TT 47: Quantum Magnets, Molecular Magnets and Skyrmions

Time: Wednesday 15:00–18:45 Location: H23

TT 47.1 Wed 15:00 H23

Electric field control of magnonic heat flow — •Benjamin Köhler and Wolfram Brenig — Institut für Theoretische Physik, Technische Universität Braunschweig, Germany

Insulating quantum magnets allow for genuine spin transport phenomena without carrier dynamics. Here we study the thermal conductivity of a two dimensional square lattice spin-1/2 Heisenberg antiferromagnet in the presence of a spatially confined, external electric field. The latter is used to alter the Dzyaloshinskii-Moriya interaction and hence the spin canting which controls the heat flow.

Using linear spin wave theory and a Kubo approach we evaluate the thermal conductivity taking into account current relaxation via intrinsic magnon-phonon scattering for finite fields and temperature. Semi-quantitative estimates for attainable variations of the heat conductivity in realistic materials will be presented as a function of the temperature, the external fields, and the size of the region the field is applied to.

TT 47.2 Wed 15:15 H23

NMR of the two-dimensional $S = 1/2$ Heisenberg antiferromagnet CuPOF — •D. Dmytriieva[1,2], Z. T. Zhang[1], M. Uhlarz[1], C. P. Landee[3], J. Wosnitza[1,2], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Clark University, Worcester, Massachusetts, USA

The metal-organic compound $[Cu(pz)_2(2\text{-}OHpy)_2](PF_6)_2$ (CuPOF) is a molecular-based analog of the two-dimensional square-lattice quantum $S = \frac{1}{2}$ Heisenberg antiferromagnet with well-isolated Cu(pz) layers and a very low $k_B T_N/J = 0.21$ ratio ($J/k_B = 6.8$ K, $T_N = 1.38$ K). We present a focus study of the low-T phase transition to long-range order, performed via ^{1}H and ^{31}P nuclear magnetic resonance (NMR) and high-field magnetometry. The very good agreement between the measured high-field magnetization and QMC simulations indicates an exceptional two-dimensionality of CuPOF, with an estimated ratio of the intra- to inter-plane exchange energies of $J'/J \propto 10^{-4}$. Within the ordered state, a splitting of the ^{1}H NMR spectra reveals commensurate AF order, presumably of checkerboard type. A strong increase of T_N in applied magnetic fields furthermore manifests the low dimensionality of CuPOF. A detailed analysis of the uniform magnetization and the ^{31}P nuclear spin-lattice relaxation rate $1/T_1$ reveals an easy-plane anisotropy and a crossover from isotropic to XY behavior. Moreover, approaching the phase transition, the ^{31}P relaxation rate indicates an exponential growth of the average inter-spin correlation length.

TT 47.3 Wed 15:30 H23

HF-EPR study on the exchange couplings in 3d-4f heterometallic complexes — •Changhyun Koo[1], Arne Bahr[1], Sebastian Schmidt[2], Yan Peng[2], Ahmed Naushad[3], Maheswaran Shanmugam[3], Annie K. Powell[2], and Rüdiger Klingeler[1,4] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Department of Chemistry, Indian Institute of Technology, Mumbai, India — [4]Center for Advanced Materials, Heidelberg University, Heidelberg, Germany

3d-4f heterometallic complexes are suggested to enhance the magnetic anisotropy barrier in metal-organic coordination complexes. Though magnetic exchange coupling between 3d and 4f ions is essential, its quantitative determination by conventional magnetometry remains challenging. Our high-frequency electron paramagnetic resonance (HF-EPR) studies enable to determine the precise values of 3d-4f exchange interaction (J_{3d-4f}) as well as anisotropy of the 3d-ions. The EPR data, analyzed in terms of a Hamiltonian involving the Ising-spin concept for Ln ions, enable to derive information on the ground state and J_{3d-4f} in the complexes. The results on several series of complexes, i.e., $[Fe_4^{III}Ln_2^{III}(Htea)_4(\mu\text{-}N_3)_4(N_3)_3(piv)_3]$, $[Ni_2^{II}Ln_2^{III}(CH_3CO_2)_3(HL)_4(H_2O)_2](NO_3)_3$ (Ln = Tb, Dy, Ho, Yb, and Gd), and $[Co_2^{II}Dy_2^{III}(L)_4(NO_3)_2X$ (X = $(MeOH)_2$ and $(DMF)_2$]) will be presented and general conclusions about magneto-structural correlations will be drawn which suggest routes to optimizing ferromagnetic J_{3d-4f}.

TT 47.4 Wed 15:45 H23

High-frequency EPR studies on 3d-4f heterometallic complexes — •Arne Bahr[1], Changhyun Koo[1], Ahmed Naushad[2], Maheswaran Shanmugam[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — [2]Department of Chemistry, Indian Institute of Technology Mumbai

In the single molecular magnets (SMMs) research field, 3d-4f heterometallic complexes are expected as a solution to enhance the anisotropy barrier with the strong exchange interaction between 3d and 4f ions. Recently synthesized $[Ni_2^{II}Ln_2^{III}(CH_3CO_2)_3(HL)_4(H_2O)_2](NO_3)_3$ (Ln = Tb, Dy, Ho, and Yb) complexes, and a NiGd complex are studied by means of high frequency electron parmagnetic resonance (HF-EPR) measurments. The overall behaviour in specra for the complexes is largely dependent on the Ni-Ln and relatively weak Ln-Ln interaction. The resonance branches within the EPR spectra provide information of the g-values as a slope and the zero field splitting. Based on the observed EPR data, the ground states and the magnetic coupling between 3d and 4f ions of complexes will be discussed.

TT 47.5 Wed 16:00 H23

Anisotropy in Mn_2- and Co-complexes studied by high-frequency EPR spectroscopy — •Lena Spillecke[1], Changhyun Koo[1], Sajedeh Shahbazi[1], Marcel Patrick Merkel[2], Sebastian Schmidt[2], Annie K. Powell[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — [2]Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany

We present high-frequency/high-field electron paramagnetic resonance (HF-EPR) and static magnetisation studies on a Mn-($[TBA]_2[Mn_2^{III}Mo_4^{VI}(\mu_2\text{-}O)_6(Ot)_8(HTea)_2]$) and a Co-$Cl_2$ metal-organic coordination complex. Magnetic susceptibility of the Mn_2-complex indicates weak ferromagnetic exchange interaction between the octahedrally coordinated Mn^{3+} ions, $S = 2$. A strong anisotropy is suggested by a zero-field splitting (ZFS) of about $\Delta = 300$ GHz observed in HF-EPR data. For the Co-monomer, our data imply high-spin Co^{2+} which is presumingly antiferromagnetically coupled to a radical in the ligand-shell, hence forming an $S = 1$ ground state. Based on the measured ZFS and g-factor as well as the temperature dependence of the linewidth, the potential of the Co-complex as single molecular magnets is discussed.

TT 47.6 Wed 16:15 H23

Coupled dynamics of long-range and internal spin cluster order in Cu_2OSeO_3 — •Rolf B. Versteeg[1], Jingyi Zhu[1], Christoph Boguschewski[1], Fumiya Sekiguchi[1], Anuja Sahasrabudhe[1], Kestutis Budzinauskas[1], Petra Becker[2], Daniel I. Khomskii[1], and Paul H.M. van Loosdrecht[1] — [1]University of Cologne, Institute of Physics 2, Zülpicher Straße 77, D-50937 Cologne — [2]University of Cologne, Institute of Geology and Mineralogy, Zülpicher Straße 49b, D-50674 Cologne

Quantum materials with multiple length scales for electronic interactions lead to the self-organization of long-range ordered "molecules" of charge, spin, and orbital nature. The order to disorder phase transition pathways in such quantum materials comprises disordering of both the order inside the individual molecules or "clusters", as well as the emerging long-range order.

Here, we reveal optically induced dual order parameter dynamics in the cluster magnet Cu_2OSeO_3 (Ref. [1,2,3]) using time-resolved spontaneous Raman spectroscopy. (Ref. [4]) Multiple ps-decade spin-lattice relaxation dynamics is observed, which evidences a separation of the magnetic order parameter dynamics into disordering of long-range and internal spin cluster order. Our study demonstrates the dual nature of long-range and internal cluster order dynamics in cluster magnets.

[1] S. Seki et al., Science **336**, 198 (2012)
[2] O. Janson et al., Nat. Commun. **5**, 5376 (2014)
[3] R. B. Versteeg et al., Phys. Rev. B **94**, 094409 (2016)
[4] R. B. Versteeg et al., Struct. Dyn. **5**, 044301 (2018)

TT 47.7 Wed 16:30 H23

Strong influence of 'bystanders' on the exchange in edge-

shared Cu-O chain compounds — •Helge Rosner[1], Dijana Milosavljevic[1], Jan Tomczak[2], Stefan-Ludwig Drechsler[3], and Oleg Janson[3] — [1]MPI CPfS Dresden, Germany — [2]TU Wien, Austria — [3]IFW Dresden, Germany

The influence of the structural features like bond angles and distances on the exchange integrals in cuprate materials has been studied in detail for many years. One of the dominating structural features is the Cu-O-Cu bond angle in chain-like compounds. However, similarly strong influence on the exchange couplings by side groups was observed recently. As an example, we analyse the origin of the huge difference $\delta_{J1} \sim 200$ K for the nearest neighbour exchange in Li_2CuO_2 and $SiCuO_3$, which have structurally nearly identical CuO_2 chains. For closely related materials, we also demonstrate the strong influence of hydrogen positions in the crystal structure for O-H groups or crystal water on the leading exchange terms, changing from strongly antiferromagnetic to moderately ferromagnetic. We elucidate the underlying microscopic mechanisms based on detailed DFT studies and subsequently derived multi-band tight-binding models. The results widely improve our understanding of magneto-structural correlations in cuprate compounds.

15 min. break.

TT 47.8 Wed 17:00 H23

Quantum tunneling and large coercivity in Fe-doped Li_3N — Manuel Fix[1], Enrique del Barco[2], and •Anton Jesche[1] — [1]EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86135 Augsburg, Germany — [2]Department of Physics, University of Central Florida, Orlando, Florida 32816, USA

The basic magnetic unit in Fe-doped Li_3N is not a cluster or a domain but the magnetic moment of single, isolated Fe ions [1]. This novel model system shows large magnetic anisotropy and allows to study quantum tunneling of the magnetization in a rather simple, inorganic material at liquid helium temperatures.

For small concentrations of roughly 0.1 % Fe, we have found an extreme field-dependence of the magnetic tunneling [2]. Applied *longitudinal* fields lift the ground-state degeneracy and destroy the tunneling condition. The relaxation time increases from $\tau \sim 10^4$ by four orders of magnitude in applied fields of only a few milliTesla, which reveals exceptionally sharp tunneling resonances. In applied *transverse* magnetic fields, on the other hand, the spin-flip probability increases, which proves the resonant character of this tunneling process. Therefore, it is possible either to freeze the orientation or to promote the flip of a spin-state by tiny applied fields.

[1] A. Jesche *et al.*, Nat. Commun. **5**:3333 (2014)
[2] M. Fix, J. H. Atkinson, P. C. Canfield, E. del Barco, A. Jesche, Phys. Rev. Lett. **120**, 147202 (2018)

TT 47.9 Wed 17:15 H23

Spiral ordering in the edge sharing chain cuprate $CuSiO_3$ — •Dijana Milosavljevic[1], Andrei Gippius[2], Michael Baenitz[1], Stefan-Ludwig Drechsler[3], Oleg Janson[3], Johannes Richter[4], and Helge Rosner[1] — [1]MPI Chemical Physics of Solids, Dresden — [2]Lomonosov Moscow State University — [3]IFW Dresden — [4]MPI Physics of Complex Systems, Dresden

$CuSiO_3$ is spin-1/2 cuprate system isostructural to the famous Spin-Peierls system $CuGeO_3$ [1]. Due to this similarity, the compound was described previously as a quasi one-dimensional $J_1 - J_2$ chain compound with strongly dominating J_2 [2]. Experimentally, the system orders antiferromagnetically at about 8 K with a propagation vector of (1/2 0 1/8) with the structural Cu-O chains running along c [3]. This spiral ordering is inconsistent with the previous parametrisation, motivating a re-investigation of the compound. Re-determining crystal structure and sample composition by synchrotron XRD and applying density functional calculations together with high temperature series expansion, we suggest a new parameter set of exchange couplings that is consistent with all experimental findings. The new magnetic model describes the compound in terms of strongly antiferromagnetically coupled $J_1 - J_2$ chains with a ferromagnetic J_1 of about 35 K and a frustration ratio $\alpha = |J_2/J_1| \sim 0.35$..

[1] H. H. Otto, M. Meibohm, Z. Kristallogr. **214**, 558 (1999)
[2] M. Baenitz et al., Phys. Rev. B **62**, 12201 (2002)
[3] H. Wolfram et al., Phys. Rev. B **69**, 144115 (2004)

TT 47.10 Wed 17:30 H23

Magnon spectrum of the noncollinear antiferromagnet Mn_3Ge — •Aleksandr S. Sukhanov[1,2], Ph. Bourges[3], H. C. Walker[4], M. S. Pavlovskii[5], K. Manna[1], C. Felser[1], and D. S. Inosov[2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [3]Laboratoire Léon Brillouin, CEA-CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette, France — [4]ISIS Facility, STFC, Rutherford Appleton Laboratory,Didcot, Oxfordshire OX11-0QX, United Kingdom — [5]Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia

We discuss the full spin-wave spectrum of the noncollinear antiferromagnet Mn_3Ge obtained using neutron time-of-flight and triple-axis spectroscopy. The sublattice of magnetic ions in hexagonal Mn_3Ge can be viewed as two adjacent kagome layers stacked along the crystallographic [001] axis. Below T_N of 370 K the Mn atoms form the coplanar triangular 120° antiferromagnetic (AFM) order. Our measurements revealed a magnon mode with a spin-wave gap of 5 meV and a very steep anisotropic dispersion. The obtained spectra allows one to build an effective model of magnetic interactions in the system. We found two coupled magnon-phonon excitations seen in the vicinity of the zone center on the energies of 14 meV and 17.5 meV. We argue that this mixed excitations represent a strong magneto-elastic coupling in Mn_3Ge.

TT 47.11 Wed 17:45 H23

Observation of two independent skyrmion phases in a chiral magnet material — •Alfonso Chacon[1], Lukas Heinen[2], Marco Halder[1], Andreas Bauer[1], Wolfgang Simeth[1], Sebastian Mühlbauer[3], Helmuth Berger[4], Markus Garst[5], Achim Rosch[2], and Christian Pfleiderer[1] — [1]Physik Department, Technische Universität München, Garching, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Köln, Germany — [3]Heinz Maier-Leibnitz (MLZ), Technische Universität München, Garching, Germany — [4]École Polytechnique Federale de Laussane, Laussane, Switzerland — [5]Institut für Theoretische Physik, Technische Universität Dresden, Dresden, Germany

Magnetic materials can host skyrmions, which are topologically nontrivial spin textures. In chiral magnets with cubic lattice symmetry, all previously observed skyrmion phases require thermal fluctuations to become thermodynamically stable in bulk materials, and therefore exist only at relatively high temperature, close to the helimagnetic transition temperature. Here, we report the identification of a second skyrmion phase in Cu_2OSeO_3 at low temperature and in the presence of an applied magnetic field, from small angle neutron scattering and magnetization measurements. Theoretical modelling provides evidence that the stabilization mechanism is given by well-known cubic anisotropy terms, and accounts for an additional observation of metastable helices tilted away from the applied field. The generic character of the underlying mechanism suggests a new avenue for the discovery, design and manipulation of topological spin textures.

TT 47.12 Wed 18:00 H23

Interaction of Skyrmions and Pearl Vortices in Superconductor-Chiral Ferromagnet Heterostructures — •Samme M. Dahir, Anatoly F. Volkov, and Ilya M. Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

We investigate a hybrid heterostructure with magnetic skyrmions (Sk) inside a chiral ferromagnet interfaced by a thin superconducting film via an insulating barrier. The barrier prevents the electronic transport between the superconductor and the chiral magnet, such that the coupling can only occur through the magnetic fields generated by these materials. We find that Pearl vortices (PV) are generated spontaneously in the superconductor within the skyrmion radius, while anti-Pearl vortices ($\overline{\text{PV}}$) compensating the magnetic moment of the Pearl vortices are generated outside of the Sk radius, forming an energetically stable topological hybrid structure. Finally, we analyze the interplay of skyrmion and vortex lattices and their mutual feedback on each other. In particular, we argue that the size of the skyrmions will be greatly affected by the presence of the vortices offering another prospect of manipulating the skyrmionic size by the proximity to a superconductor.

TT 47.13 Wed 18:15 H23

Tracing domain wall conductivity in the skyrmion-host multiferroic GaV_4S_8 — •Somnath Ghara, Korbinian Geirhos, Peter Lunkenheimer, Vladimir Tsurkan, and István Kézsmárki — Experimental Physics V, Center for Electronic Correlations and Mag-

netism, University of Augsburg, Augsburg, Germany

The lacunar spinel, GaV_4S_8, has attracted tremendous interests due to the presence of Néel-type magnetic skyrmion and its multiferroic properties. It crystallizes in a non-centrosymmetric cubic structure ($F\overline{4}3m$) at room temperature and undergoes a ferroelectric transition at 43 K, reducing the crystal symmetry to rhombohedral ($R3m$). In the rhombohedral state, the crystals usually consist of four types of polar domains, whose populations can be controlled by applying static electric fields while cooling the samples through the rhombohedral transition. To monitor the domain population, we performed pyro- and magnetoelectric polarization, resistivity and magnetization measurements. We found that the single-domain state with high resistance can be realized upon poling, while the resistance in the multi-domain state is several orders of magnitude lower, which imply the presence of highly conductive domain walls.

TT 47.14 Wed 18:30 H23

Winding up quantum spin helices: Avoided level crossing vs. topological protection — •Thore Posske and Michael Thorwart — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

A magnetic helix can be wound into a classical Heisenberg chain by fixing one end while rotating the other one. We show that in quantum Heisenberg chains, the magnetization slips back to the trivial state beyond a finite turning angle. Avoided level crossings thus undermine classical topolog- ical protection. Yet, for special values of the axial Heisenberg anisotropy, stable spin helices form again, which are nonlocally entangled. Away from these sweet spots, spin helices can be stabilized dynamically or by dissipation. For half-integer spin chains of odd length, a spin slippage state and its Kramers partner define a qubit with a non-trivial Berry connection.