TT 6: Quantum Magnets and Molecular Magnets (joint session TT/MA)

Time: Monday 9:30–13:00 Location: H 3010

TT 6.1 Mon 9:30 H 3010

Frustrated spin ladders in quasi-1D $S = \frac{1}{2}$ Heisenberg magnet balyakinite $CuTeO_3$ — •Helge Rosner[1] and Oleg Janson[2] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Deutschland — [2]Institut für Festkörperphysik, TU Wien, Österreich

Copper tellurium oxides are enjoying increasing attention as a promising playground for quantum magnetism [1]. A chemically simple compound, the natural mineral balyakinite $CuTeO_3$ features an intricate crystal structure with Cu_2O_6 dimers connected by TeO_4 tetrahedra into a 3D network. Magnetization measurements indicate a sizable spin gap which is not closed in a magnetic field of 60 T. By using DFT calculations, we show that the magnetism of balyakinite is quasi-1D, and can be described by a frustrated ladder model with four antiferromagnetic exchanges: the dominant rung exchange $J_\perp$, sizable $J_\parallel$ and weak $J'_\parallel$ that alternate along both legs, as well as the weak frustrated cross-coupling $J_\times$. Using the DFT+U estimates of the exchange integrals, we calculate the spin correlations in the ground state. Peculiarities of the magnetic excitation spectrum will be briefly discussed.
[1] M. R. Norman, arXiv:1708.05100.

TT 6.2 Mon 9:45 H 3010

Extreme field-sensitivity of the magnetic tunnelling in Fe-doped Li_3N — •Manuel Fix[1], James H. Atkinson[2], Paul C. Canfield[3,4], Enrique del Barco[2], and Anton Jesche[1] — [1]EP VI, EKM, University of Augsburg, D-86159, Germany — [2]Department of Physics, UCF, Orlando FL 32816, USA — [3]The Ames Laboratory, ISU, Ames, Iowa 50011, USA — [4]Department of Physics and Astronomy, ISU, Ames, Iowa 50011, USA

The magnetic properties of dilute $Li_2(Li_{1-x}Fe_x)N$ with $x \sim 0.001$ are dominated by the spin of single, isolated Fe atoms [1]. Below $T = 10$ K the spin-relaxation times become temperature-independent, indicating a crossover from thermal excitations to the quantum tunnelling regime.

The spin-flip probability increases tremendously in *transverse* magnetic fields, proving the resonant character of this tunnelling process. Upon application of *longitudinal* fields, on the other hand, the ground-state degeneracy is lifted and the tunnelling condition destroyed. We show time dependent magnetization measurements performed on single crystals in various longitudinal magnetic fields at temperatures $T = 2-16$ K. An increase of the relaxation time by four orders of magnitude in applied fields of only a few milliTesla reveals exceptionally sharp tunnelling resonances. This strong field dependence of the spin reversal could be employed to create stable ($\mu_0 H_z = 3$ mT) but switchable ($H_z = 0$) magnetic 'quantum bits' at elevated temperatures.
[1] A. Jesche *et al.*, Nature Comm. **5**:3333 (2014)

TT 6.3 Mon 10:00 H 3010

In- & interchain exchange constants of Li_2CuO_2: the origin of the ferromagnetic inchain ordering — •S.-L. Drechsler[1], R. Klingeler[2], W. Lorenz[2], R. Kuzian[3], L. Hozoi[1], R. Jadav[1], J. Richter[4], H. Rosner[5], U. Nitzsche[1], A. Tsirlin[6], and S. Nishimoto[1,7] — [1]IFW-Dresden, Germany — [2]Heidelberg University, Germany — [3]Inst. f. Problems of Material Science, Kiev, Ukraine — [4]MPI-PKS, Dresden, Germany — [5]MPI-CPfS, Dresden, Germany — [6]Augsburg University, Germany — [7]TU Dresden, Germany

Li_2CuO_2 takes a special place among frustrated chain compounds with edge-sharing CuO_4 units and a ferromagnetic (FM) nearest neighbor (NN) in-chain coupling J_1 due to its ideal planar CuO_2 chain structure and its well-defined 3D Neél-type ordering below $T_N \approx 9$ K of adjacent chains whose magnetic moments are aligned FM along the chains (b-axis). There are only frustrating AFM *interchain* couplings (IC) with adjacent chains *shifted* by half a lattice constant b. *No* room is left for strong unfrustrated IC in shtark contrast with a recently proposed scenario [1]. The AFM IC with dominant NNN components plays a decisive role in the stabilization of the FM alignment of the magnetic moments along b. Although weak, with 8 NNN IC it is significant enough to prevent a competing non-collinear spiral type ordering. We report realistic values of all relevant exchange constants based on two DFT and quantum chemistry calculations in full accord with a spin-wave analysis of INS, RIXS, and magnetic susceptibility $\chi(T)$ data. The large $J_1 \approx$ -230 K is ascribed to a sizable direct FM Cu-O coupling $K_{pd} \approx 100$ meV.
[1] G. Shu *et al.*, New J. Phys. **19**, 023026 (2017).

TT 6.4 Mon 10:15 H 3010

Magnetic susceptibility and high frequency EPR studies on three isostructural $Fe_2^{III}Ln_2^{III}$ complexes — •Silvia Menghi[1], Changhyun Koo[1], Yan Peng[2], Christopher Anson[2], Annie Powell[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — [2]Institute of Inorganic Chemistry, Karlsruhe Institut of Technology, Karlsruhe, Germany

Magnetic interactions and anisotropy of three 3d/4f heteronuclear metal-organic complexes are studied by means of high-frequency electron paramagnetic resonance (HF-EPR) and magnetic susceptibility measurements. All complexes under study exhibit isostructural tetranuclear core motifs $[(Fe_2^{III}Ln_2^{III}(\mu_3\text{-}OH)_2(teaH)_2(O_2CCPh)_6]\cdot 3MeCN$ (L=Y,Gd,Dy). The HF-EPR data show various resonance branches, each of which with finite zero field splitting. The static magnetic susceptibility data imply strong antiferromagnetic coupling of $J_{FeFe} = -6.71(4)$ cm^{-1} between the two Fe^{III} centers. The coupling between Fe and Ln was found to be weak and ferromagnetic. In order to gain quantitative insight into the anisotropy and the Fe-Dy exchange interaction, simulations have been performed using a proper hamiltonian which applies a Ising concept for the lanthanide ions.

TT 6.5 Mon 10:30 H 3010

Effect of radicals on coupling and anisotropy in mono- and dinuclear Ni(II) complexes with an azopyridine ligand — •Sven Spachmann[1], Roland Bischoff[2], Changhyun Koo[1], Hans-Jörg Krüger[2], and Rüdiger Klingeler[1,3] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Faculty of Chemistry, TU Kaiserslautern, Kaiserslautern, Germany — [3]Center for Advanced Materials, Heidelberg University, Heidelberg, Germany

We present static magnetization and high-frequency electron paramagnetic resonance (HF-EPR) studies on metallorganic mono- and dinuclear Ni(II)-complexes with radical and non-radical azopyridine ligands. In the monomer, the radical is coupled ferromagnetically to the Ni(II) spin, thereby forming an $S = 3/2$ ground state. In the non-radical mononuclear system, anisotropy is of the easy-plane type with $D_{Ni} = 4.0$ K and $|E| = 0.32$ K.

We observe a strong effect of the radical bridge on the dimer systems: While the non-radical azopyridine-bridged Ni(II)-dimer has a singlet ground state with a weak intradimer coupling of $J \approx 20$ K, a strong ferromagnetic coupling $J_{Ni-rad} \approx -500$ K is observed in the radical azopyridine-bridged Ni(II)-dimer between the radical and the Ni(II)-ions. The antiferromagnetic Ni-Ni coupling in the radical-bridged dimer $J_{Ni-Ni} = 25$ K is of the same order as without the radical. The HF-EPR and magnetization measurements confirm the $S = 5/2$ ground state and axial symmetry. We obtain $g_z = 2.126$ and $D_{5/2} = -0.844$ K, which corresponds to a single-ion anisotropy of $|D_{Ni}| = 4.2$ K.

TT 6.6 Mon 10:45 H 3010

Highly dispersive magnons with spin-gap like features in the frustrated ferromagnetic chain system $Ca_2Y_2Cu_5O_{10}$ by inelastic neutron scattering — M. Matsuda[1], J. Ma[1], V.O. Garlea[1], T. Ito[2], H. Yamaguchi[2], K. Oka[2], •S.-L. Drechsler[3], R. Yadav[3], L. Hozoi[3], H. Rosner[4], R. Schumann[5], R. Kuzian[6], and S Nishimoto[3,5] — [1]Quantum Matter Division, Oak Ridge, NRL, USA — [2]Natiomal Institute of AIST, Tsukuba, Japan — [3]IFW-Dresden, Germany — [4]MPI-CPfS, Dresden, Germany — [5]TU Dresden, Germany — [6]Inst. f. Problems of Material Science, Kiev, Ukraine

We report an inelastic neutron scattering study including its theoretical description for $Ca_2Y_2Cu_5O_{10}$ and map out the full large magnetic dispersion relation extending up to 53 meV. A doubly frustrated linear Heisenberg-type spin chain model with two inchain and two diagonal antiferromagnetic (AFM) interchain couplings (IC) analyzed within linear spin-wave theory reproduces well the observed strong dispersion in chain direction and q weak one perpendicularly. The large dispersion leads to a record value of the NN intrachain coupling $| J_1 | \approx 280$ K which points to a large direct FM Cu-O coupling K_{pd} value slightly above 100 meV. Our J_1-value resolves an old puzzle of FM inchain ordering vs. an improper AFM pseudo Curie-Weiss (CW) behavior for $\chi(T)$. It yields a true FM CW-regime above 1500 K, only. The

observed "gaps" at 11.5 and 28 meV stem from an interaction with a phonon mode and the synenergetic disorder influence on the CuO_2 chains by the incommensurate alternating cationic YCa-chains distorting the O positions and a specific quantum effect from the AFM IC, respectively.

TT 6.7 Mon 11:00 H 3010

Magnetism of atacamite, $Cu_2Cl(OH)_3$ — •Leonie Heinze[1], Randirley Beltran-Rodriguez[2], Gael Bastien[2], Anja U.B. Wolter[2], Manfred Reehuis[3], Jens-Uwe Hoffmann[3], Kirrily C. Rule[4], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig, Germany — [2]IFW Dresden, Dresden, Germany — [3]HZB, Berlin, Germany — [4]ANSTO, Kirrawee, Australia

Atacamite, $Cu_2Cl(OH)_3$, has been reported to exhibit magnetic behavior characteristic of a frustrated quantum magnet. Notably, an antiferromagnetic transition at $T_N = 9.0\,K$ has been observed and, further, susceptibility measurements previously carried out indicate a Curie-Weiss temperature $|\Theta_{CW}| \gg T_N$ [1,2]. So far, attempts have been undertaken to determine the symmetry of the magnetic ground state of this material by means of μSR and NMR measurements on polycrystalline material [2,3], however with contradictory results.

Starting from this given situation, we have reinvestigated the magnetic properties of atacamite [4]: Mineral single-crystals were studied by means of susceptibility and magnetization measurements along the principal crystal axes as well as elastic neutron scattering. This way, we have established the symmetry of the magnetic ground state and present new insights into the unusual magnetic properties of atacamite.

[1] X. G. Zheng, *et al.*, Solid State Commun. **130**, 107 (2004).
[2] X. G. Zheng, *et al.*, Phys. Rev. B, **71**, 174404 (2005).
[3] K. Zenmyo, *et al.*, J. Phys. Soc. Jpn., **82**, 084707 (2013).
[4] L. Heinze, *et al.*, Physica B, doi.org/10.1016/j.physb.2017.09.073 (2017).

15 min. break.

TT 6.8 Mon 11:30 H 3010

Alternating ferro- and antiferromagnetic Heisenberg chain: from dimer to Haldane limit — •Niklas Casper and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Braunschweig, Germany

We present results of a study of the $S = 1/2$ Heisenberg chain with alternating ferro- and antiferromagnetic exchange, J_2 and J_1 respectively. This system interpolates from a dimer to a Haldane chain as $j = |J_2/J_1|$ varies from 0 to ∞. Using perturbation theory (PT) and quantum Monte Carlo based on the stochastic series expansion (SSE) method, we study elementary excitations, thermodynamic properties, and the dynamic structure factor $S(\mathbf{q}, \omega)$. For $j \ll 1$ we find good agreement between PT and SSE. For arbitrary j we show that $S(\mathbf{q}, \omega)$, obtained from SSE, scales between triplons at $j \ll 1$ and a Haldane chain spectrum at $j \gg 1$. Finally, we contrast our findings for the spin gap versus j against existing literature.

TT 6.9 Mon 11:45 H 3010

Field Control of Magnonic Heat Flow — •Benjamin Köhler and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

Insulating quantum magnets allow for genuine spin transport phenomena without carrier dynamics. Controlling such transport by means of external fields is vital for potential device design. Here we study thermal conductivity of a two dimensional square lattice spin-1/2 Heisenberg antiferromagnet in the presence of an external field. The latter is used to manipulated the heat flow due to spin canting.

Using nonlinear spin wave theory and a Kubo approach we evaluate the thermal conductivity taking into account current relaxation via intrinsic magnon decay for finite fields and temperature. Semiquantitative estimates for attainable variations of the heat conductivity in realistic materials will be presented as a function of the temperature and the external fields, suggesting interesting implications for spin caloritronic applications.

TT 6.10 Mon 12:00 H 3010

Suppression of spin-crossover by dynamic Jahn-Teller effect in C_{60}^{3-} — •Dan Liu, Naoya Iwahara, and Liviu Chibotaru — Theory of Nanomaterials Group, University of Leuven, Leuven, Belgium

In conventional spin crossover systems, the vibrational degrees of freedom enhances the entropic effect in excited high-spin terms resulting from the softening of vibrations [1]. Here, we show an opposite effect of vibration on the spin crossover taking C_{60}^{3-} as an example [2]. The vibronic states resulting from dynamical Jahn-Teller effect in C_{60}^{3-} are obtained using the numerical diagonalization of the linear $p^n \otimes 8d$ Jahn-Teller Hamiltonian with the currently established coupling parameters. It is found that the Jahn-Teller effect stabilizes the low-spin states, resulting in the violation of Hund's rule. The energy gain due to the Jahn-Teller dynamics is found to be comparable to the static Jahn-Teller stabilization. The Jahn-Teller dynamics influences the thermodynamic properties via strong variation of the density of vibronic states with energy. Thus, the large vibronic entropy in the low-spin states enhances the effective spin gap of C_{60}^{3-} quenching the spin crossover. This finding is used for the rationalization of the experimental data on the spin gaps in various fullerides.

[1] P. Gütlich, A. Hauser, and H. Spiering, Angew. Chem. Int. Ed. 33, 2024 (1994).
[2] D. Liu, N. Iwahara, and L. F. Chibotaru, arXiv:1711.00340 [cond-mat.mtrl-sci].

TT 6.11 Mon 12:15 H 3010

Andreev transport through single-molecule magnets — •Filip Pawlicki and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland

Transport characteristics of a single molecule magnet coupled to two ferromagnetic and one superconducting lead are studied theoretically by means of the real-time diagrammatic technique. The coupling to the ferromagnets is assumed to be weak, while the coupling to the superconductor can be arbitrary. The quantities of interest include the Andreev current, differential conductance, tunnel magnetoresistance (TMR) and current cross-correlations. It is shown that the system exhibits splitting of Andreev states due to additional degrees of freedom of the molecule. The TMR and current cross-correlations are used to quantify the contribution of crossed and direct Andreev reflections to the current. We also compare our results to those obtained for a quantum dot in a similar three-terminal setup and discuss the possibility of using molecules for Cooper pair splitting.

TT 6.12 Mon 12:30 H 3010

Manifestations of a coherent Kondo lattice formed in adatoms — •Richard Korytár[1], María Moro Lagares[2], and David Serrate[3] — [1]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [3]Institute of Nanoscience of Aragon (INA), University of Zaragoza, Spain

In a recent experiment, chains of magnetic adatoms were constructed on a pristine metallic surface. A careful analysis by scanning-tunneling spectroscopy demonstrates that the Kondo screening overtakes magnetic interactions at all accessible chain lengths. A comparison with many-body calculations allows to address diverse real space aspects of the coherent Kondo lattice, such as: overlapping Kondo clouds, long-range mediated hybridization and Fermi surface effects. The phenomenology of the onset of heavy fermions in these systems can be discussed.

TT 6.13 Mon 12:45 H 3010

Formation of Local Magnetic Order in Atomic-Scale Ir Junctions — •Markus Ritter, Martin Keller, Torsten Pietsch, and Elke Scheer — Department of Physics, University of Konstanz, D-78467 Konstanz, Germany

The transition metals Pt, Pd, and Ir are paramagnets close to the Stoner transition of ferromagnetism. However, in reduced dimensions, such as small clusters and atomic contacts, a magnetically ordered state has been predicted [1]. In atomic contacts of the elements Pt and Pd, the emergence of local magnetic order has been experimentally confirmed recently [2, 3]. Currently there is no demonstration of such phenomena in Ir. Therefore, we investigate the magnetic properties of atomic Ir contacts and monoatomic chains [4]. The occurrence of local magnetic order is deduced from magnetoconductance (MC) and anisotropic magnetoconductance (AMC) measurements. The rich MC behavior is interpreted in the framework of a microscopic model of the local magnetic configuration and is compared to earlier findings in Pt and Pd contacts. Furthermore, in many contacts electronic transport (dI/dV) spectroscopy shows a pronounced zero-bias anomaly (ZBA) and further features, which are currently not fully understood. The ZBA is analyzed in the context of Kondo screening of the local magnetic moment in the junction.

[1] Delin, Tosatti. Phys. Rev. B **68**, 144434 (2003).
[2] Strigl et al. Nat. Commun. **6**, 6172 (2015).
[3] Strigl et al. Phys. Rev. B **94**, 144431 (2016).
[4] Thiess et al. Phys. Rev. Lett. **103**, 217201 (2009).