TT 42: Correlated Electrons: Frustrated Magnets - Cu-based Systems & FeCr

Time: Wednesday 9:30–13:00 Location: H18

TT 42.1 Wed 9:30 H18

Interplay of Spin and Lattice in a Pseudo-Kagome System — Vladimir Gnezdilov[1,2], •Peter Lemmens[2], Yurii Pashkevich[3], Alexander Vasiliev[4], and Peter Berdonosov[4] — [1]ILTPE, Kharkov, Ukraine — [2]IPKM, TU-BS, Braunschweig — [3]DonFTI, Donetsk, Ukraine — [4]MSU, Moskow, Russia

The layered cuprates, francisites $Cu_3Bi(SeO_3)_2O_2X$, with X=Br or Cl, with pseudo-kagome structure were studied across the structural and magnetic phase transitions using Raman spectroscopy. For X=Cl a soft optical mode is revealed. The temperature-dependent changes in the phononic and magnetic subsystems of these highly frustrated magnets allow proposing a microscopic magnetic model including Dzyaloshinsky-Moriya interaction to explain the nature of the observed spin-wave excitations.

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TT 42.2 Wed 9:45 H18

Peculiarities of structural distortions in kagome francisites — •Alexander A. Tsirlin[1], Danil Prishchenko[2], Vladimir Tsurkan[3], and Vladimir G. Mazurenko[2] — [1]EP VI, Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Ural Federal University, Ekaterinburg, Russia — [3]EP V, Electronic Correlations and Magnetism, University of Augsburg, Germany

Francisites $Cu_3Bi(SeO_3)_2O_2X$ (X = Cl, Br) are spin-$\frac{1}{2}$ kagome materials with predominantly ferromagnetic exchange couplings. Despite this tendency toward ferromagnetism, they entail strong magnetic frustration related to antiferromagnetic couplings between next-nearest neighbors. The infinite classical degeneracy of the ground state is lifted by anisotropic Dzyaloshinsky-Moriya couplings that stabilize canted magnetic order within the kagome planes. The canting angle θ reveals strong dependence on the halogen atom, chlorine ($\theta \simeq 70°$) or bromine ($\theta = 52°$), which is difficult to rationalize assuming that these ions are not part of the kagome planes and have no influence on relevant superexchange couplings. By combining high-resolution synchrotron x-ray diffraction with *ab initio* calculations of lattice dynamics, we show that the Cl francisite undergoes a structural phase transition triggered by the weakly bonded Cl ions located between the kagome planes. This transition has strong impact on the in-plane magnetism and alters magnetic interactions considerably. In the Br francisite, no structural phase transition is observed, and a more regular version of the kagome lattice is formed.

TT 42.3 Wed 10:00 H18

Substitutions in Cu-based frustrated spin-systems: $BaCuSi_2O_6$ and $ZnCu_3(OH)_6Cl_2$ — •Pascal Puphal[1], Denis Sheptyakov[2], Natalija Van Well[2], Raivo Stern[3], Lars Postulka[1], Bernd Wolf[1], Michael Lang[1], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe Universität Frankfurt, Germany — [2]PSI, Switzerland — [3]National Institute of Chemical Physics and Biophysics, Estonia

$BaCuS_2O_6$ is a spin dimer system presenting a 2D Bose-Einstein condensation of triplons at low temperatures and high magnetic fields. We present a structural analysis of the substituted system $(Ba_{1-x}Sr_x)CuSi_2O_6$, which reveals a stable tetragonal crystal structure down to 2 K unlike its parent compound x = 0. We explore the structural details with low-temperature neutron and synchrotron powder diffraction, room-temperature NMR, as well as magnetic- and specific-heat measurements.

$ZnCu_3(OH)_6Cl_2$ is a highly frustrated kagomé system, which has a antiferromagnetic superexchange interaction of J = 17 meV, but no magnetic transition or long-range order has been observed down to T = 50 mK. We present first results of $M_xCu_{4-x}(OH)_6Cl_2$, with a three valent ion M, which should lead to a Dirac metal as proposed by I. I. Mazin et. al. [1]. We could synthesize a Paratacamite-type (x < 1), which shows a magnetic ordering below 6.5 K. This transition can be decreased with increasing x.

[1] I. I. Mazin et. al., Nature Communications **5**, 4261 (2014)

TT 42.4 Wed 10:15 H18

Spin model of volborthite $Cu_3V_2O_7(OH)_2{\cdot}2H_2O$ revisited: coupled trimers instead of zigzag chains — •Oleg Janson[1], Shunsuke Furukawa[2], Tsutomu Momoi[3,4], Philippe Sindzingre[5], Johannes Richter[6], and Karsten Held[1] — [1]IFP, TU Wien, Austria — [2]University of Tokyo, Japan — [3]Condensed Matter Theory Laboratory, RIKEN, Japan — [4]RIKEN Center for Emergent Material Science, Japan — [5]Université Pierre & Marie Curie, Paris, France — [6]University of Magdeburg, Germany

Motivated by recent experiments on volborthite single crystals showing a wide $\frac{1}{3}$-magnetization plateau [1], we adopt the structural data and perform microscopic modeling by means of density functional theory (DFT). Using DFT+U, we find four leading magnetic exchanges: antiferromagnetic J and J_2, as well as ferromagnetic J' and J_1. Simulations of the spin Hamiltonian show good agreement with the experiment for $J{:}J'{:}J_1{:}J_2 = 1 : -0.2 : -0.5 : 0.2$ with $J \simeq 252$ K. The $\frac{1}{3}$-plateau phase pertains to polarized magnetic trimers formed by strong J bonds. An effective $J \to \infty$ model shows a tendency towards condensation of magnon bound states preceding the plateau phase [2].

[1] H. Ishikawa *et al.*, PRL **114**, 227202 (2015).
[2] O. Janson *et al.*, arXiv:1509.07333.

TT 42.5 Wed 10:30 H18

$Cu_4(OH)_6FBr$ - a structurally perfect spin-1/2 kagome system — •Bernd Wolf[1], Elena Gati[1], Nguyen Hieu Hoang[1], Harald O. Jeschke[2], Francesc Salvat-Pujol[2], Roser Valenti[2], John A. Schleuter[3], and Michael Lang[1] — [1]Physics Institute, Goethe-University Frankfurt(M), Germany, — [2]Institute for Theoretical Physics, Goethe-University Frankfurt(M), Germany, — [3]Division of Materials Research, National Science Foundation, Arlington, Virginia, USA

Spin-1/2 kagome lattices have been intensively investigated in recent years since they support the formation of quantum spin liquids (QSL). A prominent example is the natural mineral herbertsmithite $ZnCu_3(OH)_6Cl_2$ [1]. Here chemical modifications are difficult to realize and therefore new design strategies are necessary for synthesizing novel QSL. $Cu_4(OH)_6FBr$ reflects such a novel approach [2] where a structurally perfect kagome arrangement is achieved. We present a detailed magnetic characterization of small single crystals of $Cu_4(OH)_6FBr$. Measurements of the magnetization and susceptibility down to 2 K and up to 5 T reveal indications for two dominant magnetic couplings of different sign and an antiferromagnetic transition at $T_N = 15$ K exhibiting a weak ferromagnetic component. The experimental findings are in good agreement with the results of density functional theory (DFT) calculations. In addition, we present thermal expansion measurements from which the pressure dependence of T_N is determined.

[1] T.-H. Han et al., Nature **492**, 406 (2012).
[2] H. O. Jeschke et al., PRB **92**, 094417 (2015)

TT 42.6 Wed 10:45 H18

Synthesis and crystal growth of Cu-based kagome materials — •Christian Klein, Franz Ritter, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, D-60438 Frankfurt am Main

Magnetic frustration in kagome-type lattices can lead to novel type of ground states, the so-called Quantum Spin Liquids (QSLs). [1] For studying experimentally the properties of QSLs new materials in single crystalline form are essential.We report on the crystal growth under hydrothermal conditions and characterization of the new material Barlowite ($Cu_4(OH)_6BrF$). [2] Substitution of the cation on the interlayer-site enables us to modify the physical properties. Selective use of non-magnetic ions on the interlayer position leads to a quasi-two-dimensional system by decoupling the exchange between the kagome-layers. [3] We will discuss various synthetic pathways, together with thorough structural characterization.

[1] P. A. Lee, Science **321**, 1306 (2008)
[2] H. Jeschke et al., PRB **92**, 094417 (2015).
[3] Guterding et al., arXiv:1511.05686v1.

TT 42.7 Wed 11:00 H18

Interplay of magnetic sublattices in langite $Cu_4(OH)_6SO_4 \cdot 2H_2O$ — •Satoshi Nishimoto[1,2], Stefan Lebernegg[3], Alexander A. Tsirlin[4], Oleg Janson[5], Günther J. Redhammer[6], Stefan-Ludwig Drechsler[1], and Helge Rosner[3] — [1]IFW Dresden, Dres-

den, Germany — [2]TU Dresden, Dresden, Germany — [3]MPI CPfS, Dresden, Germany — [4]Institute of Physics, University of Augsburg, Germany — [5]Institute of Solid State Physics, TU Vienna, Austria — [6]University Salzburg, Austria

Magnetic and crystallographic properties of the mineral langite $Cu_4(OH)_6SO_4 \cdot 2H_2O$ are reported. Density-functional band structure calculations suggest a quasi-two-dimensional spin model consisting of two interacting subsystems: (A) Frustrated Heisenberg chains with ferromagnetic nearest-neighbor (NN) and antiferromagnetic (AFM) next-nearest-neighbor (NNN) exchange couplings, which is responsible for the magnetic ordering at $T_N \simeq 5.7\,\mathrm{K}$, and (B) weakly-coupled frustrated chains with AFM NN and NNN exchange couplings. At low temperature, the magnetic susceptibility of the former subsystem is about five times larger than that of the latter one. Therefore, the system can be regarded as a combination of isolated subsystems with respect to applied magnetic field. The subsystem (A) may give an ideal host exhibiting multipolar physics. Experimentally observed magnetic susceptibility, specific heat, and magnetization are also compared to our numerical results.

15 min. break

TT 42.8 Wed 11:30 H18

Investigation of the antiferromagnetic - ferromagnetic dimer chain compound $BaCu_2V_2O_8$ at zero and finite temperatures — •Ekaterina Klyushina[1,2], Alexander Tiegel[3], Nazmul Islam[1], Jitae Park[4], Bastian Klemke[1], Andreas Honecker[5], Salvatore Manmana[3], and Bella Lake[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [3]Georg-August-Universität Göttingen, Germany — [4]Heinz Maier-Leibnitz Zentrum, TU München, Garching, Germany — [5]Université de Cergy-Pontoise, France

Highly dimerized quantum magnets have attracted a great deal of attention in the recently due to the unconventional temperature behavior of their magnetic excitations[1,2]. Here we present our investigations of the highly dimerized antiferromagnet-ferromagnetic 1D chain $BaCu_2V_2O_8$ both at base and at finite temperatures. The single crystal inelastic neutron scattering measurements at base temperature reveal that there are two excitation branches which disperse along the L direction over the energy range of 36-46 meV. The comparison with DMRG simulations indicates that the antiferromagnetic dimers are coupled ferromagnetically along the c axis. The line shape of the excitations at the dispersion minima was found to become asymmetry with increasing temperature. Thus unconventional thermal behavior also exists in dimer compounds with ferromagnetic interdimer coupling.

[1] D. L. Quintero-Castro et al., PRL **109**, 127206 (2012)
[2] D. Tennant et al., PRB **85**, 014402 (2012).

TT 42.9 Wed 11:45 H18

Neutron diffraction on the frustrated spin-chain linarite at low temperatures and high fields — •Leonie Heinze[1], Britta Willenberg[2], Jens-Uwe Hoffmann[2], Anja U.B. Wolter-Giraud[3], Bernd Büchner[3], Kirrily C. Rule[4], Andrew Studer[4], Bachir Ouladdiaf[5], and Stefan Süllow[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig — [2]Helmholtz-Zentrum Berlin für Materialien und Energie — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden — [4]The Bragg Institute, ANSTO — [5]Institut Laue-Langevin Grenoble

The natural mineral linarite, $PbCuSO_4(OH)_2$, has been established as a model compound of the frustrated one-dimensional spin chain with ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor interactions [1]. Recently, it has been demonstrated that it exhibits a complex magnetic phase diagram in applied fields $B \parallel b$ axis up to 9.5 T for temperatures below 2.8 K [2].

Here, we present additional neutron diffraction experiments on the field induced phases of linarite, with special emphasis on the low temperature and high magnetic field regime for fields applied along the crystallographic b axis. This way, the temperature and field dependence of the magnetic moment were established for temperatures down to 50 mK and fields up to 9.5 T. As well, the nature of the phase transitions from phase IV into the surrounding phases being of first order was derived.

[1] B. Willenberg et al., PRL **108** 117202 (2012)
[2] B. Willenberg et al., arXiv:1508.02207

TT 42.10 Wed 12:00 H18

Exotic spin phases in the one-dimensional spin-1/2 quantum magnet $LiCuSbO_4$ as seen by high-field NMR and ESR spectroscopies — •Margarita Iakovleva[1,2,3], Hans-Joachim Grafe[1], Evgeniia Vavilova[3], Vladislav Kataev[1], Alexey Alfonsov[1], Hiroyuki Nojiri[4], Mihai I. Sturza[1], Sabine Wurmehl[1], and Bernd Büchner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Zavoisky Physical Technical Institute, Kazan, Russia — [4]Institute of Materials Research, Sendai, Japan

We will present our recent results of high-field NMR and sub-THz ESR studies of the quantum magnet $LiCuSbO_4$ (LCSO) that presents an excellent model system of a one-dimensional spin-1/2 quantum magnet with frustrated exchange interactions. Such networks are predicted to exhibit a plethora of novel ground states beyond classical ferro- or antiferromagnetic phases. In LCSO the absence of a long-range magnetic order down to sub-Kelvin temperatures is suggestive of the realization of a quantum spin liquid state. Our NMR and ESR measurements in strong magnetic fields up to 16 Tesla reveal clear indications for the occurrence of an exotic field-induced hidden phase which we will discuss in terms of multipolar physics.

TT 42.11 Wed 12:15 H18

Theoretical Aspects of Quantum Magnetism in $LiSbCuO_4$ — Satoshi Nishimoto[1], •Stefan-Ludwig Drechsler[1], Ullrich Roessler[1], Roman Kuzian[2], Johannes Richter[3], and Helge Rosner[4] — [1]ITF at the Leibniz Institute IFW-Dresden, 01171 Dresden, Germany — [2]IPMS, Kiev, Ukraine — [3]University of Magdeburg, Germany — [4]MPI-cPfS, Dresden, Dresden

We apply various theoretical methods (DMRG, LDA+U, equation of motion for hard-core bosons, complete diagonalizations, and a full symmetry analysis) to model the recently discovered novel frustrated edge-shared chain cuprate $LiSbCuO_4$ [1] in terms of isotropic and anisotropic interacting J_1-J_1'-J_2 chains including also interchain coupling. Special attention is paid to possible field induced multipolar phases near the saturation field and the remarkable interplay of possible nematicity with symmetric and antisymmetric exchange anisotropy. In particular, the main exchange intra and interchain couplings are estimated, the nature and the role of weak Dzyaloshinskii-Moriya interactions allowed by the low crystal symmetry as well as disorder effects caused by the Li-split positions are adressed,too. Various thermodynamic properties such as magnetization and magnetic specific heat are calculated and compare well with available experimental data. $LiSbCuO_4$ is found to be one of the most challenging edge-shared cuprates with unusual physical properties.

[1] S.E. Dutton *et al.*, PRL **108**, 187206 (2012).

TT 42.12 Wed 12:30 H18

Thermodynamic investigations of the quasi-2d triangular Heisenberg antiferromagnet $Cs_2CuCl_{4-x}Br_x$ ($x = 1, 2$) — •Ulrich Tutsch, Lars Postulka, Bernd Wolf, Michael Lang, Natalija van Well, Franz Ritter, Cornelius Krellner, and Wolf Assmus — Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TR 49

$Cs_2CuCl_{4-x}Br_x$ ($0 \le x \le 4$) is a quasi-two-dimensional Heisenberg antiferromagnet with an anisotropic triangular in-plane coupling of the spins. The ratio J'/J of the spin-spin coupling constants determines the degree of frustration in the system and has been found to be 0.34 ($x = 0$) and 0.47 ($x = 4$) for the border compounds. In ref. [1] it has been suggested that for some intermediate Br concentration an even higher degree of frustration can be reached, and indeed, some results pointing into this direction have been reported by Ono *et al.* [2].

Here, we present specific heat C and susceptibility χ measurements below 1 K in magnetic fields B up to 13.5 T for the intermediate compounds $Cs_2CuCl_2Br_2$ and Cs_2CuCl_3Br, which, due to site-selective substitution [1], show a well-ordered halide sublattice. Our results, which point to a relatively high degree of frustration for $x = 2$, as well as the derived B-T phase diagram will be discussed in the framework of the triangular spin lattice.

[1] P.T. Cong *et al.*, Phys. Rev. B **83**, 064425 (2011)
[2] T. Ono *et al.*, J. Phys. Soc. Jpn. **74** Suppl., 135 (2005)

TT 42.13 Wed 12:45 H18

Spin relaxation processes in $Cr_{1-x}Fe_x$ — •S. Säubert[1,3], P. Schmakat[2,3], J. Kindervater[1], G. Benka[1], A. Bauer[1], J. N.

Wagner[4], W. Häussler[3], O. Holderer[3], S. M. Shapiro[5], C. Pfleiderer[1], and P. Böni[2] — [1]Lehrstuhl für Topologie korrelierter Systeme, Technische Universität München, Garching, Germany — [2]Lehrstuhl für Neutronenstreuung, Technische Universität München, Garching, Germany — [3]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [4]Karlsruher Institute for Technology, IAM-WK, Eggenstein- Leopoldshafen, Germany — [5]Brookhaven National Laboratory, Department of Physics, Upton, USA

$Cr_{1-x}Fe_x$ shows reentrant spin glass behaviour below a doping dependent freezing temperature T_f. In contrast to a classical spin glass, the ground state changes from antiferromagnetic to ferromagnetic order with increasing iron concentration x [1, 2].

We report a study of the spin relaxation processes by means of neutron spin echo, magnetisation measurements and neutron depolarisation imaging for a wide range of concentrations x. This allows us to compare the relaxation process depending on the particular state at high temperatures. Our measurements provide an unprecedented combination of microscopic information on the spin dynamics and spin freezing on multiple length and time scales.

[1] S. K. Burke et al., J. Phys. F: Met. Phys. **13** 45 1-470 (1983)
[2] S. M. Shapiro et al., PRB **24**, 6661 (1981)
[3] R.M. Pickup et al., PRL **102**, 097202 (2009)