TT 18: CE: Low-dimensional Systems - Materials 1

Time: Monday 18:30–20:00 Location: HSZ 201

TT 18.1 Mon 18:30 HSZ 201

Magnetic models from DFT cluster calculations - an alternative to supercell computations? — •Stefan Lebernegg[1], Miriam Schmitt[2], Ulrike Nitzsche[3], and Helge Rosner[2] — [1]Universität Salzburg, 5081 Salzburg, Austria — [2]MPI CPfS Dresden, 01187 Dresden, Germany — [3]IFW Dresden, 01171 Dresden, Germany

For the treatment of strong electron correlation two standard approaches are commonly used: In principle, quantum chemistry can deal with strong correlations exactly, but only for small clusters. On the other hand, periodic 3D compounds can be calculated reliably in DFT codes, but the correlations are treated in a very approximate manner, often including external parameters like in the LSDA+U method. The far goal of this work is to find a way to construct reliable clusters capable to describe local properties of solids. In a first step toward this aim, magnetic properties of simple Cu^{2+} compounds with different ligands (N,O,F,Cl,Br) that exhibit edge sharing chains as their central building blocks are systematically studied. For the model clusters, effects of their finite size, embedding and termination as well as the substitution of Cu by formally nonmagnetic cations (broken chain) are investigated. The calculations are carried out within a full potential DFT code and are compared with corresponding known periodic 3D compounds (CuNCN, Li_2CuO_2, $CuCl_2$, $CuBr_2$). The presented cluster approach not only enables the application of highly accurate computational methods but might be used instead of elaborated supercell calculations. Moreover, additional degrees of freedom can provide deeper insight into magneto-structural correlations.

TT 18.2 Mon 18:45 HSZ 201

A microscopic magnetic model for the spin-1/2 Heisenberg piezoelectric ferrimagnet Cu_2OSeO_3 — •Oleg Janson, Alexander Tsirlin, and Helge Rosner — Max-Planck-Institut für Chemische Physik fester Stoffe

We present the results of band structure calculations for the piezoelectric ferrimagnet Cu_2OSeO_3. Below the $T_C = 60$ K, the compound exhibits sizable magnetocapacitance and stays metrically cubic, which excludes lattice strain from possible magnetoelastic mechanisms [1]. The crystal structure of Cu_2OSeO_3 comprises two inequivalent positions of magnetic Cu^{2+} atoms: 4 Cu(1) atoms are locally coordinated by a trigonal bipyramid of O atoms, while 12 Cu(2) atoms have a distorted 4-fold coordination, typical for cuprates. The net magnetization in the ferrimagnetically ordered ground state results from the antiparallel arrangement of Cu(1) and Cu(2) sublattices [2] and amounts to one-half of the saturation value. Based on DFT calculations, we disclose different magnetically active orbitals for Cu(1) and Cu(2) and five relevant magnetic couplings that form a complex, albeit non-frustrated 3D spin lattice. The role of quantum fluctuations will be discussed in the context of the reduced ordered moment on Cu atoms amounting to $0.61\,\mu_B$ [1] and a low $T_C/J \approx 0.6$.

[1] J.-W. G. Bos *et al.*, Phys. Rev. B 78, 094416 (2008).
[2] M. Belesi *et al.*, Phys. Rev. B 82, 094422 (2010).

TT 18.3 Mon 19:00 HSZ 201

Ferromagnetic versus helical order in edge sharing CuO_2 chains - a computational study — •Helge Rosner[1], Ulrike Nitzsche[2], Roman Kuzian[2], and Stefan-Ludwig Drechsler[2] — [1]MPI CPfS Dresden — [2]IFW Dresden

The magnetic ground state of edge sharing CuO_2 spin 1/2 Heisenberg chains with ferromagnetic nearest neighbor exchange J_1 and antiferromagnetic second neighbor exchange J_2 depends delicately on structural details of the crystal structure, like Cu-O-Cu bond angles, Cu-O distances and the position of the cations. Without taking into account a renormalization by the interchain coupling, a critical ratio $\alpha = -J_2/J_1 = 1/4$ separates a ferromagnetic from a helical ground state (FM for $\alpha < 1/4$, helical for $\alpha > 1/4$). Here, we present a density functional based band structure study that investigates the different influences of various structural parameters for Li_2CuO_2 as example compound. We find that the ferromagnetic and antiferromagnetic contributions develop rather differently for the same structural changes. Therefore, the key parameter α for the ground state is especially sensitive to small structural changes that might be induced by temperature or pressure variation.

TT 18.4 Mon 19:15 HSZ 201

The influence of inter-chain couplings on the thermodynamics of the strongly frustrated chain cuprate Li_2CuO_2 — •W.E.A. Lorenz[1], S.-L. Drechsler[1], R.O. Kuzian[2], S. Nishimoto[1], S. Petit[3], Y. Skourski[4], N. Wizent[1], R. Klingeler[5], and B. Büchner[1] — [1]Leibniz-Inst. f. Festkörper- & Werkstoffforschung, Dresden, Germany — [2]Inst. f. Problems of Materials Science, Kiev, Ukraine — [3]Laboratoire Léon Brillouin, Saclay, France — [4]Hochfeld-Magnetlabor Dresden(HLD), FZ-Dresden-Rossendorf, Dresden, Germany — [5]Kirchhoff Institute for Physics, University of Heidelberg, Heidelberg, Germany

We report on detailed experimental and theoretical studies on the magnetic properties of Li_2CuO_2. This compound serves as a simple, but representative model system for spin-chain materials in which strong nearest-neighbor ferromagnetic interactions in the chain which are frustrated by an antiferromagnetic (afm) coupling to next-nearest-neighbors. The competition of interactions can induce incommensurate correlations in the chain. On the example of Li_2CuO_2 we illustrate, that relatively weak inter-chain couplings can prevent incommensurate long-range order and determine solely the saturation field. The inter-chain coupling derived from the saturation field are in excellent agreement with inelastic neutron scattering data [1,2]. The absence of bound magnon states in Li_2CuO_2 is explained in terms of the inter-chain couplings exceeding a critical value of a few meV, only.

[1] W.E.A. Lorenz *et al.*, Europhys. Lett. **88**, 37002 (2009).
[2] S. Nishimoto *et al.*, arXiv:1004.3300v2 (2010).

TT 18.5 Mon 19:30 HSZ 201

Evidence for the opening of a spin gap in the Ca-doped S=1/2 spin chain compound $SrCuO_2$ probed by NMR — •Franziska Hammerath, Satoshi Nishimoto, Hans-Joachim Grafe, A.U.B. Wolter, Christian Hess, Vladislav Kataev, Patrick Ribeiro, S.-L. Drechsler, and Bernd Büchner — Institute for Solid State Research, IFW Dresden,

We present ^{63}Cu Nuclear Magnetic Resonance (NMR) measurements on undoped $SrCuO_2$ and Ca-doped $Sr_{0.9}Ca_{0.1}CuO_2$ single crystals. The crystal structure contains one dimensional CuO_2 double chains that are magnetically decoupled due to frustration. For $SrCuO_2$ the spin lattice relaxation rate T_1^{-1} is temperature independent as it is expected for a one dimensional S=1/2 Heisenberg spin chain. Doping with nonmagnetic, isovalent Ca takes place on the Sr sites outside the spin chains, and should not affect the magnetic properties of the compound. It is therefore very surprising that we do observe a decrease of T_1^{-1} in the Ca-doped sample for temperatures below 80K that clearly evidences the opening of a gap in the spin excitation spectrum. Density Matrix Renormalization Group (DMRG) calculations are presented to discuss the origin of this spin gap.

TT 18.6 Mon 19:45 HSZ 201

Low temperature ballistic spin transport in the $S = 1/2$ antiferromagnetic Heisenberg chain compound $SrCuO_2$ — H. Maeter[1], A.A. Zvyagin[1,2], H. Luetkens[3], G. Pascua[3], Z. Shermadini[3], C. Hess[4], N. Hlubek[4], B. Büchner[4], R. Saint-Matin[5], A. Revcolevschi[5], and •H.-H. Klauss[1] — [1]Institut für Festkörperphysik, TU Dresden — [2]Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, Kharkov, 61103, Ukraine — [3]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen, Switzerland — [4]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden — [5]Laboratoire de Physico–Chimie de L'Etat Solide, ICMMO, UMR 8182, Universite Paris-Sud, 91405 Orsay, France

For one-dimensional quantum spin chain systems recent experimental and theoretical studies indicate unexpectedly large, in some cases diverging spin and heat transport coefficients. Local probes, like e.g. muon spin relaxation (μSR) can indirectly characterize the spin transport properties of low dimensional systems via the magnetic field dependence of the spin lattice relaxation rate $\lambda(B)$. For diffusive spin transport $\lambda \propto B^{-0.5}$ is expected. For the ground state of the isotropic spin-1/2 antiferromagnetic Heisenberg chain the eigenstates of the Heisenberg Hamiltonian dominate the spin transport, which is then *ballistic*. Using the Müller ansatz $\lambda \propto B^{-1}$ is expected in this case. For $SrCuO_2$ we find $\lambda \propto B^{-0.9(3)}$. This result is temperature independent for 5 K$\leq T \leq$ 300 K. Within conformal field theory and using the Müller ansatz we conclude *ballistic* spin transport in $SrCuO_2$.