TT 22: Low-dimensional Systems - Materials

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

TT 22.1 Thu 9:30 H18

Doping effects in the low-dimensional spin-Peierls system TiOCl — •Sebastian Glawion[1], Götz Berner[1], Matthias Schlachter[1], Michael Sing[1], Markus Hoinkis[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4 and Röntgen Research Center for Complex Materials, Universität Würzburg, D-97074 Würzburg, Germany — [2]Experimentalphysik II, Universität Augsburg, D-86135 Augsburg, Germany

Due to the underlying triangular mesh of Ti atoms, which favours magnetic frustration, it has been speculated that the Mott-insulator TiOCl could show RVB-like superconductivity, provided one can induce metallic behaviour. However, the observed non-canonical transition into a dimerized spin-Peierls phase at T_{c1}=67K and a Bonner-Fisher-like susceptibility above T_{c2}=92K point to a quasi-1D behaviour discarding such frustrations. Interestingly, as was indicated, e.g., by ARPES, 2D magnetic frustrations nevertheless might be important due to a small but non-negligible interchain coupling. Searching for a metallic phase, we investigated the feasibility of doping in different ways: in situ evaporation of alkaline atoms and compositional variation by ion bombardment. We found that there are qualitative differences between the two methods, such that in the latter case the near E_f spectral weight remains essentially unchanged while the onset of its leading edge is aligned with the chemical potential, and the dispersion is lost. On the other hand, a new feature appears in the gap region upon alkaline intercalation. The overall Ti 3d dispersions are retained but the gap is not fully closed.

TT 22.2 Thu 9:45 H18

Exotic Ground State of η-$Na_{9/7}V_2O_5$ — •Dmitry Zakharov[1,2], Hans-Albrecht Krug von Nidda[1], Günter Obermeier[3], Siegfried Horn[3], and Alois Loidl[1] — [1]EP V, EKM, University of Augsburg, 86135 Augsburg, Germany — [2]Kazan State University, 420008 Kazan, Russia — [3]EP II, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

The nature of the ground gapped state in the novel quasi-one-dimensional compound η-$Na_{9/7}V_2O_5$ is rather mysterious, if one takes into account the odd number of spins on each structural element. Combining the results of specific heat, susceptibility, electron spin resonance and dielectric conductivity measurements we show that it can be understood in terms of multi-spin objects building up a linear chain. In spite of the small total spin, their spatial extent results in an exchange constant comparable to the one in the non-dimerized state.

TT 22.3 Thu 10:00 H18

Drude response and evidence of a density-wave state in the β'' – $(ET)_2SF_5CH_2CF_2SO_3$ organic superconductor — •Stefan Kaiser[1], Natalia Drichko[1], Martin Dressel[1], and John Schlueter[2] — [1]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Material Science Division, Argonne National Laboratory, Argonne, Illinois 60439-4831, U.S.A.

The quasi-two-dimensional organic superconductor β'' – $(ET)_2SF_5CH_2CF_2SO_3$ is a prominent example of highly correlated electron systems. It raises interest because it forms a density-wave state around 140 K proposed by [Nam et al., PRL **87**, 117001]. Previous optical measurements do not show a Drude contribution. Here we present reflectance measurements at frequencies down to 10 cm^{-1} and temperatures down to 1.8 K, well below the superconducting transition T_c = 5.2 K. Already at room temperature a Drude behavior is observed which grows for lower temperatures. For light polarized in the high reflecting direction a pronounced gap opens around 200 cm^{-1} for T < 125 K. This we relate to the density-wave-gap driven by the nesting of the quasi-one-dimensional Fermi surface. The gap shows a slight anisotropy.

TT 22.4 Thu 10:15 H18

Quadratic temperature dependence of the resistivity up to 50 K of transition metal dichalcogenides with distorted CdI_2-structure — •Thorsten Zandt, Helmut Dwelk, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

In this contribution we present a detailed study of the temperature dependence of the electrical resistivity and magnetoresistance of β/Td-$MoTe_2$, WTe_2, $NbTe_2$ and $TaTe_2$ single crystals between 1.7 K and 350 K. In particular, the electrical resistivity, R(T)-R(0), shows at low temperatures a gradient proportional to T^2 up to 50 K what is atypical for 'normal' metallic behavior. In contrast, the magnetoresistance shows a normal characteristics for a metal. These results will be discussed within the framework of several microscopic mechanisms, e.g. like electron-electron scattering, which include electron-electron, hole-hole, and electron-hole processes [1].

[1] T. Zandt, H. Dwelk, C. Janowitz und R. Manzke: Quadratic temperature dependence of the resistivity up to 50 K of metallic $MoTe_2$, proceedings of the 15th International Conference on Solid Compounds of Transition Elements Krakau 2006, will be published 2007 in the Journal of Alloys and Compounds

TT 22.5 Thu 10:30 H18

Quasi one-dimensional magnetism driven by unusual orbital ordering in $CuSb_2O_6$ — •Helge Rosner[1], Deepa Kasinathan[1], and Klaus Koepernik[1,2] — [1]MPI CPfS Dresden, Germany — [2]IFW Dresden, Germany

Cuprate compounds, including the family of high-T_c-superconductors, exhibit a large variety of exotic physical properties. This variety is determined by the interplay of different interactions; mainly covalency, ligand-fields and strong correlation effects. A nearly universal component of cuprate systems is a strongly elongated CuO_6-octahedron wherein the exotic behaviour finds its origin in the deceivingly simple planar Cu-O orbital lying in its basal plane. In this well established standard scenario, the involvement of the apical out-of-plane orbitals is not settled completely. The surprisingly regular CuO_6-octahedra of $CuSb_2O_6$ offer a unique opportunity to elucidate this scenario due to the changed balance of interactions in this system. Here, we present an electronic structure study resulting in an hitherto unobserved ground state originating from a competition of in- and out-of-plane orbitals. Our results show that strong Coulomb correlation drives a surprising and unique orbital ordering. This, in turn, gives rise to an unusual and strongly one-dimensional magnetic ordering that is unlike any ordering observed in conventional low-dimensional cuprates. Our results provide a unique and natural interpretation of recent neutron data and indicate a rare opportunity to study the involvement of non-planar orbital effects.

The Emmy-Noether program is acknowledged for financial support.

TT 22.6 Thu 10:45 H18

Correlation driven charge order at $LaAlO_3$/$SrTiO_3$ and $LaTiO_3$/$SrTiO_3$ Interfaces — •Rossitza Pentcheva[1] and Warren Pickett[2] — [1]Section Crystallography, Dept. of Earth and Environmental — [2]Department of Physics, University of California, Davis,

To explain recent experiments reporting metallic conductivity at the interfaces between the Mott insulator $LaTiO_3$ (LTO) and band insulator $SrTiO_3$ (STO) but also between the two simple band insulators $LaAlO_3$ (LAO) and STO we have performed density-functional theory calculations employing the FP-LAPW-method within the WIEN2k implementation including a Hubbard-type on site Coulomb repulsion (DFT+U). We find that charge mismatch at the LTO/STO IF is accommodated by the formation of a charge and orbitally ordered (CO/OO) layer with a checkerboard arrangement of Ti^{3+} and Ti^{4+} and an antiferromagnetic coupling of the Ti^{3+}-spins [1]. Lattice relaxations lead to the observed conducting behavior. An analogous diluted layer of Ti^{3+} spins is obtained for the n-type LAO/STO interface, although the corresponding bulk materials are nonmagnetic [2]. For a structurally ideal p-type LAO/STO IF strong correlations in the oxygen p states and the formation of a charge and orbitally ordered O Pπ magnetic hole render a possible explanation for the measured insulating behavior. Alternatively, charge compensation by oxygen vacancies and the formation of a charge conjugate F-center is considered.

[1] R. Pentcheva and W.E. Pickett, cond-mat/0608212.
[2] R. Pentcheva and W.E. Pickett, Phys. Rev. B. 74, 035112 (2006).

TT 22.7 Thu 11:00 H18

Optical properties of the 1D antiferromagnet $KCuF_3$ — •Joachim Deisenhofer[1], Paolo Ghigna[2], Franz Mayr[3], Alois Loidl[3], and Dirk van der Marel[1] — [1]Departement de Physique

de la Matiere Condensee, Universite de Geneve, CH-1211 Geneve 4, Switzerland, — [2]Dipartimento di Chimica Fisica, Universita di Pavia, I-27100 Pavia, Italy, — [3]Experimentalphysik V, Center for Electronic Correlations and Magnetism, Augsburg University, D-86135 Augsburg, Germany

We present measurements of the optical properties of $KCuF_3$, a paradigm for orbital ordering[1] and one of the best realizations of a quasi-one dimensional spin chain [2]. We can identify the d-d excitations on the Cu sites and the charge-transfer gap of the system. The observed level splitting and the gap value will be compared to recent results obtained by LDA+U calculations [3]. Moreover, we find anomalies in the optical properties already above the magnetic phase transition. These features appear concomitantly with a change in the orbital order parameter as reported by resonant x-ray scattering [4] and evidence a low-temperture structural change [5].

[1] K. I. Kugel and D. I. Khomskii, Sov. Phys. Usp. 25, 231 (1982). [2] B. Lake et al., Nature Materials 4, 329 (2005). [3] I. Leonov, unpublished. [4] L. Paolasini et al., PRL 88, 106403 (2002). [5] N. Binggeli and M. Altarelli, PRB 70, 085117 (2004).

15 min. break

TT 22.8 Thu 11:30 H18

Orbital Ordering in Cs_2AgF_4 - an electronic structure study — •Deepa Kasinathan[1], Klaus Koepernik[1,2], and Helge Rosner[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]IFW Dresden, P.O. Box 270016, D-01171, Germany

The argentate Cs_2AgF_4, first synthesized in 1974 has many similarities to the high-T_c cuprates, featuring AgF_2 sheets in place of CuO_2 sheets. While the undoped cuprates are antiferromagnetic, this argentate is ferromagnetic with a T_{Curie} of about 15 K. Density functional calculations in the proposed tetragonal structure produce an itenerant half-metallic ferromagnet. Recent inelastic neutron scattering experiments have suggested an orthorhombic structure that allows an orbitally ordered ferromagnetic ground state. We performed electronic structure calculations using the LDA+U method on this system and were able to obtain an orbitally ordered ground state, not only for the newly proposed orthorhombic lattice but also for the orginal tetragonal lattice by constraining the bravais lattice and allowing the change of the atomic basis. In specific, very small changes in the position of the in-plane fluorine atoms already trigger an orbital ordering. Our calculated energy scale shows that this orbitally ordered state should be stable for all temperatures, consistent with the experiment.

TT 22.9 Thu 11:45 H18

Evidence for a magnetic phase transition in the frustrated spin-1/2 Heisenberg chain compound Li_2ZrCuO_4 — •Natalia Tristan[1], Rüdiger Klingeler[1], Hubertus Luetkens[2], Hans-Henning Klauss[3], Stefan-Ludwig Drechsler[1], Yuri Skourski[4], Olga Volkova[5], Alexander Vasiliev[5], Bernd Büchner[1], and N. Leps[1] — [1]Leibniz-Institute for Solid State and MaterialsResearch, IFW-Dresden, 01171 Dresden, Germany — [2]Laboratory for Muon-Spin Spectroscopy, PaulScherrer Institut, CH-5232 Villigen, Switzerland — [3]Institute for Physics of Condensed Matter,Technical University Braunschweig, Germany — [4]HighMagnetic Field Laboratory, FZ Dresden-Rossendorf, Germany — [5]Physics Faculty, Moscow State University,Russia

The anomaly of unusual shape in the specific heat and the maximum in the derivative of the magnetic suseptibility $d\chi(T)/dT$ at around 6 K as well as magnetization behavior of the low dimensional Li_2ZrCuO_4 allude to onset of a long range order in this compound. This suggestion is also supported by results of muon spin relaxation performed on a powder sample of Li_2ZrCuO_4, which show a spontaneous muon spin precession below 5.75 K. A peculiar rectangular shape of the static field distribution in the ordered state is consistent with an incommensurate helical spin structure predicted theoretically.

TT 22.10 Thu 12:00 H18

The electronic structure of the quantum critical system Li_2ZrCuO_4 — •Miriam Schmitt[1], Jiři Málek[2,3], Stefan-Ludwig Drechsler[2], and Helge Rosner[1] — [1]MPI CPfS Dresden — [2]IFW Dresden — [3]Institute of Physics, ASCR, Praha, Czech Republic

Quasi one-dimensional magnetic chain compounds with nearest-neighbor exchange J_1 and next-nearest-neighbor exchange J_2 exhibit a quantum critical point (QCP) for the ratio J_2/J_1 = -0.25. The recently synthesized compound Li_2ZrCuO_4, which contains spin-1/2 chains of distorted, edge shared CuO_4 plaquettes, is close to this QCP and shows therefore a strong field dependence of the thermodynamical properties. From fits to the measured susceptibility and specific heat, a ratio $J_2/J_1 \sim$ -0.3 was determined.[1] Here, we present a detailed study of the electronic and magnetic properties of Li_2ZrCuO_4 based on density functional calculations. We combine results of LDA calculation, which were mapped onto an effective one-band tight-binding model and subsequently to an extended Heisenberg model with exchange integrals derived from total energy differences for constraint magnetic states using LDA+U. The influence of (i) the deviation from the standard, planar CuO_4 geometry and (ii) the experimentally observed Li disorder was carefully investigated. We find $J_2/J_1 \sim -0.25 \pm 0.03$ very close to the QCP. In addition, we obtain a sizeable inter-chain coupling $J_\perp \sim$ 7K playing an important role for the saturation field due to the vicinity of the QCP.

The Emmy-Noether program is acknowledged for financial support.

[1] S.-L. Drechsler *et al.* Phys. Rev. Lett., accepted.

TT 22.11 Thu 12:15 H18

Magnetic frustration in one dimension - the distorted diamond chain azurite$(Cu_3(CO_3)_2(OH)_2)$ - — •Bernd Wolf[1], Andreas Brühl[1], Mariano de Souza[1], Katharina Removic-Langer[1], Yeekin Tsui[1], Ulrich Tutsch[1], Jürgen Schreuer[2], and Michael Lang[1] — [1]Physikalisches Institut, Universität Frankfurt, 60438 Max-von-Laue-Strasse 1, FOR 412 — [2]Institut für Mineralogie, Ruhr-Universität-Bochum, 44780 Universitätsstrasse 150

A simple realization of a frustrated quantum-spin system is the S = 1/2 distorted diamond chain, where the ground state is strongly constrained by the ratio of the three coupling constants J_i. A theoretical phase diagram at T = 0 was examined consisting of a ferrimagnetic -, a dimerized -, as well as a spin fluid (SF) phase. The natural mineral azurite ($Cu_3(CO_3)_2(OH)_2$) represents a distorted diamond chain. We discuss thermodynamic measurements, such as specific heat, thermal expansion, elastic constant and magnetic susceptibility, some of which are also measured under hydrostatic pressure, in a wide-stretched temperature and field range. According to magnetic susceptibility and magnetization measurements, the ground state of azurite is located close to the quantum phase transition, separating the gapless SF phase from the gapped dimerized phase. We find pronounced acoustic anomalies at high fields indicating a significant spin-phonon interaction. From the enormous size of the anomalies in the sound velocity, a large magnetic Grüneisen parameter can be inferred, this possibly resulting from the proximity of the system to a quantum critical point.

TT 22.12 Thu 12:30 H18

Optical response of the ladder compound $Sr_{2.5}Ca_{11.5}Cu_{24}O_{41}$ under high pressure — •S. Frank[1], C. A. Kuntscher[1], R. Klingeler[2], and B. Büchner[2] — [1]Experimentalphysik II, Universität Augsburg, D-86159 Augsburg, Germany — [2]Leibniz-Institut für Festkörper-und Werkstoffforschung Dresden, PF 27 01 16, 01171 Dresden, Germany

Since the discovery of a pressure-induced superconducting phase, the highly Ca-doped $Sr_{14-x}Ca_xCu_{24}O_{41}$ two-leg ladder compound is intensively investigated. Based on earlier studies it was suggested that Ca doping [1,2] as well as the application of pressure [3] transfer holes from the chains to the ladders. The nature of the superconductivity, however, remains an open issue.

An important piece of information is how the dynamics of the charge carriers change upon pressure application. We therefore studied the pressure-dependent optical response of $Sr_{2.5}Ca_{11.5}Cu_{24}O_{41}$ over a broad frequency range (far-infrared to visible) at room temperature. Based on these results, we will discuss the possible occurrence of a pressure-induced dimensional crossover in $Sr_{2.5}Ca_{11.5}Cu_{24}O_{41}$ and speculate on the implications of our findings for the superconductivity in this system. *Supported by the DFG, Emmy Noether-program. Provision of beamtime at the ANKA Angströmquelle Karlsruhe is acknowledged.*

[1] T.Osafune et al., Phys. Rev. Lett. **78**, 1980 (1997)
[2] N. Nücker et al., Phys. Rev. B **62**, 14384 (2000)
[3] Y.Piskunov et al., Phys. Rev. B **72**, 064512 (2006)

TT 22.13 Thu 12:45 H18

$CuSe_2O_5$ – a new quasi one-dimensional spin-1/2 Heisenberg system — •Oleg Janson[1,2], Walter Schnelle[1], Marcus Schmidt[1], Stefan-Ludwig Drechsler[3], and Helge Rosner[1] — [1]MPI CPfS Dresden, Germany — [2]St. Petersburg State University,

Russia — [3]IFW Dresden, Germany

We report a joined experimental and theoretical study of the new quasi one-dimensional spin-1/2 Heisenberg system $CuSe_2O_5$. Its crystal structure is characterized by chains of canted isolated CuO_4 plaquettes aligned along the c axis of the monoclinic lattice, raising the question about the size of the different exchange couplings between the CuO_4 units. Combining measurements of the magnetic susceptibility χ and specific heat c_p with DFT band structure calculations, we analyze the magnetic properties and the leading exchange interactions of this compound. The single crystals of $CuSe_2O_5$ were grown by chemical vapour transport using $TeCl_4$ as transport agent. Our χ and c_p data indicate a phase transition to long range antiferromagnetic order at $T_N \sim 17$K. From a tight-binding analysis of the electronic structure and from total energy calculations for constraint magnetic states we can describe the system in good approximation by a nearest neighbour exchange $J_1 \sim 20$ meV along the structural chains and a sizable interchain coupling $J_\perp \sim 5$ meV in good agreement with the experimental results.

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