TT 78: Correlated Electrons: Poster Session

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

TT 78.1 Thu 15:00 Poster D

CT-QMC-simulations on the single impurity Anderson model with a superconducting bath — •Florian Sohn and Thomas Pruschke — Institut für theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Coupling a heavy fermion impurity to a superconducting lead induces a competition between the Kondo effect and superconductivity in the low temperature regime. This situation has been modeled with a single impurity Anderson model, where the normal state bath is replaced by a BCS-type superconducting bath in mean field approximation. We study this model using a continuous-time quantum Monte Carlo hybridization expansion algorithm. Results include the impurity Green's functions as well as the corresponding spectral functions obtained from analytic continuation. Two side bands are observed which we discuss in the light of Yu-Shiba-Rusinov states [1-3]. We gratefully acknowledge financial support by the DFG project PR293/13-1.
[1] Y. Luh, Acta Phys. Sin. **21**, 75 (1965)
[2] H. Shiba, Prog. Theor. Phys. **40**, 435 (1968)
[3] A. I. Rusinov, Sov. Phys. JETP **29**, 1101 (1969)

TT 78.2 Thu 15:00 Poster D

Dielectric and thermodynamic measurements on the magnetoelectric perovskite $EuTiO_3$ — •Johannes Engelmayer, Christoph Grams, Joachim Hemberger, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Germany

Various perovskite titanates $ATiO_3$ are known to undergo ferroelectric phase transitions, e.g., for $A = \mathrm{Ba, Pb, Cd}$. $BaTiO_3$ is the only ferroelectric alkaline-earth titanate, since ferroelectric long-range order is suppressed in $CaTiO_3$ and $SrTiO_3$ by quantum fluctuations, which is referred to as quantum paraelectric behavior. The rare-earth titanate $EuTiO_3$ is similar to $SrTiO_3$, since it has the same valencies (Eu^{2+},Ti^{4+}) and the same ionic radii. Both are cubic at room temperature and undergo a structural phase transition to tetragonal upon cooling. In contrast to the nonmagnetic Sr^{2+}, the half-filled 4f shell of Eu^{2+} with $S = 7/2$ has a large magnetic moment of $7\mu_B$. Below $T_N = 5.5$ K the localized 4f moments order antiferromagnetically, while rather small fields of 1.5 T are sufficient to saturate the magnetization. Here we present field- and temperature-dependent measurements of magnetization, specific heat, and thermal expansion, exhibiting characteristic anomalies at T_N. Broadband measurements of the permittivity reveal the dynamics of polar domain walls at the onset of the structural phase transition, as well as the materials quantum paraelectric nature that is masked by high conductivity for low frequencies.

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

TT 78.3 Thu 15:00 Poster D

Low-temperature structure and Fermi surface of (La,Ce)$TiGe_3$ — •Tobias Förster[1], Helge Rosner[2], Jacob Grasemann[1], Marc Uhlarz[1], Wolfram Kittler[3], Veronika Fritsch[4], Oliver Stockert[2], Jochen Wosnitza[1], and Hilbert v. Löhneysen[3] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Max Planck Institute f. Chemical Physics of Solids, Dresden, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]Institut für Physik, Universität Augsburg, Augsburg, Germany

$CeTiGe_3$ presents the rare case of a ferromagnetically ($T_C \approx 14$ K) ordered Kondo-lattice compound and is probably the first known example of an intermetallic hexagonal perovskite of the $BaNiO_3$ structure type. $LaTiGe_3$ may be used as its nonmagnetic reference, since both compounds crystallize in the same crystal structure [1,2]. To clarify the interplay between structural, localized, and itinerant degrees of freedom an accurate knowledge of the electronic band structure is necessary. Here, we present a detailed electronic-structure study of both compounds applying full potential density functional calculations. Since the Ge's atomic position couples strongly to the band structure at the Fermi energy, a low-temperature, high-resolution structure refinement was made. We attempt to separate the influence of different parameters on the topology of the respective Fermi surfaces and will compare our results with de Haas-van Alphen measurements.
[1] P. Manfrinetti et al., Solid State Commun. **135** (2005) 444.
[2] W. Kittler et al., PRB **88** (2013) 165123.

TT 78.4 Thu 15:00 Poster D

Thermal transport and thermodynamic properties of the Weyl monophosphide NbP — •Ulrike Stockert, Michael Baenitz, Binghai Yan, Claudia Felser, and Marcus Schmidt — Max Planck Institute for Chemical Physics of Solids, Dresden

NbP is a Weyl semimetal, which exhibits a huge positive magnetoresistance (MR) exceeding 8 x 10^5% at 2 K for an electrical current applied along b and a magnetic field of 9 T along c. The MR is further increasing roughly linearly up to at least 60 T. This finding has been attributed to an ultrahigh charge carrier mobility.

We performed thermal transport and specific heat measurements on NbP for the same configuration, namely the magnetic field B along c and the heat current along b. We find a huge change of the thermopower in magnetic fields with a maximum value of 800 μV/K at 9 T and 50 K. Such large effects have been rarely observed in bulk materials, the only example with a larger magnitude at our knowledge being the doped semiconductor InSb. We suggest that the high charge-carrier mobility held responsible for the giant magnetoresistance of NbP is also causing the large magnetothermopower. In addition, electron-phonon scattering processes may play a role, an idea which is also in line with the observation of quantum oscillations in the thermal conductivity of NbP. These are much larger than expected for the electronic contribution estimated from the Wiedemann-Franz-law. Quantum oscillations are also seen in the thermopower and specific heat data.

TT 78.5 Thu 15:00 Poster D

An integrable $S = \frac{1}{2}$ Heisenberg chain with impurity and modified density of states — •Yahya Öz and Andreas Klümper — Bergische Universität Wuppertal

Starting from the integrable Heisenberg XXZ model by use of the R-matrix a new model with impurity and modified dispersion relation is obtained. We consider the thermodynamical approach based on the well-known finite set of non-linear integral equations (NLIE) of convolution type for obtaining the integrable modification of the spinon energy-momentum dispersion for the derivation of the thermodynamic equations of this new model. In these equations, energy e and momentum p take a new dispersion relation of the form $e(p) \simeq p^\alpha$ for small momenta where $\alpha < 1$.

TT 78.6 Thu 15:00 Poster D

Quantum criticality gains long-time quantum correlations — •Rouhollah Jafari[1,2] and Alireza Akbari[1] — [1]Asia Pacific Center for Theoretical Physics, Pohang, Gyeongbuk 790-784, Korea — [2]Department of Physics, University of Gothenburg, Sweden

Using the general quantum compass model as an environmental system, the dynamical evolution of the decoherence factors, quantum correlations, and negativity of the central spins has been investigated for different initial states. The relation between the quantum-classical transition of the central system, and the occurrence of an avoided level crossing quantum phase transition in its surrounding system has been analyzed. It is well known that the gapless quantum criticality enhances the decay of decoherence factors[1], while our calculations represent a different story for the gapped critical environment. The results that have been found show that long-time quantum correlations at the critical point are an effect of gapped criticality, and maximum decaying occurs away from the critical point[2].
[1] H. T. Quanet al., PRL **96**, 140604 (2006)
[2] R. Jafari, and A. Akbari, EPL **111**, 10007 (2015)

TT 78.7 Thu 15:00 Poster D

Crystal Growth and Characterization of $CeFe_{1-x}Ru_x$ PO — •Tanita Ballé, Kristin Kliemt, and Cornelius Krellner — Goethe Universität Frankfurt, Kristall- und Materiallabor

CeRuPO is a one of the few heavy fermion systems, which order ferromagnetically at low temperatures ($T_C = 15$ K), because of dominant RKKY-interaction [1]. CeFePO on the other hand shows no long-range magnetic order even at low temperatures because of dominant Kondo effect [2] ($T_K = 10$ K). By substituting CeFePO with ruthenium we can reach a quantum critical point, at which the RKKY-interaction and the Kondo effect are equally strong [3]. To study the quantum critical

point, and to enlighten the question if the order stays ferromagnetically down to lowest temperatures, high quality crystals are needed. Here, the growth and characterization of the single crystals will be discussed. We obtained mm-sized single crystals of the unsubstituted CeRuPO and CeFePO by a modified Bridgeman method using tin as a flux. The quality of the crystals was verified by Powder-X-Ray-Diffraction, energy dispersive X-ray spectroscopy and Laue backscattering.

[1] C. Krellner et al., PRB **76**, 104418 (2007)
[2] E. M. Brüning et al., PRL **101**, 117206 (2008)
S. Lausberg et al., PRL **109**, 216402 (2012)
[3] S. Kitagawa et al., J. Phys. Soc. Jpn. **82**, 033704 (2013)

TT 78.8 Thu 15:00 Poster D

Tuning $ZrFe_4Si_2$ by Ge and Y substitution — •Katharina Weber[1,2], Nandang Mufti[1], Til Goltz[2], Theo Woike[3], Hans-Henning Klauss[2], Christoph Bergmann[1], Helge Rosner[1], and Christoph Geibel[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Institute of Solid State Physics, TU Dresden, Germany — [3]Institute for Structural Physics, TU Dresden, Germany

The intermetallic compound series AFe_4X_2 (A = Y, Lu, Zr; X = Si, Ge) presents a rare case of magnetic frustrated metallic systems. In particular $ZrFe_4Si_2$ is of strong interest because our results indicate this system to be very close to a quantum critical point (QCP) where Fe magnetic order disappears. To get a deeper insight into its ground state, we performed a detailed study of Ge and Y substituted $ZrFe_4Si_2$. The isovalent substitution of Ge for Si induces a negative chemical pressure as Ge is larger than Si. As expected from this, the substitution results in the formation of a well-defined antiferromagnetic order with Néel temperatures increasing up to 25 K at 40 % Ge. This confirms $ZrFe_4Si_2$ to be extremely close to the QCP, just on the magnetic side of it. With the second substitution series $Y_xZr_{1-x}Fe_4Si_2$ we investigate the development from the highly reduced antiferromagnetic order in $ZrFe_4Si_2$ towards the two magnetic transitions at 56 K and 76 K, which we see in YFe_4Si_2.

TT 78.9 Thu 15:00 Poster D

Unusual antiferromagnetic structure of $YbCo_2Si_2$ — N. Mufti[1,2], K. Kaneko[1,3], A. Hoser[4], M. Gutmann[5], C. Geibel[1], C. Krellner[1,6], and •O. Stockert[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [2]Department of Physics, State University of Malang, Malang, Indonesia — [3]Quantum Beam Science Center, Japan Atomic Energy Agency, Tokai, Japan — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [5]ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Didcot, United Kingdom — [6]Physikalisches Institut, Goethe-Universität Frankfurt, Frankfurt

We report on extensive powder and single crystal neutron diffraction experiments to study the magnetic structure in $YbCo_2Si_2$ below the Néel temperature $T_N = 1.7$ K in detail. Representation analysis has been used to find the possible magnetic structure models compatible with the experiments. Two different magnetically ordered phases can clearly be distinguished. At lowest temperatures a commensurate magnetic structure with a propagation vector $\mathbf{k}_1 = (0.25\ 0.25\ 1)$ and equal moments or about 1.4 μ_B/Yb is found, while the intermediate phase ($T > 0.9$ K) is characterized by an incommensurate amplitude-modulated magnetic structure with $\mathbf{k}_2 = (0.25\ 0.086\ 1)$. The magnetic structure in $YbCo_2Si_2$ is in stark contrast to all other compounds of the RCo_2Si_2 family (R = rare earth element) likely due to some itineracy of the Yb 4f states being responsible for the magnetism.

TT 78.10 Thu 15:00 Poster D

Frustrated magnetism in $Yb_2Fe_{12}P_7$ — •Kai Grube[1], Diego A. Zocco[1], Frank Weber[1], Sebastian Kuntz[1], Ryan Baumbach[2], James Hamlin[3], Ivy Lum[4], Jeff Lynn[5], Qingzhen Huang[5], Marc Janoschek[6], M. Brian Maple[4], and Hilbert von Löhneysen[1] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]National High Magnetic Field Laboratory, Tallahassee, USA — [3]Departement of Physics, University of Florida, Gainesville, USA — [4]Department of Physics, University of California, San Diego USA — [5]NIST Center for Neutron Research, Gaithersburg, USA — [6]Los Alamos National Laboratory, USA

$Yb_2Fe_{12}P_7$ is characterized by a low magnetic transition temperature of $T_N \approx 1$ K and the breakdown of Fermi-liquid behavior. These properties suggest the proximity to a quantum critical point (QCP). The non-Fermi-liquid (NFL) behavior, however, does not conform to the standard QCP scenario described by the Hertz-Millis-Moriya theory. We measured thermal expansion, magnetostriction and magnetization. The pressure dependence was studied up to 15 GPa using resistivity measurements in piston cylinder and diamond anvil cells. The measurements reveal that only a small fraction of the Yb moments participate in the long-range magnetic order. The Grüneisen ratio does not diverge for $T \to 0$ indicating that the NFL behavior is not related to a nearby pressure-induced QCP. In view of the unusual noncentrometric crystal structure, our observations might point to geometric frustration of the magnetic moments.

TT 78.11 Thu 15:00 Poster D

Fluctuation dynamics near the quantum critical point in the S=1/2 Ising chain $CoNb_2O_6$ — •Steffen Harms, Johannes Engelmayer, Thomas Lorenz, and Joachim Hemberger — II. Physikalisches Institut, University of Cologne, Germany

$CoNb_2O_6$ is a model system for quantum phase transitions in magnetic field. Its structure consists of layers of CoO_6 octhahedrons separated by non-magnetic NbO_6 layers. The edge-sharing oxygen octahedrons link the Co^{2+}spins via Co-O-Co superexchange and form 1D ferromagnetic zigzag chains along the orthorhombic c axis. Crystal field effects lead to an easy-axis anisotropy of the Co^{2+} moments in the ac plane and to an effective spin-1/2 chain system. The 1D spin system can be described by the Ising model. At T=0K a transverse magnetic field can induce a quantum phase transition from a long range ferromagnetic state into a quantum paramagnetic state. Employing measurements of the complex AC-susceptibility in the frequency range 10MHz $< \nu <$ 5GHz for temperatures down to 50mK we investigate the slowing down of the magnetic fluctuation dynamics in the vicinity of the critical field at $\mu_0 H$=5.25T [1].

Funded through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

[1]: A.W. Kinross et al. PRX **4**, 031008 (2014)

TT 78.12 Thu 15:00 Poster D

Chiral spin-orbital liquids with nodal lines — •Willian Massashi Hisano Natori[1], Rodrigo Gonçalves Pereira[1], and Eduardo Miranda[2] — [1]Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil — [2]Instituto de Física Gleb Wataghin, Unicamp, Campinas, Brazil

Quantum spin liquids (QSL) are strongly correlated systems that remain magnetically disordered down to 0 K. Although QSLs are known to be the ground state of many model Hamiltonians, their experimental discovery is debated, underlining the importance of research on spin liquid states arising from realistic Hamiltonian models. In this work, we propose a quantum spin-orbital liquid as a stable phase of a spin-orbital model in double ordered perovskites (DOP). This model accounts for antiferromagnetic interactions and strong spin-orbit coupling. We made a global SU(2) and compass symmetries explicit through a convenient representation. Afterwards, we rewrite the Hamiltonian in terms of Majorana fermion operators plus a Z_2 gauge field. A mean-field decoupling preserving the model symmetries was proposed, whose ground state is a QSL characterized by degenerate gapless Fermi lines. The fact that these lines are associated with a topological invariant and the presence of energetically separated surface states indicates that this QSL is topologically non-trivial. Some predicted results are compared with the experimental data available for the spin liquid candidate Ba_2YMoO_6.

TT 78.13 Thu 15:00 Poster D

Thermal Expansion and Magnetostriction Measurements on $PrIr_2Zn_{20}$ — •Andreas Wörl[1], Christian Stingl[1], Akito Sakai[1], Keisuke T. Matsumoto[2], Takahiro Onimaru[2], Toshiro Takabatake[2,3], and Philipp Gegenwart[1] — [1]Experimentalphysics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Graduate School of Advanced Sciences of Matter, Hiroshima University, Higashi-Hiroshima 739-8530, Japan — [3]Institute for Advanced Materials Research, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

Strong hybridization between electric quadrupole moments and conduction electrons gives rise to interesting physical phenomena such as new quantum phases and novel metallic properties. Non-fermi-liquid behavior based on the two channel Kondo effect is predicted by theory. $PrIr_2Zn_{20}$ crystallizes in the $CeCr_2Al_{20}$-type structure, where the Pr^{3+} ions are surrounded by the highly symmetric cubic crystal field of 16 Zn atoms. The ground state is the non-magnetic Γ_3 doublet and carries only electric quadrupole and a magnetic octupole moment. At $T_Q = 0.11$ K the electric quadrupole moments order in

a antiferroquadrupolar way. A superconducting transition occurs at $T_c = 0.05\,K$. The phase transition at $T_Q = 0.11\,K$ can be suppressed by high magnetic fields parallel to the [100] direction. We investigate the thermal expansion and magnetostriction at low temperatures. By applying high magnetic fields the system is tuned towards a quadrupolar quantum critical point. Furthermore the reaction of the system on breaking the cubic symmetry by compressive stress is explored.

TT 78.14 Thu 15:00 Poster D

Doping studies in hexagonal A_2IrO_3 — •Ina-Marie Pietsch, Friedrich Freund, and Philipp Gegenwart — Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86159 Augsburg, Germany

Hexagonal iridates A_2IrO_3 (A=Na or Li) are spin-orbit Mott insulators and candidate materials for the realization of the highly anisotropic bonding dependent Kitaev magnetic exchange [1]. However, details of the magnetic properties sensitively depend on the balance of various parameters such as bandwidth, Coulomb repulsion, spin-orbit coupling and the trigonal distortion of the IrO_6 octahedron. A partial substitution of Na by smaller Li as well as the partial magnetic depletion for A_2IrO_3 materials provides experimental input on the evolution of magnetic properties [2,3]. Based upon the previous results, a new series of doped A_2IrO_3 materials (including hyperhoneycomb β-Li_2IrO_3 [4]) is synthesized, characterized and magnetically investigated using SQUID magnetometry.

[1] Y. Singh et al., Phys. Rev. Lett. **108**, 127203 (2012).
[2] S. Manni et al., Phys. Rev. B **89**, 241103 (2014).
[3] S. Manni et al., Phys. Rev. B **89**, 241102(R) (2014).
[4] A. Biffin et al., Phys. Rev. B **90**, 205116 (2014).

TT 78.15 Thu 15:00 Poster D

^{7}Li and ^{23}Na NMR measurements on $(Na_{0.75}Li_{0.25})_2IrO_3$ — •Tusharkanti Dey[1], Markus Prinz-Zwick[2], Martina Schädler[2], Friedrich Freund[1], Soham Manni[1], Avinash Mahajan[2,3], Norbert Büttgen[2], and Philipp Gegenwart[1] — [1]EP-VI, Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]EP-V, Electronic Correlations and Magnetism, University of Augsburg, Germany — [3]IIT Bombay, India

An experimental realization of the proposed Kitaev spin-liquid phase in Na_2IrO_3 and Li_2IrO_3 is still a big challenge. Efforts to suppress the magnetic ordering in Na_2IrO_3 by substituting isoelectronic Li in the Na site was partially successful [1, 2]. An earlier report [1] suggests the optimum doping to be 25% where the magnetic ordering is suppressed to 6 K while the structure remains undisturbed. Interestingly, for the $(Na_{0.75}Li_{0.25})_2IrO_3$ sample Na and Li are crystallographically ordered where the Li ions reside at the centre of the Ir honeycombs [1]. We have studied the material using both ^{7}Li and ^{23}Na NMR. Results of our spectra, spin-lattice and spin-spin relaxation measurements will be discussed in the poster.

[1] S. Manni, S. Choi, I. I. Mazin, R. Coldea, M. Altmeyer, H. O. Jeschke, R. Valenti, and P. Gegenwart, Phys. Rev. B **89**, 245113 (2014)
[2] G. Cao, T. F. Qi, L. Li, J. Terzic, V. S. Cao, S. J. Yuan, M. Tovar, G. Murthy, and R. K. Kaul, Phys. Rev. B **88**, 220414(R) (2013)

TT 78.16 Thu 15:00 Poster D

Hints for a pressure-induced phase transition in the honeycomb lattice iridate Na_2IrO_3 probed by infrared microspectroscopy — •Volker Hermann[1], Jihaan Ebad-Allah[1,2], Friedrich Freund[1], Philipp Gegenwart[1], and Christine Kuntscher[1] — [1]Universität Augsburg, 86159 Augsburg, Germany — [2]Department of Physics, University of Tanta, 31527 Tanta, Egypt

Honeycomb lattice iridates A_2IrO_3 with A=Na, Li, Sr,... are discussed in terms of topological insulators and Mott insulators due to their strong spin-orbit coupling [1,2]. Na_2IrO_3 has a layered honeycomb structure with edge-sharing IrO_6 octahedra. We have carried out pressure-dependent reflection and transmission measurements on monocrystalline Na_2IrO_3 in the infrared and visible frequency ranges. With increasing pressure the phonon modes harden and the Ir 5d crystal field excitations change only slighly. Several observations suggest the occurrence of a pressure-induced phase transition, including splitting and screening of phonon modes.

[1] Ch. H. Kim et al., PRL **108**, 106401 (2012)
[2] Y. Singh and P. Gegenwart, PRB **82**, 064412 (2010)

TT 78.17 Thu 15:00 Poster D

Structural and magnetic properties of $Sr_2Y_{1+x}Ir_{1-x}O_6$ materials — •Gizem Aslan Cansever[1], Maximilian Geyer[1], Christian G.F. Blum[1], Sebastian Gass[1], Kaustuv Manna[3], Franziska Hammerath[1,2], Laura T. Corredor[1], Andrey Maljuk[1], A.U.B. Wolter[1], Sabine Wurmehl[1,2], and Bernd Büchner[1,2] — [1]IFW Dresden, Institute for Solid State Research, 01171 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01062 Dresden, Germany — [3]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Ir-based materials have attracted a lot of attention because of the competition between the spin-orbit coupling, Coulomb interaction and crystal field [1]. Sr_2YIrO_6 double perovskites with Ir^{+5} ($5d^4$) ions are generally considered to have a nonmagnetic ground state (J=0). However, Sr_2YIrO_6 double perovskites have been reported to exhibit long-range magnetic order at low temperature and the distorted IrO_6 octahedra were discussed to cause the magnetism in this compound [2]. In this study $Sr_2Y_{1+x}Ir_{1-x}O_6$ materials were investigated in relation to structural and magnetic properties with varying Y and Ir concentrations. The samples were prepared by solid-state chemical reaction method. Magnetic susceptibility measurements were performed down to 0.4 K.

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

TT 78.18 Thu 15:00 Poster D

High-field multi-frequency ESR spectroscopy of La_2CuIrO_6 — •Stephan Fuchs[1], Vladislav Kataev[1], Kaustuv Manna[1], Sabine Wurmehl[1], Anup Kumar Bera[3], Andrey Malyuk[1], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden,D-01171 — [2]Institut für Festkörperphysik, Technische Universität Dresden,D-01062 — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

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

TT 78.19 Thu 15:00 Poster D

Investigation of the Thermodynamic Properties of Insulating Pyrochlores — •J. Gronemann[1,2], E. L. Green[1], R. Schönemann[1,2], M. Uhlarz[1], H.D. Zhou[3], M. Ruminy[4], T. Fennell[4], M. Kenzelmann[4], and J. Wosnitza[1,2] — [1]HLD-EMFL, HZDR, Dresden, Germany — [2]TU Dresden, Germany — [3]Univ. of Tennessee, Knoxville, USA — [4]PSI, Villingen, Switzerland

Geometrically frustrated pyrochlores have gained interest in recent years due to their novel low temperature properties. In the insulating compounds $Pr_2Sn_2O_7$ and $Tb_2Ti_2O_7$ the magnetic Pr^{3+} and Tb^{3+} ions form corner sharing tetrahedrons and can develop long or short-range order corresponding to a spin-ice or spin-liquid state, respectively. Heat capacity was measured down to 100 mK to investigate the low temperature ground state. Despite the similarities between both samples (similar crystal structures and a non-Kramers doublet in the ground state [1-2]) our measurements show no long-range magnetic order in $Tb_2Ti_2O_7$ down to 100 mK, a possible spin-liquid candidate, while in contrast $Pr_2Sn_2O_7$ is a well-known "dynamic" spin-ice compound as evidenced by a sharp specific heat anomaly around 800 mK [2] and confirmed by our recent AC susceptibility measurements. Though in typical spin-ice compounds the anomaly is suppressed by applying high magnetic fields, in $Pr_2Sn_2O_7$, however, the peak broadens and shifts to higher temperatures with increasing field. Further investigations are underway to determine the exact nature of this state and why it differs so drastically from the isostructural $Tb_2Ti_2O_7$.

[1] L. Ventelon et al., PRB **91**, 224430 (2015)

[2] H. D. Zhou et al., PRL **101**, 227204 (2008)

TT 78.20 Thu 15:00 Poster D

Spin-strain effects in the frustrated magnet $Tb_2Ti_2O_7$ at low temperatures — •Y. Gritsenko[1,2], S. Zherlitsyn[1], J. Wosnitza[1,2], M. Ruminy[3], T. Fennell[3], and M. Kenzelmann[4] — [1]HZDR/HLD, Dresden, Germany — [2]TUD/IFP, Dresden, Germany — [3]PSI/LNS, 5232 Villigen PSI, Switzerland — [4]PSI/LDM, 5232 Villigen PSI, Switzerland

Geometrically frustrated magnets have attracted much attention, due to their tendency to build unconventional ground states with exotic excitations. $Tb_2Ti_2O_7$ possesses a pyrochlore lattice as building block of the crystallographic structure, providing a basis for geometric frustration. This cubic material features Curie-Weiss temperature of $\Theta_{CW} = -19$ K, but no long-range magnetic order has been detected down to 50 mK indicating a large frustration. The existence of a spin-liquid state has been suggested for $Tb_2Ti_2O_7$. Here, we present results of ultrasonic investigations of this material. The magnetic field was applied along the [110] direction at temperatures of 20, 150 and 300 mK. Clear anomalies were found for different acoustic modes. The temperature dependence of the sound velocity shows a softening at about 500 mK and step-like features at about 150 mK suggesting a low-temperature phase transformation. This investigation sheds new light on the role of lattice degrees of freedom and magneto-elastic interactions in this material.

This work has been partially supported by DFG through SFB 1143. We acknowledge the support of the HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL).

TT 78.21 Thu 15:00 Poster D

Magnetization of pyrochlore compounds at mK temperatures — •Lars Opherden[1,2], Thomas Herrmannsdörfer[1], Jianhui Xu[3], Nazmul Islam[3], Bella Lake[3], and Joachim Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden, HZDR, Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Abteilung Quantenphänomene in neuen Materialien, HZB, Berlin, Germany

Since spin-ice and magnetic-monopole behavior was observed in $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$, frustrated $A_2B_2O_7$ (A = rare-earth, B = transition metal) pyrochlores became a highly topical research area [1]. In this material class, magnetic A^{3+} ions sit on corner-sharing tetrahedra. The crystal electrical fields dominate the interaction. This results in the formation of Kramer doublets and the alignment of the moments along the local ⟨111⟩ direction, if the rare-earth ions have a odd number of unpaired electrons. The balance between dipole-dipole and ferro- or antiferromagnetic exchange interaction leads to the occurrence of highly frustrated magnetism with a variety of ground state configurations such as spin-ice, spin-liquid or all-in-all-out ordering [2]. Because the correlation temperature is mostly observed at $T < 1$ K, magnetization measurements at millikelvin (mK) temperatures are necessary to investigate these ground states. Here, we present measurements performed in a SQUID magnetometer, designed for the mK temperature range, on novel pyrochlore zirconates $A_2Zr_2O_7$ (A = Nd, Sm).

[1] S. T. Bramwell *et. al.*, Science **294**, 1495 (2001).
[2] J. S. Gardner *et. al.*, Rev. Mod. Phys. **82**, 5546 (2010).

TT 78.22 Thu 15:00 Poster D

NMR of the frustrated spin-ladder system copper-sulfolane — •D. Dmytriieva[1], Z. Zhang[1], M. Naumann[1], H. Kühne[1], J. Wosnitza[1], E. Wulf[2], and A. Zheludev[2] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Neutron Scattering and Magnetism, Laboratory for Solid State Physics, ETH Zürich, Switzerland

We present first results from NMR experiments on the frustrated spin-ladder compound $H_8C_4SO_2{\cdot}Cu_2Cl_4$ (copper-sulfolane). From a comparison of the ^{35}Cl NMR spectra to macroscopic susceptibility data, we demonstrate that the ^{35}Cl nuclei are suitable local probes for the magnetic correlations of the nearby Cu^{2+} $S = 1/2$ moments. At magnetic fields exceeding 3.75 T and temperatures approaching 1.6 K, we find an increase of the nuclear spin-lattice relaxation rate, signaling the onset of long-range magnetic order. For the structurally disordered version of this compound, specific-heat measurements indicate a strong suppression of the magnetic ordering temperature with surprisingly small concentrations of bromine substitution on the non-magnetic halogen site. It has been proposed that this phenomenology is driven by a novel mechanism, based on random frustration by bond disorder. In an approach to shed light on the substitution-induced modification of exchange couplings and correlations in the vicinity of the bromine sites as well as on the slow, long-range magnetic fluctuations at the transition to the ordered state, we show first results of ^{35}Cl and ^{81}Br NMR data obtained from high-quality single crystals.

TT 78.23 Thu 15:00 Poster D

Coexistence of spin frozen state and persistent spin dynamics in $NaSrCo_2F_7$ as probed by μSR and NMR — •Shanu Dengre[1], Rajib Sarkar[1], Sascha Albert Bräuninger[1], Jason W. Krizan[2], Felix Brückner[1], Philipp Materne[1], Hubertus Luetkens[3], Chris Baines[3], Hans-Henning Klauss[1], and Robert J. Cava[2] — [1]Institute for Solid State Physics, TU Dresden, D-01069, Germany — [2]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA — [3]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

^{23}Na -and ^{19}F NMR, and μSR experiments are performed to explore the microscopic properties of $NaSrCo_2F_7$, which is a newly discovered magnetically frustrated pyrochlore with weak bond disorder and with a frustration index of f = 42. While ^{23}Na and ^{19}F NMR experiments clearly suggest the presence of quasi static field distribution below ∼3 K as reflected in the huge NMR line broadening and wipe out effect of NMR signal intensity, μSR experiments on the other hand remains passive to this spin frozen state. Both NMR and μSR results indicate the slowing down of the magnetic (spin) fluctuations upon cooling towards the NMR spin frozen state. μSR relaxation rate increases slightly below ∼ 3 K, and remains not only constant down to 20 mK, but also stands independent in longitudinal magnetic field upto 4000 G implying that the spin fluctuations are dynamic. These observations suggest the coexistence of partial spin frozen state and persistent spin dynamics in $NaSrCo_2F_7$.

TT 78.24 Thu 15:00 Poster D

Spin Dynamics in the Strongly Magnetically Frustrated Compounds $YBaCo_3AlO_7$ and $YBaCo_3FeO_7$ Probed by NMR and ESR Spectroscopy — •Margarita Iakovleva[1,2,4], Julian Zeisner[1,2], Martin Valldor[3], Evgeniia Vavilova[4], Hans-Joachim Grafe[1], Stephan Zimmermann[1,2], Alexey Alfonsov[1], Vladislav Kataev[1], and Bernd Büchner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [4]E. K. Zavoisky Physical-Technical Institute, Kazan, Russia

In the Swedenborgite type compounds $YBaCo_3AlO_7$ and $YBaCo_3FeO_7$ the magnetic lattice can be described as a stacking of kagome layers, where unconventional ground states such as a spin liquid state can be expected due to the strong geometrical frustration. We performed a combined experimental study of magnetic properties of single crystals of $YBaCo_3AlO_7$ and $YBaCo_3FeO_7$ with high field ESR and high field NMR spectroscopy. The experimental results show the occurrence of short-range quasi static electron spin correlations at $T^* \approx 22$ K for $YBaCo_3AlO_7$ and $T^* \approx 60$K for $YBaCo_3FeO_7$ but not a long-range antiferromagnetic order. We compare our results with AC and DC susceptibility measurements and discuss a possible competition between a spin glass-like state due to intrinsic structural disorder and a spin liquid state arising from strong magnetic frustration in this materials.

TT 78.25 Thu 15:00 Poster D

Magnetic domains and frustration in metallic CePdAl — •Stefan Lucas[1], Zita Hüsges[1], Veronika Fritsch[2], Akito Sakai[2], Kai Grube[3], Christian Taubenheim[3], Chien-Lung Huang[1], Hilbert von Löhneysen[3], and Oliver Stockert[1] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]EP 6, Electronic Correlations and Magnetism, University of Augsburg, Germany — [3]Karlsruhe Institute of Technology, Germany

Magnetic frustration is an exciting topic in condensed matter physics, since it can lead to new ground states of materials, e.g. a spin liquid or spin glass state. Effects of magnetic frustration have been investigated intensively for insulating materials. However, the existence of magnetic frustration in metallic systems is still under debate. CePdAl is a metallic Kondo system, where geometric magnetic frustration arises from the formation of Ce ions on a distorted Kagomé lattice. Neutron scattering experiments revealed, that only two thirds of the magnetic Ce moments order antiferromagnetically below $T_N = 2.7$ K, whereas the other third remains mainly disordered. Thermodynamic as well as neutron scattering measurements are presented to verify the existence of partial magnetic frustration in CePdAl. Recently neutron diffraction experiments under magnetic fields applied along two orthogonal

directions in the magnetically hard basal plane were performed. They show opposite effects on the magnetic intensity of a selected magnetic domain depending on the field direction with respect to the propagation vector. If this is only an effect of different domain population or also due to a change in magnetic frustration shall be discussed.

TT 78.26 Thu 15:00 Poster D

Numerical evidence for quadrupolar-octopolar order in $RETM_2(Al,Zi)_{20}$ — •Jan Attig[1], Darrell Tse[2], Eric Kin-Ho Lee[2], Arun Paramekanti[2], and Yong Baek Kim[2] — [1]Institute for Theoretical Physics, University of Cologne — [2]Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada

Motivated by recent experiments on materials of the type $RETM_2(Al,Zi)_{20}$ (where RE is a rare earth and TM a transition metal element) we investigate a minimal model for the pseudo-spin degrees of freedom of the rare earth ions. The model is described by J1-J2 pseudo-spin interactions in three-dimensions where the XY part models quadrupolar order and the Ising part models octopolar order.

We use various computational methods such as simulating annealing to find the zero temperature phase digram and investigate further by using single-spin flip Monte Carlo simulations for finite temperature. One notable finding is the existence of non-coplanar spiral ordering of pseudo-spins, which may explain some of the experimental data on the electronic ordering in $RETM_2(Al,Zi)_{20}$.

TT 78.27 Thu 15:00 Poster D

Interplay of structural and magnetic properties in copper(II) sulfate hydrates $CuSO_4 \times n H_2O$ — Maria Rosner[1,2], Anne Henschel[1], Yurii Prots[1], Marcus Schmidt[1], •Helge Rosner[1], and Andreas Leithe-Jasper[1] — [1]MPI CPfS Dresden, Germany — [2]Martin-Andersen-Nexö-Gymnasium Dresden

Copper(II)-sulfate pentahydrate $CuSO_4 \times 5H_2O$ is likely the most abundant Cu(II) compound and well studied, including its quasi one-dimensional spin 1/2 magnetism. However, copper(II)-sulfates exist as a series of compounds $CuSO_4 \times nH_2O$ (n=0,1,3,5) that differ in their degree of hydration, exhibiting very distinct crystal structures and, in consequence, pronounced differences in their properties. Here, we present a systematic investigation of the series, comprising synthesis (powder and single crystals) , structural (XRD) and thermodynamical (DTA/TG, C_p, χ) characterization as well as electronic structure calculations. As the result, we obtain a consistent picture of the development of the magnetic behavior upon dehydration.

TT 78.28 Thu 15:00 Poster D

Fragmented S=1/2 alternating spin chains in layered monoclinic $Li_3Cu_2SbO_6$ — •Michael Richter[1], Changhyun Koo[1], Vladimir Nalbandyan[2], Elena Zvereva[3], Alexander Vasiliev[3], Igor Shukaev[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Chemistry Faculty, Southern Federal University, Rostov-na-Donu, Russia — [3]Faculty of Physics, Moscow State University, Moscow, Russia

We report the magnetic properties of polycrystalline layered $Li_3Cu_2SbO_6$ which reveals the coexistence of alternating $S = 1/2$ spin chains, spin chain fragments and quasi-free spins. Static magnetic susceptibility measurements show two contributions to the magnetic response, namely quasi-free spins at low-temperature and a spin-gapped magnetic subsystem with $\Delta \sim 120$ K. Quantitatively, the data imply that about half of the spins are organized in alternating Heisenberg chains with $J_1 = 75$ K and $J_2/J_1 = 0.6$. Our X-band ESR data corroborate well with this analysis by indicating three resolved resonance modes. High-frequency ESR shows powder-like spectra which are well described by an anisotropic g-factor with $g_{\parallel} = 2.31$ and $g_{\perp} = 2.05$. The magnetic response is ascribed to significant antisite disorder between Li and Cu-sites which yields quasi-free $S = 1/2$ spins at Li-sites as well as fragmentation of the spin chains in the Cu-layers.

TT 78.29 Thu 15:00 Poster D

Effect of explicit oxygen screening in the three-orbital cuprate model — •Xiaodong Cao[1], Cornelia Hille[2], Priyanka Seth[3], Thomas Ayral[3,4], Olivier Parcollet[3], Sabine Andergassen[2], and Philipp Hansmann[1] — [1]Max-Planck-Institute for Solid State Research Heisenbergstr. 1, 70569 Stuttgart , Germany — [2]Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [3]Institut de Physique Théorique(IPhT), CEA, CNRS, 91191Gif-sur-Yvette, Franc — [4]Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France

In the theoretical treatment of transition metal oxides we are always confronted with the question how important oxygen degrees of freedom are for ground state properties and low lying excitations. Different strategies have been employed in the past which can be separated into approaches that treat oxygen either implicitly as part of the effective transition metal 3d Wannier function or explicitly as non-interacting bath where correlated 3d states are "embedded". In the presented DMFT study we promote oxygen degrees of freedom to be active players for the correlated subspace by means of an RPA screening of the effective d-interaction which is now dynamic and included in a self-consistent way.

TT 78.30 Thu 15:00 Poster D

Electron Spin Resonance Spectroscopy on the Quasi-One-Dimensional Spin Chain Compound $Cu(NC_5H_5)_2(Cl_{1-x}Br_x)_2$ (x = 1.0, 0.98, 0.95) — •Julian Zeisner[1,2], Stephan Zimmermann[1,2], Vladislav Kataev[1], Michael Brockmann[3], Frank Göhmann[3], Michael Karbach[3], Andreas Klümper[3], Alexander Weisse[4], Matthias Thede[5], Andrey Zheludev[5], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Bergische Universität Wuppertal, Wuppertal, Germany — [4]Max-Planck-Institut für Mathematik, Bonn, Germany — [5]ETH Zürich, Zürich, Switzerland

Although known for decades low dimensional magnetic systems remain an active field in modern solid state physics. Among other aspects this is due to the peculiarities arising in reduced dimensions which complicated correct theoretical descriptions of such systems. Recently, however, progress was made in exact calculation of electron spin resonance (ESR) properties based on a Heisenberg-Ising Hamiltonian [1]. In our work we present a comparison of these predictions with ESR studies on the quasi-one-dimensional magnet $Cu(NC_5H_5)_2Br_2$. Measurements were performed over a wide frequency and temperature range giving insight into spin dynamics as well as spin structure and the magnetic anisotropy present in this compound. In addition the impact of a partial substitution of Br by Cl on spin dynamics is shown.

[1] M. Brockmann, F. Göhmann, M. Karbach, A. Klümper, and A. Weiße, PRB **85**, 134438 (2012)

TT 78.31 Thu 15:00 Poster D

Optical investigations on spin liquids — •Mathias Bories — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

In quantum spin liquids, localized spins interact antiferromagnetically but without long-range order down to zero temperature due to quantum fluctuations. Anderson predicted this phase to have resonating valence bonds as ground state and spin 1/2 excitations called "spinons". However, experiments provided only recently evidence for its existence in a few materials, amongst which the triangular-lattice charge transfer salts κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ and EtMe$_3$Sb(Pd(dmit)$_2$)$_2$. Various measurements on these organic materials observed no long-range magnetic order down to the lowest temperatures which supports the proposed spin liquid behavior. Still, the nature of the ground state and its origin are still under debate. Theoretical studies have recently suggested a large spinon Fermi surface that could contribute to the optical conductivity by spin-charge interactions, leading to additional absorption within the Mott gap following a power-law frequency dependence.

We performed broadband spectroscopy at low temperatures covering the range from THz frequencies up to the visible. Special emphasis was put on the investigation of various compounds, including both inorganic and organic quantum spin liquid candidates, to possibly observe similarities or differences. The comparison gives us the possibility to pin down intrinsic features and thus enhance the current understanding of this phase, and possibly also trigger theoretical progress.

TT 78.32 Thu 15:00 Poster D

Optical investigations of disorder in spin liquids — •Miriam Sanz Alonso — 1.Physikalisches Institut, Stuttgart, Deutschland

Quantum spin liquids (QSL) emerge from frustrated spins on a triangular lattice with anitferromagnetic interaction. As proposed by Anderson, frustration prevents long range magnetic order down to lowest temperatures. In his model the ground state consists of resonating valence bonds (RVB) and is therefore highly degenerate. One

of the most investigated QSL materials is the organic compound κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ which is a two-dimensional Mott insulator with triangular lattice. As it was also observed for closely related charge transfer salts, charge fluctuations may play a key role for the physical properties. Until now, this material was subject to magnetic, thermodynamic, transport and also some optical studies, supporting the proposed spin liquid behaviour. Recently, dielectric measurements observed typical fingerprints of relaxor ferroelectricity. Thus, we performed comprehensive spectroscopic investigations in the mid-infrared to track the temperature dependence of a charge-sensitive molecular vibration. As a result, sizeable charge disproportionation between the BEDT-TTF sites can be ruled out. In addition, we observed similar behavior in the closely-related compound κ-(BEDT-TTF)$_2$Ag$_2$(CN)$_3$. To examine the influence of disorder on the ground state, parameters like the cooling rate and chemical composition of the donor layer were varied.

TT 78.33 Thu 15:00 Poster D

Cluster Perturbation Theory for Spin Systems — •Benjamin Lenz, Salvatore R. Manmana, and Thomas Pruschke — Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany

Quantum cluster methods such as Cluster Perturbation Theory (CPT) or Variational Cluster Approximation (VCA) have been broadly applied to electron systems, but there are just very few applications to spin systems so far. Using Larkin's equations, a first order perturbation theory in cluster-cluster interactions can be constructed for spin systems and in a first attempt, dimerized Heisenberg chains have been addressed within CPT [1]. Here, we first benchmark the spectral functions and magnetization curves obtained for the Heisenberg XXZ chain by checking with exact Bethe ansatz results. Furthermore, we present CPT studies on Heisenberg zig-zag-ladders, which possess intriguing properties at high magnetic fields, and compare our findings with exact diagonalization.

Financial support via DFG through FOR1807 is gratefully acknowledged.

[1] A. S. Ovchinnikov, I. G. Bostrem, V. E. Sinitsyn, Theor. Math. Phys. **162**, 179 (2010).

TT 78.34 Thu 15:00 Poster D

Phase diagram of negative-hopping Bose-Hubbard model on triangular lattice — •Shijie Hu[1], Xuefeng Zhang[2], Axel Pelster[1], and Sebastian Eggert[1] — [1]Department of Physics and Research Center Optimas, Technical University Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Max Planck Institute for the Physics of Complex Systems Nöthnitzer Str. 38, 01187 Dresden, Germany

We study the phase diagram of the negative-hopping Bose-Hubbard model on the triangular lattice by using the parallel-tempering algorithm in the two-dimensional density matrix renormalization group (DMRG) method. For the integer-1 filling, we found a first-order transition from the chiral superfluild phase to the normal insulating phase where both U(1) and Z2 symmetry are spontaneously broken. Away from the integer-1 filling, we found a new phase corresponding to a kind of novel bond order. As the chemical potential increases, the negative-hopping Bose-Hubbard model undergoes two first-order transitions instead.

TT 78.35 Thu 15:00 Poster D

Variational Cluster Approximation for Iridates — •Teresa Schaller and Maria Daghofer — FMQ, Universität Stuttgart

We use the variational cluster approximation to investigate the phase diagram and one-particle spectral density of iridates, where kinetic energy, electronic interactions and spin-orbit coupling are all on comparable energy scales. The approach includes quantum fluctuations on a small cluster and exactly and included long-range order on a mean-field level. We will in particular investigate the filling of two holes in the t_{2g} subshell, as is realized in some iridium compounds. Hund's rule and spin-orbit coupling together favor then a local singlet ground state, while intersite exchange driven by the kinetic energy favors magnetism. We present the phase diagram resulting from this competition and the impact of crystal-field splitting.

TT 78.36 Thu 15:00 Poster D

Mean-field extension of the variational cluster approach — •Jan Lotze and Maria Daghofer — Universität Stuttgart, Institut für Funktionelle Materie und Quantentechnologien, Pfaffenwaldring 57, 70550 Stuttgart

The variational cluster approximation based on a self-energy approach can be used to study correlated-electron Hamiltonians: The self-energy of the system is replaced by that of a 'reference system' that has to have the same interaction, but can have different kinetic energy. In practice, the reference system consists of isolated clusters, which restricts the class of accessible models to those, where the interaction is local, e.g., as in the Hubbard model. Inter-site interactions can be included exactly within each cluster, but not on bonds connecting clusters.

We propose here to use a mean-field decoupling for these bonds. While this is an approximation that falls ouside the self-energy approach, a systematic improvement over simple mean-field treatments becomes possible, as fewer bonds are mean-field decoupled for larger directly solved clusters. We present first results of this extension for the t-J-U model.

TT 78.37 Thu 15:00 Poster D

Magnetic Excitations of Spin-Orbit and Hund's Rule Coupled Mott Insulators — •Michael Schmid and Maria Daghofer — FMQ Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

When both, Hund's-rule and spin-orbit coupling are strong, the local ground state of two electrons in d^4 iridates is a singlet. However, the triplet states are not very high in energy and kinetic-energy-driven interactions between ions can mix some triplet character into the overall ground state. We are here interested in mangetic excitaions of such compounds and complement an analytic approach based on the similarity to dimers with a numerical investigation. We make here use of a recently extension of a dynamical density-matrix embedding scheme to exciations.

TT 78.38 Thu 15:00 Poster D

Thermal transport in the Heisenberg-Kitaev model — •Alexandros Metavitsiadis and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We study the finite temperature thermal transport properties of the Kitaev-Heisenberg two-leg spin ladder, within the framework of linear response theory. For simultaneously non-vanishing Kitaev and Heisenberg exchange, we present results from numerical techniques, namely Exact Diagonalization and the Quantum Typicality, to explore the parameter space. In the absence of Heisenberg interactions, the model is exactly solvable, and we support our numerical findings with analytical results. In addition, the large number of conservation laws allows a detailed analysis of the transport properties in different Hilbert space subsectors, classified by different Z_2 gauge flux configurations. Finally we will focus on the breaking of integrability with the onset of a Heisenberg coupling on the ladder, starting from purely Kitaev exchange.

TT 78.39 Thu 15:00 Poster D

Frustration and Interaction in complex 2-dimensional Systems — •Malte Harland[1], Mikhail Katsnelson[2], and Alexander Lichtenstein[1] — [1]University of Hamburg — [2]Radboud University Nijmegen

We present a study of magnetic frustration in the Hubbard model. Frustration effects are a highly debated topic, since they are assumed to reveal new phases, e.g. spin liquids. To control the degree of frustration we interpolate the nearest-neighbour – next-nearest-neighbour hopping ratio of the square lattice. We choose a special 2d-lattice such, that the next-nearest-neighbour hopping exists only in every second square and is checkerboard-like distributed. We solve the half-filled Hubbard model and characterize different phases by means of the Cluster Dynamical Mean-Field Theory(CDMFT) for small, intermediate and large local Hubbard interactions. CDMFT maps the lattice problem onto a cluster in the Anderson-impurity model, that is solved numerically by a continuous-time quantum Monte Carlo solver (CTHYB). CDMFT enables us to investigate the non-local, short-range correlations of this frustrated system.

TT 78.40 Thu 15:00 Poster D

Dynamical mean-field and density-matrix renormalization-group studies of partial Kondo screening — •Matthias Peschke[1], Maximilian Aulbach[1], Fakher F. Assaad[2], and Michael Potthoff[1] — [1]I. Institut f. Theor. Physik, Universität Hamburg, Germany — [2]Institut f. Theor. Physik und Astrophysik, Universität Würzburg

The competition between Kondo screening and indirect magnetic exchange is studied for systems with geometrical frustration using dynamical mean-field theory (DMFT) and the density-matrix

renormalization group (DMRG). A systematic scan of the weak- to intermediate-coupling regime of the periodic Anderson model on the triangular lattice is performed for a wide range of fillings n by means of a site-dependent DMFT approach for a non-primitive unit cell containing three correlated f orbitals. The resulting phase diagram comprises different phases: a non-magnetic Kondo insulator at half-filling, a non-magnetic metallic Kondo-singlet phase for fillings slightly off half-filling and an antiferromagnetic phase at lower fillings driven by RKKY exchange. The antiferromagnetic and the Kondo-singlet phases are separated in the U-n phase diagram by an extended region of partial Kondo screening (PKS), i.e., a phase where the magnetic moment at one site in the unit cell is Kondo screened while the remaining two are coupled antiferromagnetically. The mean-field scenario is checked against numerically exact DMRG data. To this end we analyze different two- and four-point magnetic correlation functions for the Kondo-lattice on one-dimensional frustrated ladders.

TT 78.41 Thu 15:00 Poster D

Phonons in the helimagnet MnSi — •Matthias Mörtter, Frank Weber, and Daniel Lamago — Karlsruher Institut für Technologie, Institut für Festkörperphysik, Deutschland

The interactions of electronic, spin, and lattice degrees of freedom in solids result in complex phase diagrams, new emergent phenomena, and technical applications. Recently, it was shown by detailed inelastic neutron scattering measurements and ab-initio calculations that the phonon renormalization in non-centrosymmetric FeSi is intimately linked to its unconventional magnetic properties [1]. In the current study, we investigated the isostructural helimagnet MnSi over a large temperature range, 4 K $\leq$ T $\leq$ 500 K, using thermal inelastic neutron scattering. Focusing on wave vectors with clear phonon selection rules, we report phonons energies, line widths and intensities and compare them to the magnetic properties of MnSi.

[1] S. Krannich et al., Nature Comm. **6**, 9961 (2015).

TT 78.42 Thu 15:00 Poster D

Andreev transport in a correlated ferromagnet-quantum-dot-superconductor device — •Krzysztof P. Wójcik and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

In this contribution the spin-resolved Andreev transport in a hybrid ferromagnet-quantum-dot-superconductor device is discussed. In particular, the Andreev transmission and the resulting linear response conductance, calculated by means of the numerical renormalization group method, are analyzed. We show that, generally, the transport properties are conditioned by the interplay of correlations leading to the Kondo effect, superconducting proximity effect and the ferromagnetic-contact-induced exchange field. The exchange field greatly affects the low-energy behavior of the Andreev transmission by splitting the Kondo resonance. Moreover, it leads to a nonmonotonic dependence of the Andreev conductance on the dot level position. At low temperatures, the conductance has a peak at the particle-hole symmetry point, which however becomes quickly suppressed with increasing the temperature.

TT 78.43 Thu 15:00 Poster D

Magnetic Linear Dichroism of Collective Spin Excitations in a Chiral Magnet — •Ioannis Stasinopoulos[1], Stefan Weichselbaumer[1], Andreas Bauer[2], Helmuth Berger[3], Johannes Waizner[4], Markus Garst[4], Christian Pfleiderer[2] und Dirk Grundler[1,5] — [1]Physik-Department E10, TU München, Garching, Germany — [2]Physik-Department E51, TU München, Garching, Germany — [3]IMX, EPFL, Lausanne, Switzerland — [4]Institute for Theoretical Physics, Univ. Köln, Köln, Germany — [5]LMGN, IMX, EPFL, Lausanne, Switzerland

Skyrmions are spin whirls emerging in chiral-magnets and arranging in a hexagonal lattice with typical lattice constants of several tens of nm. Collective spin excitations in chiral magnets have generated large interest due to their potential for magnetologic and microwave applications. We describe the dynamics of the mean magnetization of the spin helix by considering the ellipticity and gyrotropy of its precession where we find magnetic linear dichroism over a remarkably large parameter range. Combining our calculations with broadband microwave spectroscopy on the insulator Cu_2OSeO_3, we demonstrate how to deliberately address different skyrmion or spin helix modes and induce finite wavevector transfer by using different coplanar waveguides and appropriate sample shapes. This detailed understanding allows to tailor the GHz response of chiral magnets for magnonic and spintronic devices.

Financial support by the DFG via TRR80 and NIM is acknowledged.

TT 78.44 Thu 15:00 Poster D

Correlations of magnetic crystalline order in critical chiral paramagnets — •Laura Köhler, Achim Rosch, and Markus Garst — Institute for theoretical physics, University of Cologne, Cologne, Germany

The formation of magnetic long-range order in chiral magnets like MnSi or Cu_3OSeO_3 corresponds to a so-called weak-crystallization process where strong interactions between critical paramagnons result in a fluctuation-induced first-order transition [1,2,3]. In these materials, the helimagnetic order and the Skyrmion lattice realize a one- and two-dimensional magnetic crystal, respectively. We explore crystalline correlations above the critical temperature T_c by considering the two-loop self-energy that involves three paramagnons with vanishing total momentum. In this case, the momenta of the paramagnons form a triangle. We discuss the importance of various triangular configuration and, in particular, equilateral triangles which are building blocks for two- as well as three-dimensional crystalline order.

[1] M. Janoschek et al., PRB **87**, 134407 (2013).
[2] A. Bauer, M. Garst and C. Pfleiderer, PRL **110**, 177207 (2013).
[3] J. Kindervater et al., PRB **89**, 180408(R) (2014).

TT 78.45 Thu 15:00 Poster D

Spin-wave excitations of magnetic skyrmion crystals — •Johannes Waizner and Markus Garst — Institute for Theoretical Physics, University of Cologne, Cologne, Germany

The cubic chiral magnets realize magnetic skyrmion crystals that correspond to topologically non-trivial, two-dimensional magnetic textures within the plane perpendicular to the applied field. The magnon excitations form, according to Bloch's theorem, a two-dimensional band structure. First, we focus on the magnetic resonances at the Gamma point [1] and discuss their properties, in particular, their ellipticity and gyrotropy. Second, we evaluate the energy- and momentum-dependent cross section expected in inelastic neutron scattering experiments. Third, we discuss the non-trivial topology of the magnon band structure that is reflected in finite Chern numbers of some of the bands.

[1] T. Schwarze, J. Waizner, M. Garst, A. Bauer, I. Stasinopoulos, H. Berger, C. Pfleiderer, and D. Grundler, Nat. Mater. **14**, 478 (2015).

TT 78.46 Thu 15:00 Poster D

Skyrmion caloritronics — •Sarah Schroeter, Achim Rosch, and Markus Garst — Institute for Theoretical Physics, Cologne, Germany

Skyrmions in insulating chiral magnets can be manipulated by applying a magnon current, for example, with the help of a temperature gradient. In turn, the scattering of spin-waves off skyrmions results in an emergent Lorentz force that leads to a topological magnon Hall effect. Based on our previous work [1,2], we discuss thermal transport of magnons in the presence of a dilute gas of skyrmions in a two-dimensional chiral magnet. Using the Boltzmann equation, we derive the thermal transport coefficients for the magnons as well as the effective equation of motion for the skyrmion positions.

[1] C. Schütte and M. Garst, PRB **90**, 094423 (2014).
[2] S. Schroeter and M. Garst, Low Temp. Phys. **41**, 817 (2015).

TT 78.47 Thu 15:00 Poster D

Spin chains with weak dissipation and pumping — •Florian Lange, Zala Lenarčič, and Achim Rosch — Universität zu Köln

We consider one-dimensional spin chains weakly coupled to the environment. The coupling is described by a Lindblad equation. Such a setup could, for example, be spin chains coupled to a bath of nuclear spins, by ultracold atoms or by atoms in cavities. In the limit of weak coupling, the steady state density matrix is approximately described by a (generalized) Gibbs ensemble. The parameters of this ensemble are obtained by tracking the evolution of the (approximate) conservation laws of the system arising from the coupling to the bath. Details of the couplings strongly influence the steady state and the system can be tuned to low, high or negative temperatures. Integrable and non-integrable spin chains show qualitatively different behaviour.

TT 78.48 Thu 15:00 Poster D

The Fermi surface of Sr_2RuO_4: spin-orbit and anisotropic

Coulomb interaction effects — Guoren Zhang, Evgeny Gorelov, •Esmaeel Sarvestani, and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Juelich, D-52425 Juelich, Germany

The topology of the Fermi surface of Sr_2RuO_4 is well described by local density approximation calculations with spin-orbit interaction, but the relative size of its different sheets is not. By accounting for many-body effects via dynamical mean-field theory, we show that the standard isotropic Coulomb interaction worsen or does not correct this discrepancy. In order to reproduce experiments, it is essential to include the Coulomb anisotropy. The latter is small but has strong effects; it competes with the Coulomb-enhanced spin-orbit coupling and with the isotropic Coulomb term. This mechanism is likely to be at work in other multi-orbital systems. Finally, we find a strong spin-orbital entanglement. This supports the view that the conventional description of Cooper pairs via factorized spin and orbital part might not apply to Sr_2RuO_4.

TT 78.49 Thu 15:00 Poster D

Highly Anisotropic Magnon Dispersion in Ca_2RuO_4: Evidence for Strong Spin Orbit Coupling — •Stefan Kunkemöller[1], Daniel Khomskii[1], Paul Steffens[2], Andrea Piovano[2], Augustinus Agung Nugroho[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut Laue Langevin, Grenoble, France — [3]Institut Teknologi Bandung, Indonesia

Ca_2RuO_4 is a key material for the understanding of the impact of spin-orbit coupling in 4d and 5d compounds, which is intensively studied at present. We have studied the magnon dispersion in Ca_2RuO_4 by inelastic neutron scattering on large single crystals containing 1

TT 78.50 Thu 15:00 Poster D

Temperature and polarization dependent Raman measurements of Ca_2RuO_4 — •Raphael German — II.Physikalisches Institut Köln

Ca_2RuO_4 is a Mott-like insulator, which undergoes a metal-insulator transition at 357 K and antiferromagnetic ordering at $T_N = 110$ K. Here, we report a temperature and polarization dependent Raman scattering study. Earlier studies claimed a Raman active two-magnon excitation around 100 cm^{-1}. This, however, is incompatible with the results from recent inelastic neutron scattering measurements, which suggest that this mode might be of single magnon nature. Instead, it is more likely that the feature which appears at $\sim$ 650 cm^{-1}, previously claimed to be due to a charge gap, has a two-magnon origin. Another open question in the interpretation of the Raman spectra is the origin of the high-energy peak at $\sim$ 1360 cm^{-1}. We will discuss the origin of the Raman peaks in terms of one- and two-magnon processes; magnon-phonon coupling, and possible crystal field excitations.

TT 78.51 Thu 15:00 Poster D

Field-induced ordered phases in the tetragonal quasi-2d dimer system $Ba_{0.9}Sr_{0.1}CuSi_2O_6$ — •Lars Postulka, Bernd Wolf, Pascal Puphal, Natalija Van Well, Franz Ritter, Cornelius Krellner, and Michael Lang — Goethe-Univeristät, Physikalisches Institut SFB/TR49, D-60438 Frankfurt(M),Germany

Magnetic compounds built of antiferromagnetically-coupled S = 1/2 dimers, allow to study finite-temperature critical phenomena under well-controlled conditions, including Luttinger-liquid, Berezinskii-Kosterlitz-Thouless-type topological order as well as Bose-Einstein-condensation of triplons. A material of high interest within this context is the quasi-2d coupled-dimer system $BaCuSi_2O_6$, which shows a field-induced ordered state exhibiting the signatures of a dimensional reduction [1]. This has been assigned to perfectly frustrated interlayer couplings, but has been questioned by Sheptyakov et al. since the system undergoes a tetragonal to orthorhombic phase transition at 100 K below which two different types of dimer layers exist [2]. Here we report magnetic properties of $Ba_{0.9}Sr_{0.1}CuSi_2O_6$ where the structural phase transition has been suppressed by strontium doping. We show results on magnetic susceptibility measurements as a function of temperature between 2 K < T < 300 K as well as field-dependant measurements up to B < 50 T at T = 1.5 K. We estimate the magnetic couplings and compare the results with those of the well-known parent compound $BaCuSi_2O_6$.

[1] S. E. Sebastian et al., Nature **441**, 617 (2006)
[2] D. V. Sheptyakov et al., PRB **86**, 014433 (2012)

TT 78.52 Thu 15:00 Poster D

Dimensional crossover in manganese based analogues of iron pnictides — •Manuel Zingl, Elias Assmann, and Markus Aichhorn — Institute of Theoretical Physics and Computational Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

The manganese pnicitides $BaMn_2As_2$ and LaOMnAs crystallize in the same structure as the extensively studied iron pnictide high-temperature superconductors $BaFe_2As_2$ and LaOFeAs. In contrast to the d^6 configuration of the iron systems, the manganese d-shell is only half-filled (d^5). As a consequence, electronic correlations are much stronger, placing these compounds at the verge of the Mott metal-insulator transition. In this region of the phase diagram materials are prone to enhanced magnetism, apparent in the remarkably high Néel temperature of 625 K for $BaMn_2As_2$. We demonstrate that the experimentally observed differences in the Néel temperatures, the band gap, and the optical properties of the manganese compounds under consideration can be traced back to their effective dimensionality. Our fully charge self-consistent DFT+DMFT calculations show excellent agreement with experiments, especially measured optical spectra.

TT 78.53 Thu 15:00 Poster D

Electronic structure of Mo and W investigated with positron annihilation — •Markus Dutschke[1], Michael Sekania[1,3], Diana Benea[4,5], Hubert Ceeh[6], Joseph-A. Weber[6], Christoph Hugenschmidt[6], and Liviu Chioncel[1,2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [3]Andronikashvili Institute of Physics, Tamarashvili 6, 0177 Tbilisi, Georgia — [4]Faculty of Physics, Babes-Bolyai University, Kogalniceanustr 1, Ro-400084 Cluj-Napoca, Romania — [5]Department of Chemistry, Ludwig Maximilian University of Munich, Butenandstr. 5-13, D-81377 München, Germany — [6]FRM II, Technische Universität München, Lichtenbergstrasse 1 D-85748 Garching, Germany

We perform electronic structure calculations to analyze the momentum distribution of the transition metals molybdenum and tungsten. We study the influence of positron-electron and the electron-electron interactions on the shape of the two-dimensional angular correlation of positron annihilation radiation (2D-ACAR) spectra. Our analysis is performed within the framework of the combined Density Functional (DFT) and Dynamical Mean-Field Theory (DMFT). Computed spectra are compared with recent experimental investigations.

TT 78.54 Thu 15:00 Poster D

Infrared study of the electronic phase diagram of $Cr_{1-x}V_xN$ — Fabian Meggle[1], •Jihaan Ebad-Allah[1,2], Francisco Rivadulla[3,4], and Christine Kuntscher[1] — [1]Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — [2]Department of Physics, University of Tanta, 31527 Tanta, Egypt — [3]Center for Research in Biological Chemistry and Molecular Materials, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain — [4]Department of Physical Chemistry, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain

Transition-metal nitrides have attracted great interest due to their mechanical and physical properties, which are useful for improving technological applications [1]. Several studies suggested that doping CrN with vanadium could lead to thermoelectric materials, which have optimal mechanical and chemical properties. CrN is a narrow gap, correlation-induced, semiconductor. Increasing vanadium doping in $Cr_{1-x}V_xN$ leads to a gradual suppression of the resistivity and a transition to itinerant-electron behavior through several phases including superconductivity in VN [2].

Here we report the results of a study on the electronic and vibrational properties of $Cr_{1-x}V_xN$ powder pellets by reflection measurements in the infrared and visible frequency ranges at ambient conditions. Furthermore, we carried out resistivity measurements to confirm the behaviour of the optical conductivity at low energy.

[1] P. F. McMillan, Nature Materials **1**, 19 (2002)
[2] C. X. Quintela, F. Rivadulla, and J. Rivas, PRB **82**, 245201 (2010).

TT 78.55 Thu 15:00 Poster D

Crystal growth and characterization of Ir-Te compounds — •Philipp Kurzhals, Frank Weber, Diego Zocco, Peter Adelmann, Michael Merz, Thomas Wolf, Sebastian Kuntz, and Kai Grube — Karlsruhe Institute of Technology, Institute for Solid State

Physics, Karlsruhe, Germany

$IrTe_2$ is distinguished by a structural phase transition whose origin is not understood up to the present day [1]. We grew crystals using the self-flux method starting from the reagents iriudium and tellurium and got specimen with varying amounts of $IrTe_2$ and Ir_3Te_8, analyzed by x-ray powder diffraction. We studied the transition near T = 280 K in magnetization measurements down to T = 1.8 K probing also for superconductivity, which was reported for intercalated samples [2]. Results indicate that the structural transition happens over an extended range in temperature and superconductivity is absent in our samples.

Ir_3Te_8 is not studied to such an extent as $IrTe_2$. In previous publications a structural phase transition is reported [3]. We characterized the transition by performing magnetization measurements and X-ray diffraction.

[1] G. L. Pascut et al., PRL **112**, 086402 (2014)
[2] J. J. Yang et al., PRL **108**, 116402 (2012)
[3] L. Li et al., PRB **87** (2013).

TT 78.56 Thu 15:00 Poster D

Angle-Resolved Photoemission Spectroscopy of rare earth $LaSb_2$ — Matteo Michiardi[1], •Fabian Arnold[1], G. Shwetha[2], V. Kanchana[2], Vaitheeswaran Ganapathy[3], Karl Frederik Faerch Fisher[1], Axel Svane[1], Marco Bianchi[1], Bo Brummerstedt Iversen[1], and Philip Hofmann[1] — [1]Aarhus University, Denmark — [2]IIT-Hyderabad, India — [3]University of Hyderabad, India

Several rare earth diantimonides have been found to exhibit intriguing electronic properties such as anisotropic linear and non-saturating magnetoresistance. Among these materials, $LaSb_2$ is not only considered for application in magnetoresistive devices but it is also found to be superconducting at low temperatures and it is investigated as candidate material to host charge density wave phases. Despite the several studies on its transport properties, the electronic structure of $LaSb_2$ is still largely unknown. Here we present an angle-resolved photoemission spectroscopy and ab-initio calculation study of $LaSb_2(001)$. The observed band structure is found to be in good agreement with theoretical predictions. Our results reveal that $LaSb_2$ is a semimetal with a strongly nested two-dimensional Fermi surface. The low energy spectrum is characterized by four massive hole pockets and by four shallow, strongly directional, electron pockets that exhibit Dirac-like dispersion. We speculate on the possibility that this peculiar electronic structure drives the magnetoresistance to its quantum limit, explaining its unconventional behavior.

TT 78.57 Thu 15:00 Poster D

Ground state properties of MnB_4 — •Jan Lennart Winter[1], Nico Steinki[1], Dirk Schulze Grachtrup[1], Dirk Menzel[1], Stefan Süllow[1], Arno Knappschneider[2], and Barbara Albert[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, TU Darmstadt, Germany

Recently, single crystalline MnB_4 was synthesized for the first time, yielding microscale crystals with dimensions of the order of 200 μm [1]. Based on band structure calculations, it was argued that the material is semiconducting as result of a Peierls distortion. Conversely, in a study of polycrystalline material it was concluded that the material is a weakly ferromagnetic metal [2].

To establish if MnB_4 is a semiconductor we have carried out single crystal four point resistivity measurements. For this purpose a setup for measuring microscale samples was developed and characterized. Qualitatively, we find semiconducting behavior (increasing resistivity for decreasing temperature), although a band gap could not be derived because of a non-linear Arrhenius plot. Our data are consistent with MnB_4 being a pseudogap/small gap material as proposed in [1]. A pronounced sample dependence of the transport properties points to the presence of impurity states. For the single crystals no ferromagnetic signatures could be obtained, suggesting an extrinsic cause of it in polycrystalline material.

[1] A. Knappschneider et al., Angew. Chem. **126**, 1710 (2014)
[2] H. Gou et al., PRB **89**, 064108 (2014)

TT 78.58 Thu 15:00 Poster D

Scaling of the Optical Conductivity in the Transition from Thermal to Many-Body Localized Phases — •Robin Steinigeweg[1], Jacek Herbrych[2], Frank Pollmann[3], and Wolfram Brenig[4] — [1]University of Osnabrück — [2]CCQCN and University of Crete — [3]MPIPKS Dresden — [4]Technical University Braunschweig

We study the frequency dependence of the optical conductivity $\mathrm{Re}\,\sigma(\omega)$ of the Heisenberg spin-1/2 chain in the transition from thermal to many-body localized phases induced by the strength of a spatially random magnetic field. Using the method of dynamical quantum typicality, we calculate the real-time dynamics of the spin-current autocorrelation function and obtain the Fourier transform $\mathrm{Re}\,\sigma(\omega)$ in high frequency resolution and for system sizes L much larger than $L \sim 14$ accessible to standard exact-diagonalization approaches. We unveil that the low-frequency behavior of $\mathrm{Re}\,\sigma(\omega)$ is well described by $\mathrm{Re}\,\sigma(\omega) \approx \sigma_{\mathrm{dc}} + a\,|\omega|^{\alpha}$, with $\alpha \approx 1$ in a wide range of the thermal phase and up to the many-body localized phase. We particularly detail the decrease of σ_{dc} as a function of increasing disorder for strong exchange anisotropies. We further find that the temperature dependence of σ_{dc} is consistent with the existence of a mobility edge.

TT 78.59 Thu 15:00 Poster D

Non-Equilibrium transport study in strongly correlated hetero structures — •Milos Radonjic[1,2], Ivan Rungger[3], and Liviu Chioncel[1] — [1]Center for Electronic Correlations and Magnetism, TP III, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [3]Mathematics and Modelling, National Physical Laboratory, Hampton Rd, Teddington, Middlesex, UK, TW11 0LW

The effects of local electronic interactions and finite temperatures upon the non-equilibrium transport properties across the metallic heterostructure Cu_4CoCu_4 are studied. Results are obtained by combining DFT and equilibrium DMFT solver on one side, and DFT and non-equilibrium steady state impurity solver based on second order perturbation in Hubbard interaction U, on the other side. Results of these two methods are compared for the transmission. It is shown that local, but dynamical electronic correlations reduce the total transmission at the Fermi level, and also increase the spin polarization. The multi-orbital non-equilibrium steady state impurity solver is formulated in the Keldysh Green's function formalism and allows us an access to all non-equilibrium quantities, such as non-equilibrium steady state current.

TT 78.60 Thu 15:00 Poster D

Self-consistent Born approach to strongly correlated electron systems in non-equilibrium — •Gerhard Dorn — TU Graz, Austria

The self-consistent Born master equation method is apt to describe the non-equilibrium behaviour of strongly correlated electron systems which are weakly coupled to non-interacting leads.

The poster compares the self-consistent Born approach with different other methods, like Born Markov master equation or Cluster Perturbation Theory (CPT), and shows the improvements according to correct representation of the Coulomb blockade or of the lead induced level broadening.

TT 78.61 Thu 15:00 Poster D

Boundary-driven dissipative quantum chains in large external fields — •Zala Lenarcic[1] and Tomaz Prosen[2] — [1]Institute for theoretical physics, University of Cologne, D-50937, Germany — [2]Faculty for mathematics and physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia

We treat the nonequilibrium transport as a consequence of a combined driving: from a pseudo-force, originating in the bias in Markovian processes at the system's boundaries, and from a real force due to an external field gradient g. For strong field gradients a systematic perturbation theory of the steady state current and slowest decay modes of the density matrix can be formulated for a general inhomogeneous XXZ spin 1/2 chain. From the explicit asymptotic expression for the current it is clear that by combining both drivings arbitrarily large current rectification can be achieved under $g \to -g$ in the presence of interaction. Moreover, via tailored field profiles one can obtain further control over the strength of stationary current.

[1] Z. Lenarčič and T. Prosen, PRE **91**, 030103(R) (2015).

TT 78.62 Thu 15:00 Poster D

Combining ab initio wavefunction methods with dynamical mean-field theory: A feasibility study with NiO — •Daniil Tolloui-Mantadakis, Marc Hoeppner, Theodoros Tsatsoulis, Andreas Grueneis, and Philipp Hansmann — Max Planck Institute for Solid State Research, Stuttgart, Germany

In materials science, Density Functional Theory has been proved to be, so far, the most reliable and efficient tool for computational simulations of compounds. Effects of electronic correlations, however, conflict with the effective single particle picture of DFT. The first step beyond - by means of perturbation theory - emerges in various implementations of the so called GW method, but also here computations are questionable in non-perturbative regimes, e.g., close to the Mott-Hubbard metal to insulator transition. Only computationally costly non-perturbative methods like dynamical mean-field theory can help to provide answers on reduced Hilbert spaces of effective Hamiltonians. The widely used combination of DMFT with DFT methods is, however, always confronted with the conceptual difference between the two approaches and the so called double counting errors cannot be avoided. In our study we replace DFT with Hartree-Fock or Hartree-Fock+MP2 theory which does not pose this problem when connected with DMFT. Retaining non-local self energies on a static mean field level we perform a feasibility study of fully self consistent HF+MP2+DMFT for the example of NiO.

TT 78.63 Thu 15:00 Poster D

Spin-Orbit functional renormalization for unconventional Fermi surface instabilities — •Mario Fink — Institut für Theoretische Physik und Astrophysik Lehrstuhl für Theoretische Physik I Am Hubland 97074 Würzburg

The functional renormalization group has been successfully employed to describe the pairing mechanism in e.g. the cuprates and iron pnictides. For the latter, the expansion to multi-orbital models proved both necessary and revealing, providing a concise microscopic understanding of the extended s-wave order parameter. As another aspect of complexity of the electronic band structure, spin-orbit coupling (SOC) has been identified as an essential ingredient for the appearance of topological superconductors and further intricate unconventional Fermi surface instabilities. We present an expanded scheme of the functional renormalization group that incorporates the coupling between orbital and spin degrees of freedom. We consider atomic SOC as well as Rashba SOC in order to explore unconventional phases that mix singlet and triplet pairing instabilities in the particle-particle and the particle-hole channel. We illustrate our approach at the example of representative multi-orbital spin-orbit models.