TT 11: CE: Low-dimensional Systems - Materials 2

Time: Tuesday 9:30–12:45 Location: H18

TT 11.1 Tue 9:30 H18

Electron Energy-Loss Spectroscopy on the Transition-Metal Dichalchogenide $2H$-$TaSe_2$ — •Andreas König[1], Roman Schuster[1], Helmuth Berger[2], Martin Knupfer[1], and Bernd Büchner[1] — [1]Institute for Solid State Research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Insitut de Physique de la Matière Complexe, EPFL, CH-1051 Lausanne, Switzerland

$2H$-$TaSe_2$ is one of the various polytypes of the transition-metal dichalchogenide (TMDC) $TaSe_2$. It consists of hexagonal layers with weak interlayer van-der-Waals bonding. It shows phase transitions to a charge-density wave (CDW) and to a superconducting state. Although there is strong evidence for the competition of these two ordering effects as well as for a Peierls transition scenario for the origin of the CDW, a theoretical understanding of the mechanism leading to the phase transitions is still subject of discussions. What is already proved for $2H$-$TaSe_2$ and a few other TMDCs is a negative dispersion of the bulk plasmon in the normal state and an even larger bandwidth of this negative dispersion in the CDW state, which is altogether not a common metal behavior [1]. We performed Electron Energy-Loss Spectroscopy in transmission on thin films of $2H$-$TaSe_2$ for different temperatures above and below the CDW transition temperature to investigate the connection of the CDW phase transition to the plasmon dispersion.

[1] Schuster et al., Phys. Rev. B. **79**, 045134 (2009)

TT 11.2 Tue 9:45 H18

Raman scattering evidence for a cascade-like evolution of the charge-density-wave collective amplitude mode — •Hans-Martin Eiter[1], Michela Lavagnini[2], Leonardo Tassini[1], Bernhard Muschler[1], Jiun-Haw Chu[3], Nancy Ru[3], Ian R. Fisher[3], Leonardo Degiorgi[2], and Rudi Hackl[1] — [1]Walther Meissner Institute, Bavarian Academy of Sciences and Humanities, 85748 Garching — [2]Laboratorium für Festkörperphysik, ETH - Zürich, CH-8093 Zürich, Switzerland — [3]GLAM, Stanford University, CA 94304, USA

We report results of Raman scattering experiments as a function of temperature on the charge-density-wave (CDW) systems $DyTe_3$ and on $LaTe_3$ at 6 GPa applied pressure. We clearly identify the unidirectional collective CDW amplitude excitation and follow their temperature dependence in the range from 6 K to 311 K. Surprisingly, we discover that the amplitude mode develops as a succession of two mean-field, BCS-like transitions at two different temperatures.

Tri-tellurides with heavier rare-earth atoms (i.e. Tm, Er, Ho, Dy) undergo another phase transition to a bidirectional CDW at low temperatures. In $DyTe_3$ we find spectroscopic evidence for the amplitude mode excitation associated with the bidirectional CDW occuring below 50 K.

This work is supported by the DFG under Grant No. Ha2071/5-1.

TT 11.3 Tue 10:00 H18

LDA+Slave-boson mean-field theory: a powerful low-energy tool for realistic strongly correlated systems — •Christoph Piefke and Frank Lechermann — I. Institut fuer Theoretische Physik, Universitaet Hamburg, Jungiusstrasse 9, 20355 Hamburg

The rotationally invariant slave-boson mean-field theory (RISB) has proven to be a powerful tool to investigate large parameter spaces of arbitrary strongly interacting systems [1,2]. In this approach, complex fermionic interactions are described by means of an electon-operator decoupling into a quasiparticle part and localized bosonic degrees of freedom. A set of constraints ensures that this mapping does not leave the Hilbert space of the original problem. At saddle-point, a self-consistent mean-field solution is obtained.

As an efficent method for demanding problems, RISB is used to investigate LDA-based models for realistic materials with strong electronic correlations. Resulting physical quantities like the quasiparticle weight or the local spin correlations for, e.g., the Na_xCoO_2 system [3], are in very good agreement with more accurate many-body approaches. Moreover the additionally extracted multiplet weights for atoms and clusters in the strongly correlated regime provide further important insight into the competition between itinerancy and localization.

[1] T. Li, P. Wölfle, and P. J. Hirschfeld, Phys. Rev. B **40**, 6817 (1989).

[2] F. Lechermann, A. Georges, G. Kotliar and O. Parcollet, Phys. Rev. B **76**, 155102 (2007).

[3] F. Lechermann, Phys. Rev. Lett. **102**, 046403 (2009).

TT 11.4 Tue 10:15 H18

Ground state description of $BiCu_2PO_6$ and $BiCu_2AsO_6$ — •Deepa Kasinathan, Alexander Tsirlin, Oleg Janson, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Low dimensional spin systems have always been of interest to the physics community due to their inherent exotic magnetic properties. A further impetus for the study of low-dimensional spin systems was given by the discovery of spin-ladder materials, due to the fact that they are intermediate objects between 1D and 2D systems. Recent experiments by two groups [1,2] on a spin-ladder material $BiCu_2PO_6$ exhibited a gapped singlet ground state with a spin gap of about 34 K, though the strength of the spin-exchange interactions have remained controversial. No consensus has been reached on the correct spin-ladder model to describe this compound. We will report on our re-investigations of $BiCu_2PO_6$ and the related material $BiCu_2AsO_6$ using density functional theory based electronic structure calculations and as well as Transfer Matrix Renormalization Group (TMRG) calculations. Our results necessitate the inclusion of previously neglected exchange couplings to describe the spin-ladder model more appropriately.

[1] B. Koteswararao, *et. al.*, Phys. Rev. B **76**, 052402 (2007).

[2] O. Mentré, *et. al.*, Phys. Rev. B **80**, 180413 (2009).

TT 11.5 Tue 10:30 H18

Unraveling the 1/2 magnetization plateau: a new microscopic magnetic model for $CdCu_2(BO_3)_2$ — •Oleg Janson[1], Alexander Tsirlin[1], Johannes Richter[2], Yurii Skourski[3], and Helge Rosner[1] — [1]MPI CPfS Dresden — [2]University of Magdeburg — [3]Dresden High Magnetic Field Laboratory (HLD)

Copper(II) cadmium borate $CdCu_2(BO_3)_2$ is a spin-1/2 Heisenberg system showing a remarkable 1/2 plateau in the magnetization curve. Based on experimental studies of this compound ($\chi(T)$, $C_p(T)$, $M(H)$), a phenomenological model for its magnetism has been suggested [1]. According to this model, the system can be described as consisting of spin chains and dimers, formed by structurally different atoms Cu1 and Cu2, respectively. However, recent neutron diffraction experiments [2] evidence an inconsistency of this simple chain-dimer model, since both Cu positions show sizable magnetic moments in the ordered state.

We have studied this system using DFT calculations. Typically for Cu^{2+} materials, the magnetism of $CdCu_2(BO_3)_2$ can be described by an effective one-orbital approach. Based on the tight-binding fit of the relevant LDA bands, we estimate the antiferromagnetic contribution to the magnetic exchange. The total exchange is obtained by LSDA+U supercell calculations. Exact diagonalization studies of the parameterized Heisenberg model evidence that the new microscopic model consistently describes all existing thermodynamical data. The results of new $M(H)$ measurements and NMR experiments will be briefly discussed.

[1] Hase et al., Phys. Rev. B **72** 172412 (2005).

[2] Hase et al., Phys. Rev. B **80** 104405 (2009).

TT 11.6 Tue 10:45 H18

Magnetic properties of the spin chain compound Li_2CuO_2 — •W.E.A. Lorenz[1], S.-L. Drechsler[1], R.O. Kuzian[2], W.-D. Stein[3], N. Wizent[1], G. Behr[1], A. Hiess[4], W. Schmidt[5], S. Petit[6], K. Nenkov[1], M. Loewenhaupt[3], R. Klingeler[1], and B. Büchner[1] — [1]Leibniz-Inst. f. Festkörper- & Werkstoffforschung, Dresden, Germany — [2]Inst. f. Problems of Materials Science, Kiev, Ukraine — [3]Inst. f. Festkörperphysik, TU Dresden — [4]Inst. Laue Langevin, Grenoble, France — [5]Jülich Centre f. Neutron Science — [6]Laboratoire Léon Brillouin, Saclay, France

We report recent experiments on Li_2CuO_2 single crystals. The magnetic phase diagram we have derived from magnetization, specific heat, thermal expansion and magnetostriction data is discussed in view of a new detailed inelastic neutron scattering study [1]. Li_2CuO_2 represents a simple, strongly frustrated spin chain material close to the 3D ferromagnetic (FM)-helical critical point. At low temperatures weak antiferromagnetic inter-chain exchange interactions are found to cause FM in-chain ordering. Above the ground state low-lying helical

excitations are observed. Implications - esp. of the relatively large nearest neighbor exchange interaction - for the frustrated akin ferromagnetic spin chain compound $Ca_2Y_2Cu_5O_{10}$ and the helical system Li_2ZrCuO_4 are pointed out.

[1] W.E.A. Lorenz *et al.*, Europhys. Lett. **88**, 37002 (2009).

15 min. break

TT 11.7 Tue 11:15 H18

Spectroscopic ellipsometry study of the edge-sharing CuO_4 chain cuprate Li_2CuO_2 — •Yulia Matiks[1], A.V. Boris[1], J. Malek[2], S. Nishimoto[2], S.-L. Drechsler[2], P. Horsch[1], N. Wizent[2], G. Behr[2], M. Knupfer[2], B. Buchner[2], and B. Keimer[1] — [1]Max-Planck-Inst. f. Festkörperforschung, Stuttgart, Germany — [2]Leibniz-Inst. f. Festkörper- & Werkstoffforschung, Dresden, Germany

Motivated by observation of a double-peak structure in the edge-sharing chain cuprate $LiCuVO_4$, assigned to the Zhang-Rice exciton states [1], we report detailed ellipsometric measurements on Li_2CuO_2. This compound is characterized by different ratio between the near-neighbor J_1 and the next-near-neighbor J_2 exchange integrals, $\alpha = -J_2/J_1 = 0.33$ [2]. Temperature dependence of the interband transition peaked at 3.7 eV in the optical conductivity along the chains follows spin correlations and becomes apparent below $T_N \approx 9K$. This excitation is assigned to the Zhang-Rice singlet excitation and modelled within a five band Cu $3d$ O2 p extended Hubbard model including long range Coulomb interactions. Applying exact diagonalization and DMRG studies to Cu_nO_{2n+2} chains and corresponding rings a strong intersite Coulomb interaction of about V_{pd}=2.2 eV is found. The main in-chain exchange integrals obtained from a mapping onto a spin-1/2 Hamiltonian are in agreement with the spin wave analysis of the new detailed inelastic neutron scattering study [2].

[1] Y. Matiks *et al.*, Phys. Rev. Lett. **103**, 187401 (2009).
[2] W.E.A. Lorenz *et al.*, Europhys. Lett. **88**, 37002 (2009).

TT 11.8 Tue 11:30 H18

Longitundinal magnon in the AF chain system $KCuF_3$ — Vladimir Gnezdilov[1], •Peter Lemmens[2], Dirk Wulferding[2], Paolo Ghigna[3], and Joachim Deisenhofer[4] — [1]ILTP, Kharkov, Ukraine — [2]IPKM, TU-BS, Braunschweig — [3]DCF, Univ. Pavia, Italy — [4]Exp. Phys. V, CECM, Univ. Augsburg

The low energy longitudinal magnon in $KCuF_3$ was observed and studied for the first time in Raman scattering at temperatures below the Neel temperature. The observation of a spinon continuum and this longitudinal mode reveals the coexistence of antiferromagnetic ordering and quantum fluctuations in $KCuF_3$ for T<T_N. Work supported by DFG.

TT 11.9 Tue 11:45 H18

Ballistic heat transport of quantum spin excitations — •Nikolai Hlubek[1], Patrick Ribeiro[1], Romuald Saint-Martin[2], Surjeet Singh[1], Alexandre Revcolevschi[2], Georg Roth[3], Günter Behr[1], Bernd Büchner[1], and Christian Hess[1] — [1]IFW-Dresden, Germany — [2]Université Paris-Sud, Orsay, France — [3]RWTH Aachen, Germany

We provide experimental evidence for ballistic heat transport in the spin chain material $SrCuO_2$. In particular, we investigate high purity samples of this double chain cuprate and observe a huge magnetic heat conductivity $\kappa_{\rm mag}$. An extremely large spinon mean free path of more than a micrometer demonstrates that $\kappa_{\rm mag}$ is only limited by extrinsic scattering processes which is a clear signature of ballistic transport in the underlying spin model. Furthermore we study the influence of magnetic Ni and non-magnetic Mg impurities on $\kappa_{\rm mag}$ of $SrCuO_2$. While Ni-doping has a large impact on the magnetic thermal conductivity, Mg-doping shows no influence. In order to clarify this surprising behavior we compare $\kappa_{\rm mag}$ to measurements of the single chain compound Sr_2CuO_3.

TT 11.10 Tue 12:00 H18

Ferromagnetic zigzag chains in $CdVO_3$: the role of cadmium — •Alexander Tsirlin and Helge Rosner — Max-Planck Institute CPfS, Dresden, Germany

Most of the low-dimensional spin systems show antiferromagnetic ground states or ground states with low net magnetization due to a weak asymmetry of the exchange couplings. Low-dimensional ferromagnets are rare, yet they show interesting low-temperature properties. These properties can be affected by quantum fluctuations, although entirely ferromagnetic systems with isotropic exchange couplings are not subject to the magnetic frustration. In this contribution, we present a band structure-based microscopic model for the low-dimensional spin-$\frac{1}{2}$ compound $CdVO_3$. The crystal structure of $CdVO_3$ shows zigzag chains of VO_5 square pyramids. These chains can be considered as spin chains with nearest-neighbor (J_1) and next-nearest-neighbor (J_2) couplings, both being ferromagnetic: $J_1 \simeq J_2 \simeq -50$ K. Moreover, the interchain couplings are also ferromagnetic and lead to ferromagnetic ordering at $T_C = 24$ K. From the structural point of view, the exclusively ferromagnetic couplings in $CdVO_3$ are highly counter-intuitive. However, band structure calculations explain these couplings by an effect of low-lying Cd $5s$ states that mix with V $3d$ states and mediate hoppings between the half-filled V d_{xy} and the empty V d_{xz}, d_{yz} orbitals. The severe violation of the conventional superexchange scenario should be a general feature of Cd-containing compounds and can be used for the design of new low-dimensional magnets.

TT 11.11 Tue 12:15 H18

Quantum evolution from spin-gap to AF state in a low-dimensional spin system — Vladimir Gnezdilov[1], •Peter Lemmens[2], Dirk Wulferding[2], Reinhard Kremer[3], Collin Broholm[4], and Helmuth Berger[5] — [1]ILTP, Kharkov, Ukraine — [2]IPKM, TU-BS, Braunschweig — [3]MPI-FKF, Stuttgart — [4]DPA, Johns Hopkins Univ., Baltimore, USA — [5]EPFL Lausanne

The low-dimensional spin systems α- and β-$TeVO_4$ share the same monoclinic crystal symmetry while having a different connectivity of VO_4 octahedra and long range order vs. a quantum disordered ground state, respectively. We report a rich magnetic Raman spectrum and phonon anomalies that evidence strong spin-lattice coupling in both systems. Work supported by DFG.

TT 11.12 Tue 12:30 H18

Spin-Jahn-Teller Effect in the Antiferromagnetic Molecular Wheel $CsFe_8$ — •Johannes Lotze[1], Oliver Waldmann[1], Anne-Christine Chamayou[2], Christoph Janiak[2], Ayuk M. Ako[3], Annie K. Powell[3], and Ilya Sheikin[4] — [1]Physikalisches Institut, Universität Freiburg, Germany — [2]Institut für Anorganische und Analytische Chemie, Universität Freiburg, Germany — [3]Institut für Anorganische Chemie, Universität Karlsruhe, Germany — [4]Grenoble High Magnetic Field Laboratory, CNRS Grenoble, France

Antiferromagnetic molecular wheels are ring-like arrangements of exchange-coupled magnetic metal ions. As a function of a magnetic field, the Zeeman splitting leads to a series of level-crossings (LCs) at characteristic fields, where the ground state changes from total spin $S = 0$ to $S = 1$, $S = 2$, and so on. Previous magnetic torque and ^{1}H-NMR measurements on $CsFe_8$ single crystals demonstrated phase transitions at the LCs at low temperatures [PRL 96, 027206 (2006), PRL 99, 087201 (2007)]. They were explained by a field-induced spin-Jahn-Teller effect (JTE) due to a magneto-elastic coupling between the spins in the wheel and the lattice. Some models for this process were developed, but a full microscopic understanding is lacking. New high-field torque data were recorded, which provide a comprehensive picture of the angular as well as temperature dependence of the phase transition. A strong angle dependence of the critical fields and temperatures with two qualitatively different regimes was observed, which allows us to distinguish the relative contributions of zero-field splitting and Dzyaloshinsky-Moriya interactions to the spin-JTE.