Bätge, Ka Chun Chan, and Michael Thoss — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Germany

A variety of interesting transport phenoma exist in nanoelectronic systems. Recently, quantization of heat transport has been observed [1] and counterintuitive thermal stabilization in molecular junctions has been predicted [2]. In this context, we investigate voltage and temperature driven electron and heat transport from a theoretical point of view. In particular, we are interested in the interplay of electronic and vibrational degrees of freedom. For this purpose, we use the hierarchical quantum master equation method [3], which generalizes perturbative master equation methods by including higher-order contributions as well as non-Markovian memory and allows for the systematic convergence of the results.

[1] L. Cui *et al.*, Science **355**, 1192 (2017).
[2] R. Härtle *et al.*, Phys. Rev. B **98**, 081404(R) (2018).
[3] C. Schinabeck *et al.*, Phys. Rev. B **94**, 201407(R) (2016).

TT 64.8 Thu 15:00 Poster D

Quantum Transport through Single-molecule Junctions: Non-adiabatic Effects — •Christoph Kaspar, Christian Schinabeck, and Michael Thoss — Albert-Ludwigs-Universität, Freiburg, Germany

The coupling of electronic and nuclear degrees of freedom is an important mechanism in non-equilibrium charge transport in molecular junctions and may result in a variety of interesting phenomena such as decoherence, switching and local cooling or heating [1]. While the effect of adiabatic polaron-type coupling has been studied in great detail, new phenomena are expected for non-adiabatic coupling scenarios which correspond to a breakdown of the Born-Oppenheimer approximation. In this contribution, we present results of a model study of non-adiabatic effects employing the hierarchical quantum master equation approach [2, 3]. This method generalizes perturbative master equation methods by including higher-order contributions as well as non-Markovian memory and allows for the systematic convergence of results. In particular, we observe a quantum transport behavior strongly influenced by the interaction with the vibrational modes.

[1] Härtle *et al.*, Phys. Rev. B **98**, 081404 (2018)
[2] Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008)
[3] Schinabeck *et al.*, Phys. Rev. B **94**, 201407R (2016)

TT 64.9 Thu 15:00 Poster D

Thermal conductivity and thermal diffusivity of suspended few-layer h-BN using the 3ω method — •Sofia Blanter, Nicola Paradiso, Denis Kochan, and Christoph Strunk — Institut für experimentelle und angewandte Physik, Universität Regensburg, Universitätstr. 31, 93053 Regensburg

We present measurements of thermal conductivity and thermal diffusivity for few-layer suspended hexagonal boron nitride. The measurements are performed on 15 nm thick suspended h-BN flakes using the 3ω method.

The flakes are exfoliated and transferred on top of a SiN membrane with an etched slit, using the all-dry viscoelastic stamping method [1].

We use the 1D diffusion model [2], that allows us to extract the thermal conductivity and thermal diffusivity of our flakes between 25 and 300 K. The temperature dependence of the thermal conductivity is consistent with previous measurements using a different technique [3], and demonstrates the reliability of the method. First results on few-layer $MoSe_2$ flakes are presented.

[1] A. Castellanos-Gomez et al., 2D Materials **1** (2014), 011002
[2] A. Sikora et al., Rev. Sci. Instrum. **83** (2012), 054902
[3] I. Jo et al., Nano letters **13.2** (2013), 550-554

TT 64.10 Thu 15:00 Poster D

Zero-dimensional contacts to carbon nanotubes encapsulated by hexagonal boron nitride — Christian Bäuml, •Michaela Eichinger, Nicola Paradiso, and Christoph Strunk — University of Regensburg, Regensburg, Germany

Edge contacts to carbon nanotubes (CNTs) have a contact interface of only a handful of atoms. Nevertheless, they display a resistance less than 30 kΩ, comparable to the most transparent contacts obtained with previous techniques [1].

In this work we present an alternative method for edge contacting CNTs. Unlike the method demonstrated by Huang et. al., we do not pick up the CNT. Instead we grow CNTs directly on few-layer hexagonal boron nitride (hBN) by chemical vapor deposition. We cover the interesting CNT portion by a second hBN layer by simple dry stamping in nitrogen atmosphere. Edge contacts are then fabricated using a similar recipe as for the production of graphene edge contacts. The simplicity of our approach is particularly suited for the fabrication of hybrid 2D-1D material structures based on ultra-clean CNTs.

[1] J.-W. Huang et. al. Nano Lett. **15**, 6836 (2015)

TT 64.11 Thu 15:00 Poster D

Lab::Measurement – measurement control with Perl — Simon Reinhardt[1], Christian Butschkow[1], Stefan Geissler[1], Alois Dirnaichner[1], Florian Olbrich[1], Charles E. Lane[2], and •Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany — [2]Department of Physics, Drexel University, Philadelphia, USA

`Lab::Measurement` is a collection of Perl 5 modules providing control of test and measurement devices. It allows for quickly setting up varying and evolving complex measurement tasks with diverse hardware. Instruments can be connected by means such as GPIB (IEEE 488.2), USB-TMC, or VXI-11 / raw network sockets via Ethernet. Internally, third-party backends as, e.g., Linux-GPIB, National Instruments' NI-VISA library, or Zurich Instruments' LabOne API are used, as well as lightweight drivers for USB and TCP/IP-based protocols. The wide range of supported connection backends enables cross-platform portability. Dedicated instrument driver classes relieve the user from taking care of internal or vendor-specific details. A high-level layer provides fast and flexible creation of nested measurement loops, where, e.g., several input variables are varied and output data is logged into a customizable folder structure. `Lab::Measurement` has already been successfully used in several low temperature transport spectroscopy setups. It is free software and available at `http://www.labmeasurement.de/`

[1] S. Reinhardt *et al.*, Comp.Phys.Comm. **234**, 216 (2019)

TT 64.12 Thu 15:00 Poster D

Optomechanics of a suspended carbon nanotube quantum dot coupled to a coplanar microwave resonator — Stefan Blien, Patrick Steger, •Niklas Hüttner, Richard Graaf, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

A clean, suspended single wall carbon nanotube is the ultimate limit of a nanomechanical beam resonator, where the fundamental transversal vibration mode reaches resonance frequencies on the order of 100MHz – 1 GHz and mechanical quality factors up to 10^6. Placing a nanotube next to a coplanar resonator at cryogenic temperatures results in a microwave optomechanical system with dispersive coupling. This system, however, has a fundamentally new property: the nanotube is also

a quantum dot, and strong interaction of motion and single electron tunneling dominates its behaviour.

We have implemented a transfer technique to integrate such a nanotube into a superconducting circuit, and present measurements on a combined device coupling a suspended quantum dot to a microwave resonator mode at millikelvin temperatures. The dispersively coupled optomechanical system is characterized via two-tone spectroscopy (red side band photon upconversion) as well as optomechanically induced transparency (OMIT). The interaction of charge transport and vibration, via Coulomb blockade and single electron tunneling, leads to a strongly enhanced, tunable optomechanical coupling.

TT 64.13 Thu 15:00 Poster D

Carbon nanotube transfer into complex devices with commercial quartz tuning forks — •Patrick Steger, Niklas Hüttner, Richard Graaf, Alexander Albang, Stefan Blien, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040, Regensburg, Germany

Our work focuses on coupling suspended, clean carbon nanotubes (CNTs) to a superconducting coplanar waveguide (CPW) resonator for experiments in the field of optomechanics. However, device fabrication is challenging. To increase our fabrication yield we separate the CVD process for CNT growth from the rest of the device fabrication. CNTs are then transferred to the device in a second step. Our transfer setup allows in situ precharacterization of the CNT during the transfer process. When a suitable CNT is found, the transfer process is finished by cutting the tube with current pulses at both ends.

Using commercial quartz tuning forks as CNT growth substrate produces high quality samples with a good yield and relatively low fabrication effort. Fabrication of customized fork structures might help to further enhance the yield.

TT 64.14 Thu 15:00 Poster D

Proximity induced superconductivity in normal metal/h-BN encapsulated graphene/superconductor junctions — •Preeti Pandey[1], Romain Danneau[1], Ralph Krupke[1,2], and Detlef Beckmann[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Materials and Earth Sciences, Technical University Darmstadt, Darmstadt, Germany

We present an electronic transport study of multiterminal normal metal/graphene/superconductor (NGS) junctions. In these junctions, the monolayer graphene sheet was encapsulated between two h-BN crystals. The graphene channel contacts the superconductor and the normal metal electrodes in orthogonal SGS and NGN junction configuration. We have observed clear signs of Josephson effect in the SGS junction when the graphene channel is driven to the n-doped as well as to the p-doped regime using a gate electrode. We have investigated the effect of the current through the NGN junction, which acts as a controlling parameter, on the Josephson current through the SGS junction.

TT 64.15 Thu 15:00 Poster D

Correlation Effects on the Electronic Structure of Graphene Nanoribbon Heterojunctions — •Jan-Philip Joost, Niclas Schlünzen, and Michael Bonitz — Institute of Theoretical Physics and Astrophysics, Kiel University, 24098 Kiel, Germany

Due to their tunable band gap graphene nanoribbons (GNRs) emerged as a promising candidate for various applications in nanoelectronics and optoelectronics [1]. Compared to macroscopic graphene, in GNRs electron–electron correlations are enhanced by the quantum confinement of the electrons. An accurate description, therefore, has to go beyond the often used mean-field approaches [2]. Here, we decribe the GNRs using an extended Hubbard model that improves the common tight-binding models by taking into account electron–electron interactions. The model is solved by a nonequilibrium Green functions [3] (NEGF) approach combined with the GW self-energy to account for electron correlations. As a particular application we study the electronic structure of GNR heterojunctions and compare to the experimental observations of Ref. [4].

[1] J. P. Llinas *et al.*, Nat. Commun. **8**, 633 (2017)
[2] J.-P. Joost *et al.*, Phys. Status Solidi B, in press
[3] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[4] D. J. Rizzo *et al.*, Nature **560**, 204 (2018)

TT 64.16 Thu 15:00 Poster D

Thermal-induced currents and spin caloritronics in a graphene nanostructure — •Thi Thu Phùng[1,2], Andreas Honecker[1], and Javad Vahedi[1] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy Pontoise, 95302 Cergy-Pontoise, France — [2]University of Science and Technology of Ha Noi, 18 Hoang Quoc Viet, Ha Noi, Vietnam

We study a spin caloritronics device based on a heterostructure consisting of a hexagonal graphene flake with anti-ferromagnetic zigzag edges as central region connecting two leads [1] using the non-Equilibrium Green's Function (NEGF) technique combined with a mean-field approximation for the Hubbard model. Spin-up and spin-down currents are simultaneously generated and flow in opposite directions when leads are at different temperatures. Thanks to the magnetization at the zigzag-edges of the graphene flake, the resulting spin-up current is much larger such that both total spin current and net charge current are obtained. The key ingredients are the imbalance of charge carrier concentrations which is determined by the Fermi distribution at the source and drain, transmission spectra and on-site Coulomb repulsion U. These currents not only exhibit a negative differential thermoelectric resistance, but also can be modulated easily by the gate voltage. By adjusting parameters suitably, the efficiency of the spin-filtering effect might achieve nearly 100%. These findings make the proposed device a promising candidate for spin caloritronics applications.

[1] A. Valli, A. Amaricci, V. Brosco, and M. Capone, Nano letters **18**, 2158 (2018).

TT 64.17 Thu 15:00 Poster D

Structural and electronic properties of graphene/MoS_2 bilayer heterostructures — •Somepalli Venkateswarlu, Andreas Honecker, and Guy Trambly de Laissardière — Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy-Pontoise, France

Graphene and two-dimensional materials based on transition metal dichalcogenides have gained increasing attention because of their fascinating features in electronics and optical properties [1]. Combining a single layer of graphene with a transition metal dichalcogenide layer in a Van der Waals heterostructure offers an intriguing means of controlling the electronic properties through these bilayer heterostructures [2]. Here, we report the structural and electronic properties of graphene/MoS_2 bilayer heterostructures. For the theoretical calculations, we use Density Functional Theory with Van der Waals corrections, as implemented in the Abinit package [3]. We analyze the interlayer spacing between the graphene and MoS_2 layers and also the location of Dirac points near the Fermi level. In particular, we focus on the structural and electrical properties of bilayer heterostructures with different supercell geometries and give particular attention to the effect of relaxing the lattice structure. These heterostructures are based on different supercell geometries (4:3, 5:4, and 9:7), having different magnitudes of the lattice mismatch.

[1] E. S. Kadantsev, P. Hawrylak, Solid State Comm. **152**, 909 (2012)
[2] S. Singh, C. Espejo, A. H. Romero, Phys. Rev. B **98**, 155309 (2018)
[3] X. Gonze et al., Comp. Mat. Sci. **25**, 478 (2002); https://www.abinit.org

TT 65: Annual General Meeting of the Low Temperature Physics Division

Time: Thursday 18:30–20:00 Location: H7

Duration 90 min.

TT 66: Ultrafast Dynamics of Light-Driven Systems

Time: Friday 9:30–12:45 Location: H2

Invited Talk TT 66.1 Fri 9:30 H2

Non-equilibrium superconductivity: from post-quench dynamics to controlling competing orders — •Peter P. Orth — Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

Understanding and controlling the non-equilibrium behavior of correlated quantum systems is one of the major research goals in condensed matter physics. It holds promise to dynamically tune material properties on ultrafast timescales. One route to optical control of correlated matter is via excitation of optical phonons. Another avenue is to excite acoustic phonons, which, due to their low excitation energies, generally leads to less heating. We demonstrate that driving acoustic phonons to a non-equilibrium state results in the remarkable phenomenon of a momentum-dependent effective temperature, by which electronic states at different regions of the Fermi surface are subject to distinct local temperatures. This has a profound effect on the delicate balance between competing ordered states in unconventional superconductors, opening a new avenue to control correlated phases. We also report on a joint theory-experiment study of THz pump-probe spectroscopy of superconductors Nb_3Sn and NbN. To quantitatively describe the superconducting gap dynamics, we present a semi-phenomenological approach that captures not only the coherent BCS gap dynamics at sub-picosecond timescales but also dissipative processes beyond BCS. Finally, we explore gap dynamics in two-band systems, where we find that the presence of two gap scales leads to the appearance of a new exponent in the universal power-law decay of the oscillations.

TT 66.2 Fri 10:00 H2

Floquet behavior of correlated systems with light-matter coupling — •Mona Kalthoff[1], James Freericks[2], Götz Uhrig[3], Dante Kennes[4], Angel Rubio[1], and Michael Sentef[1] — [1]Max-Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Georgetown University, Washington, D.C., United States of America — [3]Technische Universität Dortmund, Dortmund, Germany — [4]Freie Universität Berlin, Berlin, Germany

Periodically driven nonequilibrium many-body systems have a quasi-energy spectrum which can be tailored by external driving fields, known as Floquet engineering of desired system properties[1]. However, continuous periodic driving is not realizable in pump-probe experiments in solids. For instance it is not clear which criteria a pulse has to meet for a system exposed to a pulsed drive to approach the Floquet limit of a periodically driven system. However, there are analytical results for noninteracting band electrons in infinite dimensions[2]. Moreover we discuss t-DMRG results for interacting 1D chains in the charge density wave phase to study the emergence of Floquet behavior for realistic pulse shapes. This builds on the recently proposed Floquet engineering in quantum chains[3].

[1] Sentef et al., Nat. Comm. 6, 7047 (2015); Uhrig et al, arXiv:1808.10199 (2018)
[2] Kalthoff et al., Phys. Rev. B 98, 035138 (2018)
[3] Kennes et al., Phys. Rev. Lett. 120, 127601 (2018)

TT 66.3 Fri 10:15 H2

Transient Floquet engineering of superconductivity — •Nagamalleswara Rao Dasari and Martin Eckstein — Department of Physics, University of Erlangen-Nuremberg, 91058 Erlangen, Germany

Intense time-periodic laser fields can transform the electronic structure of a solid into strongly modified Floquet-Bloch bands. While this suggests multiple pathways to induce electronic orders such as superconductivity or charge density waves, the possibility of preparing low-energy phases of Floquet Hamiltonians remains unclear because of the energy absorption at typical experimentally accessible driving frequencies. Here we investigate a realistic pathway towards laser control of electronic orders, which is the transient enhancement of fluctuating orders. Using a conserving Keldysh Green's function formalism, we simulate the build-up of short range Cooper-pair correlations out of a normal metal in the driven attractive Hubbard model. Even for frequencies only slightly above or within the bandwidth, a substantial enhancement of correlations can be achieved before the system reaches a high electronic temperature. This behavior relies on the non-thermal nature of the driven state. The effective temperature of the electrons at the Fermi surface, which more closely determines the superconducting correlations, remains lower than an estimate from the global energy density. Even though short ranged, the fluctuations can have marked signatures in the electronic spectra.

TT 66.4 Fri 10:30 H2

Ultrafast dynamics of superconductors: Cooper-pair Dephasing or Thermalization? — •Christopher Stahl and Martin Eckstein — Lehrstuhl für Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Deutschland

We investigate the ultrafast dynamics of superconductivity in a BCS model. The reduction of the gap after different excitation protocols, which has been observed in various theoretical and experiential studies, may in principle be due to dephasing of the pair correlations at individual momenta, or due to thermalization to a hot electron state. While in time-dependent BCS theory it is clear that the gap would only dephase, we show, using non-equilibrium dynamical mean-field theory, that dephasing and thermalization can be clearly distinguished on short times even beyond mean-field theory. Furthermore we propose an experimental protocol to obtain the pair correlations at individual momenta and thus distinguish the two scenarios. This scheme, which is based on a measurement of the statistical variance of the number of photoelectrons in each momentum state in time-resolved pump-probe photoemission spectroscopy, can more generally provide a way to obtain two-particle quantities in a time-resolved fashion. The technique requires only a small bandwidth of the probe pulse in frequency space and can therefore yield a high time-resolution.

TT 66.5 Fri 10:45 H2

Light induced transient dynamics of the charge transfer insulator La_2CuO_4 — •Amrit Raj Pokharel[1], Markus Beyer[2], Steinn Ymir Agustsson[1], Manuel Obergfell[1,2], Tao Dong[1], Gennady Logvenov[3], Ivan Bozovic[3], Zala Lenarcic[4], Peter Prelovsek[4,5], and Jure Demsar[1,2] — [1]Institute of Physics, University of Mainz, Germany — [2]Department of Physics, University of Konstanz, Germany — [3]Brookhaven National Laboratory, USA — [4]Jozef Stefan Institute, Slovenia — [5]University of Ljubljana, Slovenia

We investigate the transient dynamics of La_2CuO_4, the parent compound of the Lanthanum based cuprate high temperature superconductors, upon photo excitation with UV photons across the charge transfer (CT) gap of 2.1 eV. The resulting transient state is studied for extracting the time-evolution of the broadband complex dielectric function in the spectral range of 0.5 - 2.6 eV. Experiments are performed as a function of the excitation density over several orders of magnitude, up to 0.1 absorbed photons/Cu-atom. Modeling the changes in the complex dielectric function with the (induced) Drude - Lorentz model reveals a pronounced renormalization of the CT gap, accompanied by the light-induced mid-gap absorption, resembling the evolution of optical properties by chemical doping. The data provide strong constraints on the possible photogenerated free carrier (Drude) response. We demonstrate, that even at the highest excitation densities, where in the case of comparable chemical doping a metallic state is realized, photodoping results in a negligible density of free carriers, underscoring the underlying Mott physics.

TT 66.6 Fri 11:00 H2

Excitation Dynamics in the Antiferromagnetic Mott Insulator Ca_2RuO_4 — •Parmida Shabestari[1,2], Anita Mahinpei[1,2], Min-Jae Kim[1,2], Hao Chu[1,2], Maximillian Krautloher[1], Joel Bertinshaw[1], Bernhard Keimer[1], and Stefan Kaiser[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]4th Physics Institute, Stuttgart University, Stuttgart, Germany

Among ruthenates, the antiferromagnetic Mott insulator Calcium Ruthenate, Ca_2RuO_4, has shown remarkable complexity in spin, orbital and phonon correlations. Strong spin-orbit coupling manifests in the form of a complex Phonon, Magnon and collective Higgs mode spectrum. Here we report on the transient dynamics after photo-excitation across the Mott gap, revealing saturation and depletion regimes. In addition we find a so far unknown coherent low frequency mode, which we characterize by Impulsive Stimulated Raman and Terahertz spectroscopy as a possible paramagnon.

15 min. break.

TT 66.7 Fri 11:30 H2

Enhancement of superconductivity in MgB_2 by narrow-band THz pumping — •Nilabha Bhattacharjee[1], Amrit Raj Pokharel[1], Tao Dong[1,2], Alexej Pashkin[3], Stephan Winnerl[3], Manfred Helm[3], Zi Zhao Gan[4], Yue Wang[4], Li Yu Shi[4], Nan Lin Wang[4], and Jure Demsar[1] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, Mainz — [2]International Center For Quantum Materials (ICQM), Peking University — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [4]Institute of Condensed Matter Physics, School of Physics, Peking University

First observations of amplified superconductivity by electromagnetic radiation at sub-gap frequencies date back to late 1960's [1]. These works reported an increase of the gap and the superconducting transition temperature in type-I superconductors Al and Sn. Recently, enhancement effects have also been observed in NbN by using picosecond narrow-band THz pulses, tuned to the vicinity of the superconducting gap frequency [2]. Here we report on systematic studies of the superconducting gap dynamics in MgB_2. Tuning the pump frequency between the two superconducting gap energies in this two-band superconductor we observe strong superconducting enhancement effects competing with THz driven pair-breaking. For temperatures close to the transition temperature (T_c = 36 K) the enhancement effects seem to dominate, giving rise to a global amplification of superconductivity.
[1] A. F. G. Wyatt, et al., Phys. Rev. Lett. 16, 1166 (1966)
[2] M. Beck, et al, Phys. Rev. Lett. 110, 267003 (2013)

TT 66.8 Fri 11:45 H2

Collective modes in non-equilibrium in unconventional superconductors with competing ground states — •Marvin A. Müller[1], Pavel A. Volkov[1,2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey, 08854, USA

Motivated by the recent development of terahertz pump-probe spectroscopy, we investigate the short-time dynamics and collective modes in superconductors with multiple attractive pairing symmetries. We consider a single-band square lattice model with nearest neighbor attraction. This interaction decouples into $s-$, $d-$ and $p-$wave channels and by variation of band filling this yields strong competition between these channels. Driving the system out of equilibrium, we find signatures of collective states of symmetries different from the groundstate symmetry, which are called Bardasis-Schrieffer modes in the context of $s-$wave groundstate. We show that, depending on the polarization direction, additional order parameter symmeries can be excited in pump-probe experiments and the collective 'Bardasis-Schrieffer' modes can be observed.

TT 66.9 Fri 12:00 H2

All-optical nonequilibrium pathway to stabilizing magnetic Weyl semimetals in pyrochlore iridates — •Gabriel E. Topp[1], Nicolas Tancogne-Dejean[1], Alexander F. Kemper[2], Angel Rubio[1,3], and Michael A. Sentef[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany — [2]Department of Physics, North Carolina State University, Raleigh, NC, USA — [3]Center for Computational Quantum Physics (CCQ), Flatiron Institute, 162 Fifth Avenue, New York NY 10010

The 227 pyrochlore iridates were conjectured to exhibit an antiferromagnetically ordered Weyl semimetallic (AF-WSM) phase provided that one could tune the ordered magnetic moment. In our work [1] we propose an ultrafast nonequilibrium pathway to engineering a nonequilibrium AF-WSM phase with short laser pulses. Relying on ab initio TDDFT+U calculations, we investigate the open-system dynamics after an interaction quench in a mean-field dynamics simulation starting from the AFI phase. By computational time- and angle-resolved photoemission spectroscopy (tr-ARPES) measurements, we track the emergence of nonequilibrium Weyl fermions on a femtosecond timescale.
[1] G. E. Topp et al., Nature Communications 9, 4452 (2018)

TT 66.10 Fri 12:15 H2

Ultrafast spin dynamics and high-harmonic generation in multilayer systems based on graphene — •Dominik Schulze and Jamal Berakdar — Institute for physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle (Saale), Germany

High harmonic generation in solids is attracting considerable research due to prospect application in solid-state based emitting devices and ultrafast optoelectronics.

Our research interest is devoted to the role of spin and its exploitation in ultrafast spintronics. In this talk, we present our research on high-harmonic generation in spin-orbital coupled systems such as multilayer systems based on graphene.

The goal is twofold: 1) to utilize these systems as a local radiation source, and 2) to analyze the emitted, time-dependent spectra that may carry footprints of internal spin-dependent mechanism that are important for the operation of spintronic devices.

We present results on multilayer systems composed of graphene on a substrate which induces a strong spin-orbit coupling into the graphene layer. This leads to various interesting effects resulting from the sublattice potential, the Rashba type spin-orbit coupling and a time-reversal symmetry breaking. Full-fledge calculations show how the gap opening at the K and K' points of the graphene affects the high harmonic generation of inter band excitations.

TT 66.11 Fri 12:30 H2

Spin-orbit induced dynamics in a driven single molecule junction — •Moritz Frankerl, Milena Grifoni, and Andrea Donarini — Institut für Theoretische Physik, Universität Regensburg, 93035 Regensburg, Germany

Recent experiments based on THz-STM have shown how to obtain both space and time resolution of molecular dynamics on its intrinsic length and time scales [1]. The average transmitted charge is recorded as a function of tip position and pump-probe pulse delay. We report here on the theoretical investigation of the combined spin and orbital dynamics of a single molecule copper-phthalocyanine junction. The dynamics is studied directly in the time domain, with the full pump-probe scheme simulated within a generalized master equation approach. The spin-orbit coupling on the metallic center is responsible for intertwined spin and orbital dynamics. Control and electrical read out can be achieved respectively via an external magnetic field and coupling to ferromagnetic leads.
[1] T. L. Cocker et al., Nature **539**, 263 (2016)

TT 67: Cryogenic Particle Detectors and Other Superconducting Electronics

Time: Friday 9:30–12:00 Location: H4

TT 67.1 Fri 9:30 H4

Towards microcalorimetry with sub-eV energy resolution: Metallic magnetic calorimeters with direct sensor readout — •Matthäus Krantz, Andreas Fleischmann, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Metallic magnetic calorimeters (MMCs) are energy dispersive single particle detectors typically operated at temperatures below 50 mK. By using a paramagnetic temperature sensor strongly coupled to a matching absorber, state-of-the-art MMCs convert the energy input into a magnetic flux change that is measured by a current-sensing dc-SQUID via a superconducting flux transformer. However, transformer losses and parasitic inductances within the transformer result in a signal reduction ultimately limiting the achievable energy resolution. To challenge this limit we develop MMCs with direct sensor readout for enhanced signal coupling. There, the temperature sensor is placed on top of or within the SQUID loop. Our most recent prototype comprises a gradiometric meander-shaped SQUID inductance and gives reason to expect to significantly lower our current MMC world record energy resolution of 1.6 eV (FWHM) for soft X-rays. We describe the design, microfabrication and optimization of our prototype and discuss the presently achieved performance indicating that we will be able to reach sub-eV energy resolution in the near future.

TT 67.2 Fri 9:45 H4

Development of a Beta Spectrometry Setup using Metallic Magnetic Calorimeters — •Michael Paulsen[1,2], Jörn Beyer[1], Lina Bockhorn[3], Christian Enss[2], Sebastian Kempf[2], Karsten Kossert[3], Martin Loidl[4], Riham Mariam[4], Ole Nähle[3], Philipp Ranitzsch[3], and Matias Rodrigues[4] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [3]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — [4]CEA, LIST, Laboratoire National Henri Becquerel, Saclay, France

The precise knowledge of beta spectrum shapes is relevant in radionuclide metrology, e.g. when determining the activity of samples containing beta emitting isotopes, as well as in fundamental research or applications such as nuclear medicine. Employing Metallic Magnetic Calorimeters (MMCs) with the radionuclide sample embedded in a 4π absorber geometry has proven to be among the best beta spectrometers in terms of energy resolution, notably for low energy beta transitions. This presentation discusses a new MMC-based beta spectrometer that is being developed within the MetroBeta project that operates at temperatures < 20 mK. We present initial beta spectra measurements of Cl-36 (Emax = 709.5 keV) using the newly developed setup, including a discussion of the data acquisition and evaluation used.

TT 67.3 Fri 10:00 H4

Gamma spectroscopy to measure the ^{229}Th isomer energy using a 2-dimensional array of metallic magnetic microcalorimeters — •Jeschua Geist[1], Daniel Hengstler[1], Christian Schötz[1], Sebastian Kempf[1], Loredana Gastaldo[1], Andreas Fleischmann[1], Christian Enss[1], Georgy A. Kazakov[2], Simon Stellmer[2], and Thorsten Schumm[2] — [1]Heidelberg University — [2]Vienna University of Technology

The isotope ^{229}Th has a nuclear isomer state with the lowest presently known excitation energy, which possibly allows to connect the fields of nuclear and atomic physic with a potential application in a nuclear clock. In order to verify and improve the accuracy of the currently most accepted energy value for this isomere energy, (7.8 ± 0.5) eV, we plan to resolve the 29.18 keV doublet in the γ-spectrum following the α-decay of ^{233}U, corresponding to the decay into the ground and isomer state, to measure the isomer transition energy without additional theoretical input parameters.

We developed the detector array maXs-30 consisting of 8x8 metallic magnetic calorimeters with an expected energy resolution below 6 eV, providing a large detection area of 16 mm^2 to face the low rate of the 29.18 keV transitions. We present a new value for the isomere energy with a detector performance of 11 eV FWHM for photons up to 60 keV, show latest recorded ^{229}Th spectra and discuss different ways to derive the isomer energy from these spectra.

TT 67.4 Fri 10:15 H4

Saturation power measurement for a non-degenerate parametric amplifier based on a dispersion engineered SQUID array. — •Ivan Takmakov[1,2], Patrick Winkel[1], Farshad Foroughi[3,4], Luca Planat[3,4], Javier Puertas Martinez[3,4], Wolfgang Wernsdorfer[1,2], Alexey Ustinov[1,2,5], Ioan Pop[1,2], and Nicolas Roch[3,4] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [3]Universite Grenoble Alpes, Institut NEEL, France — [4]CNRS, Institut NEEL, France — [5]Russian Quantum Center, National University of Science and Technology MISIS, Russia

Saturation power is one of the most important characteristics of an amplifier. For a Josephson Parametric Amplifier (JPA) its accurate measurement imposes a challenge. A JPA is typically operated at 20mK and the attenuation of coaxial cables changes when they are cooled down. Thus a calibration is required to know the power of a microwave signal at the input of a JPA.

We present measurements of saturation power of a Dimer Josephson Junction Array Amplifier (DJJAA). The amplifier is based on a dispersion engineered SQUID array. In order to measure the amplifier's saturation power, in front of a DJJAA we connect a transmon qubit coupled to a transmission line. The transmission through this chip depends on the power of a signal. Using this dependence we can measure the signal power at the qubit sample and thus perform a calibration for the saturation power measurements.

TT 67.5 Fri 10:30 H4

Towards a SQUID-based Traveling Wave Parametric Amplifier — •Luca Planat, Arpit Ranadive, Karthik Bharadwaj, Olivier Buisson, Rémy Dassonneville, Farshad Foroughi, Wiebke Guichar, Sébastien Léger, Cécile Naud, Javier Puertas-Martínez, and Nicolas Roch — Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France

Superconducting Parametric Amplifiers are key to research fields involving microwave signals in the quantum regime, such as superconducting qubits or NEMs because of the large gain they provide and their noise performance. Large interaction time between a weak microwave signal, a strong coherent pump tone and a non-linear medium is required to obtain enough gain. Up to now, this was achieved by coupling the non-linear medium to a resonator. But this is also possible by using distributed non-linear media and working in transmission, thus overriding issues of limited bandwidth due to resonant cavities. When the medium is a Josephson junction, this new class of amplifier is called Josephson Traveling Wave Parametric Amplifier (J-TWPA) [1]. We will present our on-going effort to develop a SQUID-based TWPA. It will allow to tune in situ the characteristic impedance of the TWPA to have a perfect impedance match with the rest of the electronic setup, despite the uncertainty of the electrical properties of the device due to the fabrication process.

This work was supported by the French Agence Nationale de la Recherche (ANR CLOUD project No. ANR-16-CE24-0005).

[1] C. Macklin et al., Science 350, 6258 (2015)

TT 67.6 Fri 10:45 H4

Microwave SQUID Multiplexing of Metallic Magnetic Calorimeters — •Mathias Wegner, Daniel Richter, Felix Ahrens, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

To our present knowledge the most suitable device for reading out large-scale detector arrays consisting of hundreds or thousands of metallic magnetic calorimeters (MMCs) is a microwave SQUID multiplexer (μMUX). Each channel of a μMUX consists of a non-hysteretic rf-SQUID which is used for detector readout and which is inductively coupled to a superconducting microwave $\lambda/4$ resonator with unique resonance frequency. Due to the magnetic flux dependence of the SQUID inductance as well as the mutual interaction between the SQUID and the associated resonator, the signal of the MMC is transduced into a resonance frequency shift of the related resonator.

While the basic multiplexer model developed in the context of transition edge sensors was sufficient for developing our first prototype

μMUX devices, it does not include important aspects which need to be considered for an optimized MMC readout. In particular, the model does not describe the readout power dependence as well as the impact of the parasitic shunts of the Josephson junction and the influence of the MMCs on the μMUX characteristics.

In this contribution we present a refined version of the μMUX model which includes these aspects. Besides, we show that we gain a very good agreement between measured data and our refined multiplexer model.

TT 67.7 Fri 11:00 H4

Efficient Filter Solutions for Frequency Demultiplexing of Microwave-SQUID coupled Metallic Magnetic Calorimeters — •Nick Karcher, Oliver Sander, and Marc Weber — Karlsruhe Institute for Technology, Eggenstein-Leopoldshafen, Germany

For the Electron Capture in Ho^{163} (ECHo) experiment, metallic magnetic calorimeters deliver the required energy resolution of ≤ 5 eV for the Holmium decay energy spectrum. To gather the statistics for the spectrum 12000 calorimeters are planned. Microwave SQUID multiplexing can be used to connect several hundred metallic magnetic calorimeters via a single coax pair to a room temperature DAQ system.

We will show an FPGA based software-defined radio DAQ system which can generate the required stimulation frequency comb and is capable of processing the sensor modulated signals. The multiplex bandwidth of a channel is between 4 – 8 GHz with a complex baseband of 800 MHz. It relies on five 1 GS/s, 16 Bit DA and 14 Bit AD converters. For a large number of channels (>100) the necessary channelization hardware resources within the FPGA drives the cost. We will present a novel channelization scheme. Compared to a purely digital down conversion (DDC) based solution it reduces the required resources by almost 85% by utilizing a combination of poly-phase filtering, and DDC at a clock rate of 500 MHz.

TT 67.8 Fri 11:15 H4

Quantum discord in squeezed microwaves — •Kirill G. Fedorov[1,2], Stefan Pogorzalek[1,2], Minxing Xu[1,2], Michael Fischer[1,2,3], Edwar Xie[1,2,3], Qi-Ming Chen[1,2], Achim Marx[1], Frank Deppe[1,2,3], and Rudolf Gross[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, Technische Universitaet Muenchen, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), Schellingstrasse 4, 80799 Muenchen, Germany

Quantum discord is known as a general measure for quantum correlations in bipartite systems. It encompasses all nonclassical correlations including entanglement. Quantum discord has many intriguing fundamental properties many of which require experimental verification such as the asymptotic robustness towards environmental noise. We experimentally investigate quantum discord in propagating two-mode squeezed (TMS) microwave states generated with the help of superconducting Josephson parametric amplifiers. We exploit asymmetric noise injection into these TMS states which allows us to demonstrate the robustness of quantum discord as opposed to the sudden death of entanglement. Finally, we discuss the relevance of quantum discord as a resource in quantum communication and sensing , in particular with respect to remote state preparation and quantum radar protocols.

We acknowledge support by the German Research Foundation through FE 1564/1-1, Elite Network of Bavaria through the program ExQM, EU Quantum Flagship project QMiCS, and Excellence Cluster MCQST.

TT 67.9 Fri 11:30 H4

Quantum one-time pad with propagating squeezed microwaves — •Stefan Pogorzalek[1,2], Kirill G. Fedorov[1,2], Qi-Ming Chen[1,2], Michael Fischer[1,2,3], Michael Renger[1,2], Edwar Xie[1,2,3], Achim Marx[1], Frank Deppe[1,2,3], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

Quantum communication protocols employ nonclassical correlations as a resource for an efficient transfer of quantum states. The closely related field of quantum cryptography deals with the secure transfer of information by exploiting quantum correlations. As a fundamental quantum communication protocol, remote state preparation (RSP) achieves both an efficient and secure transfer of a quantum state. We focus on the latter property by relating the RSP scheme to an extension of the cryptographic protocol known as the one-time pad to the quantum regime. In particular, we achieve the transfer of a quantum squeezed state with 1.6 dB of squeezing below the vacuum over a distance of 35 cm of superconducting cable. At the same time, the classically communicated signal reveals nearly no information about the transferred quantum state.

We acknowledge support by the German Research Foundation through FE 1564/1-1 and the Excellence Cluster MCQST, the Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (Grant No 820505).

TT 67.10 Fri 11:45 H4

Quantum Fourier Transform in Oscillating Modes — •Qi-Ming Chen[1,2], Frank Deppe[1,2,3], Michael Renger[1,2], Michael Fischer[1,2,3], Stefan Pogorzalek[1,2], Edwar Xie[1,2,3], Kirill G. Fedorov[1,2], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

Quantum Fourier transform (QFT) is a key ingredient for many kinds of quantum algorithms. Traditional realizations of QFT requires a large number of qubits or a moderate number of qubits with a complex procedure of qubit recycling mechanism, which limit its application in present-day platforms. We address this problem by mapping the qubit state to an oscillating mode with an infinite-dimensional Hilbert space, and realize QFT in two coupled oscillating modes through cross-Kerr interaction. This method provides the possibility of realizing high-precision QFT without scaling up the dimension of the quantum circuit, which paves the way for realizing various quantum algorithms in the near future.

We acknowledge support by the German Research Foundation through FE 1564/1-1 and the Excellence Cluster MCQST, the Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (Grant No 820505).

TT 68: Topology: Other Topics

Time: Friday 9:30–12:15 Location: H22

TT 68.1 Fri 9:30 H22

Interaction-driven quantum Hall plateau transition between a $|C| > 1$ Chern Insulator and a $\nu = 1/3$ Laughlin state in the Hofstadter model — •Leon Schoonderwoerd[1], Frank Pollmann[2], and Gunnar Möller[1] — [1]Functional Materials Group, School of Physical Sciences, University of Kent, Canterbury CT2 7NZ, United Kingdom — [2]Department of Physics, TFK, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany

We present numerical evidence of an interaction-driven quantum Hall plateau transition between a $|C| > 1$ Chern Insulator and a $\nu = 1/3$ Laughlin state in the Hofstadter model. We study the model using DMRG at flux densities p/q, where the lowest Landau level (LLL) manifold is made up of p magnetic sub-bands. First, we show explicit evidence that a $\nu = 1/3$ Laughlin state can be stabilised in situations where the LLL consists of multiple bands, when the interaction strength V is sufficiently high. Matching the number of magnetic subbands to $1/\nu$, the model also realises a Chern insulator at low interaction strength. We show evidence for a direct transition between these two phases at some flux densities, and we characterise the transition in terms of its critical, topological and entanglement properties.

TT 68.2 Fri 9:45 H22

Superconducting proximity effect in a fractional quantum Hall edge state — •Andreas B. Michelsen[1], Solofo Groenendijk[1], Patrik Recher[2], Tobias Meng[3], Bernd Braunecker[4], and Thomas Schmidt[1] — [1]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxem-

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Parafermions have emerged as a promising platform for topological quantum computation. Current proposals for their experimental realization are usually centered around inducing them in topological edge states. This can be achieved through the application of the superconducting proximity effect to a fractional quantum Hall edge state, where Cooper pairs tunnel to form Laughlin quasiparticles, which retain the pair-correlation on a significant length scale.

While induced superconductivity is rather well understood in topological insulator or integer quantum Hall edge states, the theoretical understanding of this phenomenon in fractional quantum Hall edge states is so far rudimentary. We thus expand on the understanding of this process through a microscopic investigation of the proximity effect in such edge states.

TT 68.3 Fri 10:00 H22

Ground state splitting and robust braiding of parafermions in fractional quantum hall states — •Solofo Groenendijk[1], Alessio Calzona[1,2], Edvin Idrisov[1], Hugo Tschirhart[1], and Thomas Schmidt[1] — [1]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg — [2]Dipartimento di Fisica, Università di Genova, Via Dodecaneso 33, 16146 Genova, Italy

Parafermion bound states generalize the exchange statistics of Majorana fermions and can appear as zero-energy bound states by inducing superconductivity in fractional quantum Hall states. It has been shown that braiding them in edge states can be achieved via a series of nucleation and fusion processes, and can be useful for topological quantum computation. We study analytically and numerically the effect of the chemical potential and a finite length on such braiding protocols.

We show using a combination of bosonization and refermionization that a nonzero chemical potential μ can lift the ground state degeneracy by a factor $\delta E \propto e^{-L/\xi}\cos(\frac{\mu L}{v})$, where L is the distance between two parafermions, ξ is a correlation length and v the Fermi velocity. This generalizes a previous result which was based on a semi-classical approach. This effect destroys the robustness of the proposed braiding protocols because it causes level crossings during the braiding process.

We investigate those avoided crossings for $\mathbb{Z}_3$ parafermions and show that multiple Landau-Zener transitions occur when using conventional braiding protocols even for slow braiding speeds. We mitigate this effect by proposing a new protocol which is robust to these diabatic transitions.

TT 68.4 Fri 10:15 H22

Error-Analysis of the Chern Number in the Haldane-Hubbard Model — •Thomas Mertz, Karim Zantout, and Roser Valentí — Institut für Theoretische Physik, Goethe Universität, 60438 Frankfurt am Main, Germany

In correlated models such as the Hubbard model, the exact form of the self-energy has proven to be elusive, even to the most state-of-the-art numerical techniques. Successors to dynamical mean field theory have been developed to treat the momentum-dependent corrections, however, there is still no general consensus among these improvements.

Here, we discuss the effects of different sources of error in the self-energy on the Chern number. Our discussion puts a particular emphasis on the non-local corrections obtained on top of the dynamical mean field self-energy. In our analysis we study the Haldane-Hubbard model, however, our results should be applicable to similar models as well.

TT 68.5 Fri 10:30 H22

Spectral analysis of the finite Kitaev chain — •Nico Leumer, Milena Grifoni, and Magdalena Marganska — Institut of Physics, Regensburg

Nearly two decades ago, Kitaev published his famous toy model about the emergence of Majorana fermions in the context of spinless electrons on a chain with p-wave superconducting pairing ([1], [2]). Due to its simplicity this model is often used to explain the concepts of topological superconductors.

Despite its popularity, not much is known about the spectrum of a *finite* Kitaev chain. We report here on a spectral analysis yielding the spectrum E(k) and the eigenvectors of the finite chain in analytic form. By mapping the Kitaev chain to a system of two coupled SSH-chains, a non trivial quantisation condition for the allowed k values is found.

[1] A. Y. Kitaev, Phys. Usp. 44, (2001)
[2] R. Aguado, Riv. Nuovo Cimento 40, 16, (2017)

TT 68.6 Fri 10:45 H22

Edge spin correlations driving topological phase transition in an 1D interacting model — •Daniel Duarte, Daniela Pfannkuche, and Marta Prada — Universität Hamburg, I. Institut für Theoretische Physik, Jungiusstrasse 9, 20355 Hamburg

We study a one-dimensional Su-Schrieffer-Heeger like dimerized chain of interacting fermions by means of density matrix renormalization group on the MPS ansatz. The different spin correlation functions are studied and a phase diagram is obtained as a function of dimerization and on site interaction parameters. We find finite spin edge correlations at the transition region of the trivial topological phase and the non-trivial one. Next we characterise the topology in terms its quantum topological phase and the existence of localized spin edge states when the phase is non-trivial. We discuss the connection between the appearance of edge-spin correlations and the phase, the calculation of the phase itself and provide an extended phase diagram, complementing existing ones [1,2]

[1] B.-T. Ye, L.-Z. Mu, and H. Fan, Phys. Rev. B 94, 165167 (2016)
[2] Da Wang, S. Xu, Yu Wang and C. Wu, Phys. Rev B 91, 115118 (2015)

15 min. break.

TT 68.7 Fri 11:15 H22

Non-Hermitian systems and topology: A transfer matrix perspective — •Vatsal Dwivedi[1] and Flore Kunst[2] — [1]Institut für theoretische Physik, Zülpicher Straße 77a, 50937 Köln — [2]Department of Physics, Stockholm University, AlbaNova University Center, 106 91 Stockholm

Non-Hermitian systems are known to exhibit features strikingly different from their Hermitian counterparts, a quintessential example being the lack of a bulk-boundary correspondence in the conventional sense. In this talk, I will describe a transfer matrix approach to these systems. The algebraic structure of the transfer matrix and a Riemann surface associated with the complex energies provide a clear and intuitive picture of various topological aspects of these systems.

TT 68.8 Fri 11:30 H22

Breakdown of the topological fracton order in the X-Cube model — •Matthias Mühlhauser and Kai Phillip Schmidt — Institut für Theoretische Physik I FAU Erlangen-Nürnberg, Erlangen, Deutschland

We investigate the robustness of type-I topological fracton order under zero-temperature quantum fluctuations. To this end the exactly solvable three-dimensional X-cube model is studied in the presence of an external homogeneous magnetic field using high-order series expansions and variational techniques. It is found that the ground-state phase diagram displays first-order phase transitions between the topologically-ordered fracton phase and the polarized phase for all studied field directions. Furthermore, the spectral properties of the low-energy excitations in the fracton phase, especially so-called lineons and planons, are determined.

TT 68.9 Fri 11:45 H22

Measuring beyond the resolution limit of a detector — •Roman-Pascal Riwar — JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, Germany

We recently made the unexpected prediction that the non-equilibrium transport statistics of conventional sequential electron tunneling are indistinguishable from those of fractional charges – in the sense that the statistics are effectively equivalent to fractional charges, measured with a detector that can resolve only integer charges. This effect is due to a topological transition of the system-detector dynamics. Here, we consider a potential application of this effect, when we turn it on its head: if we indeed expect to have a detector with insufficient resolution, the presence of fractional processes might not be effective, but in fact real. We propose, that this could lead to the intriguing possibility of measuring discrete stochastic processes that are smaller than the resolution limit. We provide a proof of principle at the practical example of charge detectors measuring transport through localized charge islands, where the detectors are too large to resolve individual islands. Finally, we show that the effect is indeed protected, by explicitly tak-

ing into account likely sources of perturbations or measurement errors in the setup.

TT 68.10 Fri 12:00 H22

Bulk-boundary correspondence for non-Hermitian Hamiltonians — •Heinrich-Gregor Zirnstein[1], Bernd Rosenow[1], and Gil Refael[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]Institute of Quantum Information and Matter, California Institute of Technology, USA

For sufficiently strong gain and loss, genuinely non-Hermitian topological phases can be realized and characterized by generalized topological invariants. In such phases, the Hamiltonian cannot be deformed into a gapped Hermitian Hamiltonian without the energy bands touching each other. Since the so-called non-Hermitian skin effect causes localization of all eigenstates at a boundary of the system, we discuss topological properties by focusing on response functions, which are experimental observables. In particular, a comparison of Green functions for periodic and open boundary conditions shows that in general there is no correspondence between topological invariants computed for periodic boundary conditions, and edge states observed for open boundary conditions. We prove these statements for one-dimensional systems in several symmetry classes, and discuss generalizations to higher spatial dimensions. In particular, in more than one spatial dimension, every Hamiltonian whose bands do not touch each other is topologically equivalent to a Hermitian one, and non-Hermitian topological indices are only possible when bands touch each other.

TT 69: Cold Atomic Gases and Superfluids

Time: Friday 9:30–11:30 Location: H23

TT 69.1 Fri 9:30 H23

Diagrammatic Large-N approach to the Unitary Fermi Gas — •Gunnar Möller and Christopher R. Winterowd — University of Kent, Canterbury, UK

We explore a large-N, many fermion flavour, generalisation of the unitary Fermi gas [1] using diagrammatic Monte-Carlo techniques. Seminal work on the unitary Fermi gas problem has established a diagrammatic Monte-Carlo (diagMC) approach [2], which needs to be supplemented by exploring the high-order asymptotics of the series expansion [3]. Here, we extend the problem by introducing the inverse number of flavours as a small parameter via a large-N generalisation of the unitary gas [4,5], and we then apply diagMC. Using the Borel resummation technique developed by Rossi et al [3], we show that the convergence radius in the Borel plane is enlarged as a function of fermion flavours, thus facilitating the convergence of the series in the vicinity of the transition into the superfluid phase.

More generally, the combination of large-N field theory techniques with high-order numerical resummations opens up a new avenue for investigations of strongly interacting systems.

[1] W. Zwerger, Springer (2012)
[2] K. Van Houcke et al., Nat Phys 8, 366 (2012);
Van Houcke, et al., arXiv:1305.3901 (2013)
[3] R. Rossi, et al., PRL 121, 130405 (2018)
[4] M. Y. Veillette, et al., PRA 75, 043614 (2007)
[5] P. Nikolic and S. Sachdev, PRA 75, 033608 (2007)

TT 69.2 Fri 9:45 H23

Mechanical resonances of mobile impurities in a one-dimensional quantum fluid — •Thomas Schmidt[1], Karyn Le Hur[2], and Peter Orth[3] — [1]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg — [2]Centre de Physique Theorique, Ecole Polytechnique, CNRS, Universite Paris-Saclay, F-91128 Palaiseau, France — [3]Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

We study a one-dimensional interacting quantum liquid hosting a pair of mobile impurities causing backscattering. We determine the effective retarded interaction between the two impurities mediated by the liquid. We show that for strong backscattering this interaction gives rise to resonances and antiresonances in the finite-frequency mobility of the impurity pair. At the antiresonances, the two impurities remain at rest even when driven by a (small) external force. At the resonances, their synchronous motion follows the external drive in phase and reaches maximum amplitude. Using a perturbative renormalization group analysis in quantum tunneling across the impurities, we study the range of validity of our model. We predict that these mechanical antiresonances are observable in experiments on ultracold atom gases confined to one dimension.

TT 69.3 Fri 10:00 H23

Floquet induced superfluidity — •Shijie Hu[1], Xue-Feng Zhang[2], Tao Wang[1,2,3], Axel Pelster[1], and Sebastian Eggert[1] — [1]Technische Universität Kaiserslautern — [2]Chongqing University — [3]Wuhan Institute of Technology

We consider two states of hard-core bosons with periodically modulated Rabi driving in a one dimensional (1D) optical lattice, which is equivalent to the 1D Hubbard model with time-periodic interactions. Using Floquet theory the model can be mapped to an effective Hamiltonian for high frequencies, which is described by a static interactions and hopping parameters that depend on the local densities. In particular, if the density difference of one species is non-zero on neighboring sites, the effective hopping of the other species is reduced and can even take on negative values. Using a combination of analytic calculations and different advanced numerical simulations we establish the full quantum phase diagram for half-integer filling for this system. Surprisingly, the density-dependent reduction of hopping drives a quantum phase transition into a superfluid phase. For negative hopping a previously unknown state is found, where one species induces a gauge phase of the other species, which leads to a superfluid phase of gauge-dressed particles. The corresponding experimental signatures in time-of-flight experiments are calculated and show characteristic signatures of the different phases. The phase transition line between the two superfluid phases corresponds to an exactly solvable model with high degeneracy.

TT 69.4 Fri 10:15 H23

New probes of the t-J model in quantum gas microscopes — •Annabelle Bohrdt[1,2], Christie Chiu[2], Geoffrey Ji[2], Muqing Xu[2], Daniel Greif[2], Markus Greiner[2], Eugene Demler[2], Fabian Grusdt[1,2], and Michael Knap[1] — [1]Department of Physics and Institute for Advanced Study, Technical University of Munich, 85748 Garching, Germany — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

Quantum gas microscopes for ultracold atoms can provide high-resolution real-space snapshots of complex many-body systems. We implement machine learning to analyze and classify such snapshots of ultracold atoms. Specifically, we compare the data from an experimental realization of the two- dimensional Fermi-Hubbard model to two theoretical approaches: a doped quantum spin liquid state of resonating valence bond type, and the geometric string theory, describing a state with hidden spin order. This approach considers all available information without a potential bias towards one particular theory by the choice of an observable and can therefore select the theory which is more predictive in general. Up to intermediate doping values, our algorithm tends to classify experimental snapshots as geometric-string-like, as compared to the doped spin liquid. Our results demonstrate the potential for machine learning in processing the wealth of data obtained through quantum gas microscopy for new physical insights.

TT 69.5 Fri 10:30 H23

Gross-Neveu-Wilson model and correlated symmetry-protected topological phases — Alejandro Bermudez[1], •Emanuele Tirrito[2], Matteo Rizzi[3], Maciej Lewenstein[4], and Simon Hands[5] — [1]Departamento de Fisica Teórica, Universidad Complutense, 28040 Madrid, Spain — [2]ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain — [3]Johannes Gutenberg-Universität, Institut für Physik, Staudingerweg 7, 55099 Mainz, Germany — [4]ICREA, Lluis Companys 23, 08010 Barcelona, Spain — [5]Department of Physics, College of Science, Swansea University, Singleton Park, Swansea SA2 8PP, United Kingdom

We show that a Wilson-type discretization of the Gross-Neveu model, a fermionic N-flavor quantum field theory displaying asymptotic freedom and chiral symmetry breaking, can serve as a playground to ex-

plore correlated symmetry-protected phases of matter using techniques borrowed from high-energy physics. A large- N study, both in the Hamiltonian and Euclidean formalisms, yields a phase diagram with trivial, topological, and symmetry-broken phases separated by critical lines that meet at a tri-critical point. We benchmark these predictions using tools from condensed matter and quantum information science, which show that the large-N method captures the essence of the phase diagram even at N = 1. Moreover, we describe a cold-atom scheme for the quantum simulation of this lattice model, which would allow to explore the single-flavor phase diagram.

TT 69.6 Fri 10:45 H23

Rhombi-chain Bose-Hubbard model: Geometric frustration and interactions — Christine Cartwright[1], Gabriele De Chiara[1], and •Matteo Rizzi[2] — [1]Centre for Theoretical Atomic, Molecular and Optical Physics, Queen's University Belfast, Belfast BT7 1NN, United Kingdom — [2]Institut für Physik, Johannes Gutenberg Universität, Staudingerweg 7, 55099 Mainz, Germany

We explore the effects of geometric frustration within a one-dimensional Bose-Hubbard model using a chain of rhombi subject to a magnetic flux. The competition of tunneling, self-interaction, and magnetic flux gives rise to the emergence of a pair-superfluid (pair-Luttinger liquid) phase besides the more conventional Mott-insulator and superfluid (Luttinger liquid) phases. We compute the complete phase diagram of the model by identifying characteristic properties of the pair-Luttinger liquid phase such as pair correlation functions and structure factors and find that the pair-Luttinger liquid phase is very sensitive to changes away from perfect frustration (half-flux). We provide some proposals to make the model more resilient to variants away from perfect frustration. We also study the bipartite entanglement properties of the chain. We discover that, while the scaling of the block entropy pair-superfluid and of the single-particle superfluid leads to the same central charge, the properties of the low-lying entanglement spectrum levels reveal their fundamental difference.
[1] Phys. Rev. B 98, 184508 (2018)

TT 69.7 Fri 11:00 H23

The longitudinal and transverse structure factors in impurity-doped spin chains with a magnetic field — Imke Schneider[1], Kevin Jägering[1], Annabelle Bohrdt[2], Sofia Brenner[1], Daniel Wessel[1], and •Sebastian Eggert[1] — [1]Technische Universität Kaiserslautern — [2]Technische Universität München

We consider the dynamic structure factor in impurity doped spin-1/2 chains for general anisotropy, magnetic field and momentum. The impurities lead to effectively isolated finite chain segments with a discrete spectrum and characteristic correlations, which have distinct effects on the longitudinal and transverse structure factors. We present very accurate results for the low energy spectral weight obtained by numerical Density Matrix Renormalization Group techniques and identify the character of dominant excitations for a large range of doping concentrations, anisotropies, and fields. In comparison with bosonization and find surprisingly good agreement with the numerical results. This has direct relevance for recent experiments on spin chains and ultracold gases and shows that, contrary to expectations, bosonization works especially well for short chains and in the vicinity of divergences.

TT 69.8 Fri 11:15 H23

Phonon-mediated Casimir interaction between finite mass impurities — Andrei Pavlov, Jeroen van den Brink, and •Dmitri Efremov — IFW Dresden

The Casimir effect, a two-body interaction via vacuum fluctuations, is a fundamental property of quantum systems. In solid state physics it emerges as a long-range interaction between two impurity atoms via virtual phonons. In the classical limit for the impurity atoms in D dimensions the interaction is known to follow the universal power-law $U(r) \sim r^{-D}$. However, for finite masses of the impurity atoms on a lattice, it was predicted to be $U(r) \sim r^{-2D-1}$ at large distances. We examine how one power-law can change into another with increase of the impurity mass and in presence of an external potential. We provide the exact solution for the system in one-dimension. At large distances it indeed $U(r) \sim r^{-3}$ for finite impurity masses, while for the infinite impurity masses or in an external potential it crosses over to $U(r) \sim r^{-1}$. At short distances the Casimir interaction is not universal and depends on the impurity mass and the external potential.