TT 72: Poster Session: Correlated Electrons

Time: Wednesday 15:00–19:00 Location: Poster B

TT 72.1 Wed 15:00 Poster B

Fermi Surface determination of $CeAl_2$ via de Haas-van Alphen oscillations — •Michael Petrov, Chris Franz, Schorsch Sauther, Andreas Bauer, Mark Wilde, and Christian Pfleiderer — Physik-Department, Technische Universitaet Muenchen, 85748 Garching, Germany

In this work, we revisit the Fermi surface properties of $CeAl_2$, a prototypical heavy-fermion compound that has attracted interest [1,2] because it promises tractable conditions for investigating the emergence of the heavy electron state in an f-electron system and its evolution across metamagnetic phase transitions [3]. In particular, the aim of the current research is a comprehensive picture of the Fermi surface properties, both, above and below the metamagnetic transitions. Torque magnetometry is used as a measurement technique for the de Haas-van Alphen (dHvA) effect that is complementary to the previously employed modulation technique. First results regarding both dHvA oscillations and the magnetic state via the non-oscillatory torque components are presented. The dHvA orbits are compared to the results of density functional theory calculations.

[1] Reinders *et al.*, JMMM **79**, 295 (1989)
[2] Pricopi *et al.*, Physica B: Condensed Matter **294**, 276 (2001)
[3] Schefzyk *et al.*, Solid State Communications **54**, 525 (1985)

TT 72.2 Wed 15:00 Poster B

Low-temperature properties of the non-centrosymmetric heavy-fermion compound $CeTAl_3$ (T = Cu, Ag, Au, Pd, Pt) — Christian Franz[3], Stefan Weber[1], •Jan Spallek[1], Alexander Regnat[1], Petr Cermak[2], Astrid Schneidewind[2], Andreas Bauer[1], Anatoly Senyshyn[2], and Christian Pfleiderer[1] — [1]Physik Departement, Technische Universität München, Garching, Deutschland — [2]JCNS-MLZ PANDA, Forschungszentrum Jülich, Garching, Deutschland — [3]Forschungsreaktor München 2, Garching, Deutschland

We report a comprehensive study of the series of non-centrosymmetric heavy-fermion compounds $CeTAl_3$ (T = Cu, Ag, Au, Pd, and Pt). Large single crystals have been prepared by means of optical floatzoning. The single-crystal ingots were characterized using Laue x-ray scattering, powder x-ray diffraction, and energy dispersive x-ray spectroscopy. For T = Cu, Au, Pd, and Pt the system crystallizes in the non-centrosymmetric I4mm crystal structure, while we observe a slight orthorombic distortion for T = Ag. Subsequently, the magnetization, specific heat, and electrical resistivity were investigated down to temperatures of 200 mK and in magnetic fields of up to 14 T revealing typical heavy-fermion behavior. At low temperatures, $CeCuAl_3$ and $CeAuAl_3$ order antiferromagnetically, whereas $CeAgAl_3$ is a ferromagnet. Indications of magnetic order are observed in $CePdAl_3$. Inelastic neutron scattering studies indicate the presence of so-called vibron modes, i.e., coupled modes of phonons and crystal electric field excitations.

TT 72.3 Wed 15:00 Poster B

Pressure and field dependent entropy of the heavy-fermion system CePdAl — •Kai Grube[1], Sebastian Kuntz[1], Chien-Lung Huang[2], Veronika Fritsch[3], and Hilbert von Löhneysen[1,4] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [2]Department of Physics and Astronomy, Rice University, Houston, Texas 77005, United States — [3]Experimentalphysik VI, Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86159 Augsburg, Germany — [4]Physikalisches Institut, Karlsruher Institut für Technologie, 76049 Karlsruhe, Germany

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

TT 72.4 Wed 15:00 Poster B

Evolution of magnetic order in $HoIn_{1-x}Cd_xCu_4$ — Christina Baumeister[1], Oliver Stockert[2], and •Veronika Fritsch[1] — [1]EP 6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

$HoInCu_4$ is a partially frustrated metal, crystallizing in the cubic $AuBe_5$ structure. The Ho ions carrying the magnetic moment form a fcc lattice, with alternating antiferromagnetic planes along [100], which are separated by frustrated planes as shown by neutron scattering experiments [1]. The partial frustration is manifested in magnetization and specific heat data, leading to a frustration parameter $f = 14.3$ [2]. In contrast, no signatures of magnetic frustration are found in isotructural $HoCdCu_4$ [3]. Here, Neutron scattering experiments point to a magnetic structure of ferromagnetic planes, which are stacked antiferromagnetically along the [111] direction [4]. We will present detailed measurements of magnetization and specific heat on the alloying series $HoIn_{1-x}Cd_xCu_4$ tracking the evolution of the magnetic order and the magnetic frustration as function of Cd content.

[1] O. Stockert *et al.*, Experimental Report, HMI B 612 (2006).
[2] V. Fritsch *et al.*, Phys. Rev. B, **71**, 132401 (2005).
[3] V. Fritsch *et al.*, Phys. Rev. B, **73**, 094413 (2006).
[4] O. Stockert *et al.*, Experimental Report, MLZ Garching (2017).

TT 72.5 Wed 15:00 Poster B

Crystal structure and magnetic properties of $CeMg_{3-x}Ag_x$ — •Alexander Engel[1], Georg Eickerling[2], Ernst-Wilhelm Scheidt[2], Philipp Gegenwart[1], and Veronika Fritsch[1] — [1]EP 6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Chemical Physics and Materials Science, Augsburg University, Germany

$CeMg_3$ crystallizes in a BiF_3 cubic heusler-phase type structure and is a heavy-fermion antiferromagnet with $T_N = 3.4$ K. Gradually substituting Mg with Ag makes it possible to tune the exchange interaction and hereby the antiferromagnetic order. Furthermore a structural phase transition accompanied by a charge density wave occurs for $x \geq 1.5$. This structural phase transition was confirmed by temperature dependent single crystal x-ray diffraction. Moreover we show measurements of electrical resistivity and heat capacity on polycrystals tracking the magnetic order and structural phase transition in the alloy-series of $CeMg_{3-x}Ag_x$ and discuss a possible structural quantum critical point.

TT 72.6 Wed 15:00 Poster B

3D topological Kondo insulators: effects of strong correlations onthe stability of topological phases — •Paul Züge[1], Soroush Arabi[1], Francisco Meirinhos[1], and Johann Kroha[1,2] — [1]Physikalisches Institut and Bethe Center for TheoreticalPhysics, Universität Bonn, Germany — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, China

Topological Kondo insulators (TKI) are heavy-fermion (HF) materials where strong correlations generate a HF band with a hybridization gap around the Fermi level and the strong spin-orbit coupling in the 4f orbitals on the rare-earth sites, hybridizing with the light conduction electron band, induces non-trivial topology with conserved topological invariants in these bands. Since in all relevant energy scales, the HF band width, the gap and quasiparticle decay rates are of comparable size, the Kondo temperature T_K, TKIs are ideal systems to study the stability of topological phases in the presence of interactions. However, most theoretical studies have been on the effective single-particle (mean-field) level up to now. We use the slave boson (SB) representation for the HF band and systematically expand around the SBMF saddle point, taking the Gaussian fluctuations of the SB field into account. Feeding the resulting self-energies back into the boson and fermion propagators, this leads to self-consistent saddle-point equations, which imply a finite spectral width for the HF states. We solve these equations self-consistently for the bulk of three-dimensional TKIs. We compute the HF and conduction electron spectral functions and analyse the stability of the topological hybridization gap.

TT 72.7 Wed 15:00 Poster B

Slave Boson Mean Field - revisited — •Jannis Seufert, David

Riegler, Michael Klett, and Ronny Thomale — Institute for Theoretical Physics, University of Würzburg, Germany

Considering correlated electron systems where interactions constitute the dominant energy scale is a challenging problem in solid state physics. The Slave-boson mean field method provides an exact mapping of fermionic Hamiltonians into a description, where the interaction terms become bilinear in bosonic auxiliary fields, whereas terms which are bilinear in the original Hamiltonian transform to a mix of auxiliary bosonic and fermionic fields. A consecutive mean field treatment is therefore especially suitable to incorporate the impact of strong interactions, and yields a non-interacting effective band structure. Experimentally relevant quantities such as heat capacity or effective mass can be derived from the mean field variables, while dynamic quantities such as susceptibilities can be obtained from fluctuations around the saddle point. Evaluating susceptibilities allows to obtain phase diagrams, especially talking incommensurate magnetism by means of a magnetic, momentum dependent mean field into account. We provide a fresh look on the method of spin rotation invariant Slave-boson mean field with fluctuations around the saddle point, and its applications to investigate incommensurate magnetism and heavy fermion systems.

TT 72.8 Wed 15:00 Poster B

Towards the crystal growth of nuclear spin tuned $YbRh_2Si_2$ — •Thanh Duc Nguyen, Doan-My Tran, Sebastian Witt, and Cornelius Krellner — Physikalisches Insitut, Goethe-Universität Frankfurt am Main, D-60438 Frankfurt

The investigation of the heavy fermion compound $YbRh_2Si_2$ allows new insights concerning the interplay of quantum phase transitions and superconductivity. The compound shows at 70mK antiferromagnetic order which can be further suppressed to a quantum critical point. Recently, at 2mK a superconducting state was discovered [1]. Due to the ordering of the nuclear spin of ^{171}Yb and ^{173}Yb before the superconducting state emerges it is a matter of particular interest to investigate the evolution of the superconductivity in single crystals with pure zero and non-zero nuclear spins of the Yb-isotopes. To this end, we first need to optimize the metallothermic reduction of the rare earth element as the isotopes are only available as oxides. Furthermore, we present the optimization of down-scaling in mass the single crystal growth and we report two ways to regaining ytterbium from foreign phase $YbRhIn_5$.
[1] E. Schuberth et al., Science 351, 485 (2016).

TT 72.9 Wed 15:00 Poster B

High-Pressure studies on the quasi-one-dimensional heavy fermion metal $YbNi_4P_2$ — •Takaki Muramatsu[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

$YbNi_4P_2$ is very unique system among correlated electron compounds due to the quasi-one-dimensional nature. The crystal structure is tetragonal $ZrFe_4Si_2$ type structure ($P4_2/mnm$) in which Yb chains along c-axis are separated by chains of edge-shared Ni tetrahedra. Below 0.17K, $YbNi_4P_2$ orders ferromagnetically (FM) with small ordered magnetic moment of $0.05\mu_B$ [1]. $YbNi_4P_2$ is a rare expample where a ferromagnetic quantum critical point can be accessed [2]. Here, we present high-pressure studies of $YbNi_4P_2$ using a diamond-anvil pressure cell. Application of pressure on strongly correlated electron system plays an important role to discuss the quantum criticality and to study the detailed properties of the system. In this work, temperature dependence of the electrical resistivity of $YbNi_4P_2$ was measured under high pressure to understand the basics of competing nature among 4f valence of Yb ion, long range magnetic order and Kondo effect.
[1] C. Krellner et al., New J. Phys, **13**, 103014 (2011).
[2] A. Steppke et al., Science, **339**, 933 (2013).

TT 72.10 Wed 15:00 Poster B

Crystal Growth with Flux Method and Characterization of $CeRu_2P_2$ — •Fabian Feldmann, Kristin Kliemt, and Cornelius Krellner — Physikalisches Inst., Goethe Univ., DE

$CeRu_2P_2$ is a rare-earth ternary phosphide with the tetragonal $ThCr_2Si_2$ type crystal structure. The electrical resistivity in [100] direction of $CeRu_2P_2$ shows a broad maximum at T = 180 K and metallic behavior for lower temperatures [1], indicative of a slightly intermediate valent system, which was confirmed recently in RIXS measurements [2]. Here, we report a crystal growth method for $CeRu_2P_2$. The single crystals have been grown in Sn-flux with temperatures up to 1500 °C. We have characterized the grown crystals with EDX and powder x-ray diffraction measurements. Furthermore, we present measurements of electrical resistivity, specific heat and magnetic susceptibility.
[1] T. Fujiwara et al., J. Phys.: Conf. Ser. **273**, 012112 (2011)
[2] A. Amorese et al., Phys. Rev. B **93**, 165134 (2016)

TT 72.11 Wed 15:00 Poster B

Characterization of Hf and Sc substituted $YbNi_4P_2$ single crystals — •Paul Denck, Kristin Kliemt, and Cornelius Krellner — Institute of Physics, Goethe-University Frankfurt, D-60438 Frankfurt, Germany

The low lying Curie temperature, $T_C = 0.17$ K, of the heavy-fermion compound $YbNi_4P_2$ can be further suppressed by substituting P by As. The rare case of a ferromagnetic quantum critical point occurs in the substitution series $YbNi_4(P_{1-x}As_x)_2$ at $x \approx 0.1$ [1,2]. Single crystals $Yb_{1-x}Hf$, $Sc_xNi_4P_2$, with various hafnium and scandium concentrations were grown by the Czochralski method [3,4]. We characterized the room temperature crystal structure by powder x-ray diffraction and determined the change in the lattice constants for increasing content of the subtituent. Furthermore, these crystals were characterized by electrical transport, heat capacity, and magnetization measurements to investigate the effect of the substitution on the ferromagnetic order.
[1] C. Krellner et al., New J. Phys. **13**, 103014 (2011)
[2] A. Steppke et al., Science **339**, 933 (2013)
[3] K. Kliemt, C. Krellner, J. Cryst. Growth **449**, 129 (2016)
[4] K. Kliemt, C. Krellner, J. Phys.: Conf. Series **807**, 032005 (2017)

TT 72.12 Wed 15:00 Poster B

Hydrostatic-pressure tuning of the magnetic states in the frustrated itinerant system YFe_4Si_2 — •C. Thurn[1], B. Wolf[1], C. Krellner[1], N. Mufti[2], C. Geibel[2], and M. Lang[1] — [1]Physikalisches Institut, Goethe Uni, Frankfurt/M., SFB/TR49, Germany — [2]MPI CPfS, Dresden, Germany

Magnetic frustration can enhance quantum fluctuations which are supposed to be the key in creating exotic states. Whereas frustration is often found in insulators, frustrated magnetic metals are rare. The family of intermetallic AFe_4X_2 with A=Y, Lu, Zr and X=Ge, Si represents such frustrated itinerant systems in which the Fe ions are arranged on slightly distorted, edge-linked tetrahedra which promote the frustration. The properties of these compounds cover a wide range, including frustrated antiferromagnetic order and potentially paramagnetic states close to quantum-critical points. The substitution on the A and X sites here modifies the unit-cell parameters, suggesting a significant influence of chemical pressure on the ground-state properties. In order to mimic and fine-tune the effect of chemical pressure, we present a study of the magnetic properties of YFe_4Si_2 under hydrostatic pressures up to 4 kbar. This compound shows two consecutive magnetic phase transitions at ambient pressure which are strongly coupled to structural degrees of freedom. Our results indicate moderate pressure dependences of the two phase transitions. In order to investigate the interplay of the structure with magnetic frustration in more detail, we also discuss pressure tuning of the distinctly more frustrated system $ZrFe_4Si_2$ which might be located close to a quantum-critical point.

TT 72.13 Wed 15:00 Poster B

Higher order transport mechanisms using matrix product — •Simon Kothe, Lars-Hendrik Frahm, and Daniela Pfannkuche — 1. Institut für Theoretische Physik, Universität Hamburg

We investigate different methods to approach the Kondo regime of an atom that is coupled to two reservoirs. In our model the atom is simplified as a spin, that is biased by a magne- tocrystalline anisotropy field and the exchange interaction to electrons in the reservoirs. As our first approach we use a perturbation ansatz to obtain equations of motion for the reduced density matrix of the spin. This allows us to calculate dynamics of the atom as well as trans- port properties. In our second approach we use matrix product states (MPS) to describe the state of the system and apply the density matrix renormalization group (DMRG) algorithm. The resulting transport properties show the importance of higher order coupling mechanisms.

TT 72.14 Wed 15:00 Poster B

Effective interactions between rotating impurities immersed in a bosonic bath — •xiang li and mikhail lemeshko — IST, Klosterneuburg, Austria

As first reported in [1], an impurity exchanging angular momentum with the environment can be described as a new quasiparticle, the an-

gulon. The outcome of the angulon theory has been shown to be in good agreement with experiments on molecules rotating in quantum solvents [2]. Here, we study the direct and bath -mediated interactions between two rotating molecular impurities in a bosonic bath. A theory of bi-angulon quasiparticle is proposed.
[1] R. Schmidt and M. Lemeshko, Phys. Rev. Lett. 114, 203001 (2015)
[2] M. Lemeshko, Phys. Rev. Lett. 118, 095301 (2017)

TT 72.15 Wed 15:00 Poster B

Emergence of non-abelian magnetic monopoles in a quantum impurity problem — •Enderalp Yakaboylu, Andreas Deuchert, and Mikhail Lemeshko — IST Austria (Institute of Science and Technology Austria), Am Campus 1, 3400 Klosterneuburg, Austria

Recently it was shown that molecules rotating in superfluid helium can be described in terms of the angulon quasiparticles [1]. Here we demonstrate that in the experimentally realized regime the angulon can be seen as a point charge on a 2-sphere interacting with a gauge field of a non-abelian magnetic monopole. Unlike in several other settings, the gauge fields of the angulon problem emerge in the real coordinate space, as opposed to the momentum space or some effective parameter space. Furthermore, we find a topological transition associated with making the monopole abelian, which takes place in the vicinity of the previously reported angulon instabilities. These results pave the way for studying topological phenomena in experiments on molecules trapped in superfluid helium nanodroplets, as well as on other realizations of orbital impurity problems [2].
[1] M. Lemeshko, Phys. Rev. Lett. 118, 95301 (2017).
[2] E. Yakaboylu, A. Deuchert, and M. Lemeshko, arXiv:1705.05162.

TT 72.16 Wed 15:00 Poster B

Thomas Fermi regime of neutrons stars at finite temperature — •Kouidri smail — Departmet of Physics University of Saida Algeria

We present our numerical calculations to study the behavior of a neutron stars at finite temperature and in Thomas Fermi limit. This system of BEC is described by the famous Gross- Pitaevskii equation, which can be solved numerically using several method [1]. The term which contains the gravitational contribution is described by Poisson equation, that can be solved by iterative processus. Our work combines these two methods to study the time evolution of a self-gravitating.

TT 72.17 Wed 15:00 Poster B

Evolution of the order parameter close to the CDW quantum critical point in $Lu(Pt_{1-x}Pd_x)_2In$ — •Stefan Lucas[1], Thomas Gruner[1], Andreas Hoser[2], Manfred Reehuis[2], Karin Schmalzl[3], Michael Marek Koza[3], Christoph Geibel[1], and Oliver Stockert[1] — [1]Max Planck Institute for Chemichal Physics of Solids, Dresden, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Institut Laue-Langevin, Grenoble, France

In contrast to magnetic quantum phase transitions being studied for many years, those driven by an instability of the crystal structure are hardly investigated so far. The intermetallic alloying series $Lu(Pt_{1-x}Pd_x)_2In$ represents a model system to study a Charge-Density-Wave (CDW) quantum critical point (QCP) occurring at $x \approx 0.58$ [1]. A strong and well defined maximum of the superconducting transition temperature right in the vicinity of the QCP indicates a close connection between the low-energy order parameter fluctuations and superconductivity. The important role of the structural fluctuations is already suggested in specific heat and resistivity measurements and was now investigated by neutron diffraction. We present the evolution of the superstructure (i.e. the order parameter) for different concentrations of $Lu(Pt_{1-x}Pd_x)_2In$ and discuss the role of critical fluctuations in this system.
[1] T. Gruner *et al.*, *Nat. Phys.* **13**, 967 (2017)

TT 72.18 Wed 15:00 Poster B

Crystal growth and soft phonon mode of the quantum critical CDW system $Lu(Pt_{1-x}Pd_x)_2In$ — •Thomas Gruner[1], Stefan Lucas[1], Satoshi Tsutsui[2], Koji Kaneko[3], Oliver Stockert[1], and Christoph Geibel[1] — [1]MPI CPfS, Dresden, Germany — [2]JASRI, SPring-8, Sayo, Hyogo, Japan — [3]JAEA Quantum Beam Science Center, Tokai, Ibaraki, Japan

The connection between a charge density wave (CDW) quantum critical point (QCP) and superconductivity (SC) is presently a hot topic. We recently reported the discovery of a CDW in $LuPt_2In$ at $T_{CDW} = 490\,K$, which can be continuously tuned to $T = 0$ by partially substituting Pd for Pt [1]. Moreover, $Lu(Pt_{1-x}Pd_x)_2In$ shows a sharp peak in the x dependence of the superconducting T_c just at the QCP, indicating a very unusual coupling between CDW and SC [1]. Here, we discuss the growth of large high-quality single crystals across the whole composition range. The challenge in growing them is the combination of high-melting elements with the low-melting In. We used these crystals for a series of momentum (Q) resolved inelastic x-ray scattering experiments. They provided a first insight into the Q, T and x dependence of the phonon softening connected with the CDW. In one phonon branch the phonon energy drops towards zero when T decreases towards $T_{CDW}(x)$ and Q approaches the CDW propagation vector. Our results provide an essential basis for analyzing the critical behaviour in this system. Furthermore, we present an improved structure model of the CDW state.
[1] T. Gruner et al., Nature Physics **13**, 967-972 (2017)

TT 72.19 Wed 15:00 Poster B

Ising tricriticality in the extended Hubbard model with bond dimerization — •Florian Lange, Satoshi Ejima, and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, D-17489 Greifswald, Germany

We explore the quantum phase transition between symmetry protected topological and charge-density-wave insulating states in the one-dimensional, half-filled, extended Hubbard model with explicit bond dimerization. We show that the critical line of the continuous Ising transition terminates at a tricritical point, belonging to the universality class of the tricritical Ising model with central charge $c = 7/10$. Above this point, the quantum phase transition becomes first order. Employing a numerical matrix-product-state based (infinite) density-matrix renormalization group method we determine the ground-state phase diagram, the spin and two-particle charge excitations gaps, and the entanglement properties of the model with high precision. Performing a bosonization analysis we can derive a field description of the transition region in terms of a triple sine-Gordon model. This allows us to derive field theory predictions for the power-law (exponential) decay of the density-density (spin-spin) and bond-order-wave correlation functions, which are found to be in excellent agreement with our numerical results.

TT 72.20 Wed 15:00 Poster B

Fluctuation effects at the onset of $2k_F$ density wave order with one pair of hot spots 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 connecting a single pair of hot spots on the Fermi surface. We compute the momentum and frequency dependence of the fermion self-energy near the hot spots to leading order in a fluctuation expansion (one loop). Non-Fermi liquid behavior with anomalous frequency scaling, a vanishing quasi-particle weight, and a logarithmically divergent renormalization of the Fermi velocity are obtained. Going beyond the leading order calculation we find that the one-loop result is not self-consistent. Moreover, we show that any self-energy with a non-Fermi liquid frequency exponent wipes out the peak of the polarization function at the $2k_F$ wave vector, and thus destroys the mechanism favoring $2k_F$ density waves over those with generic wave vectors.

TT 72.21 Wed 15:00 Poster B

Non-linear integral equations for the XXX-$\frac{1}{2}$-chain with off-diagonal boundary conditions — •Dennis Wagner and Andreas Klümper — Bergische Universität Wuppertal, Wuppertal, Germany

The off-diagonal Bethe-Ansatz is a method to solve integrable models that lack U(1)-symmetry and hence do not have a reference state for the application of the coordinate or algebraic Bethe ansatz. Within this work, it is tried to use an inhomogeneous T-Q relation for the XXX-$\frac{1}{2}$-chain with off-diagonal boundary conditions as well as the fusion hierarchy to derive non-linear integral equations. For concrete tests, the system size is reduced to $N = 4$, under the assumption, that the general procedure also holds for larger system sizes. To test the derivation of non-linear integral equations via this procedure, an inhomogeneous T-Q relation for the XXX-$\frac{1}{2}$-chain with periodic boundary conditions is investigated. Finally, for the chain with off-diagonal

boundary fields a system of three non-linear integral equations is presented.

TT 72.22 Wed 15:00 Poster B

Quantum Monte Carlo simulations of quantum critical fermions — •Carsten Bauer[1], Yoni Schattner[2], Erez Berg[3], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]Department of Physics, Stanford University, Stanford, CA 94305, USA — [3]Department of Physics, University of Chicago, Chicago IL 60637, USA

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 fermionic excitations on a Fermi surface. When driving the metal through a phase transition, this interplay can give rise to superconductivity and non-Fermi liquid behavior.

Fortunately, for certain classes of metallic quantum critical points this rich physics can be studied by determinant quantum Monte Carlo simulations, without suffering from the notorious fermion "sign problem". I will show numerically exact studies of different Fermi surfaces coupled to antiferromagnetic SU(2) order in two spatial dimensions. I will further demonstrate that Julia, a new dynamical programming language, is excellently suited for conducting such studies both with regards to speed and code complexity.

TT 72.23 Wed 15:00 Poster B

High-field ESR studies of the honeycomb-lattice material α-$RuCl_3$ — •Alexey N. Ponomaryov[1], E. Schulze[1,2], J. Wosnitza[1,2], P. Lampen-Kelley[3,4], A. Banerjee[3], J.Q. Yan[3], C.A. Bridges[3], D.G. Mandrus[3], S.E. Nagler[3], A.K. Kolezhuk[5], and S.A. Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]TU Dresden, Germany — [3]Oak Ridge National Laboratory, Oak Ridge, TN, USA — [4]University of Tennessee, Knoxville, TN, USA — [5]T. Shevchenko National University of Kyiv, Ukraine

We present high-field electron spin resonance (ESR) studies of the honeycomb-lattice material α-$RuCl_3$, a prime candidate to exhibit Kitaev physics. Two modes of antiferromagnetic resonance were detected in the zigzag ordered phase, with magnetic field applied in the *ab* plane. A very rich excitation spectrum was observed in the field-induced quantum paramagnetic phase. The obtained data are compared with results of recent numerical calculations, strongly suggesting a very unconventional multiparticle character of the spin dynamics in α-$RuCl_3$. The frequency-field diagram of the lowest-energy ESR mode is found consistent with the behavior of the field-induced energy gap, revealed by thermodynamic measurements.

This work was supported by DFG (project ZV 6/2-2).

TT 72.24 Wed 15:00 Poster B

RIXS on the j = 1/2 double perovskite Ba_2CeIrO_6 — •Chin Chyi Loo[1], Alessandro Revelli[1], Anna Efimenko[2], Marco Moretti Sala[2], Giulio Monaco[3], Thomas Koethe[1], Petra Becker[4], Ladislav Bohatý[4], Paul H. M. van Loosdrecht[1], and Markus Grüninger[1] — [1]II, Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, D-50937 Köln, Germany — [2]ESRF-The European Synchrotron, 71 Avenue des Martyrs, 38000 Grenoble, France — [3]Physics Department, University of Trento, Via Sommarive 14, 38123 Povo (TN), Italy — [4]Institute of Geology and Mineralogy, Section Crystallography, University of Cologne, Köln, Germany

Spin-orbit-entangled j=1/2 iridates were predicted to show novel quantum states of matter. However, real materials deviate from a pure j=1/2 state due to, e.g., a non-cubic crystal field. Resonant inelastic x-ray scattering (RIXS) at the Ir L edge is ideally suited to study the j = 1/2 character and to determine the non-cubic crystal field. In the double perovskite Ba_2CeIrO_6, the Ir ions form an fcc lattice and the local symmetry is close to cubic, with a monoclinic angle β = 89,986° [1]. The RIXS spectra establish the local j =1/2 ground state as well as a crystal-field splitting of the excited j = 3/2 state of less than 100 meV, the smallest observed thus far in iridates.

[1] M. Wakeshima, D. Harada, Y. Hinatsu, *J. Mater. Chem.* **10** (2000) 419.

TT 72.25 Wed 15:00 Poster B

RIXS on $5d^5$ $Ba_3CeIr_2O_9$ and $Ba_3Ti_xIr_{3-x}O_9$ — •Alessandro Revelli[1], Marco Moretti Sala[2], Giulio Monaco[3], Petra Becker[4], Ladislav Bohatý[4], Thomas Koethe[1], Tobias Fröhlich[1], Maria Hermanns[5], Paul H.M. van Loosdrecht[1], Jeroen van den Brink[6], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]ESRF, Grenoble — [3]Dipart. di Fisica, Universita di Trento — [4]Abt. Kristallographie, Institut für Geologie & Mineralogie, Universität zu Köln — [5]Institut für Theoretische Physik, Universität zu Köln — [6]IFW, Dresden

Spin-orbit entangled $j = 1/2$ Mott insulators set the stage for fascinating novel quantum states of matter. In corner-sharing geometry of the IrO_6 octahedra, one finds strong Heisenberg exchange between $j = 1/2$ moments, while edge-sharing geometry features bond-directional Kitaev exchange. However, the case of face-sharing octahedra has hardly been explored. Using resonant inelastic x-ray scattering (RIXS), we study the $5d^5$ compound $Ba_3CeIr_2O_9$ with face-sharing octahedra forming triangular layers. Both hopping and spin-orbit coupling are large. The RIXS data reveal the first and exceptionally clean realization of the quasi-molecular-orbital scenario that was debated extensively (but refuted) for Na_2IrO_3. The ground state shows a total $j = 0$ singlet predominantly built from $j = 1/2$ moments with the corresponding triplet excitation lying at an extraordinarily large energy. For M=Ti, the compound $Ba_3Ti_xIr_{3-x}O_9$ exists for different values of x and shows Ti/Ir site disorder. In RIXS we observe a coexistence of $j = 1/2$ moments and quasi-molecular singlets.

TT 72.26 Wed 15:00 Poster B

Influence of the mixed-valence state of Ir on the structural properties of $Ba_3MIr_2O_9$ (M= In, Lu, Mg) — •Georg Bothmann[1], Tusharkanti Dey[1], Anatoliy Senyshyn[2], Philipp Gegenwart[1], and Alexander Tsirlin[1] — [1]Lehrstuhl für Experimentalphysik VI, Zentrum für Elektronische Korrelationen und Magnetismus, Univesität Augsburg, Deutschland — [2]FRM-II, Technische Universität München, Deutschland

Mixed-valence iridates are a new platform for frustrated magnetism as shown in [1]. It is suspected that the mixed-valence state may evolve with temperature. Here we used x-ray diffraction (using radiation from a synchrotron) and neutron powder diffraction in a broad temperature range to compare the mixed-valence In and Lu compounds of the $Ba_3MIr_2O_9$ family of hexagonal perovskites with the integer-valence Mg compound of the same family.

The temperature dependence of the structural parameters, including lattice constants and Ir-Ir distances, will be reported. Additionally the instability toward a monoclinic distortion will be discussed.

[1] T. Dey, Phys. Rev. **B 96** (2017) 174411

TT 72.27 Wed 15:00 Poster B

Honeycomb Kitaev iridate and rhodate thin films — •Maximilian Uhl[1], Sebastian Esser[1], Vladimir Roddatis[2], Vasily Moshnyaga[3], and Philipp Gegenwart[1] — [1]Experimentalphysik VI, Universität Augsburg, 86159 Augsburg, Germany — [2]Institut für Materialphysik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [3]1. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Recently materials realizing the honeycomb Kitaev exchange attracted considerable attention (for a review see [1]). Li-based heavy transition metal oxides Li_2IrO_3 [2] and Li_2RhO_3 [3] are prototype systems in this class. For the latter material, up to now only polycrystals are available which display a spin-glassy ground state. Epitaxial thin films are thus of particular interest, as they could reveal the true ground state and its dependence on strain. We utilize the metal-organic aerosol deposition (MAD) technique [4] and report the successful growth of thin films of both materials, as well as their structural and magnetic characterization. This work is supported by the German Science Foundation through SPP 1666 and TRR 80.

[1] S.M. Winter *et al.*, J. Phys.: Condens. Matter **29** (2017) 493002.
[2] Y. Singh *et al.*, Phys. Rev. Lett. **108**, (2012) 127203.
[3] P. Khuntia *et al.*, Phys. Rev. B **96**, (2017) 094432.
[4] M. Jungbauer *et al.*, Appl. Phys. Lett. **105**, 251603 (2014)

TT 72.28 Wed 15:00 Poster B

Magnetization and specific heat of Cr-doped α-$RuCl_3$ — •Mohammad Hossein Haghighi[1,2], Gaël Bastien[1], Anja U. B. Wolter[1], Maria Roslova[3], Anna Isaeva[3], Thomas Doert[3], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Department of Chemistry and Food Chemistry, TU Dresden, 01069 Dresden, Germany

α-$RuCl_3$ crystallizes in a layered honeycomb structure and has been

proposed as a candidate to realize a fractionalized Kitaev model with strongly frustrated, bond-dependent, anisotropic interactions between Ru^{3+} magnetic moments ($j = \frac{1}{2}$). By introducing Cr as dopant to this Mott insulator ($S = \frac{3}{2}$ at the Ru sites), one can investigate changes of the long-range order in the ground state of α-$RuCl_3$ as well as of the anisotropic Kitaev interactions and field-induced effects which appear upon doping. We report on susceptibility and specific heat measurements of $Ru_{1-x}Cr_xCl_3$, probing the effect of different doping levels on the magnetic and thermodynamic properties on single crystals for the full range $0 \leqslant x \leqslant 1$.

TT 72.29 Wed 15:00 Poster B

Influence of Negative Charge Carrier Doping in $Nd_2Ir_2O_7$ on Structure and Magnetic Behavior — •Sebastian Selter[1], Ameya Prabhune[1], Anja U. B. Wolter[1], Saicharan Aswartham[1], and Bernd Buechner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany

We present the influence of negative charge doping on the structure and magnetic behavior of rare earth iridate pyrochlore $(Nd_{1-x}Ca_x)_2Ir_2O_7$ and $Nd_2(Ir_{1-x}Ga_x)_2O_7$ with x = 0..0.2.

$Nd_2Ir_2O_7$ possesses a hyperkagome lattice of corner-shared IrO_6 and edge-shared NdO_8 units. This gives rise to magnetic frustration and an all-in-all-out (AIAO) ordering is observed at low temperatures. Further, this material undergoes a metal-to-insulator transition (MIT) at around 30 K. MIT is a phenomenon observed in all rare earth iridate pyrochlores, except for $Pr_2Ir_2O_7$ which is metallic down to lowest temperatures. However, $Nd_2Ir_2O_7$ shows the lowest MIT temperature compared to other rare earth iridate pyrochlores and therefore is nearest to a possible quantum MIT. Furthermore, band structure calculations suggest that a Weyl semimetallic state with broken time reversal symmetry may be stabilized by the AIAO order in $Nd_2Ir_2O_7$. Recently, a dependency of the magnetic behavior and the MIT on the oxygen position in the rare earth iridate pyrochlores was proposed from theoretical side. A strong coupling of the physical properties to the crystal structure in $Nd_2Ir_2O_7$ can be concluded.

TT 72.30 Wed 15:00 Poster B

Spin-orbital superexchange and spin-orbit coupling — •Pascal Strobel and Maria Daghofer — Universität Stuttgart Institut für funktionelle Materie und Quantentechnologie, 70569 Stuttgart, Deutschland

In recent years t_{2g} spin-orbital models on a honeycomb lattice have been studied with either strong or no spin-orbit coupling. In both cases the ground state was investigated in dependency of Hund's coupling as well as the ratio of superexchange and direct exchange. With nonexistent spin-orbit coupling one obtains exotic phases like dimer states, while in the case of strong SOC one can find a Kitaev spin liquid phase.

However the phase diagram for intermediate spin-orbit coupling is yet relatively unknown. While [1] proposed a phase diagramm for the superexchange limit, we still need to explore the direct exchange limit as well as the influence of crystal deformation.

In this work we investigate the influence of moderate SOC, Hund's coupling, as well as the ratio of superexchange and direct exchange on several ordered states, which might be candidates for a ground state at some point in the phase diagram. The analytical results of the superexchange limit can then be compared to the numerical ones of [1]. Of particular interest in this work is whether we can find exotic phases like a spin liquid even without strong spin orbit coupling.

[1] A. Koga, S. Nakauchi, J. Nasu, arXiv:1705.09659

TT 72.31 Wed 15:00 Poster B

Excitation spectra of hard-core bosons in strongly spin-orbit coupled Van Vleck-type d^4 Mott insulators — •Friedemann Aust and Maria Daghofer — Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

In spin-orbit coupled Mott insulators with a t_{2g}^4 electron configuration, the interplay of spin-orbit coupling, Hund's rule and Kugel-Khomskii superexchange can be mapped to an effective singlet-triplet model [1]. For honeycomb or triangular lattice geometries, as found in e.g. delafossite, interactions have a bond selective structure reminiscent of the Kitaev honeycomb model. However, the local degrees of freedom are not given by a spin but by a singlet ground state and low-lying triplet excitations, which can be seen as hard-core bosons.

We discuss this model in the presence of direct exchange in addition to inter-orbital superexchange. Going beyond analytic considerations, we use cluster perturbation theory (CPT) and the variational cluster approximation (VCA), where the hard-core constraint can be taken into account, to obtain magnetic excitation spectra in regimes dominated by Heisenberg, Kitaev, or less symmetric couplings.

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

TT 72.32 Wed 15:00 Poster B

Variational Cluster Approximation for d^4 systems — •Teresa Feldmaier and Maria Daghofer — Institut für funktionelle Materie und Quantentechnologien, Universität Stuttgart, Deutschland

We use the variational cluster approximation to investigate the phase diagram and one-particle spectral density of multi-band Hubbard models with strong spin-orbit coupling. The approach includes quantum fluctuations on a small cluster exactly, where frustration can be treated without additional complications, and long-range order on a mean-field level.

We will in particular investigate systems with four electrons per site, where a local singlet competes with itinerant triplet excitations that can condense into magnetic order. Further, the competition of Hund's rule and spin-orbit coupling with crystal-field splitting leads to various phases which are realized in some iridium and ruthenium compounds.

TT 72.33 Wed 15:00 Poster B

The Kitaev-Heisenberg bilayer: a series expansion analysis — •Erik Wagner and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Braunschweig, Germany

We study two layers of a honeycomb Kitaev spin-model, coupled by additional interlayer Heisenberg exchange J to form a bilayer. Focusing on the limit of strong interlayer coupling, we present results of zero temperature series expansion calculations, based on the flow equation method. Allowing for anisotropic intralayer exchange $J_{x,y,z}$ and two types of layer stackings, we calculate the evolution of the ground state energy and the dispersion of the elementary triplon excitations in powers of $J_{x,y,z}$ up 9th order. The stability of the dimer phase with respect to triplon gap closure will be analyzed, based on Padé approximants. Additionally we will compare our results with bond-operator theory using the Holstein-Primakoff approximation.

TT 72.34 Wed 15:00 Poster B

Coexistence of phase transitions and hysteresis near the onset of Bose-Einstein condensation — Michael Maennel[4] and •Klaus Morawetz[1,2,3] — [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]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Informatik DV,Petersstr. 14,04109 Leipzig, Germany

Multiple phases occurring in a Bose gas with finite-range interaction are investigated [2]. In the vicinity of the onset of Bose-Einstein condensation (BEC), the chemical potential and the pressure show a van der Waals-like behavior indicating a first-order phase transition for weak interactions like Hartree-Fock or Popov approximation. However, for strong interactions there remains a multivalued region for the T-matrix approximation even after the Maxwell construction, which is interpreted as a density hysteresis [1]. This unified treatment of normal and condensed phases becomes possible due to the recently found scheme to eliminate self-interactions in the T-matrix approximation, which allows one to calculate properties below and above the critical temperature [3,4].

[1] Phys. Rev. A 87 (2013) 053617
[2] New J. Phys. 12 (2010) 033013
[3] J. Stat. Phys. 143 (2011) 482
[4] Phys. Rev. B 84 (2011) 094529

TT 72.35 Wed 15:00 Poster B

Quantum transport and response with spin-orbit coupling in magnetic fields — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Electronic transport in spin-polarized systems with impurity interactions and spin-dependent meanfields is discussed. The coupled quantum kinetic equations for the scalar and spin components for SU(2) are derived with special consideration of spin-orbit coupling and magnetic

fields. Linearizing, the RPA spin and density dynamical responses to electric fields (polarized light) are presented for arbitrary magnetic fields, Several known effects are described: spin-Hall, anomalous Hall and optical Hall effect, spin-heat coupling. New transport coefficients occur due to the selfconsistent precession direction. Clarifying the relative importance of meanfield and scattering correlations, new modes due to magnetic fields and spin-orbit coupling are found and terahertz out-of plane resonances are predicted.

[1] Europhysics Letters, 104 (2013) 27005
[2] Phys. Rev. **B 92** (2015) 245425
[3] errata Phys. Rev. **B 93** (2016) 239904(E)
[4] Phys. Rev. **B 92** (2015) 245426
[5] Phys. Rev. **B 94** (2016) 165415

TT 72.36 Wed 15:00 Poster B

Magnetic ground state of the cubic perovskite $Ba_3NiNb_2O_9$ — •Sh. Yamamoto[1], G. Aslan Cansever[2], T. Gottschall[1], M. Uhlarz[1], C. G. F. Blum[2], A. Wolter-Giraud[2], S. Aswartham[2], S. Wurmehl[2], T. Herrmannsdörfer[1], S. Seiro[2], B. Büchner[2], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]IFW-Dresden, Germany

We investigated the magnetic spin-1 perovskite $Ba_3NiNb_2O_9$ by means of complex ac susceptibility measurements at extreme sample conditions. $Ba_3NiNb_2O_9$ with cubic perovskite structure (Pm-3m) has a random occupation of Nb(66 %)/Ni(33 %) at the center of the cubic perovskite unit cell. Different from the isostoichiometric sister compound, $Ba_3NiNb_2O_9$ with P-3m1 structure which shows both uud-spin configuration and multiferroicity, the magnetic properties of the investigated system have not been studied below 2 K yet. For our single crystals, we observe a spin freezing transition at around 0.7 K. Furthermore, the peak of χ' is suppressed by applying an external dc field of 200 mT and χ" shows a sudden onset near the freezing temperature.

TT 72.37 Wed 15:00 Poster B

Magnetism of the effective spin-1/2 chain compound $Cs_2CoCl_{4-x}Br_x$ — •Severin Kopatz[1], Oliver Breunig[1], Daniel Brüning[1], Ladislav Bohatý[2], Petra Becker[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Kristallographie, Universität zu Köln, Germany

Cs_2CoCl_4 contains $CoCl_4$ tetrahedra, which form one-dimensional chains along the crystallographic b axis. The orbital groundstate of Co^{2+} ($3d^7$, S=3/2) is split by a crystal field anisotropy D into two doublets and an easy-plane anisotropy of the magnetization is established and a description as an effective spin-1/2 XXZ chain arises. By considering thermal as well as virtual excitations of higher crystal field states, we find that the spin chain is in the XY-limit with an anisotropy $J_z/J_\perp \approx 0.12$ substantially smaller than previously believed [1]. Below 300 mK antiferromagnetic order evolves and several new phases are induced in magnetic fields [2]. Cs_2CoCl_4 is isostructual to $Cs_2CuCl_{4-x}Br_x$ where site-selective doping was used to characterize quasi 2D quantum antiferromagnets with different degrees of magnetic frustration [3]. Here, we present specific-heat studies on bromine doped $Cs_2CoCl_{4-x}Br_x$ for different x. Funded by the DFG via CRC 1238 Projects A02 and B01.

[1] O. Breunig *et al.*, Phys. Rev. Lett. **111**, 187202 (2013)
[2] O. Breunig *et al.*, Phys. Rev. B **91**, 024423 (2015)
[3] P. T. Cong *et al.*, Phys. Rev. B **83**, 064425(2011)

TT 72.38 Wed 15:00 Poster B

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

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

TT 72.39 Wed 15:00 Poster B

Frustrated magnetism in the Eu-based intermetallic system $EuIr_2P_2$ — •Diego Gaspar Franco and Christoph Geibel — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Deutschland

Frustration in magnetic systems is a topic of strong current interest, since it can result in unusual ground states. The majority of studies on frustration in magnetic systems have been performed on insulating spin systems, while frustrated metallic systems remain largely unexplored. Interesting effects may be expected for the later case from the interplay between itinerant electrons and frustrated magnetic degrees of freedom.

$EuIr_2P_2$ was in an early work proposed to order ferromagnetically based on the positive Curie-Weiss temperature, estimated from the high-temperature susceptibility [1]. However, our recent measurements conclusively show that it orders antiferromagnetically at $T_{N1} = 5$ K, in spite of the positive Curie-Weiss temperature. Besides there is a second magnetic transition at $T_{N2} = 3$ K. The size of the specific heat anomaly at TN1 is small compared to other S=7/2 systems. Furthermore we observe a large tail in the specific heat above T_{N1} indicative of strong magnetic fluctuations. These effects point to a magnetic structure with a significant degree of frustration due to different competing magnetic interactions.

[1] C. Lux, et al., J. Alloys and Comp. 200 (1993) 135

TT 72.40 Wed 15:00 Poster B

Magnetic properties of single crystalline clinoatacamite — •Jan Lennart Winter[1], Leonie Heinze[1], Dirk Menzel[1], Stefan Süllow[1], Pascal Puphal[2], Cornelius Krellner[2], Manfred Reehuis[3], and Ralf Feyerherm[3] — [1]Institute for Condensed matter pyshics, TU Braunschweig, Germany — [2]Physikalisches Institut, Goehte-Universität Frankfurt, Germany — [3]HZB Materialien und Energie, Berlin, Germany

In recent years, clinoatacamite $Cu_2Cl(OH)_3$ has been studied in the context of geometric magnetic frustration in a quantum spin system. Only, previous research has been performed on synthetic powder samples, raising questions about sample quality and (residual) magnetic anisotropy [1,2]. Here, for the first time, we report a detailed investigation on single crystalline clinoatacamite by presenting studies of the magnetic susceptibility/magnetization and by means of neutron scattering. Based on these measurements we derive the magnetic phase diagram, revealing a complex magnetic behavior with a multitude of different (field induced) phases. We discuss our results with respect to the role of magnetic frustration on the properties of clinoatacamite.

[1] Zheng X.G., Kawae T., Kashitani Y., Li C. S., Tateiwa N., Takeda K., Yamada H., Xu C. N., and Ren Y., Phys. Rev. B **71** 052409 (2005)
[2] H. Morodomi, K. Ienaga, Y. Inagaki, T. Kawae, M. Hagiwara, and X. G. Zheng, J. Phys.: Conf. Ser. **200**, 032047 (2010).

TT 72.41 Wed 15:00 Poster B

Crystal growth in aqueous solution of Cs_2CuCl_4 and $Cs_2ZnCl_{4-x}Br_x$ using the evaporation method — •Susanna Rongstock, Nazia Kaya, Franz Ritter, and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt, D-60438 Frankfurt

In recent years, Cs_2CuCl_4 and Cs_2CuBr_4 have been extensively investigated both experimentally and theoretically, as they represent model systems for quasi-2D triangular-lattice quantum antiferromagnets. They attracted much attention due to their unconventional magnetic properties resulting from the interplay of strong quantum fluctuations in reduced dimensions, geometrical frustration and effects of spin-lattice interactions close to the field-induced quantum critical point (QCP). In triangular antiferromagnetis the heat capacity is a capable measurement technique to study the magnetism. To obtain the magnetic contribution, it is necessary to subtract the phononic contribution, by measuring the heat capacity of $Cs_2ZnCl_{4-x}Br_x$. Due to the high number of possible phases different preliminary phases are built during the crystal growth of the Cs_2CuCl_4-crystal. Hence to develop

a solution which creates a preliminary phase free growing of the crystals is of interest. In this contribution we will present the preliminary phase development of the Cs_2CuCl_4-crystal at 30°C in dependence to the pH-value and the resulting modification of the solution as well as the heat capacity measurements of the Cs_2ZnCl_4-crystal. Additionally we will present the crystal growth method and the structural analysis of both systems.

TT 72.42 Wed 15:00 Poster B

Kagome systems - The search for new quantum spin liquid candidates — •Katharina M. Zoch, Pascal Puphal, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main

Kagome systems serve as the ideal candidates to obtain a realization of a quantum spin liquid (QSL), a class of matter where the spins do strongly fluctuate down to lowest temperatures thus preventing order. Two-dimensional Cu-based quantum spin systems are very promising to understand their physics. Hence high-quality single crystals with minimal amount of disorder are essential to investigate the intrinsic properties of QSLs. Two closely related systems realizing a kagome lattice are $YCu_3(OH)_6Cl_3$ and $Y_3Cu_9(OH)_{19}Cl_8$ which both show strong frustration. However, while having a similar structure the magnetic ground state is different [1]. This poster addresses the synthesis and properties of these and other kagome compounds analyzed with diffraction, VSM and specific heat.
[1] P.Puphal et al. J. Mater. Chem. C 5 (2017) 2629

TT 72.43 Wed 15:00 Poster B

Exploring the magnetic phase diagram of a metal-organic S = 1 triangular spin system. — •Sumanta Chattopadhyay[1], Thomas Herrmannsdörfer[1], Sudipta Kanungo[3], Sergei Zvyagin[1], Marc Uhlarz[1], Kaustuv Manna[4], Walter Schnelle[4], Jhuma Sannigrahi[5], Joachim Wosnitza[1], and Ranjan Patra[2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Panjab University, Chandigarh, India — [3]Department of Physics, IIEST, Howrah, India — [4]Max Planck Institute for Chemical Physics of Solids Dresden, Germany — [5]ISIS Facility, Rutherford Appleton Laboratory, Didcot, OX11 0QX, U.K.

We report on magnetic properties of a novel metal-organic S = 1 antiferromagnetic triangular spin compound with isolated Ni2+ triangles entitled as BHAP-Ni3. Specific heat measurements reflect an onset of magnetic correlation at low temperatures without any long-range order down to 300 mK, indicating the presence of an unusual magnetic ground state. ESR measurements performed at 1.5 K advocate this ground state to be a gapped one. Field-dependent magnetization measured on the single crystal shows anisotropic behavior with field applied parallel and perpendicular to the triangle plane. However, a clear plateau-like region is seen in both directions above 8 T which corresponds to half of the fully polarized value of Ni2+ moment. The presence of such half-magnetization plateau is quite unusual in the family of triangular magnets. High-field magnetization measurements using pulsed magnet show another field-induced plateau above 30 T corresponding to the fully polarized state of S = 1 triangles.

TT 72.44 Wed 15:00 Poster B

Magnetic and thermodynamic characterization of single crystals of $La_2MM'O_6$ (M = Mg, Zn, Co and M'=Ru, Ir) — •Randirley Beltrán[1], Gaël Bastien[1], Sebastian Gass[1], Anja U.B. Wolter[1], Ryan Morrow[1], Michael Vogl[1], Mihai Sturza[1], Sabine Wurmehl[1], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW-Dresden, Germany — [2]TU Dresden, Germany

In compounds with 4*d* and 5*d* transition metal oxides, among them the double perovskites $A_2MM'O_6$, strong magnetic frustration can be expected due to different origins: competing magnetic interactions and strong spin-orbit coupling. The arrangement of MO_6 and $M'O_6$ corner-sharing octahedra provide two (magnetic) sub-lattices that results in a variety of magnetic properties related with the competing exchange interactions. For nonmagnetic M ions, the fcc lattice structure of the magnetic M' ions has been theoretically proposed for hosting Kitaev interactions. In this work we probe the magnetic and thermodynamic properties of the double perovskite single crystals $La_2MM'O_6$ with M = Mg, Zn, Co and M' = Ir, Ru. We study the magnetic susceptibility and specific heat as function of different parameters, such as temperatue, magnetic field and orientation. Additionally, we use the application of hydrostatic pressure in the mixed 3*d*-5*d* compound La_2CoIrO_6 to tune the magnetic ground state of this system, because pressure leads to changes of the magnetic exchange couplings.

TT 72.45 Wed 15:00 Poster B

A SUSY-connection between classical spin spirals and free fermions — •Jan Attig[1], Krishanu Roy Chowdhury[2], Michael Lawler[2], and Simon Trebst[1] — [1]University of Cologne — [2]Binghamton University / Cornell University

The formation of coplanar spin spirals is a common motif in the magnetic ordering of many frustrated magnets. For classical antiferromagnets, geometric frustration can lead to a massively degenerate ground state manifold of spirals whose propagation vectors can be described, depending on the lattice geometry, by points (triangular), lines (fcc), surfaces (frustrated diamond) or completely flat bands (pyrochlore). Here we demonstrate an exact mathematical correspondence of these spiral manifolds of classical antiferromagnets with the Fermi surfaces of free-fermion band structures. We provide an explicit lattice construction relating the frustrated spin model to a corresponding free-fermion tight-binding model. We discuss implications of topological band structures in the fermionic system to the corresponding classical spin system and further expand this mapping by employing concepts from super symmetric quantum mechanics to extent the present work for quantum spin systems.

TT 72.46 Wed 15:00 Poster B

Frustrated magnetism in the Kondo lattice on a zig-zag ladder — •Lena Woelk, Matthias Peschke, and Michael Potthoff — I. Institut für Theoretische Physik

We study the magnetic phase diagram of the Kondo lattice model on the half-filled zig-zag chain as a function of the exchange coupling J and the hopping amplitudes t, t' in both the classical-spin and the quantum-spin case using a quantum-classical hybrid approach and the density matrix renormalization group (DMRG).

The competition between RKKY, superexchange, and the geometric frustration yields a complex phase diagram: We find multiple spiral phases, an antiferromagnetic phase as well as a small ferromagnetic region. In both the classical- and the quantum-spin case, we also find an extended region with a dimerized ground state, which consists of alternating ferro- and antiferromagnetic spin correlations along the rungs of the ladder. This alleviates the geometric frustration and is a precursor of quasi-long-range magnetic order.

The strong coupling limit $J \gg t$ can be described with perturbation theory. The spin correlations in both the classical- and the quantum-spin case are captured by an effective classical Heisenberg model. In the weak coupling limit one expects the spin correlations to be governed by RKKY theory, this is checked against our results.

TT 72.47 Wed 15:00 Poster B

Spin liquid behaviour in the disordered double perovskite $BaTi_{1/2}Mn_{1/2}O_3$ — M. R. Cantarino[3], •R. Sarkar[1], R.S. De Freitas[3], H. Luetkens[2], C. Baines[2], R. Lora-Serrano[4], R.P. Amaral[4], S. Brauninger[1], V. Grinenko[1], H.-H. Klauss[1], E. C. Andrade[5], and F. A. Garcia[3] — [1]Institute of Solid State and Materials Physics, TU Dresden, D-01062 Dresden, Germany — [2]Laboratory for Muon-Spin Spectroscopy, PSI, 5232 Villigen PSI, Switzerland — [3]IFUSP, Univ. de São Paulo, 05508-090, São Paulo-SP, Brazil — [4]Univ. Fed. de Uberândia, Instituto de Física, 38400-902, Uberlrândia-MG, Brazil — [5]Instituto de Física de São Carlos, Universidade de São Paulo, C.P. 369, São Carlos, SP, 13560-970, Brazil.

We present bulk susceptibility, heat- capacity and μSR experiments of the disordered double perovskite $BaTi_{1/2}Mn_{1/2}O_3$. Heat capacity investigations down to $T = 0.1$ K and in magnetic fields up to 9 T exhibits a field dependent broad anomaly around $T = 3 - 7$ K, and no long range ordering. Macroscopic magnetic properties, measured down to $T = 0.5$ K, do not display as well any sign for phase transition. The zero field (ZF) and longitudinal field dependence μ^+ time spectra shows the absence of any static magnetism down to 20 mK. However, ZF μ^+ relaxation rate λ display a steep increase in the T interval $1.5 < T < 10$ K and levels up as a constant value indicating a correlated fluctuating ground state. Our experimental data and analysis suggests that $BaTi_{1/2}Mn_{1/2}O_3$ is a suitable candidate to host a spin liquid ground state.

TT 72.48 Wed 15:00 Poster B

Magnetisation of lithium nitridometalates and magnetite nanoparticles upon electrochemical cycling — •Elisa Thauer[1], Michael Richter[1], Manuel Fix[2], Anton Jesche[2], and Rüdiger Klingeler[1,3] — [1]Kirchhoff Institute for Physics,, Heidelberg Univer-

sity, 69120 Heidelberg, Germany — [2]EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany — [3]Center for Advanced Materials, 69120 Heidelberg University, Heidelberg, Germany

We report *in-situ* and *ex-situ* studies of the magnetic properties of lithium nitridometalates and magnetite nanoparticles upon electrochemical treatment. In $Li_2Li_{1-x}M_xN$ with M = Fe or Ni, the effect of delithiation, i.e. electrochemical change of the valence of the transition metal ions, on the magnetic properties was studied by means of *ex-situ* SQUID magnetometry. In case of $Li_{2.7}Fe_{0.3}N$ the initial hard magnetic ground state is suppressed by delithiation. In addition, a re-usable *in-situ* electrochemical cell was designed for operation in the SQUID magnetometer. Studies on Fe_3O_4 nanoparticles prove significant changes of the magnetisation upon electrochemical lithiation and delithiation.

TT 72.49 Wed 15:00 Poster B

Electron spin resonance studies on the frustrated tripod-Kagome material $Mg_2Gd_3Sb_3O_{14}$ — •Christoph Wellm[1,2], Julian Zeisner[1,2], Mihai Sturza[2], 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 consisting of a modified pyrochlore lattice with nonmagnetic interlayers have been suggested as an interesting target of experimental investigation. Since the Kagome planes in these compounds are well separated from each other, two-dimensional magnetic behavior is expected. 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 classical Heisenberg magnet, in which the magnetic Gd^{3+} centres are devoid of spin-orbit coupling. Measurements were conducted over a frequency range of 70-420 GHz and temperatures ranging from 3-50 K. The Gaussian shape of the spectra is consistent with a model where dipolar spin-spin interaction plays a dominant role, while the growing asymmetry of the lineshape upon decrease of temperature signifies an effective internal field building up, an indication of increasing short-range spin-spin-correlations. 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 72.50 Wed 15:00 Poster B

Probing the Kitaev-Heisenberg material α-$RuCl_3$ via field-dependent microwave absorption — •Christoph Wellm[1,2], Julian Zeisner[1,2], Alexey Alfonsov[2], Anja Wolter[2], Maria Roslova[3], Anna Isaeva[3], Thomas Doert[3], Matthias Vojta[4], 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 — [3]Fachrichtung Chemie und Lebensmittelchemie, TU Dresden, D-01062 — [4]Institut für Theoretische Physik, TU Dresden, D-01062

Topologically ordered states of matter have recently gained much attention due to their novel physical properties, the signatures of which can be experimentally probed. A prime example is the spin liquid realized in the Kitaev honeycomb lattice compass model, where fractionalization of particles leads to broad continuum-like features in the magnetic response. We will present the high-field microwave absorption results on the Mott-Hubbard-insulating material α-$RuCl_3$ which is, due to its structure and strong spin-orbit coupling, a promising candidate for the realization of Kitaev physics. Measurements on a single-crystal were conducted over a frequency range of ν = 70-660 GHz at temperatures ranging from 3-30 K. Strikingly, in addition to previously observed conventional gapped magnon modes, we find a highly unusual broad continuum characteristic of fractionalization which extends to energies below the lowest sharp mode and to temperatures significantly higher than the ordering temperature.

TT 72.51 Wed 15:00 Poster B

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 – in contrast to electronic nodal-line semimetals – 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 explore the stability of these highly degenerate bands in the presence of additional interactions.

TT 72.52 Wed 15:00 Poster B

Thermodynamics of Kitaev magnets — •Bahareh Ghannad and Simon Trebst — University Of Cologne

Kitaev spin models are prototypical frustrated magnets that exhibit low-temperature spin liquid physics. This is true independent of whether the constituent spin degrees of freedom are classical O(3) Heisenberg spins or quantum SU(2) spin-1/2 spins. Here, we will discuss thermodynamic signatures of a variety of Kitaev spin models for different lattice geometries and contrast them for the classical and quantum case. Of particular interest are two-spin and four-spin correlation functions that reveal the nature of the spin liquid regime. We report results from both analytical approaches and large-scale numerical Monte Carlo simulations.

TT 72.53 Wed 15:00 Poster B

Majorana zero modes in the Kitaev honeycomb model — •Daniel Otten, Ananda Roy, and Fabian Hassler — JARA- Institute for Quantum Information, RWTH Aachen University, D- 52056 Aachen, Germany

Kitaev's honeycomb model is a quantum spin liquid that gives rise to an emergent static $\mathbb{Z}_2$ gauge field coupled to Majorana fermions. In presence of an applied external magnetic field, the system is, dependent on the choice of interaction strength, in a gapped, non-abelian phase. In this phase, the vortex excitations of the emergent $\mathbb{Z}_2$ gauge field have Majorana zero modes bound to them. We investigate the properties of these Majorana zero modes. Using Jordan-Wigner transformation, we map the effective Hamiltonian to that of a chiral p-wave superconductor. We analytically calculate the wave functions of the Majorana zero modes in the continuum limit and the energy splitting that arises when two vortices approach each other. Furthermore, to understand the implications of the zero modes in the original spin model, we calculate the spin-spin correlator and the dynamical structure factor in presence of these vortices. These results are relevant for possible experimental observations and characterizations of the Majorana zero modes in systems that are dominated by the interaction of the Kitaev honeycomb model.

TT 72.54 Wed 15:00 Poster B

Disorder and Correlations in 3D Kitaev Models — •Kevin O'Brien[1], Maria Hermanns[2], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]Department of Physics, University of Gothenburg, SE 412 96 Gothenburg, Sweden

Kitaev's honeycomb model is an example of an exactly solvable interacting spin-1/2 model with exchange frustration, providing theorists with the rare opportunity to study the physics of spin fractionalization in its quantum spin liquid groundstate with full analytical control. In their groundstate, the spin-1/2 moments fractionalize into a static, gapped Z2 gauge field as well as into fermionic excitations which may be gapped or gapless. The nature of the gapless phase depends both on the dimension of the underlying lattice and on the projective nature of certain discrete symmetries. The resulting nodal structure of the fermionic excitations ranges from nodal lines to Dirac nodes in 2D and from full Fermi surfaces to nodal lines and even Dirac/Weyl nodes in 3D. While spin-spin correlations in the Kitaev model are short-ranged in general, there are certain long-ranged four-spin correlations which are sensitive to the nodal structure of the fermionic excitations. In this work we investigate the nature in which these correlation functions are determined by the gapless fermionic excitations. Additionally, we examine the role which disordering of the Z2 gauge field plays in altering these correlations. Finally, we explore the connection between the gauge-disordered Kitaev spin liquid and finite temperature calculations.

TT 72.55 Wed 15:00 Poster B

Thermodynamics of a gauge-frustrated Kitaev spin liquid — •Tim Eschmann[1], Petr A. Mishchenko[2], Yasuyuki Kato[2], Yukitoshi Motome[2], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne — [2]Department of Applied Physics,

University of Tokyo

Kitaev spin models are prototypical frustrated magnets in which the spin degrees of freedom fractionalize and the emergent spin liquid ground state can be described in terms of Majorana fermions coupled to a $\mathbb{Z}_2$ gauge field. It is by now well known that varying the underlying lattice structure, these spin liquids can be described as Majorana metals with a topological band structure that includes the formation of Dirac or Weyl nodes, nodal lines, or entire Majorana Fermi surfaces. Here our focus will be on the physics of the concurrently forming $\mathbb{Z}_2$ gauge field. Typically, this (static) gauge field orders at low temperatures, with a finite-temperature (inverted Ising) transition occurring in three-dimensional settings. We will discuss an explicit example that goes beyond this paradigmatic situation where the gauge field is found to be subject to geometric frustration, the thermal ordering transition is suppressed, and a residual zero-temperature entropy arises. We discuss a variety of thermodynamic signatures of this physics obtained from large-scale, sign-free quantum Monte Carlo simulations of the underlying Kitaev model.

TT 72.56 Wed 15:00 Poster B

Splitting of the magnetic monopole excitation energy in spin ice — •Jacob Hornung[1,2], Tino Gottschall[1], Mathis Antlauf[3], Lars Opherden[1,2], Thomas Herrmannsdörfer[1], and Jochen Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik,TU Dresden, Germany — [3]Institut für Anorganische Chemie, TU Bergakademie Freiberg, Germany

We present a new model for the magnetic monopole excitation process in spin-ice systems. In this approach, we include the interactions of the electric dipole moments which where priviously predicted to emerge in consequence of the formation of magnetic monopoles. By that, the model allows for describing the temperature-dependent spin relaxation time. We compare this relaxation-time behavior with data received for the three spin-ice systems $Dy_2Sn_2O_7$, $Dy_2Ti_2O_7$ and $Dy_2Ge_2O_7$. By that we also determine the magnitude of their electrical dipole interactions.

TT 72.57 Wed 15:00 Poster B

ESR on the $S = 1/2$ triangular magnet $NaYbS_2$ — •Jörg Sichelschmidt[1], Michael Baenitz[1], Philipp Schlender[2], and Thomas Doert[2] — [1]MPI for Chemical Physics of Solids, Dresden — [2]TU Dresden, Dept. of Chemistry and Food Chemistry

$NaYbS_2$ is one of a few spin 1/2 triangular quantum magnets for which a quantum spin-liquid picture is invoked. It has a delafossite structure with a planar triangular spin arrangement which leads to a low-temperature magnetism determined by exchange frustration effects. The crystal electric field (CEF) in $NaYbS_2$ allows an effective spin $S = 1/2$ in contrast to other delafossites materials which contain Cr^{3+} ($S = 3/2$), for instance. There, extensive electron spin resonance (ESR) measurements of Cr^{3+} could verify a Z_2 ordering scenario for triangular Heisenberg antiferromagnets [1].

We present first results of the Yb^{3+}-ESR in single-crystalline $NaYbS_2$. Well-defined spectra could be only observed for temperatures below $\approx$ 70 K because of the increasing influence of the relaxation via the higher CEF levels of Yb^{3+} towards higher temperatures. The spectra show a large anisotropy, as determined by the CEF, similar to what has been observed in other Yb-systems [2]. Towards low temperatures we observed a moderate increase of the linewidth. This may indicate a spin-liquid state in agreement with NMR results where the increase of the spin-spin relaxation towards low temperatures is discussed as a signature of a quantum spin-liquid.

[1] M. Hemmida et al., J. Phys. Soc. Jpn. 80, 053707 (2011)
[2] A. Kutuzov et al., J. Phys. Cond. Mat. 20, 455208 (2008)

TT 72.58 Wed 15:00 Poster B

From Kitaev exchange towards quantum disorder: A pressure dependent optical study on α-$RuCl_3$ — •Tobias Biesner[1], Weiwu Li[1], Yohei Saito[1], Andrej Pustogow[1], Martin Dressel[1], Anja Wolter-Giraud[2], Bernd Büchner[2], Maria Roslova[3], and Thomas Doert[3] — [1]1. Physikalische Institut, Universität Stuttgart, Germany — [2]IFW-Dresden, Germany — [3]Dept. Chem. and Food Chem., TU-Dresden, Germany

The j_{eff}=1/2 Mott insulator α-$RuCl_3$ is a promising Kitaev quantum spin liquid candidate due to its layered, almost ideal honeycomb lattice with a high degree of frustration. While the pure Kitaev physics is commonly hampered by a magnetic state, external pressure could suppress antiferromagnetic order.

We present a comprehensive study of the optical properties of α-$RuCl_3$ powder and single crystals by infrared spectroscopy in a broad range of frequencies down to low temperatures and under hydrostatic pressures in order to elucidate a pressure-induced new quantum state. Due to the large energy scales of α-$RuCl_3$, moderate pressures ($p < 1.8$ GPa) do not significantly affect the Mott insulating state. However, afm order is suppressed by pressure resulting in a transition to a quantum spin liquid like state and unveiling pure Mott physics. In the optical response we see signatures of enhanced symmetric anisotropic exchange, and evolution of the band structure; providing evidence for a strong coupling of electronic and magnetic correlations. The potential of optical studies for pressure-induced exotic quantum states is shown for α-$RuCl_3$ and discussed for other Kitaev candidates.

TT 72.59 Wed 15:00 Poster B

Comparative thermal expansion study on organic quantum-spin-liquid-candidate systems — •S. Hartmann[1], R. S. Manna[2], J. Schlueter[3], Y. Yoshida[4], and M. Lang[1] — [1]Physikalisches Institut, SFB/TR 49, Goethe-Universität Frankfurt, Germany — [2]Dept. of Physics, Indian Institute of Technology Tirupati, India — [3]Div. of Materials Research, National Science Foundation, Arlington, Virginia, USA — [4]Dept. of Chemistry, Kyoto University, 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 ground 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-TTF)$_2X$. We present a comparative study of ultra-high-resolution thermal expansion measurements on the QSL-candidates $X = Cu_2(CN)_3$ and $X = Ag_2(CN)_3$. The $X=$ $Cu_2(CN)_3$ system shows a mysterious anomaly around 6 K, frequently assigned to a QSL instability, the origin of which is still an open question. The shape and size of this effect are attributed to a second-order phase transition [2]. In contrast, we do not find any indications for a phase transition for $X=$ $Ag_2(CN)_3$. In addition, we discuss effects of applying a magnetic field and pay attention to sample-to-sample variations in the materials' low-temperature lattice effects.

[1] Balents, Nature 2010
[2] Manna et al., PRL 2010

TT 72.60 Wed 15:00 Poster B

Phase diagram of chiral antiferromagnets — •Benjamin Wolba[1], Sebastian Mühlbauer[2], and Markus Garst[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany

Chiral antiferromagnets are characterized by a Dyzaloshinskii-Moriya interaction that stabilizes spatially modulated phases of the staggered order parameter. In the framework of a Ginzburg-Landau theory, we determine the phase diagram as a function of temperature and magnetic field. In zero magnetic field, a phase with spiral antiferromagnetic order is present. A finite field naturally leads to an easy-plane anisotropy that induces a spinflop transition into a topological phase consisting of a square-lattice of vortices and antivortices. We discuss the relevance of our results for the chiral antiferromagnet $Ba_2CuGe_2O_7$.

TT 72.61 Wed 15:00 Poster B

Interface-driven Skyrmions in $SrRuO_3$ based heterostructures — •Sven Esser[1], Sebastian Esser[1], Anton Jesche[1], Vladimir Roddatis[2], and Philipp Gegenwart[1] — [1]Experimentalphysik VI, Universität Augsburg, 86159 Augsburg, Germany — [2]Institut für Materialphysik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Formation of Néel-type skyrmions at oxide interfaces is supported by Dzyaloshinskii-Moriya (DM) interaction through introducing a break of inversion symmetry. Recently artificial perovskite bilayers of the ferromagnetic metal $SrRuO_3$ (SRO) and spin-orbit semimetal $SrIrO_3$ (SIO) have been proposed to host two-dimensional Néel-type skyrmions [1].

By using a metal-organic aerosol deposition technique we have grown $[(SrIrO_3)_2/(SrRuO_3)_5]_k$ bilayers with $k = 1, 5, 10$ repetitions on cubic (001)-oriented $SrTiO_3$ substrate to investigate the interface induced

changes of the electronic and magnetic properties. The fully epitaxially strained state of the thin films was verified by X-ray diffraction patterns in combination with reciprocal space mapping and TEM images. Measurement of the in-plane magnetization indicate a relation to the number of interfaces between SRO and SIO layers. A contribution of the topological Hall effect to the Hall resistance can be observed near 80K, which may be a hint for the formation of skyrmions.
[1] J. Matsuno *et al.*, Science Adv. **2** (2016) e1600304.

TT 72.62 Wed 15:00 Poster B

High-frequency EPR and magnetization studies on azopyridine-bridged transition metal dinuclear complexes — •Felix Spathelf[1], Marco Hoffmann[1], Changhyun Koo[1], Roland Bischoff[2], Hans-Jörg Krüger[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Faculty of Chemistry, TU Kaiserslautern, Kaiserslautern, Germany

The magnetic properties of azopyridine-bridged transition metal dinuclear complexes ($[\{M(L-N_4Me_2)\}_2(\mu-apy^{2-})](SbF_6)_2$ with $M = Fe^{2+}, Cu^{2+}$) are studied by means of high-frequency electron paramagnetic resonance (HF-EPR) and magnetization measurements. Magnetization data show that the Cu_2-complex exhibits a singlet ground state associated with an intra-dimer coupling of $J = 155$ K. Accordingly, at low temperatures we observe no EPR resonances up to 700 GHz. In contrast, magnetic susceptibility of the Fe_2-complex obeys a Curie-Weiss-like behaviour at $T \leq 80$ K. Upon further heating, the data imply spin crossover from the $S = 2$ to a $S = 4$ state. Furthermore, we observe weak antiferromagnetic coupling of the Fe-ions ($J = (1.0 \pm 0.5)$ K). The HF-EPR spectra at $T = 2$ K show two resonance branches ω_1 and ω_2 with effective g-factors of 9.8 ± 0.4 and 1.986 ± 0.008, respectively, and no zero-field splitting. While the ω_1-branch can be attributed to forbidden dimer transitions, the origin of ω_2 is yet unclear. It may be either due to intrinsic transitions or result from paramagnetic impurities.

TT 72.63 Wed 15:00 Poster B

high frequency EPR studies on lanthanide monomers in different ligand structures — •sajedeh shahbazi[1], johannes werner[1], julian butscher[1], changhyun koo[1], asha roberts[2], peter comba[2], denis gorbunov[3], and rüdiger klingeler[1] — [1]Kirshhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — [2]Anorganisch-Chemisches Institut, Universität Heidelberg, Heidelberg, Germany — [3]Hochfeld-Magnetlabor Dresden, Institution Helmholtz-Zentrum, Dresden, Germany

The magnetic properties of lanthanide monomers (Ln=Dy(III) and Tb(III)) in two different ligand structures but similar coordination geometries ([Ln(x-1,2-HOPO)$_2$]PyH (x = 2Li,5Li)) are reported in order to investigate ligand field effects. The ground states of the complexes were estimated by using high-field electron paramagnetic resonance (HF-EPR) and pulsed-field magnetization studies. The slopes of the resonance branches seen in the HF-EPR data on the Tb-complexes correspond to g-factors much larger than 2 implying a forbidden transition. Based on the HF-EPR data and the saturated magnetization value at $B = 58$ T, the ground states of the Tb-complexes are derived. Finite zero-field splitting observed in [Tb(III)(2Li-1,2-HOPO)$_2$]PyH indicates lifting of the degeneracy in a non-Kramers doublet. From the obtained experimental results, the ligand field effect on the ground state in the studied complexes is discussed.

TT 72.64 Wed 15:00 Poster B

Thermal and thermal-Hall conductivity study of $SrCu_2(BO_3)_2$ — •Stevan Arsenijević[1], Hanna Dabkowska[2], Bruce Gaulin[2], Raivo Stern[3], and Jochen Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

We present measurements of the thermal and the thermal-Hall conductivity as a function of temperature and magnetic field in the two-dimensional dimer spin system $SrCu_2(BO_3)_2$. The thermal conductivity in zero magnetic field shows a pronounced peak around 4 K which is ascribed to a spin-gap opening. The low-temperature maximum is strongly suppressed by the application of magnetic field. This result implies that the majority of heat is conducted by phonons which interact with the magnetic excitations. Furthermore, a theoretical study predicted a strong thermal Hall signature due to anisotropies originating from the Dzyaloshinskii-Moriya interactions which lead to a topological character of triplon excitations [1]. Our detailed experimental investigation did not reveal such effect disproving the existence of topological transitions in the triplon band structure.
[1] J. Romhányi, K. Penc, R. Ganesh, Nat. Commun. **6** (2015) 6805

TT 72.65 Wed 15:00 Poster B

Magnetic and Structural Properties of the Trirutile-type 1D Heisenberg Antiferromagnet $CuTa_2O_6$ — •A. Golubev[1], R. E. Dinnebier[1], A. Schulz[1], R.K. Kremer[1], H. Langbein[2], A. Senyshyn[3], J. M. Law[4], T. Hansen[5], H.-J Koo[6], and M.-H. Whangbo[7] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institut für Anorganische Chemie der Technischen Universität Dresden, Dresden, Germany — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany — [4]Dresden High Magnetic Field Laboratory (HLD), Dresden, Germany — [5]Institut Laue-Langevin, Grenoble, France — [6]Kyung Hee University, Seoul, Republic of Korea — [7]North Carolina State University, North Carolina, USA

$CuTa_2O_6$ crystallizes with a monoclinically distorted trirutile structure type. By detailed high temperature neutron and x-ray powder diffraction measurements we mapped the structural phase transition to the tetragonal trirutile structure-type at 500 K. The structural phase transition was ascertained by Raman scattering experiments. ab-initio GGA+U density functional calculations of the spin exchange parameters, magnetic susceptibility and isothermal magnetization measurements constitute $CuTa_2O_6$ as one-dimensional Heisenberg quantum antiferromagnet with predominant nearest-neighbor spin exchange interaction $J - nn$ 50 K. Long-range magnetic order was not detected down to 0.4K.

TT 72.66 Wed 15:00 Poster B

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 quantum $S = \frac{1}{2}$ Heisenberg antiferromagnet (2D QHAF) 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-temperature phase transition to long-range order performed via ^{1}H and ^{31}P nuclear magnetic resonance (NMR), as well as high-field magnetometry. A low-temperature minimum of the temperature-dependent local and uniform magnetizations at T_{min} indicates a presence of the magnetic order. Within the ordered state, a splitting of the ^{1}H NMR spectra reveals commensurate AF order, presumably of checkerboard type. The phase transition, manifested as a sharp maximum of the temperature-dependent ^{31}P nuclear spin-lattice relaxation rate $1/T_1$, occurs at temperatures slightly lower than T_{min}, indicating an easy-plane anisotropy as well as a crossover between isotropic and XY behavior.

TT 72.67 Wed 15:00 Poster B

Superposition of FM and AFM Cu(II) spin-1/2 chains in $BaAg_2Cu[VO_4]_2$ studied by magnetic resonance spectroscopies — •Y. Krupskaya[1], M. Schäpers[1], A.U.B. Wolter[1], H.-J. Grafe[1], E. Vavilova[1,2], A. Möller[3], B. Büchner[1], and V. Kataev[1] — [1]IFW Dresden, Dresden, Germany — [2]Zavoisky Physical-Technical Institute, Kazan, Russia — [3]Johannes Gutenberg University Mainz, Mainz, Germany

$BaAg_2Cu[VO_4]_2$ contains Cu(II) S=1/2 ions in a distorted two-dimensional triangular lattice interconnected via non-magnetic $[VO_4]$ entities. The theoretical analysis and the magnetization measurements show that the magnetism of this compound is determined by a superposition of ferromagnetic (FM) and antiferromagnetic (AFM) uniform spin-1/2 chains. In order to probe the local magnetic properties we have performed the study of $BaAg_2Cu[VO_4]_2$ by High-Field/Frequency Electron Spin Resonance (HF-ESR) and Nuclear Magnetic Resonance (NMR) spectroscopies. In the HF-ESR measurements, we observe an anisotropic ESR spectrum typical for the Cu(II) ions and determine the g-tensor. The detailed analysis shows that the shape of the low-temperature ESR spectrum is defined by the development of the anisotropic internal fields corresponding to FM and AFM correlations in the respective Cu spin chains. The NMR study has

identified the signals from ^{51}V nuclei in the two types of chains, which strongly supports the ESR results. Altogether, the HF-ESR and NMR results confirm theoretical predictions of the superposition of FM and AFM Cu(II) spin-1/2 chains in $BaAg_2Cu[VO_4]_2$.

TT 72.68 Wed 15:00 Poster B

High-Pressure Transport Studies in 2H-$NbSe_2$ — •Owen Moulding and Sven Friedemann — University of Bristol, Bristol, UK

The transition metal dichalcogenide 2H-$NbSe_2$ has well-documented charge density wave (CDW) and superconducting transitions at 33K and 7K at ambient pressure. The CDW transition is suppressed under high pressure and is absent beyond the quantum critical point (QCP) at 4.6 GPa [1]. 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 and X-ray measurements have explored the vicinity of this QCP, and they indicate only 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. We use patterned moissanite anvil cells for pressures well beyond the QCP.
[1] Feng, Y., et al. PNAS, **109**, 7224 (2012).

TT 72.69 Wed 15:00 Poster B

Resistance peak at the superconducting transition of $SrTiO_3/Al_2O_{3-x}$-heterostructures — •Daniel Arnold, Roland Schäfer, Dirk Fuchs, and Karsten Wolff — Karlsruhe Institute of Technology, Institute for Solid State Physics

When an anisotropic system undergoes a superconducting transition the resistance is often peaking before it drops to zero. This effect is well documented for low- and high-T_c materials.

We have studied the resistive transition in the superconducting interface of (001)-oriented $SrTiO_3$ and Al_2O_{3-x} as a function of temperature and magnetic field using a Van-der-Pauw sample geometry. Our sample shows a distinct difference for the two orthogonal directions of current flow indicating a preferential direction for supercurrents. In one of the direction an especially large peak effect is present.

We discuss our experimental data by comparing it to the results of numerical simulations and analytical calculations.

TT 72.70 Wed 15:00 Poster B

Investigation of LAO/STO nanostructures — •Mithun S Prasad[1], Mohzin Minhas[1], Alexander Müller[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, $LAlO_3$ (LAO) and $SrTiO_3$ (STO) provides new opportunities to explore nano electronic devices. Recently our group has developed an industry compatible nano patterning technique [1] for the LAO/STO interface. Some recent studies on this interface have revealed that at low temperature the current transport in LAO/STO heterostructures is mainly through the domain boundaries which results in the formation of numerous current carrying filaments [2]. This fact also results massive changes in conductivity when a few filaments are confined in nanostructures. We investigate the dependence of the effect on the orientation of nanostructures with respect to the crystalline structure of the substrate at different temperatures and under application of a back-gate voltage.

TT 72.71 Wed 15:00 Poster B

Tuning the electric interface properties of amorphous $AlO_x/SrTiO_3$ interfaces — •Berengar Leikert[1], Judith Gabel[1], Martin Stübinger[1], Philipp Scheiderer[1], Matthias Schmitt[1], Tien-Lin Lee[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM) — [2]Diamond Light Source, Beamline I09, Didcot, England

Two dimensional electron systems (2DESs) at the interfaces of oxide heterostructures are considered a promising platform for future microelectronic technology which may utilize the rich electronic behavior of transition metal oxides. A simple and cost-effective method to create a 2DES is to deposit Al on the surface of $SrTiO_3$. It reduces the first oxide layers and leads to an n-doping of the oxide surface. By changing the Al redox potential via growth in oxygen atmosphere we can tune the electronic interface properties, as probed by hard x-ray photoelectron spectroscopy of the film as well as the substrate core levels. Emission angle resolved film and core level spectra are used to determine the band bending behaviour and the sheet carrier concentration as function of growth parameters. By comparison to the spectroscopic data, transport experiments offer information on carrier trapping in this oxygen vacancy dominated material.

TT 72.72 Wed 15:00 Poster B

Investigating the charge transfer in $LaVO_3/SrTiO_3$ heterostructures by photoemission spectroscopy — •Martin Stübinger[1], Judith Gabel[1], Philipp Gagel[1], Christoph Schlueter[2], Tien-Lin Lee[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Diamond Light Source Ltd., Didcot, Oxfordshire OX11 0DE, United Kingdom

Akin to the well known oxide heterostructure $LaAlO_3/SrTiO_3$ (LAO/STO) a conducting interface is found also between the strongly correlated, polar Mott insulator $LaVO_3$ (LVO) and the non-polar band insulator STO. A possible mechanism for this behavior is an electron transfer to the interface caused by the polar discontinuity. Since in LVO/STO the transition metals Ti as well as V can have different oxidation states, they both may act as hosts for the transferred electrons. In particular, a charge transfer to V would lead to a band-filling controlled Mott insulator-to-metal transition. By means of photoemission spectroscopy with synchrotron radiation we investigate the valence band structure of LVO/STO and the band alignment at the interface. In accordance with resonant photoemission at the V-L and the Ti-L edge we arrive at the conclusion that it is energetically more favorable for transferred electrons to occupy Ti than V sites. Therefore, a Mott insulator-to-metal transition is not observed in LVO.

TT 72.73 Wed 15:00 Poster B

Strain-induced metal-to-insulator transition in LiV_2O_4 thin films — •Ulrike Niemann[1], Daigorou Hirai[2], and Hidenori Takagi[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Tokyo, Tokyo, Japan

The spinel compound LiV_2O_4 is well-known for its exotic heavy fermion behaviour and has therefore been subject to several studies, addressing the origin of the heavy fermion phase [1]. Repeatedly, geometric frustration with regard to the charge and spin arrangement on the vanadium sides was discussed as a possible alternative to a dense Kondo system scenario. However, the difficulties in growing significantly large single crystals of high quality, limit the verification of discussed models. We fabricated single-crystalline thin films of LiV_2O_4 on $SrTiO_3$, LSAT and MgO substrates using pulsed laser deposition [2]. The heavy fermion behaviour of bulk LiV_2O_4 is well-reproduced in relaxed films on $SrTiO_3$ substrates, giving the opportunity to explore the heavy fermion phase in area-vice significantly larger single crystals. In contrast, an insulating phase was found in strained LiV_2O_4 thin films on MgO substrates, supporting the importance of geometric frustration for the appearance of heavy fermions in this particular compound. On the poster, we discuss the thin film fabrication and the effect of epitaxial strain on heavy fermions in LiV_2O_4 in detail.
[1] C. Urano et al., Phys. Rev. Lett. 85, 1052 (2000).
[2] U.Niemann, D. Hirai, H. Takagi (submitted)

TT 72.74 Wed 15:00 Poster B

Electronic Structure of Palladium Measured by Compton Scattering and Electron-Positron Annihilation. — •Josef Helmut Schmidbauer[1], Michael Leitner[1], and Christoph Pascal Hugenschmidt[1,2] — [1]Physik Department E21, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

Compton scattering and measurements of the angular correlation of electron-positron annihilation radiation (ACAR) offer two unique possibilities for the investigation of the bulk electronic structure. Although both methods allow the measurement of the electron momentum distribution (EMD) various differences are inherent to the respective technique. While a single ACAR spectrum provides a two-dimensional projection of the EMD a Compton scattering profile corresponds to a one-dimensional projections. Besides dissimilar experimental reso-

lution further differences originate from the influence of the positron wave function and the enhancement of different electron states (probe effects). We applied both techniques to the correlated system Palladium in order to study its electronic structure, and we present the specific features inherent to Compton scattering and ACAR.

TT 72.75 Wed 15:00 Poster B

Electronic structure of the B20 compound CrGe — •J. Klotz[1,2], K. Götze[1,2], J. Bruin[3], C. Geibel[4], K. Weber[4], M. Schmidt[4], H. Rosner[4], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]High Magnetic Field Laboratory, Radboud University, Netherlands — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

CrGe is a nonmagnetic transition-metal germanide with the B20 noncentrosymmetric cubic structure. In contrast, the isostructural MnGe and FeGe both show a helical spin order. We present dHvA-effect data on CrGe that were obtained employing capacitive torque magnetometers in a 18 T/30 mK and a 33 T/340 mK system. In combination with our fplo calculations, we provide a detailed picture of the Fermi-surface topology of CrGe. Furthermore, by comparing the calculated band structures of CrGe and MnGe, we discuss possible reasons for the absence of magnetic order in CrGe. Finally, our calculations indicate that substituting Ge by As or Sn will not lead to magnetic order.

TT 72.76 Wed 15:00 Poster B

Interplay of spin-orbit coupling, crystal-field and electronic correlations in ruthenate oxides — •Esmaeel Sarvestani[1], Guoren Zhang[1], Evgeny Gorelov[1,2], and Eva Pavarini[1,3] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany — [2]European XFEL GmbH, Hamburg, Germany — [3]JARA High-Performance Computing, RWTH Aachen, Aachen, Gemany

We investigate the effects of spin-orbit (SO) coupling, crystal-field and Coulomb interaction on the electronic properties of the t_{2g}^4 layered ruthenates Sr_2RuO_4 and $Sr_3Ru_2O_7$. We calculate effective masses, life-times and optical conductivity via the LDA+DMFT approach, using the general implementation of the continuous-time interaction-expansion QMC impurity solver of Refs.[1,2]. We find that the effect of SO coupling on the mass-enhancements depends on the parameter range. We explain this via a two-site t_{2g} Hubbard model. We additionally find that for a realistic description of the optical conductivity, it is important to include the effects of SO interaction. We show that the effects of low-symmetry terms of Coulomb interaction on the total spectral function and in-plane conductivity are small; however, they have a strong effect on the mass-enhancement anisotropy [3].

[1] E. Gorelov et. al., Phys. Rev. Lett. **104**, 226401 (2010).
[2] G. Zhang et. al., Phys. Rev. Lett. **116**, 106402 (2016).
[3] E. Sarvestani et. al., submitted to Phys. Rev. B.

TT 72.77 Wed 15:00 Poster B

Spin-Orbit Coupling and Electronic Corrleations in Ca_2RuO_4 — •Michael T. Schmid[1], Philipp Hansmann[2], and Maria Daghofer[3] — [1]michael.schmid@fmq.uni-stuttgart.de — [2]p.hansmann@fkf.mpg.de — [3]maria.daghofer@fmq.uni-stuttgart.de

Transition metal oxides of the 4d and 5d series with large spin orbit coupling (SOC) such as Iridates and Ruthenates are currently under intensive investigation [1]. Especially in the 4d systems the absence of a clear hierarchy of energy scales between crystal field (CF) and SOC splittings (e.g. in Ca_2RuO_4) poses a significant challenge for standard methods like the merger of density functional theory with dynamical mean-field theory (DFT+DMFT). With state-of-the-art DMFT impurity solvers [2], however, effective low energy models that include both CF and SOC contributions can be tackled. Here we present most recent results for Ca_2RuO_4 on the level of the magnetic susceptibilities. In contrast to mere single particle spectral functions the magnetic two particle response sheds significantly more light on the nature of the correlated magnetic phases in the considered materials.

[1] C. G. Fatuzzo et al., Phys. Rev. B, **91**, 1155104 (2015)
[2] O. Parcollet et al., Computer Physics Communications, **196**, 398 (2015)

TT 72.78 Wed 15:00 Poster B

Spin dynamics in a honeycomb compound probed by magnetic resonance technique — •Margarita Iakovleva[1,2], Hans-Joachim Grafe[1], Angela Möller[3], T. Taetz[4], Evgeniia Vavilova[2], Bernd Büchner[1], and Vladislav Kataev[1] — [1]IFW Dresden, Dresden, 01069, Germany — [2]KPhTI, Kazan, 420029, Russia — [3]IAAC, JGU Mainz, Mainz, 55128, Germany — [4]Institut für Anorganische Chemie, Universität zu Köln, Köln, 50939, Germany

The S=1/2 Heisenberg antiferromagnet $InCu_{2/3}V_{1/3}O_3$ appears to be a rare model of a honeycomb lattice compound with very weak interlayer couplings. Previous magnetization and Electron Spin Resonance (ESR) studies on this compound have revealed signatures of an antiferromagnetic transition at $T_N = 38$ K [1,2]. In our study, we used Nuclear Quadrupolar Resonance (NQR) and Nuclear Magnetic Resonance (NMR) techniques to investigate the local magnetic properties of $InCu_{2/3}V_{1/3}O_3$. The ^{115}In NMR as well as NQR spectra show a line splitting at $T<T_N$ which is a signature of the development of local magnetic fields in the vicinity of a magnetic phase transition. The T-dependence of the longitudinal relaxation rate T_1^{-1} shows a characteristic sharp peak upon approaching $T_N = 38$ K. Remarkably, with further decreasing temperature a second peak develops at $T^* = 15$ K. We discuss this peculiar feature and possible scenarios of magnetic order in $InCu_{2/3}V_{1/3}O_3$.

[1] V. Kataev, et al., JMMM 290-291, 310 (2004)
[2] M. Yehia, et al., Phys. Rev. B, 81, 060414 (2010)

TT 72.79 Wed 15:00 Poster B

Strong electronic correlations: the example of VO_2 — •Elham Khorasani[1], Malte Schüler[2], Bálint Aradi[1], and Peter Deák[1] — [1]BCCMS, Universität Bremen, Bremen, Germany. — [2]Institut für Theoretische Physik, Universität Brememen, Germany.

The metal-insulator transition in VO_2 has been a controversial issue for several decades. It is at the boundary between band theory and many-body physics and forms an important benchmark problem in theoretical solid state physics. To understand the metal-insulator mechanism across the VO_2 in B-phase, GGA+U calculations based on density functional theory have been done. Our results reveal that GGA+U can not predict the proper ground state of VO_2 in the B-phase.

Our study based on static cluster dynamical mean field theory(sC-DMFT), which is proved itself valuable in the M-phase (J. M. Tomczak et .al,J.Phys. Condens Matter, 19, 365206(2007)), did not lead to the experimentally known gap in the insulator VO_2 in B-phase. So, in the next step, in order to elucidate the correlated electronic structure of the B-phase, the full C-DMFT(P. Werner et al, Phys. Rev. Lett., 97, 076405(2006))have been done. Our results for M-phase show that the implementation of Continues-Time Quantum Monte Carlo based on hybridization expansion (CT-Hyb) as a solver makes a sign problem in full C-DMFT.To overcome the sign problem in CT-Hyb , cluster DMFT using exact agonalisation (ED) has been implemented. We compare ED and CT-QMC results for R-phase and explore properties of B-phase using ED.

TT 72.80 Wed 15:00 Poster B

Lattice dynamics of palladium in the presence of many-body effects — •Wilhelm Appelt[1,3], Andreas Östlin[2], Ivan Leonov[2], Michael Sekania[2], and Liviu Chioncel[2,3] — [1]Theoretical Physics II, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [3]Augsburg Center for Innovative Technologies, University of Augsburg, 86135 Augsburg, Germany

We present theoretical results on the phonon spectrum of palladium. A combination of the local density approximation (LDA) and dynamical mean-field theory (DMFT) is employed in order to investigate the interplay between correlated electrons and lattice degrees of freedom. A good agreement with experimental dispersion curves is found for the realistic local Coulomb interaction ($U = 1\,\mathrm{eV}$) and the local Hund's rule coupling ($J = 0.3\,\mathrm{eV}$). The Kohn anomaly along the Σ-line is observed on the level of LDA when computed at the experimental volume. When supplement with local electronic interactions, of Hubbard-type, we find that the kink along the Σ-line in the phonon dispersion curve is smoothened. Corrections in lowest order perturbation theory are used in order to study the influence of non-adiabatic self-energy effects on the phonon propagtor. This simple correction to the Born-Oppenheimer approximation allows us to access phonon lifetimes in the LDA+DMFT study.

TT 72.81 Wed 15:00 Poster B

Flavor-twisted Boundary Conditions for calculation of two-particle correlation functions — •Jonas Heverhagen and Maria Daghofer — University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Germany

We generalize the simulation technique flavor-twisted boundary condition (FTBC) combined with exact diagonalization (ED) to gain continuous momentum resolution for two-particle correlation functions. To validate this technique, we compare the results with cluster perturbation theory calculations and identify the strength and weaknesses of both techniques. Hereby, we focus on one-dimensional spin-orbital systems, where first CPT is well established and second results from only ED calculations can easily be compared with FTBC calculations. However, we stress that this technique can also be applied in higher dimensions.

TT 72.82 Wed 15:00 Poster B

CT-1/2-HYB-QMC: a new solver for time-dependent Anderson impurity — •Patryk Kubiczek[1], Alexey N. Rubtsov[2,3], and Alexander I. Lichtenstein[1] — [1]I. Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany — [2]Department of Physics, Lomonosov Moscow State University, Moscow, Russia — [3]Russian Quantum Centre, Skolkovo, Russia

We report on the progress of the development of a modified real-time continuous-time hybridization-expansion quantum Monte Carlo solver for a time-dependent single-orbital Anderson impurity model: CT-1/2-HYB-QMC. In the proposed method the diagrammatic expansion is performed only for one out of the two spin channels, while the resulting effective single-particle problem for the other spin is solved explicitly for each diagrammatic term. We show that the CT-1/2-HYB-QMC method alleviates the dynamical sign problem by reducing the order of sampled diagrams and makes it possible to reach twice as long time scales in comparison to the standard CT-HYB method. Moreover, the structure of CT-1/2-HYB perturbative expansion leads to an easier and less computationally expensive measurement of the charge current.

TT 72.83 Wed 15:00 Poster B

Variational approach to models with strongly correlated electrons — •Philip Mirbach[1], Malte Schüler[1,2], Tim Wehling[1,2], and Gerd Czycholl[1] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany

Electronic systems with strong interactions are promising materials for a wide variety of applications. These strongly correlated electron systems are often described by lattice models such as the Hubbard model. However, they are difficult to treat numerically.

We use Feynman's Variational Principle to determine optimal effective model systems that can be solved exactly, for example by ED-methods. We divide the original model into exactly solvable clusters, where the partition and the parameters are optimized by the variational principle. Internal correlation effects are correctly considered in these clusters. In addition, they maintain effective influences of the originally neglected interactions through the variation. The trivial case of completely decoupled clusters is equal to the Hartree-Fock (HF) approximation. Therefore, more complex effective model systems lead to systematic improvements beyond HF. By an optimal choice of the representation of the model, e. g. in real or momentum space, particularly effective parameters for describing the original model can be found.

Using the one-dimensional Hubbard model with four sites as an example, we show the possibilities of this method and compare the results with HF and the exact solution.

TT 72.84 Wed 15:00 Poster B

The finite-temperature Lanczos method as solver for the variational cluster approach — •Jan Lotze and Maria Daghofer — Universität Stuttgart, Institut für Funktionelle Materie und Quantentechnologien, Pfaffenwaldring 57, 70569 Stuttgart

The variational cluster approximation (VCA) based on self-energy functional theory (SFT) [1] can be used to study correlated-electron Hamiltonians: Instead of the original systems self-energy, that of a 'reference system' is considered. While full diagonalisation suffices for small reference systems, larger systems require the Lanczos method or a quantum Monte Carlo method [2] to be tractable. Considering systems at finite temperature increases the numerical burden even further. Demanding on top of this the resolution of degenerate states in the reference system requires to switch from the regular Lanczos method to the Band Lanczos method.

Here, thermodynamic and dynamical properties of the one- and two-dimensional Hubbard model at finite temperature are presented to illustrate the finite-temperature Lanczos and Band Lanczos method as solver of the reference system. The effect of degeneracies onto the results is discussed.

[1] M. Potthoff, 'Self-Energy-Functional Theory', in Strongly Correlated Systems – Theoretical Methods (Springer, 2012).
[2] G. Li, W. Hanke, A. N. Rubtsov, S. Bäse, M. Potthoff, Phys. Rev. B **80**, 195118 (2009).

TT 72.85 Wed 15:00 Poster B

Theoretical investigation of excitonic agnetism in $LaSrCoO_4$ — •juan fernandez afonso, andrii sotnikov, and jan kunes — Institute of Solid State Physics TU Wien, Vienna, Austria

We use the LDA+U approach to search for possible ordered ground states of $LaSrCoO_4$. We find a staggered arrangement of magnetic multipoles to be stable over a broad range of Co $3d$ interaction parameters. This ordered state can be described as a spin-density-wave-type condensate of $d_{xy} \otimes d_{x^2-y^2}$ excitons carrying spin $S = 1$. Further, we construct an effective strong-coupling model, calculate the exciton dispersion and investigate closing for the exciton gap, which marks the exciton condensation instability. Comparing the layered $LaSrCoO_4$ with its pseudo cubic analog $LaCoO_3$, we find that for the same interaction parameters the excitonic gap is smaller (possibly vanishing) in the layered cobaltite.

TT 72.86 Wed 15:00 Poster B

Anisotropy crossover in the frustrated Hubbard model on four-chain cylinders — •Georg Ehlers[1], Benjamin Lenz[2,3], Salvatore R. Manmana[3], and Reinhard M. Noack[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, 91128 Palaiseau, France — [3]Institut für Theoretische Physik, Universität Göttingen, 37077 Göttingen, Germany

Motivated by dimensional crossover in Bechgaard and layered organic κ salts, we investigate the metal-insulator transition in the anisotropic frustrated Hubbard model on four coupled Hubbard chains.

Using the hybrid-space density matrix renormalization group (DMRG) and the variational cluster approximation (VCA), we map out the phase diagram as a function of the anisotropy and interaction strength. The phase diagram, as seen by the hybrid-space DMRG, features a quasi-one-dimensional anti-ferromagnetic phase, a two dimensional anti-ferromagnetic phase, a metallic phase, and an incommensurate spin-density wave phase [1]. The phases are characterized through their magnetic ordering, dielectric response, and dominant static correlations.

We use DMRG in a formulation for lattices with cylindrical geometry utilizing the conserved transverse lattice momentum [2] and corroborate our findings with VCA calculations using a cluster geometry corresponding to the cylindrical lattice. As an outlook, we make contact with work studying dimensional crossover in the full two-dimensional system.

[1] G. Ehlers et al., arXiv:1705.04450 (2017)
[2] G. Ehlers et al., Phys. Rev. B 95, 125125 (2017)

TT 72.87 Wed 15:00 Poster B

Doublon Formation by Ions Impacting a Strongly Correlated System — Karsten Balzer, •Niclas Schlünzen, Maximilian Rodriguez Rasmussen, and Michael Bonitz — CAU Kiel, Germany

Strongly correlated systems of fermions have a number of exciting collective properties. Among them, the creation of a lattice that is occupied by doublons, i.e. two fermions with opposite spins, offers interesting electronic properties. In the past a variety of methods has been proposed to control doublon formation both spatially and temporally. Here, a recently proposed[1] mechanism is described and verified by computer simulations – doublon creation by the impact of energetic ions[1,2]. The theoretical characterization is based on exact diagonalization calculations for small systems and is extended to larger systems via a Nonequilibrium Green Functions description[3]. Finally, we present an idea how this concept can be realized with atoms in an optical lattice.

[1] K. Balzer, M. Rasmussen, N. Schlünzen, M. Bonitz, submitted
[2] K. Balzer, N. Schlünzen, M. Bonitz, Phys. Rev. B 94, 245118 (2016)
[3] S. Hermanns, N. Schlünzen, M. Bonitz, Phys. Rev. B 90, 125111 (2014)

TT 72.88 Wed 15:00 Poster B

Analytical Evidences for Particle Induced Doublons in Strongly Correlated Systems — •Maximilian Rodriguez Rasmussen, Karsten Balzer, Niclas Schlünzen, 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. Recently, a new mechanism has been proposed[1] – doublon creation by the impact of energetic ions. Here, these processes are described and verified by analytical results for a two-site model that is shown to capture the basic features and allows for a systematic analysis of the main trends[2]. The findings are additionally supported by a Landau–Zener description of the doublon state.

[1] K. Balzer, M. Rasmussen, N. Schlünzen, and M. Bonitz, submitted for publication (2017)

[2] M. Rasmussen, "Particle Induced Doublons in Strongly Correlated Systems", bachelor thesis (2017)

TT 72.89 Wed 15:00 Poster B

Prethermalization after a short electric field pulse — •Marc Alexander and Marcus Kollar — Theoretische Physik III, Universität Augsburg

We study the nonlinear current response to a short electric field pump pulse [1]. For weakly interacting Hubbard models we find that a prethermalization plateau develops after the pulse, in contrast to the noninteracting case. While this behavior is analogous to the prethermalization plateau that occurs after weak interaction quenches [2], the details of the metastable state now depend on the details of the bandstructure and the length, shape, and frequency of the pump pulse.

[1] V. Turkowski and J. K. Freericks, Phys. Rev. B **71**, 085104 (2005)
[2] M. Moeckel and S. Kehrein, Phys. Rev. Lett. **100**, 175702 (2008)

TT 72.90 Wed 15:00 Poster B

Generalized Gibbs ensembles in weakly open quantum systems — •Florian Lange, Zala Lenarcic, and Achim Rosch — Universität zu Köln

We consider weakly driven and weakly open quantum systems in the situation when the unperturbed system has a set of conservation laws. If the perturbation is sufficiently weak the non-equilibrium steady state can be in the thermodynamic limit efficiently described by a generalized Gibbs ensemble (GGE) characterized by one Lagrange parameter for each approximate conservation law. The values of those are determined by rate equations for the approximately conserved quantities. We extend the concept of GGEs by showing that an ensemble with time-dependent Lagrange parameters can capture the relaxation towards the steady state.

TT 72.91 Wed 15:00 Poster B

Single-hole dynamics in two-leg t-J ladder systems with matrix product states (MPS) — •Alexander Osterkorn[1], Fabian Grusdt[2], Sebastian Paeckel[1], Thomas Köhler[1], and Salvatore Manmana[1] — [1]Institut für Theoretische Physik, Universität Göttingen, 37077 Göttingen, Germany — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

We study the time evolution of a single hole in two-leg t-J-ladder systems at zero temperature using time-dependent matrix product states (MPS). We prepare the system with one fermion per lattice site with neither interaction nor tunneling between the legs. At time t = 0 one particle is removed from one of the legs and the tunneling amplitude between the two legs is set to a nonzero value. This allows us to study the separation of spinons and holons as a function of the rung-tunneling and compare to predictions from effective theories. We discuss implications for realizations with ultracold gases on optical lattices.

TT 72.92 Wed 15:00 Poster B

EPR studies of the triangular-lattice antiferromagnet Cs_2CuBr_4 — •Erik Schulze[1,2], Alexey N. Ponomaryov[1], Jochen Wosnitza[1,2], Hidekazu Tanaka[3], and Sergei A. Zvyagin[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Dresden, Germany — [3]Tokyo Institute of Technology, Tokyo, Japan

The spin dynamics of the spin-1/2 triangular-lattice antiferromagnet Cs_2CuBr_4 is probed by means of high-frequency electron paramagnetic resonance (EPR) spectroscopy. Temperature dependences of EPR parameters are studied in a broad temperature range between 1.4 and 200 K for different orientations of the applied magnetic field. In the high-temperature regime ($T \gg J/k_B$), an unusually broad and anisotropic resonance line is detected, suggesting a sizeable Dzyaloshinskii-Moriya interaction. Employing the theory of exchange narrowing, the ratio of the Dzyaloshinskii-Moriya vector components, $Dc/Da \approx 0.3$, is estimated.

This work was partially supported by Deutsche Forschungsgemeinschaft (project ZV 6/2-2) and by the HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL).

TT 72.93 Wed 15:00 Poster B

NMR study in the expected spin nematic state in Linarite — •Gaël Bastien[1], Quentin Goutaland[1], Hans Joachim Grafe[1], Edwin Kermarrec[2], Fabrice Bert[2], Philippe Mendels[2], Stefan Ludwig Drechsler[1], Satoshi Nishimoto[1], Stefan Süllow[3], Kirrily Rule[4], Anja U. B. Wolter[1], and Bernd Büchner[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, Germany — [2]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, Orsay, France — [3]Institute for Physics of Condensed Matter, TU Braunschweig, Germany — [4]The Bragg Institute, ANSTO, Kirrawee DC, Australia

The $J_1 - J_2$ Heisenberg chain is a frustrated magnetic system with competing first and second nearest neighbor interactions along a 1D chain. A new exotic state i.e. the spin nematic state is predicted to occur under magnetic field in this model. The linarite $PbCuSO_4(OH)_2$ is such a $J_1 - J_2$ Heisenberg chain with a relatively low saturation field H_{sat} ≈10T. It shows a long range magnetic spiral order below T_N=2.7K. Under a magnetic field applied along the b axis, it is changed into a collinear antiferromagnetic state and then to a collinear spin density wave, which is finally suppressed around 9.4T. We perform NMR measurement in the spin density wave state and in the narrow field interval between this spin density wave state and the saturation down to dilution temperature, to measure both the NMR spectrum and the relaxation rate. The relaxation rate was also measured at higher temperature in the paramagnetic state to investigate the fluctuations around the expected spin nematic state.

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Non-linear optical response in $SrCuO_2$ — •Philipp Warzanowski[1], Eva Benckiser[2], Dalila Bounoua[3], Paul H. M. van Loosdrecht[1], Christian Hess[4], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]ICMMO-Université Paris Sud — [4]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden

$SrCuO_2$ is regarded as a model system realizing a 1D $S = 1/2$ antiferromagnetic Heisenberg chain with a charge-transfer gap of about 1.6 eV and a large exchange constant of $J > 0.2$ eV. Optical spectroscopy allows us to study spinons by means of phonon-assisted absorption. We find $J = 225$ meV, in good agreement with neutron scattering results [1]. At low temperatures, the optical data reveal an additional non-linear absorption feature around 0.8 eV which originates from photoexcited states and depends on the incident light intensity. From time-resolved measurements we observe the temporal dynamics for the saturation and relaxation of this feature in the order of seconds to minutes. Above 160 K, this feature vanishes. Based on a three-level scheme, we describe the intensity dependence and time dependence in terms of rate equations. Similar findings in $LaSrAlO_4$ by Demsar *et al.* [2] suggest a scenario of excited carriers trapped in long-lived states related to oxygen vacancies.

[1] I. A. Zaliznyak *et al.*, Phys. Rev. Lett. 93, 087202 (2004)
[2] J. Demsar *et al.*, Phys. Rev. B 76, 054304 (2007)

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Flat bands in fractal-like geometry — •Biplab Pal and Kush Saha — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

We report the presence of multiple flat bands in a class of two-dimensional (2D) lattices formed by Sierpinski gasket (SPG) fractal geometries as the basic unit cells. Solving the tight-binding Hamiltonian for such lattices with different generations of a SPG network, we find multiple degenerate and non-degenerate *completely flat* bands, depending on the configuration of parameters of the Hamiltonian. Moreover, we find a generic formula to determine the number of such bands as a function of the generation index ℓ of the fractal geometry. We show that the flat bands and their neighboring dispersive bands have

remarkable features, the most interesting one being the spin-1 conical-type spectrum at the band center without any staggered magnetic flux, in contrast to the Kagome lattice. We furthermore investigate the effect of the magnetic flux in these lattice settings and show that different combinations of fluxes through such fractal unit cells lead to richer spectrum with a single isolated flat band or gapless electron- or hole-like flat bands. Finally, we discuss a possible experimental setup to engineer such fractal flat band network using single-mode laser-induced photonic waveguides.

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Automated construction of U(1)-invariant matrix-product operators from graph representations — •Sebastian Paeckel, Thomas Köhler, and Salvatore Manmana — Institut für Theoretische Physik, Georg August Universität Göttingen, Germany

We present an algorithmic construction scheme for matrix-product-operator (MPO) representations of arbitrary $U(1)$-invariant operators whenever there is an expression of the local structure in terms of a finite-states machine (FSM). Given a set of local operators as building blocks, the method automatizes two major steps when constructing a $U(1)$-invariant MPO representation: (i) the bookkeeping of auxiliary bond-index shifts arising from the application of operators changing the local quantum numbers and (ii) the appearance of phase factors due to particular commutation rules. The automatization is achieved by post-processing the operator strings generated by the FSM. Consequently, MPO representations of various types of $U(1)$-invariant operators can be constructed generically in MPS algorithms reducing the necessity of expensive MPO arithmetics. This is demonstrated by generating arbitrary products of operators in terms of FSM, from which we obtain exact MPO representations for the variance of the Hamiltonian of a $S = 1$ Heisenberg chain.

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Multiferroicity in Ni_3TeO_6 and $PbNi_6Mn_2Te_3O_{18}$ - a comparative Raman study — •Florian Büscher[1], Dirk Wulferding[1,2], Peter Lemmens[1,2], Raman Sankar[3], and Fang-Cheng Chou[3] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]NTU, Taipei, Taiwan

We report a comparative Raman study on the layered, 2D multiferroic compounds Ni_3TeO_6 and $PbNi_6Mn_2Te_3O_{18}$. The emergence of 2-magnon scattering enables a characterization of their magnetic subsystems. Phonon anomalies below the magnetic ordering temperatures evidence a strong coupling between lattice and spin degrees of freedom in both systems. Work supported by the Quantum- and Nanometrology initiative "QUANOMET" within Project NL-4 and NTH School "Contacts in Nanosystems".

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Magnetic properties of the spin-1 chain compound $NiCl_3C_6H_5CH_2CH_2NH_3$ — Ferdinand Lipps[1], Anke Arkenbout[2], Alexey Polyakov[2], Marco Günter[3], Timur Salikhov[4], Eugeniia Vavilova[4], Hans-Henning Klauss[3], Bernd Büchner[1], Thomas Palstra[2], and •Vladislav Kataev[1] — [1]IFW Dresden, 01069 Dresden, Germany — [2]University of Groningen, 9747 AG Groningen, The Netherlands — [3]TU Dresden, 01069 Dresden, Germany — [4]Zavoisky Physical Technical Institute, 420029 Kazan, Russia

We report experimental results of the static magnetization, ESR and NMR spectroscopic measurements of the Ni-hybrid compound $NiCl_3C_6H_5CH_2CH_2NH_3$. In this material $NiCl_3$ octahedra are structurally arranged in chains along the crystallographic a-axis. According to the static susceptibility and ESR data Ni^{2+} spins $S = 1$ are isotropic and are coupled antiferromagnetically (AFM) along the chain with the exchange constant $J = 25.5\,\mathrm{K}$. These are important prerequisites for the realization of the so-called Haldane spin-1 chain with the spin-singlet ground state and a quantum spin gap. However, experimental results evidence AFM order at $T_\mathrm{N} \approx 10\,\mathrm{K}$ presumably due to small interchain couplings. Interestingly, frequency-, magnetic field-, and temperature-dependent ESR measurements, as well as the NMR data, reveal an inhomogeneous ground state of co-existent mesoscopically spatially separated AFM ordered and spin-singlet state regions.