TT 40: Correlated Electrons: Low-dimensional Systems - Materials 3

Time: Thursday 15:00–18:15 Location: H 0104

TT 40.1 Thu 15:00 H 0104

Large quantum fluctuations in the strongly coupled spin-$\frac{1}{2}$ chains of green dioptase: a magic message from birds and trees — Oleg Janson, Alexander Tsirlin, Miriam Schmitt, and •Helge Rosner — Max-Planck-Institut für Chemische Physik fester Stoffe

We present a microscopic magnetic model for the natural mineral (green) dioptase $Cu_6Si_6O_{18}{\cdot}6H_2O$. Based on full-potential DFT calculations, we find two relevant exchange couplings in this compound: an antiferromagnetic coupling J_c, forming spiral chains along the hexagonal axis, and a ferromagnetic interchain coupling J_d within the structural Cu_2O_6 dimers. To corroborate the proposed spin model, we perform quantum Monte-Carlo simulations for the dioptase spin lattice. The evaluated ground-state (the propagation vector and the sublattice magnetization) and thermodynamic properties [$\chi(T)$] are in remarkably good agreement with the experimental data. The refined model parameters are $J_c = 78\,\mathrm{K}$ and $J_d = -37\,\mathrm{K}$ with $J_d/J_c \simeq -0.5$ [1]. Despite the lack of frustration and the 3D nature of the spin lattice, the low coordination number of 3 suffices to cause strong quantum fluctuations, as evidenced by the experiments. Alterations of the J_c–J_d model in closely related compounds will be briefly discussed.

[1] O. Janson, A. A. Tsirlin, M. Schmitt, and H. Rosner, Phys. Rev. B 82, 014424 (2010); arXiv:1004.3765.

TT 40.2 Thu 15:15 H 0104

DFT-based microscopic modeling for the spin-$\frac{1}{2}$ kagome systemherbertsmithite γ-$Cu_3Zn(OH)_6Cl_2$ — •Oleg Janson and Helge Rosner — Max-Planck-Institut für Chemische Physik fester Stoffe

Herbertsmithite γ-$Cu_3Zn(OH)_6Cl_2$ is a real material realization of the $S = 1/2$ kagome Heisenberg model. Extensive experimental characterization of this compound evidences the absence of long-range magnetic ordering down to 70 mK despite a leading exchange coupling of 190 K [1]. To account for the experimental data, a sizable structural Cu–Zn disorder was suggested. Very recent single crystal experiments revealed that these defects are confined to the interplane sites, while the magnetic kagome layers are almost defect-free [2].

Following the DFT-based study of the closely related compounds kapellasite α-$Cu_3Zn(OH)_6Cl_2$ and haydeeite α-$Cu_3Mg(OH)_6Cl_2$ [3], we apply our computational approach to the more complex case of herbertsmithite. Taking the idealized structure as a starting point, we investigate the influence of the Cu–Zn disorder onto the magnetic coupling regime. The numerical results are compared to the recent single-crystal experiments.

[1] J. S. Helton *et al.*, Phys. Rev. Lett. **98**, 107204 (2007).
[2] T. Imai *et al.*, Phys. Rev. B **84**, 020411(R) (2011).
[3] O. Janson, J. Richter, and H. Rosner, Phys. Rev. Lett. **101**, 106403 (2008); J. Phys.: Conf. Ser. **145**, 012008 (2009).

TT 40.3 Thu 15:30 H 0104

$Ca_2Y_2Cu_5O_{10}$: the first authentic frustrated quasi-1D ferromagnet and a particular rehabilitation of spin wave theory based analysis — •Stefan-Ludwig Drechsler[1], Roman Kuzian[1,2], Satoshi Nishimoto[1], Jiri Malek[1,3], Jeroen van den Brink[1], Miriam Schmitt[4], Helge Rosner[4], Masaaki Matsuda[5], Kunihiko Oka[6], Hirotaka Yamaguchi[6], and Toshimitsu Ito[6] — [1]IFW-Dresden, ITF, D01171 Dresden, Germany — [2]Inst. f. Problems of Material Sciences, NASU, Kiev, Ukraine — [3]Inst. of Physics, ASCR, Prague, Czech Republic — [4]MPI-CPFS, Dresden, Germany — [5]Quantum Cond. Division, Oak Ridge National Lab., Oak Ridge, USA — [6]AIST, Tsukuba, Ibaraki, Japan

We reexamine the magnetic excitations (ME) for $Ca_2Y_2Cu_5O_{10}$ with edge-shared CuO_2 chains (ESC). For this aim we report inelastic neutron scattering data and present the ME dispersion along $\mathbf{Q} = (H, 0, 1.5)$, unaffected by the main interchain couplings. This allows a precise extraction of the inchain couplings (IC) $J_1 \approx -170\,\mathrm{K}$, $J_2 \approx 32\,\mathrm{K}$. Their ratio $\alpha = |J_2/J_1| \approx 0.19$ indicates an exceptional position in the ESC family: close to the critical point (CP) of the J_1-J_2 spin model $\alpha_c = 1/4$, but on the *ferromagnetic* (FM) side of its phase diagram. The obtained J's agree with the results obtained for a realistic 5-band extended Hubbard *pd* model and L(S)DA+U calculations. We predict Zhang-Rice singlet features in RIXS, EELS and optics visible at 300 K for sizable frustration only. This is the signature of a frustrated FM near a CP. The weak IC determine the predicted saturation field of 65 T and J_1 gives the width of the ME dispersion.

TT 40.4 Thu 15:45 H 0104

NMR measurements on T'-La_2CuO_4, a parent compound of electron-doped cuprate superconductors — •Katharina Weber[1], Marco Günther[1], Hubertus Luetkens[2], Gwendolyne Pascua[2], Roland Hord[3], Barbara Albert[3], Lambert Alff[4], and Hans-Henning Klauss[1] — [1]Institut für Festkörperphysik, TU Dresden — [2]Laboratory for Muon Spin Spectroscopy, PSI — [3]Eduard-Zintl-Institut, TU Darmstadt — [4]Institute of Materials Science, TU Darmstadt

The study of La_2CuO_4 in the metastable T' phase is important for the understanding of the cuprate superconductors, for it allows a direct comparison to its counterpart T-La_2CuO_4, a parent compound of hole-doped cuprates. We present our mircoscopic study of the antiferromagnetically ordered phase of T'-La_2CuO_4. Pulsed ^{139}La-NMR was used to obtain spectra and relaxation rates in a temperature range from 10 to 240 K in an external field of about 5 T. The comparison of the spectra to a simulation allows us to determine the hyperfine field on the La site. The NMR measurements reveal static magnetic order below $T_N = 207$ K in contrast to previous moun spin rotation experiments on the same sample, indicating static order below 115 K [1]. However the NMR spin-lattice relaxation rates imply a change of spin dynamics at 120 K.

[1] R. Hord, H. Luetkens, G. Pascua, A. Buckow, K. Hofmann, Y. Krockenberger, J. Kurian, H. Maeter, H.-H. Klauss, V. Pomjakushin, A. Suter, B. Albert, and L. Alff, Phys. Rev. B 82, 180508(R) (2010).

TT 40.5 Thu 16:00 H 0104

High temperature magnetic heat transport of low-dimensional quantum antiferromagnets — •Oleg Mityashkin[1], Ashwin Mohan[1], Nikolai Hlubek[1], Mahmoud Abdel-Hafiez[1], Christian Hess[1], Bernd Büchner[1], Surjeet Singh[2], Romuald Saint-Martin[3], and Alexandre Revcolevschi[3] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany — [2]Indian Institute of Science Education and Research (IISER), NCL Innovation Park, Pune, India — [3]Laboratoire de Physico-Chimie de L'Etat Solide, Universite Paris-Sud, 91405 Orsay, France

We have investigated the magnetic heat transport of several cuprate materials realizing low dimensional $S = 1/2$ quantum antiferromagnets, in the temperature range [7, 650] K. The results at low temperatures have been obtained using a four-point steady state method, whereas for high temperatures a dynamical laser flash analysis has been employed. In particular, we have studied the spin chain material $SrCuO_2$ and the 2D AFM square lattice La_2CuO_4. We observe a strong suppression of the magnetic heat conductivity with increasing temperature. We analyze and discuss the behavior of the heat conductivity by considering several scattering processes, in particular defect scattering and phonon scattering. Surprisingly, the results for these compounds obtained with the dynamical laser flash method vary with sample thickness. We associate this with a fundamental problem of this measurement technique.

TT 40.6 Thu 16:15 H 0104

Single Crystal Growth and Physical properties of $La_8Cu_7O_{19}$ — •Ashwin Mohan[1], Surjeet Singh[2], Christian Hess[1], Sabine Wurmehl[1], and Bernd Büchner[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany — [2]Indian Institute of Science Education and Research (IISER), NCL Innovation Park, Pune, India.

The cuprate $La_8Cu_7O_{19}$ is an example of a low dimensional system having five-leg ladders in its spin structure. It is an interesting candidate to explore the whole range of phenomena occurring in such low dimensional systems and to investigate the resemblance of these odd leg ladders to one dimensional spin chains by probing spin excitations. Here, we present the single crystal growth of this compound and discuss first experimental data of basic physical properties of our crystal.

15 min. break.

TT 40.7 Thu 16:45 H 0104

Exotic Magnetization Plateaux in a Quasi-2D Shastry-Sutherland System — •Gregor Raphael Foltin[1], Salvatore Manmana[2], Frédéric Mila[3], and Kai Phillip Schmidt[1] — [1]Lehrstuhl Theoretische Physik 1, Technische Universität Dortmund , D-44221 Dortmund , Germany — [2]JILA , University of Colorado at Boulder, Colorado 80302 U.S.A. — [3]Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne , Switzerland

We report our findings for a quasi-2D approximation to the Shastry-Sutherland lattice which we refer to as a 4-leg Shastry-Sutherland tube. This system consists of mutually orthogonal $S = 1/2$ Heisenberg dimers which are coupled via an inter-dimer coupling J'. Using pCUTs and the DMRG, we identify as a function of J' and the magnetic field a series of magnetization plateaux. Here we focus on the ones at 1/8 and 1/4. In contrast to previous findings for coupled dimer systems, quantum fluctuations induced by correlated hopping terms influence significantly the nature of these Mott insulating states. We characterize the state at 1/4 to be a semi-classical one, and the one at 1/8 to possess a stripe structure caused by an interplay of the peculiar geometry and the inter-dimer couplings. This particular finding suggests the system to be in an insulating state in the longitudinal, but a maximally entangled state in the transverse direction. We discuss possible relations of our findings to the full 2D system, which is the underlying model for the description of the quantum magnetic material $SrCu(BO_3)_2$.

TT 40.8 Thu 17:00 H 0104

Pressure evolution of the Shastry-Sutherland magnet $SrCu_2(BO_3)_2$ — •Alexander Tsirlin and Helge Rosner — Max-Planck Institute CPfS, Dresden, Germany

We investigate the evolution of crystal structure and individual magnetic couplings in the spin-$\frac{1}{2}$ Shastry-Sutherland magnet $SrCu_2(BO_3)_2$ under hydrostatic pressure. Our results based on *ab initio* electronic structure calculations suggest the highly anisotropic compressibility of the structure that strongly shrinks along the interlayer c direction, while only weakly changing in the ab plane. This leads to a moderate change in the intralayer exchange couplings J and J' within the Cu_2O_6 dimers and between the dimers, respectively. Above 4.5 GPa, $SrCu_2(BO_3)_2$ transforms into a monoclinic phase that has been scarcely characterized experimentally. We propose an improved structural model of this phase, and identify its spin system as an anisotropic Shastry-Sutherland lattice featuring inequivalent inter-dimer couplings J'_1 and J'_2. Our results compare well to the available experimental data, and call for a further investigation of the spin-lattice coupling phenomena in $SrCu_2(BO_3)_2$.

TT 40.9 Thu 17:15 H 0104

Microscopic mechanism for the 1/8 magnetization plateau in $SrCu_2(BO_3)_2$ — •Mike Nemec, Gregor Raphael Foltin, and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, Tu Dortmund, Germany

The frustrated quantum magnet $SrCu_2(BO_3)_2$ shows a remarkably rich phase diagram in an external magnetic field which is not fully understood theoretically so far. The experimental results show a sequence of magnetization plateaux where the most prominent magnetization plateau is the one at 1/8. Theoretically, one expects that this frustrated quantum magnet should be well described by the Shastry-Sutherland model but recent calculations did not find the same sequence of magnetization plateaux as in experiments. In particular, no 1/8 plateau is found in theory. Here we study the effects of additional magnetic coupling terms like a finite Dzyaloshinskii-Moriya interaction. Most interestingly, the quantum fluctuations induced by such additional magnetic couplings lead very naturally to a stabilization of the 1/8 plateau for realistic values of the magnetic exchange constants.

TT 40.10 Thu 17:30 H 0104

Effect of bond disorder on weakly-coupled spin-1/2 antiferromagnetic Heisenberg chains — •Matthias Thede[1,2], Fan Xiao[3], Elvezio Morenzoni[1], Christopher Landee[3], and Andrey Zheludev[2] — [1]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland — [2]Paul Scherrer Institut, Villigen-PSI, Switzerland — [3]Department of Physics and Carlson School of Chemistry, Clark University, USA.

We study the effect of chemical disorder on magnetic ordering in the quasi-one-dimensional antiferromagnets $Cu(py)_2(Cl_{1-x}Br_x)_2$. The two end compounds are S = $\frac{1}{2}$ linear-chain systems with J = 2.3 meV and J = 4.5 meV, for x = 0 and x = 1, respectively. Weak inter-chain interactions lead to long range order at T_N = 1.1 K and T_N = 0.7 K, respectively. Partial substituting Br for Cl randomizes the bond strength in the spin chains. We probe magnetic and thermodynamic properties of $Cu(py)_2(Cl_{1-x}Br_x)_2$ with susceptibility, specific heat and MuSR measurements. For all samples, the temperature dependence of the magnetic susceptibility follows expectations for a S=$\frac{1}{2}$ Heisenberg chain. Specific heat data reveals more interesting behavior. While at the Cl end a very slow decrease of T_N with x is observed, on the Br side, suppression of T_N relative to x=1 is much more rapid. This disparity in the behavior samples is consistent with MuSR measurements. For the two end-compounds and $Cu(py)_2(Cl_{0.95}Br_{0.05})_2$, there is a clear evidence of static magnetic behavior below T_N. However, $Cu(py)_2(Cl_{0.94}Br_{0.06})_2$ show totally different muon spectra, indicating a strong in homogeneity of the static magnetization.

TT 40.11 Thu 17:45 H 0104

Field driven ordering in a frustrated spin ladder with bond randomness — •Erik Wulf[1], Sebastian Mühlbauer[1], Tatiana Yankova[1,2], and Andrey Zheludev[1] — [1]Neutron Scattering and Magnetism Group, Laboratory for Solid State Physics, ETH Zürich, Zürich, Switzerland — [2]Chemistry Department, M. V. Lomonosov Moscow State University, Moscow, Russia

We studied the influence of bond randomness on field driven magnon ordering in a frustrated 4-leg ladder. Weak interladder interactions and strong coupling along the ladder legs characterize the almost perfect 1D behavior of $H_8C_4SO_2 \cdot Cu_2Cl_4$. By overcoming the critical field of H_c=3.7T the gap between singlet ground state and excited triplet state is closed. The material undergoes a phase transition from spin liquid to long-range spiral order. Chemical substitution of the nonmagnetic Cl^- ions by Br^- ions causes bond disorder in $H_8C_4SO_2 \cdot Cu_2(Cl_{1-x}Br_x)_4$. The effect on the phase transition was characterized by measurements of the magnetization and the specific heat [1]. It was shown that already low Br^- concentrations of x=1% replace the phase transition by a crossover. While the specific heat data of the pure material exhibit a sharp λ-anomaly the data measured at x $\geq$ 1% show a broad peak. The same behavior is observed in the susceptibility data. In contrast to the transition the critical field itself is almost unaffected.

This work is partially supported by the Swiss National Science Foundation under project 6 of the Materials with Novel Electronic Properties program.

[1] E. Wulf, S. Mühlbauer, T. Yankova and A. Zheludev, Phys. Rev. B **85**, 174414 (2011).

TT 40.12 Thu 18:00 H 0104

ESR studies of the quasi-2D frustrated Cs_2CuBr_4 — •S.A. Zvyagin[1], D. Kamensky[1], J. Wosnitza[1], M. Ikeda[2], T. Fujita[2], M. Hagiwara[2], O.A. Starykh[3], R. Hu[4,5], H. Ryu[4], and C. Petrovic[4] — [1]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01328 Dresden, Germany — [2]KYOKUGEN, Osaka University, Toyonaka, Osaka 560-8531, Japan — [3]Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA — [4]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, USA — [5]University of Maryland, Center for Nanophysics and Advanced Materials, College Pk, MD 20742 USA

We report low-temperature electron spin resonance (ESR) studies of single-crystalline samples of Cs_2CuBr_4, a spin-1/2 antiferromagnet with a triangular spin-lattice structure. A remarkable angular dependence of the resonance field, including the splitting of the ESR line for some orientations of the magnetic field, and the presence of a gap in the ESR excitation spectrum at temperatures above the Neel temperature, T_N = 1.3 K, have been revealed. Our observations suggest that uniform Dzyaloshinskii-Moriya interaction affects the low-energy excitation spectrum in this frustrated compound. The results are compared with that obtained recently for the isostructural material Cs_2CuCl_4 [1].

The work was supported in part by DFG and EuroMagNET II (EU Contract No. 228043).

[1] Povarov et al., Phys. Rev. Lett. 107, 037204 (2011)