TT 20: Correlated Electrons: Spin Systems and Itinerant Magnets - Frustrated Magnets II

Time: Monday 15:00–18:00 Location: HSZ 304

TT 20.1 Mon 15:00 HSZ 304

Magnetic properties of $VOMoO_4$ and Li_2VOSiO_4: an LDA+DMFT study — •Amin Kiani and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

By using the local density approximation+dynamical mean field theory and local vertex approximation we calculate the static magnetic response function overall the Brillouin zone for the two highly correlated materials $VOMoO_4$ and Li_2VOSiO_4. We show that the vertex function is crucial to understand the magnetic properties. From the **q**−dependent spin susceptibility we identify the magnetic instabilities related to anti-ferromagnetic and collinear order for $VOMoO_4$ and Li_2VOSiO_4, respectively. Furthermore we determine the local magnetic moment and the Neel temperature from the high temperature uniform magnetic susceptibility. We also investigate the role of the magnetic coupling in the third dimension.

TT 20.2 Mon 15:15 HSZ 304

Magnetic anisotropies in the Ising spin-chain compound $BaCo_2V_2O_8$ and the effect of substitution — •Sandra Niesen[1], Gerhard Kolland[1], Michael Seher[1], Oliver Breunig[1], Martin Valldor[1], Markus Braden[1], Beatrice Grenier[2], and Thomas Lorenz[1] — [1]II. Phys. Institut, Universität zu Köln — [2]SPSMS, CEA-INAC/UJF-Grenoble, France

The effective Ising spin-1/2 system $BaCo_2V_2O_8$ consists of CoO_6 octahedra that form screw chains along the c axis. Long-range antiferromagnetic order is observed below $T_N = 5.5$ K in zero magnetic field with the spins aligned along c. Within the ab plane the spin arrangement is known to be frustrated with a ferromagnetic alignment of neighbouring spins along [100] and an antiferromagnetic one along [010]. Our zero field thermal expansion data show that the Néel order is accompanied by a structural transition from tetragonal to orthorhombic, which lifts the magnetic frustration [1]. Consequently, the magnetic-field influence is anisotropic within the ab plane as seen in, *e.g.* measurements of the magnetization, thermal expansion, specific heat, and thermal conductivity. A detailed study of this anisotropy and the resulting magnetic phase diagrams will be presented. In addition, we will discuss the influence of partial substitution of Ba by Sr and of Co by either magnetic or nonmagnetic ions.

This work has been supported by the DFG via SFB 608 and through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

[1] S. Niesen *et al.*, PRB **87**, 224413 (2013)

TT 20.3 Mon 15:30 HSZ 304

Spin-lattice coupling in the frustrated S=1/2 compound $Cu_7Te_6O_{18}F_2$ — Vladimir Gnezdilov[1,2], •Peter Lemmens[1], Azat Sharafeev[1], Angela Möller[3], Shichao Hu[4] und Mats Johnsson[4] — [1]IPKM, TU-BS, Braunschweig — [2]ILTPE NAS, Ukraine — [3]Dept. Chem., Univ., Houston, USA — [4]DMEC, Stockholm, Sweden

We present a Raman scattering study of the novel spin-frustrated S=1/2 compound $Cu_7Te_6O_{18}F_2$. The phonons of this compound display evidence for strong spin-lattice coupling. Furthermore, there exists a broad magnetic scattering continuum that markedly changes with the onset of long-range ordering. Work supported by DFG and B-IGSM.

TT 20.4 Mon 15:45 HSZ 304

The 2D Shastry-Sutherland model and $SrCu_2(BO_3)_2$ in Magnetic Fields up to 118T — •Andreas Honecker[1], Philippe Corboz[2], Frédéric Mila[3], HongYu Yang[3], Salvatore R. Manmana[1], Kai P. Schmidt[4], Gregor R. Foltin[4], Hiroshi Kageyama[5], Nozomu Abe[6], Shojiro Takeyama[6], and Yasuhiro Matsuda[6] — [1]Georg-August-Universität Göttingen, Germany — [2]ETH Zürich, Switzerland — [3]Ecole Polytechnique Fédérale de Lausanne, Switzerland — [4]TU Dortmund, Germany — [5]Kyoto University, Japan — [6]ISSP, University of Tokyo, Japan

The magnetization process of the orthogonal-dimer antiferromagnet $SrCu_2(BO_3)_2$ is investigated in high magnetic fields of up to 118T. A 1/2 plateau is clearly observed in the field range 84 to 108T in addition to 1/3, 1/4, and 1/8 plateaux at lower fields. Using a combination of state-of-the-art numerical simulations, the main features of the high-field magnetization curve are shown to agree quantitatively with the Shastry-Sutherland model for a ratio of inter- to intra-dimer exchange interactions $J'/J = 0.63$. It is further predicted that the intermediate phase between the 1/3 and 1/2 plateau consists of a 1/3 supersolid followed by a non-plateau 2/5 supersolid. As a byproduct, we obtain estimates for the boundaries of a zero-field plaquette phase based on exact diagonalization with up to $N = 40$ sites.

TT 20.5 Mon 16:00 HSZ 304

NMR on the Frustrated Spin-chain Compound $PbCuSO_4(OH)_2$ - Linarite — •M. Schäpers[1], A. U. B. Wolter[1], B. Willenberg[2,4], S.-L. Drechsler[1], H. Rosner[3], S. Süllow[4], and B. Büchner[1] — [1]Leibniz-Institut IFW Dresden, Dresden, Germany — [2]HZB, Berlin, Germany — [3]MPI CPfS, Dresden, Germany — [4]IPKM, TU Braunschweig, Braunschweig, Germany

We present an extensive microscopic magnetic study of the quasi-one-dimensional frustrated $s = \frac{1}{2}$ spin-chain compound linarite. Angular dependent susceptibility and ^{1}H-NMR measurements were performed at various temperatures in the paramagnetic state. All relevant NMR parameters, viz., the chemical, dipolar, and Fermi-contact contribution, were extracted to analytically calculate the local magnetic fields at the ^{1}H sites. From this analysis, a significant total spin transfer of ∼10.5 % from the magnetic copper ions onto the two oxygen ligands was derived. The magnetically ordered spin-spiral ground state below $T_N = 2.8$ K was investigated by ^{1}H-NMR for fields $\mu_0 H = 2.0$ T along the three crystallographic main directions. With the derived NMR parameters in the paramagnetic regime it is possible to model the NMR spectrum for $H \parallel c$, which is in agreement with previous neutron studies [1]. Furthermore, we compare our results with density functional band structure calculations and subsequent cluster calculations applying a *pd* model.

This work has partially been supported by the DFG under Contracts No. WO 1532/3-1 and No. SU229/10-1.

[1] B. Willenberg *et al.*, Phys. Rev. Lett. **108,** 117202 (2012).

TT 20.6 Mon 16:15 HSZ 304

Multipolar states in coupled frustrated spin-1/2 chains with exchange anisotropy — •Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], Roman Kuzian[1,2], Johannes Richter[3], and Jeroen van den Brink[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Institute for Problems of Materials Science NASU, 03180 Kiev, Ukraine — [3]Universität Magdeburg, Institut für Theoretische Physik, Germany

We studied coupled frustrated spin-1/2 Heisenberg chains at high magnetic field. The effects of inter-chain couplings and easy-axis exchange anisotropy on the multipolar states were considered using the spin-wave theory and density-matrix renormalization group method. We quantified the instability towards the formation of multipolar states against various kinds of antiferromagnetic and ferromagnetic inter-chain couplings, and also found that an easy-axis anisotropy of the ferromagnetic in-chain nearest-neighbor exchange significantly enhances the multipolar stability region [1]. We will discuss the relevance to edge-shared cuprate spin-chain compounds such as $LiVCuO_4$, $PbCuSO_4(OH)_2$ [2], etc, which are found to be possible candidates for multipolar physics.

[1] S. Nishimoto, S.-L. Drechsler, R.O. Kuzian, J. Richter, J. van den Brink, arXiv:1303.1933v1.
[2] M. Schäpers, A.U.B. Wolter, S.-L. Drechsler, S. Nishimoto, R. Vogel, W. Schottenhamel, B. Büchner, J. Richter, B. Ouladdiaf, M. Uhlarz, R. Beyer, Y. Skourski, J. Wosnitza, K.C. Rule, M. Reehuis, B. Willenberg, S. Süllow, Phys. Rev. B **88**, 195138 (2013).

15 min. break.

TT 20.7 Mon 16:45 HSZ 304

Electronic structure and magnetism of libethenite - Cu_2PO_4OH — Miriam Schmitt[1], Oleg Janson[2], Stefan Lebernegg[2], and •Helge Rosner[2] — [1]Universität Kaiserslautern, 67663 Kaiserslautern — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden

The spin 1/2 compound Cu_2PO_4OH attracted interest not only by its unusual crystal structure containing a combination of edge shared CuO_4 chains linked by Cu_2O_8 dimers, but also by the formation of a

spin gap at low temperatures. Recently, a tetramer model was suggested in a combined experimental and theoretical study [1]. Based on density functional band structure calculations we suggest that the simple tetramer model should be refined by additional intra- and inter-tetramer exchange couplings for an accurate description of the magnetic properties of libethenite.

TT 20.8 Mon 17:00 HSZ 304

Hindered magnetic order from multiple dimensionalities in CuP_2O_6 — •Alexander A. Tsirlin[1], Ramesh Nath[2], Jörg Sichelschmidt[3], Fabien Alet[4], and Ioannis Rousochatzakis[5] — [1]NICPB, Tallinn, Estonia — [2]Indian Institute of Science Education and Research, Trivandrum, India — [3]MPI CPfS, Dresden, Germany — [4]Universite de Toulouse, France — [5]IFW Dresden, Germany

We report magnetic properties of CuP_2O_6, where spin systems of different dimensionalities coexist and lead to a strong suppression of the magnetic ordering transition. This compound features spin planes formed by the Cu1 sites (2D) and spin chains formed by the Cu2 sites (1D), with the antiferromagnetic couplings $J_{2D} \simeq 40$ K and $J_{1D} \simeq 3$ K, respectively. The estimates obtained from density-functional band structure calculations are verified by quantum Monte-Carlo fits to the experimental magnetization data. The magnetic ordering transition at $T_N \simeq 8$ K results in the formation of a very weak net moment arising from Dzyaloshinsky-Moriya anisotropy in the Cu1 planes. However, the ESR signal does not vanish below T_N. We ascribe this peculiar effect to the drastic difference between the two sublattices: in the weakly coupled 1D sublattice, the ordered moment grows very slowly, hence the behavior of this sublattice is largely paramagnetic even below T_N. This physics is captured by a mean-field theory showing that the Néel temperature of CuP_2O_6 is determined by the geometrical mean value of staggered susceptibilities in the 1D and 2D sublattices.

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TT 20.9 Mon 17:15 HSZ 304

The interplay of crystal structure, electronic structure and magnetism in $SrCo_2P_2$ — •Helge Rosner, Deepa Kasinathan, Inga Kraft, Vivien Lorenz, Christoph Bergmann, and Christoph Geibel — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden

Since the discovery of high temperature superconductivity in doped iron pniktides, in particular AFe_2As_2 systems of the $ThCr_2Si_2$ structure type, the intricate interplay of crystal structure, magnetism and superconductivity in these compounds has attracted broad attention. It is widely believed that the superconductivity of this compound family is closely related tho spin fluctuations. A clear picture of the coupling scenario, however, has not yet emerged. $SrCo_2P_2$ is a structural homologue of the AFe_2As_2 compound series. Experimental investigations indicate a paramagnetic ground state of the system, but a closed vicinity to a (quantum) critical point. We studied the electronic structure and magnetic properties of this compound applying DFT calculations in different approximations. In all setups, we find a pronounced peak in the electronic density of states close to the Fermi level originating from Co-3d states, indicating an instability towards magnetic order. However, structural details have a surprisingly strong influence on details of the band structure and the topology of the Fermi surface. Our calculational results are compared with thermodynamic measurements and de-Haas-van-Alphen data.

TT 20.10 Mon 17:30 HSZ 304

Hour-glass magnetic spectrum in a stripeless insulating transition metal oxide — •Jan Yvo Drees[1], Daniel Lamago[2], Andrea Piovano[3], and Alexander C. Komarek[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Physics of Correlated Matter, Nöthnitzer Street 40, D-01187 Dresden, Germany — [2]Laboratoire Léon Brillouin, CEA/CNRS, F-91191 Gif-sur Yvette, France — [3]Institut Laue-Langevin (ILL), 6 Rue Jules Horowitz, F-38043 Grenoble, France

An hour-glass-shaped magnetic excitation spectrum appears to be a universal characteristic of the high-temperature superconducting cuprates. Fluctuating charge stripes or alternative band structure approaches are able to explain the origin of these spectra. Recently, an hour-glass spectrum has been observed in an insulating cobaltate, thus favouring the charge stripe scenario. Here we show that neither charge stripes nor band structure effects are responsible for the hour-glass dispersion in a cobaltate within the checkerboard charge-ordered regime of $La_{2-x}Sr_xCoO_4$. The search for charge stripe ordering reflections yields no evidence for charge stripes in $La_{1.6}Sr9.4CoO_4$, which is supported by our phonon studies. With the observation of an hour-glass-shaped excitation spectrum in this stripeless insulating cobaltate, we provide experimental evidence that the hour-glass spectrum is neither necessarily connected to charge stripes nor to band structure effects, but instead, probably intimately coupled to frustration and arising chiral or non-collinear magnetic correlations.

TT 20.11 Mon 17:45 HSZ 304

Magnetic properties of intermetallic AT_4X_2 compounds — •Vivien Lorenz, Inga Kraft, Christoph Bergmann, Katharina Weber, Nandang Mufti, Christoph Geibel, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Magnetic systems with reduced dimensionality or frustration attract strong interest because these features lead to an increase of quantum fluctuations and often result in unusual properties. The vicinity of magnetic and non magnetic states can further increase the fluctuations. Here, we present a detailed density-functional-based study of the electronic, magnetic and structural properties of the intermetallic AT_4X_2 compounds (A=Sc,Y,Lu,Zr,Hf; T=Fe,Ni,Re; X=Si,Ge,P,As) crystallizing in the $ZrFe_4Si_2$ structure type. Magnetic and structural transitions were previously reported for YFe_4Ge_2 and closely related compounds with trivalent A-site occupation. However, transition temperatures, nature of the transition as well as the relation between structural and magnetic transitions change significantly with the A element. Our calculational results evidence that: (i) all investigated T=Fe compounds have a magnetic ground state; (ii) all investigated T=Ni systems are non magnetic, but several of them are very close to magnetism; (iii) the magnetic properties of these compounds can be "tuned" by partial substitution on the T and X site. We also study the instability towards a structural distortion related to strong magneto-elastic coupling. Our findings will be compared to recent experimental results.