TT 28: Correlated Electrons: Low-dimensional Systems - Materials 2

Time: Wednesday 15:00–18:30 Location: H 0104

TT 28.1 Wed 15:00 H 0104

One-dimensional quantum spin magnetism of the $CrVO_4$ structure-type — •Joseph Law and Reinhard Kremer — Max Planck Institute for Solid State Research Heisenbergstraße 1, D-70569 Stuttgart

In recent years we have investigated and characterized many new and interesting 1D quantum spin systems, as of late we have concentrated on compounds that crystallize in the $CrVO_4$ structure-type.

Here we will present new results for materials that adopt this structure-type, ranging from spin-spiral long-range magnetic order and Multiferroicity to two stage spin-Peierls transitions.

TT 28.2 Wed 15:15 H 0104

***S*=5/2 spin-chain Heisenberg systems $SrMn_2V_2O_8$ and $BaMn_2V_2O_8$** — •Sandra Niesen, Gerhard Kolland, Oliver Heyer, Martin Valldor, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln

Low-dimensional magnetic systems are commonly studied due to their interesting magnetic properties. For small spin values ($S = 1/2$ or 1), the groundstate and the low-lying excitations are often dominated by strong quantum fluctuations, while a more classical behavior is expected for systems with larger spins. In this context, the series $AM_2X_2O_8$ (A = Ba, Sr, Pb; M = Cu, Co, Ni, Mn; X = V, As) are of particular interest. Depending on the transition metal, different spins are realized and the structure contains screw chains of octahedrally coordinated M^{2+} ions along the c axis of the tetragonal structure. These chains are spatially separated by a nonmagnetic matrix, resulting in a quasi-1D magnetic system. The Heisenberg $S = 5/2$ system $BaMn_2V_2O_8$ shows low-dimensional behavior with a broad maximum of $\chi(T)$ around 170 K but finally orders antiferromagnetically at 37 K. Up to now only few studies of polycristalline $BaMn_2V_2O_8$ were available [1]. Large single crystals of $BaMn_2V_2O_8$ and of the new compound $SrMn_2V_2O_8$ were prepared. The crystal structure and the basic physical properties of this new compound will be presented [2].
This work is supported by the DFG through SFB 608.
[1] Z. He *et al.* Solid State Comm. **141** (2007) 22
[2] S.K. Niesen *et al.* J. Mag. Mag. Mat. **323** (2011) 2575

TT 28.3 Wed 15:30 H 0104

Magnetic properties of alternating spin-1/2 chain compound $AgVOAsO_4$ — •Ramesh Nath[1], Alexander Tsirlin[2], Panchanana Khuntia[2], Michael Baenitz[2], Yurii Skourski[3], Christoph Geibel[2], and Helge Rosner[2] — [1]School of Physics, IISER, Thiruvananthapuram-695016 Kerala, India — [2]MPI CPfS, Nöthnitzer Str. 40, 01187 Dresden, Germany — [3]HLD, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

We investigate the magnetic properties of a one-dimensional (1D) spin-1/2 alternating chain compound $AgVOAsO_4$ via magnetic susceptibility, high-field magnetization, and ^{75}As NMR measurements. Temperature dependence of the magnetic susceptibility ($\chi(T)$) and NMR shift ($K(T)$) were fitted well by the expression for the 1D spin-1/2 alternating chain. The exchange couplings along the chain are estimated to be $J \simeq 40$ K and $J' \simeq 25$ K, with a spin gap $\Delta \simeq 13$ K. The high-field magnetization measurement at 1.4 K confirms the ground state to be a non-magnetic singlet, and reveals the critical field $H_c \simeq 10$ T of the gap closing and a saturation field $\mu_0 H_s \simeq 48.5$ T. These values are largely consistent with the estimated Δ and (J, J') values based on the fit of $\chi(T)$ and $K(T)$. The ^{75}As spin-lattice relaxation rate ($1/T_1$) follows an activated behavior at low temperatures giving rise to the same Δ value. Our experimental investigations are supported by band structure calculations that additionally reveal weak and frustrated interchain couplings, thus making this compound a promising candidate for Bose-Einstein condensation of magnons in high magnetic fields.

TT 28.4 Wed 15:45 H 0104

Evidence for a Kosterlitz-Thouless transition in the quasi-2D square-lattice compound $Pb_2VO(PO_4)_2$ — •Tobias Förster, Jörg Sichelschmidt, Enrique Kaul, Christoph Geibel, and Frank Steglich — Max Planck Institute f. Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

The layered vanadium-oxide-bis(phosphates) AA'$VO(PO_4)_2$ (AA'=Pb_2, SrZn, BaCd) present an interesting class of quasi-2D compounds. The crystal structure is dominated by layers of VO_5-pyramids and PO_4-tetrahedra forming a $S = 1/2$-square lattice of V^{4+} ions. In contrast to the majority of square lattice compounds these vanadium systems present a significant amount of frustration, because the ferromagnetic exchange along the sides of the squares is of the same order of magnitude as the antiferromagnetic exchange along the diagonals. Therefore one finds a good agreement of the bulk properties with the $S = 1/2$ Heisenberg J_1-J_2-model [1].
In such 2D $S = 1/2$ square-lattices quantum Monte Carlo simulations suggest that a small easy-plane anisotropy results in a crossover from Heisenberg to XY behavior [2]. With Electron Spin Resonance (ESR) measurements on single crystals of $Pb_2VO(PO_4)_2$ we show that this compound indeed presents an easy-plane anisotropy and that the spin dynamics measured via the ESR linewidth is well described by the occurrence of a Kosterlitz-Thouless transition at a temperature slightly below T_N.
[1] E. E. Kaul *et al.* J. Magn. Magn. Mater. **272-76**, 922 (2004)
[2] A. Cuccoli *et al.* Phys. Rev. Lett. **90**, 167205 (2003)

TT 28.5 Wed 16:00 H 0104

Thermodynamic properties of the 1-dimensional Spin-$\frac{1}{2}$ compound Cs_2CoCl_4 in transverse magnetic fields — •Oliver Breunig[1], Eran Sela[2], Benjamin Buldmann[2], Markus Garst[2], Petra Becker[3], Ladislav Bohatý[3], Christian Dax[1], Ralf Müller[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln — [3]Institut für Kristallographie, Universität zu Köln

Cs_2CoCl_4 is known as a an example of a spin-$\frac{1}{2}$ XXZ model crystal. It contains $CoCl_4$ tetrahedra, which form one-dimensional chains along the crystallographic b axis. The orbital groundstate of Co^{2+} is split by the crystal field into doublets and an easy-plane anisotropy of the magnetization is established. The ground-state doublet is separated from the first excited doublet state by approximately 15 K, in a way that at low-enough temperatures the system can be described by the one-dimensional spin-$\frac{1}{2}$ XXZ model. In literature, this model is typically studied for magnetic fields perpendicular to the easy-plane. For structural reasons, however, in Cs_2CoCl_4 the only principal magnetic field direction which is experimentally accessible lies within the easy-plane. Only few studies of the corresponding transverse field case are available so far. We compare experimental data of specific heat and thermal expansion in a temperature range from about 50 mK to 20 K to numerical calculations.

This work was supported by the DFG through SFB 608.

TT 28.6 Wed 16:15 H 0104

Combined DFT and many-body studies of charge transfer salts — •Kateryna Foyevtsova, Johannes Ferber, Harald O. Jeschke, and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Frankfurt am Main, Germany

Charge transfer salts are a class of strongly correlated low-dimensional organic materials which have recently gained revived attention. The appealing properties of these materials are a highly controlled quality of grown samples and a rich phase diagram where phase transitions are driven by variation of temperature and pressure (physical or chemical). We study the effects of strong electronic correlations in some representative charge transfer salts in the framework of the density functional theory combined with many-body methods. In particular, we perfom a comparative analysis for the isostructural compounds κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br, an unconventional superconductor with $T_c \sim 15$ K, and κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl, an antiferromagnetic Mott insulator, in a range of temperatures and interaction strengths.

TT 28.7 Wed 16:30 H 0104

An *ab initio* Comparison of the Properties of Fabre-Bechgaard Charge Transfer Salts — •Anthony Jacko, Harald O. Jeschke, and Roser Valentí — Institut für Theoretische Physik, Universität Frankfurt, 60438 Frankfurt, Germany

The Fabre-Bechgaard family of charge transfer salts have a rich phase diagram as a function of both physical and chemical pressure, due to strong electronic correlations and frustration [1]. We investigate the structural and electronic properties of several members of this family with density functional theory (DFT) calculations. By understanding

the similarities and differences between these salts at the level of DFT, we can gain an understanding of how the choice of anion influences the effects of strong correlations and frustration on the properties of these systems, leading to the many interesting phases observed.
[1] J. Moser, M. Gabay, P. Auban-Senzier, D. Jérome, K. Bechgaard, and J.M. Fabre. Euro. Phys. J. B, 1:39-46, 1998.

15 min. break.

TT 28.8 Wed 17:00 H 0104

$(TMTTF)_2SbF_6$ at the Metal-Insulator Transition: Bulk-Sensitive Photoemission Facilitated by Aluminum Coating — Katerina Medjanik[1], Dmytro Kutnyakhov[1], Hans-Joachim Elmers[1], •Gerd Schönhense[1], Andrei Gloskovskii[2], Wolfgang Drube[3], Mariano de Souza[4], Jens Müller[5], and Michael Lang[5] — [1]Inst. f. Physik, Univ. Mainz — [2]Inst. f. Anorg. und Anal. Chemie, Univ. Mainz — [3]Deutsches Elektronen-Synchrotron, Hamburg — [4]Universidade Estadual Paulista, Rio Claro, Brazil — [5]Physikalisches Inst., Goethe Universität Frankfurt

The metal-insulator transition (MIT) in the title compound has been studied using hard X-ray photoelectron spectroscopy (HAXPES) at PETRA III (beamline P09). This material undergoes a transition from a correlated metal at ambient temperature to a Mott-Hubbard insulator at T=154 K. The latter is marked by a pronounced increase in resistivity by > 3 orders of magnitude and accompanied by a charge-order phase transition. Photoelectron spectroscopy for the bare material is hampered by strong non homogeneous surface charging visible by the sudden appearance of shifted lines in addition to the main line at the transition. The large information depth (about 20nm) of HAXPES allows coating the material by a thin (5 nm) conductive Al-layer in order to avoid charging. In this way, the intrinsic change of the spectra at the metal-insulator/charge-order transition can be observed. At the transition temperature, the S 2p signal exhibits a satellite shifted from the main line by 7.2 eV towards higher kinetic energies. Funded through Transregio SFB TR49, graduate school MAINZ and COMATT.

TT 28.9 Wed 17:15 H 0104

Analysis of the temperature dependence of the structural and electronic properties of the spin liquid candidate κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ — •Harald O. Jeschke[1], Mariano de Souza[2], Rudra Sekhar Manna[2], Michael Lang[2], Roser Valentí[1], and John A. Schlueter[3] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [3]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, United States

The interplay of the effects of electronic correlations, low dimensionality and spin frustration in the organic charge transfer salt κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ is of great interest experimentally as well as theoretically. Besides the spin liquid property at very low temperatures, the material has interesting anomalies at 6K, 60K and 150K. Even though the structure of the material has been determined several times over the past 20 years, complete structural data are only available at room temperature. In our work, we precisely determine the structure at 300K, 250K, 200K, 150K, 100K, 20K and 5K. We analyze the structures using density functional theory and tight binding methods. We show that the triangular lattice Hubbard Hamiltonian parameters are temperature dependent, with the interaction strength increasing with decreasing temperature and with the frustration going through a minimum at 150 K. Our results point to the fact that the experimental determination of structures at various temperatures may be important for realistic many-body theoretical investigations of complex materials.

TT 28.10 Wed 17:30 H 0104

Single crystals and thin films of the new organic charge transfer compound (BEDT-TTF)-DTF — •Kai Ackermann[1], Milan Rudloff[1], Michael Bolte[2], Harald Jeschke[3], Matthias Wagner[2], Roser Valenti[3], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Straße 1, 60438 Frankfurt am Main — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität, Max-von-Laue-Straße 7, 60438 Frankfurt am Main — [3]Institut für Theoretische Physik, Goethe-Universität, Max-von-Laue-Straße 1, 60438 Frankfurt am Main

We investigate the structural and electronic properties of the semiconducting organic charge transfer system (BEDT-TTF)-DTF [bis(ethylenedithio)-tetrathiafulvalene - 9-dicyanomethy-lene-2,4,7-trinitrofluorene]. Crystal structure analysis and X-ray diffractometry show two different phases with monoclinic and triclinic symmetry. Both have a mixed stack configuration with a 1:1 ratio of BEDT-TTF to DTF. A characteristic of the triclinic phase is the layered structure of donor and acceptor molecules. Single crystals of both phases, which are grown from solution, were characterized by temperature-dependent (1.5K - 300K) conductivity measurements in three crystallographic directions and IR-spectroscopy for determining the charge transfer degree. First results of thin film deposition experiments by using organic molecular beam deposition are presented. These films allow to measure the frequency-dependent (20Hz - 100kHz) dielectric constant. The experimental results are discussed in view of band structure calculation within the framework of density functional theory.

TT 28.11 Wed 17:45 H 0104

Field-induced length changes in the spin-liquid candidate κ-$(ET)_2Cu_2(CN)_3$ — •Rudra Sekhar Manna[1], Mariano de Souza[1,3], John A. Schlueter[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA — [3]Present address: Departamento de Fisica, Unesp - Universidade Estadual Paulista, CEP 13500-970, Rio Claro (SP), Brazil

Thermal expansion measurements on the spin-liquid compound κ-$(ET)_2Cu_2(CN)_3$ show a pronounced and strongly anisotropic anomaly at 6 K, a clear signature of a second-order phase transition [1]. In order to study the effect of a magnetic field on the low-temperature spin-liquid state [2], dilatometric measurements under magnetic field have been performed. Interestingly, we find that besides the 6 K anomaly, which is insensitive to magnetic fields $B \leq 10$ T, the maximum field applied, field-induced anomalies show up for fields aligned along the crystallographic b-axis. The effects become particularly clear in measurements of the magnetostriction where two step-like anomalies were observed. One of these anomalies lies close to the phase boundary between quantum critical (QC_H) and weak antiferromagnetic (WAF_H) phases derived from μSR measurements [2].
[1] R. S. Manna et al., PRL **104**, 016403 (2010).
[2] F. L. Pratt et al., Nature **471**, 612 (2011).

TT 28.12 Wed 18:00 H 0104

Charge-carrier dynamics at the multiferroic transition in the organic charge-transfer salt κ-$(ET)_2$-$Cu[N(CN)_2]Cl$ studied by fluctuation (noise) spectroscopy — •Benedikt Hartmann[1], Robert Rommel[1], John Schlueter[2], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt (M) — [2]Argonne National Laboratory, Materials Science Division, Argonne, IL, USA

The organic molecular conductors $(BEDT\text{-}TTF)_2X$ are model systems for low-dimensional metals exhibiting both strong electronic correlations and electron-phonon interactions. The quasi-2D triangular lattice Mott insulator κ-$(ET)_2Cu[N(CN)_2]Cl$ (κ-Cl) undergoes an antiferromagnetic transition at $T_N \approx 27\,K$. Recently, clear evidence for charge-order driven ferroelectircity coinciding with the onset of magnetic-ordering has been found [1], making κ-Cl a multiferroic material.
We report on fluctuation (noise) spectroscopy, a suitable technique to study the low-frequency charge-carrier dynamics of κ-Cl. We discuss the temperature dependence of the $1/f$-type fluctuations in order to get insight in the electronic energy scale involved in the ordering mechanism. We observe deviations of $1/f$ noise at temperatures around 27 K which may be attributed to the formation of charge-order domains.
[1] P. Lunkenheimer, J. Müller et al., arXiv:1111.2752v2 (2011)

TT 28.13 Wed 18:15 H 0104

The anomalous metallic properties of quasi two-dimensional organic superconductors studied by non-linear transport — •Robert Rommel[1], Benedikt Hartmann[1], Jens Brandenburg[1], John Schlueter[2], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt am Main — [2]Argonne National Laboratory, Materials Science Division, Argonne, IL, USA

In ac transport measurements the technique of measuring higher harmonics, in particular the third ($R_{3\omega}$), may be used as an additional, powerful tool probing the microgeometry of the current distribution in a bulk sample. $R_{3\omega}$ has been used, e.g., to determine the superconducting transition temperature of high-T_c cuprates or to estimate

the number of correlated polarons in manganites. We apply this technique to the quasi two-dimensional organic charge-transfer salt κ-$(H_8$-$ET)_2Cu[N(CN)_2]Br$ and its fully deuterated analogue. We studied the dependence of $R_{3\omega}$ on temperature, current, frequency, magnetic field and the degree of disorder and analyze the data with respect to the vicinity of the 1^{st} order Mott metal-insulator transition line in the complex phase diagram of this class of materials. We show that the signal allows for an accurate determination of $T_c(B)$ and found a good estimate for the upper critical magnetic field B_{c2} of these extreme type-II superconductors. We furthermore gain information about changes in the transport mechanism, which we will discuss in terms of the anomalous properties of the metallic state in these materials.