TT 30: Correlated Electrons: Spin Systems and Itinerant Magnets – Frustrated Magnets 3 (jointly with MA)

Time: Tuesday 9:30–13:00 Location: H 0110

TT 30.1 Tue 9:30 H 0110

Collinear order in the frustrated spin-$\frac{1}{2}$ antiferromagnet $Li_2CuW_2O_8$ — •Alexander A. Tsirlin[1], Ramesh Nath[2], Kumar Ranjith[2], Deepa Kasinathan[3], and Markos Skoulatos[4] — [1]NICPB, Tallinn, Estonia — [2]Indian Institute of Science Education and Research, Trivandrum, India — [3]MPI CPfS, Dresden, Germany — [4]Laboratory of Neutron Scattering, PSI, Villigen, Switzerland

$Li_2CuW_2O_8$ is a three-dimensional spin-$\frac{1}{2}$ antiferromagnet that features collinear spin order despite abundant magnetic frustration that would normally trigger a non-collinear incommensurate order, at least on the classical level. Using density-functional calculations, we establish the spin lattice comprising two non-coplanar triangular networks that introduce frustration along all three crystallographic directions. Magnetic susceptibility and heat capacity reveal a 1D-like magnetic response, which is, however, inconsistent with the naive spin-chain model. Moreover, the high saturation field of 29 T compared to the susceptibility maximum at as low as 8.5 K give strong evidence for the importance of interchain couplings and the magnetic frustration. Below $T_N \simeq 3.9$ K, $Li_2CuW_2O_8$ develops collinear magnetic order with parallel spins along a and c and antiparallel spins along b. The ordered moment is about 0.7 μ_B according to neutron powder diffraction. This qualifies $Li_2CuW_2O_8$ as a unique three-dimensional spin-$\frac{1}{2}$ antiferromagnet, where collinear magnetic order is stabilized by quantum fluctuations.

Financial support of the Mobilitas program (ESF) is acknowledged.

TT 30.2 Tue 9:45 H 0110

Magnetism of the effective spin-1/2 compound Cs_2CoCl_4 — •Oliver Breunig[1], Markus Garst[2], Eran Sela[2], Achim Rosch[3], Benjamin Buldmann[3], Petra Becker[4], Ladislav Bohatý[4], Ralf Müller[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University — [3]Institut für Theoretische Physik, Universität zu Köln — [4]Institut für Kristallographie, Universität zu Köln

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. We measured specific heat and thermal expansion at temperatures down to 50 mK and in magnetic fields applied along different crystallographic axes. At temperatures between 0.3 and 4 K a description as an effective spin-1/2 XXZ chain arises. By considering both, thermal as well as virtual excitations of higher crystal field states, we find that the spin chain is in the XY-limit with an anisotropy $J_z/J_\perp \approx 0.12$ substantially smaller than previously believed. Magnetic order arises at a field-dependent temperature $T_C(H)$ due to inter-chain couplings which form a frustrated triangular lattice. Depending on the orientation of the magnetic field we observe various ordered phases. We present phase diagrams for different field directions and discuss the origin of the phases.

TT 30.3 Tue 10:00 H 0110

Equivalence of chemical and external pressures in RCoLnO — •Giacomo Prando[1], Gianni Profeta[2], Samuele Sanna[3], Carmine Ortix[1], Rustem Khasanov[4], Anand Pal[5], Veer Awana[5], Vladislav Kataev[1], Bernd Büchner[1,6], and Roberto De Renzi[7] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany — [2]SPIN-CNR and Dipartimento di Fisica, Universitá dell'Aquila, Italia — [3]Dipartimento di Fisica, Universitá di Pavia, I-27100 Pavia, Italia — [4]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [5]National Physical Laboratory (CSIR), New Delhi, India — [6]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — [7]Dipartimento di Fisica, Universitá di Parma and CNISM, Italia

We report on the local magnetic properties of the series of ferromagnetic (FM) materials RCoLnO (R = La, Pr, Nd, Sm; Ln = As, P) as investigated by means of muon spin spectroscopy under pressure P and electron spin resonance (ESR). The effect of P is shown to be quantitatively equivalent to the chemical lattice shrinkage triggered by the different ionic radii of R ions. This is verified for both experimental-dependent quantities (i. e., magnetic field at the muon site [1]) and for intrinsically material-dependent properties (i. e., FM critical temperature T_C). Results of ESR in a wide range of temperature and magnetic field clearly display that magnetism is of localized nature, despite the overall metallic behaviour of these materials.

[1] G. Prando et al., *Phys. Rev. B* **87**, 064401 (2013)

TT 30.4 Tue 10:15 H 0110

Stabilisation of the tetragonal structure in (Ba,Sr)$CuSi_2O_6$ — •Pascal Puphal[1], Natalija Van Well[1], Franz Ritter[1], Wolf Assmus[1], Denis V. Sheptyakov[2], Christian Rüegg[2,3], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Uni. Frankfurt — [2]Lab. for Neutron Scattering and Imaging, PSI, Switzerland — [3]Dep. of Quantum Matter Physics, Uni. of Geneva, Switzerland

$BaCuSi_2O_6$ is a spin dimer system presenting a 2D Bose-Einstein condensation of triplons at low temperatures and high magnetic fields. $BaCuSi_2O_6$ undergoes a structural phase transition below 100 K into an orthorhombic structure with two different dimer layers, leading to a complex Hamiltonian. Presently, the role of frustration in the orthorhombic structure is under debate. We present results for strontium substitution on the barium side and investigate the structural transition with low temperature x-ray and neutron powder diffraction. In addition the results of magnetic and specific-heat measurements are discussed. Surprisingly, we found that already small amounts of Sr (x = 0.05) lead to a suppression of the structural phase transition and the higher symmetric tetragonal crystal structure with only one sort of Cu-dimers is stable down to lowest temperatures. With increasing Sr-content the unit cell volume decreases and the intra-dimer spacing increases. Therefore, $(Ba_{1-x}Sr_x)CuSi_2O_6$ is a spin dimer system in a well-defined tetragonal crystal structure with the possibility to control the exchange interactions. Further manipulation is possible in substituting silicon by germanium (especially considering co-substitution) resulting in an increased cell volume and intra-dimer spacing.

TT 30.5 Tue 10:30 H 0110

Non-linear bond operator theory and 1/d expansion for coupled dimer magnets — •Darshan G. Joshi and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

For coupled-dimer Heisenberg magnets, a paradigm of magnetic quantum phase transition, we develop a systematic expansion in 1/d, where d is spatial dimension, using bond operators. We apply this technique to a model of dimers on a hyper-cubic lattice, a generalization of the square-lattice bilayer Heisenberg model to arbitrary d. We calculate physical observables at zero temperature in both the quantum paramagnetic and anti-ferromagnetic phases and show that the 1/d expansion consistently describes the entire phase diagram including the quantum critical point. In particular, we determine the dispersion and spectral-weight distribution of the elementary excitations, including the Higgs mode of the anti-ferromagnetic phase.

TT 30.6 Tue 10:45 H 0110

Magnetic properties in hexagonal iridates — •Friedrich Freund, Soham Manni, and Philipp Gegenwart — EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Hexagonal iridates A_2IrO_3 (A=Na or Li) are promising candidates for the realization of the Kitaev interaction, which is an anisotropic and bonding dependent interaction that can lead to novel types of spin liquid behavior. We report the synthesis, characterization and magnetic properties of poly- and single crystals of Na_2IrO_3 and two polytypes of Li_2IrO_3 [1,2]. All three materials have a threefold coordination of edge sharing IrO_6 octahedra giving rise to Kitaev exchange. While Na_2IrO_3 and α-Li_2IrO_3 form planar honeycomb layers a three-dimensional network is realized in β-Li_2IrO_3. At high temperatures, the magnetic susceptibility of all systems displays Curie-Weiss behavior with fluctuating effective 1/2 moments while at low temperatures differently ordered states are found whose properties have been investigated by neutron powder diffraction, resonant x-ray diffraction and inelastic neutron scattering [3,4].

Work in collaboration with A. Biffin, R. D. Johnson, Sungkyun Choi, A. Bombardi, P. Manuel, R. Coldea, A. Jesche and Y. Singh.

[1] Y. Singh et al., PRL **108**, 127203 (2012).
[2] T. Takayama et al., arXiv:1403.3296 (2014).
[3] A. Biffin et al., PRB **90**, 205116 (2014).
[4] S.K. Choi et al., PRL **108**, 127204 (2012).

TT 30.7 Tue 11:00 H 0110

Analysis of the optical conductivity for A_2IrO_3 (A = Na, Li) from first principles — •Ying Li[1], Kateryna Foyevtsova[2], Harald O. Jeschke[1], and Roser Valentí[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada

In this talk we will present results for the optical conductivity of Na_2IrO_3 obtained within density functional theory by including spin-orbit (SO) and correlation effects (U) as implemented in GGA+SO+U. We identify the various interband transitions and show that the underlying quasi-molecular-orbital nature of the electronic structure in Na_2IrO_3 translates into distinct features in the optical conductivity. Most importantly, we will discuss that the parity of the underlying quasi-molecular orbitals built out of Iridium t2g orbitals appears to be the main factor in determining strong and weak optical transitions. We will also present optical conductivity calculations for Li_2IrO_3 and discuss the similarities and differences with Na_2IrO_3.

15 min. break.

TT 30.8 Tue 11:30 H 0110

Raman scattering on the Honeycomb Lattice Iridates A_2IrO_3 (A=Na,Li) — Vladimir Gnezdilov[1,2], Robert Bohle[1], •Peter Lemmens[1], Soham Manni[3], Friedrich Freund[3], and Philipp Gegenwart[3] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE NAS, Ukraine — [3]IP, Univ. Augsburg

Inelastic light scattering studies on single crystals of $(Na_{1-x}Li_x)_2(Ir_{1-y}Ti_y)O_3$ (x = 0, 0.1, 0.2; y = 0, 0.025) show a polarization and temperature dependent broad band as well as phonon anomalies. We discuss these observations with respect to the relevance of the Kitaev-Heisenberg model and Majorana Fermions for A_2IrO_3.

Work supported by RTG-DFG 1953/1, Metrology for Complex Nanosystems.

TT 30.9 Tue 11:45 H 0110

Magnetic heat transport in Sr_2IrO_4 — •Frank Steckel[1], Hidenori Takagi[2], Bernd Buechner[1,3], and Christian Hess[1,3] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden — [2]Max-Planck-Institute for Solid State Research, 70569 Stuttgart — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden

The layered perovskite Sr_2IrO_4 is a $5d$ transition metal oxide with an enhanced spin-orbit coupling leading to a Mott insulating ground state with $J_{\text{eff}} = \frac{1}{2}$. It exhibits canted antiferromagnetism below $T_N = 240$ K with an antiferromagnetic coupling constant of about $J = 0.1$ eV. Thermal conductivity measurements along the ab plane of a Sr_2IrO_4 single crystal provide evidence for a contribution of magnons (below T_N) to the thermal conductivity, similar to that of the isostructural 2D $S = \frac{1}{2}$ Heisenberg antiferromagnet La_2CuO_4, where a significant magnonic contribution to the heat transport is known.

TT 30.10 Tue 12:00 H 0110

Relation between structural evolution and effective Ir moments upon applied pressure during synthesis in $Ba_3YIr_2O_9$ — •Hannes Stummer, Tusharkanti Dey, Sabine Wurmehl, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden, Germany.

The intensively investigated material class of Iridium oxide based materials provides a variety of new and unknown combinations of magnetic properties with interesting novel or exotic ground states [1]. These Iridate compounds often appear in a perovskite type structure or a related derivative which are very favorable for crystal structure modifications under high pressure. High pressure synthesis therefore can be used to tune or change the magnetic properties appearing under normal pressure [2]. The Iridate $Ba_3YIr_2O_9$ crystallizes under ambient pressure synthesis in a hexagonal structure and exhibits magnetic ordering below 4 K. A synthesis pressure of 8 GPa advances the material to form a cubic double perovskite structure which is (meta-)stable at ambient pressure. For this high pressure configuration the magnetic ordering is suppressed [3]. We will present our recent results about the systematic high pressure synthesis and characterization of $Ba_3YIr_2O_9$ samples grown under different growth pressure. The main focus will be on the correlation between structural and magnetic properties depending on the applied pressure during the synthesis process.

[1] B. J. Kim et al., PRL 101, 076402 (2008).
[2] J.G. Cheng et al., PRB 88, 205114 (2013).
[3] T. Dey et al., Phys. Rev. B 88, 134425 (2013).

TT 30.11 Tue 12:15 H 0110

Propagation of the spin-orbit exciton due to the Jahn-Teller effect in systems with strong on-site spin-orbit coupling — •Ekaterina Plotnikova[1], Maria Daghofer[2], Jeroen van den Brink[1], and Krzysztof Wohlfeld[3,4] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]University of Stuttgart Pfaffenwaldring 57 D-70550 Stuttgart — [3]Stanford University and SLAC National Accelerator Laboratory, 2575 Sand Hill Rd, Menlo Park, CA 94025 USA — [4]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland

In this work we study the interplay between the strong spin-orbit coupling and electron-phonon interaction in the strongly correlated transition metal oxides with partially filled 5d shells. We show that even relatively weak electron-phonon coupling may lead to qualitatively different physics of the 5d oxides than the one discussed so far. Thus, we derive the effective interaction between the j 'spin-orbit' coupled isospins which follows from the orbital-only interaction induced by the cooperative Jahn-Teller effect. Next, we show that such interaction may lead to a novel type of propagation of the j = 3/2 spin-orbit exciton in the ordered j = 1/2 antiferromagnet which, unlike in the pure superexchange model does not require coupling to the j =1/2 'magnon' excitations.

TT 30.12 Tue 12:30 H 0110

Anisotropic Ru^{3+} - $4d^5$ - magnetism in the α-$RuCl_3$ honeycomb system: susceptibility, specific heat and Zero field NMR — •Michael Baenitz[1], Mayukh Majumder[1], Helge Rosner[1], Alexander Tsirlin[2], Hiroshi Yasuoka[1], and Markus Schmidt[1] — [1]MPI for the Chemical Physics of Solids, 01187 Dresden, Germany — [2]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

Low dimensional $4d$- and $5d$-magnets show a wide variety of magnetic ground states due to crystal electric field (CEF) splitting and strong spin-orbit coupling (SOC). The Heisenberg-Kitaev model was applied for the competing bond-dependent magnetic exchange interactions in the $5d$-honeycomb lattices (Li_2IrO_3, Na_2IrO_3). α-$RuCl_3$ turns out to be an excellent candidate for that model because the low-spin 3+ state of Ru ($4d^5$) is equivalent to the low-spin 4+ state of Ir ($5d^5$). Hexagonal α-Ru trichloride single crystals exhibit a strong magnetic anisotropy and we show that upon applying fields up to 14 T in the honeycomb plane the successive magnetic order at $T_1 = 14$ K and $T_2 = 8$ K could be completely suppressed whereas in the perpendicular direction the magnetic order is robust. Furthermore the field dependence of χ(T) implies coexisting ferro- and antiferromagnetic exchange between in-plane components of Ru^{3+}-spins, whereas for out-of-plane components a strong antiferromagnetic exchange becomes evident. ^{101}Ru zero-field nuclear magnetic resonance evidence a complex (probably chiral) long-range magnetic order below 14 K. The large orbital moment on Ru^{3+} is found in density-functional calculations.

TT 30.13 Tue 12:45 H 0110

Local and non-local correlation effects on the frustration degree in $VOMoO_4$ and Li_2VOSiO_4 — •Amin Kiani and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

$VOMoO_4$ and Li_2VOSiO_4 are considered a realization of the two-dimensional J_1-J_2 quantum antiferromagnetic Heisenberg model. In order to study their magnetic properties we calculate the static lattice spin susceptibility $\chi(\mathbf{q}, T)$ by using the local density approximation+dynamical mean field theory (LDA+DMFT) and its cluster extension; we adopt the local vertex approximation. We show that both systems undergo a phase transition to a three-dimensional ordered state with in-plane antiferromagnetic Neel order for $VOMoO_4$ and in-plane antiferromagnetic collinear order for Li_2VOSiO_4. We extract the effective magnetic couplings from the high temperature magnetic susceptibility. For both materials we discuss the frustration degree and local and non-local correlations effects.