TT 19 Correlated Electrons: Low-dimensional Materials

Time: Tuesday 14:00–19:00 Room: HSZ 301

TT 19.1 Tue 14:00 HSZ 301

Heat transport of spin chains in $CaCu_2O_3$ — •A. Waske[1], H. ElHaes[2], C. Hess[1], N. Wizent[1], M. Apostu[1], G. Behr[1], C. Sekar[1], G. Krabbes[1], B. Büchner[1], F. Heidrich-Meisner[3], and W. Brenig[3] — [1]IFW Dresden, Germany — [2]RWTH Aachen, Germany — [3]Institut für Theoretische Physik, TU-Braunschweig, Germany

We present experimental results for the magnon thermal conductivity $\kappa_{\rm mag}$ of the ladder-like material $CaCu_2O_3$. Due to the small Cu-O-Cu bonding angle within the ladders ($\sim 120°$) the magnetic rung coupling is much weaker than the magnetic coupling along the legs. Hence, at sufficiently high temperatures the material is expected to behave like independent spin chains. In our experiments, we find a strong signature of magnetic heat transport above ~ 50 K, which appears to be linear in temperature. We estimate the magnetic mean free path which turns out to be of the order of 25 Å.

TT 19.2 Tue 14:15 HSZ 301

Revisiting the magnetism of hole-doped CuO_2 spin chains in $Sr_{14-x}Ca_xCu_{24}O_{41}$ — •Jürgen Schnack[1], Rüdiger Klingeler[2], Vladik Kataev[2], and Bernd Büchner[2] — [1]Universität Osnabrück, Fachbereich Physik — [2]Leibniz-Institute for Solid State and Materials Research IFW Dresden, Germany

Magnetization measurements of $Sr_{14-x}Ca_xCu_{24}O_{41}$ with $0 \leq x \leq 12$ in magnetic fields up to 16 T show that the low temperature magnetic response of the CuO_2 spin chains changes strongly upon doping [1]. For $x = 0$ quantum statistical simulations [2] yield that the temperature and field dependence of the magnetization can be well described by an effective Heisenberg model in which the ground state configuration is composed of spin dimers, trimers, and monomers [3]. Reduction of the number of holes in the chains through Ca-doping leads to an additional contribution to the magnetization, which depends linearly on the magnetic field. Remarkably, the slope of this linear contribution increases with the Ca content. We discuss this behavior in the context of an effective Heisenberg model for hole-doped spin chains [2].

[1] R. Klingeler *et al.*, cond-mat/0511110
[2] J. Schnack, Eur. Phys. J. B **45** (2005) 311
[3] R. Klingeler *et al.*, cond-mat/0508626

TT 19.3 Tue 14:30 HSZ 301

Electronic structure of the incommensurate composite crystal $Sr_{14}Cu_{24}O_{41}$ — •Cosima Schuster and Udo Schwingenschlögl — Institut für Physik, Universität Augsburg, 86135 Augsburg

The incommensurate composite systems $(Ca,Sr)_{14}Cu_{24}O_{41}$ are based on two different structural units, CuO_2 ladders and CuO chains, where the Cu ions have the average valence 2.25. In the Sr compound nearly all Cu^{2+} ions (with $S = 1/2$) are found on the ladders, and nearly all Cu^{3+} ions are located on the chains. The latter form Zhang-Rice singlets, socalled holes. Substitution of Sr by Ca leads to a transfer of holes from the chains to the ladders. The spin order on the chains likewise depends on the doping and ranges from dimers to antiferromagnetic order.

Our calculations are based on density functional theory and take into account the details of the crystal structure [1] by means of an unit cell including 10 chain and 7 ladder units. The LDA results show that the chains and ladders can be treated independently. We present systematic investigations of the local density of states at the chain sites by studying a reduced unit cell without CuO_2 ladders. The crystal structures of the Ca and Sr-rich compound differ in a symmetric or asymmetric alignment of the CuO chains. We find that two bands contribute to the d_{xz}-states near E_F in the asymmetric case, whereas they are degenerate in the symmetric case. A tight binding fit shows that the orbital overlap between nearest and next-nearest neighbours is of the same order of magnitude. Details of the magnetic ordering and the role of electronic correlations result from spin-polarized and LDA+U calculations.

[1] Y. Gotoh et al., Phys. Rev. B 68, 224108 (2003)

TT 19.4 Tue 14:45 HSZ 301

Optical response of the low-dimensional insulator TiOCl under pressure — •S. Frank[1], A. Pashkin[1], C. A. Kuntscher[1], M. Hoinkis[2,3], M. Klemm[2], M. Sing[3], S. Horn[2], and R. Claessen[3] — [1]1.Physikalisches Institut, Universität Stuttgart, Germany — [2]Experimentalphysik 2, Universität Augsburg, Germany — [3]Experimentelle Physik 4, Universität Würzburg, Germany

The role of lattice, spin, and orbital degrees of freedom for the properties of the low-dimensional Mott insulator TiOCl is currently under debate. Upon cooling, the compound undergoes a transition to a nonmagnetic ground state, most probably a spin-Peierls state. The role of the orbital degree of freedom is much less clear: The occurrence of a second phase transition was discussed in terms of strong orbital fluctuation; this picture was questioned by transmission measurements, showing strong absorption features which were interpreted in terms of transitions between the crystal field-split Ti t_{2g} levels [1]. To obtain more information on the orbital excitations in TiOCl and to add new facets to its properties, we studied the polarization-dependent optical response as a function of pressure. The measurements were performed over a broad frequency range (mid-infrared to visible) on very thin crystals, which allowed to determine the position and lineshape of the absorption features as a function of pressure. We also discuss the possibility of a pressure-induced phase transition.

Supported by the DFG, Emmy Noether-program.

[1] R. Rückamp et al., Phys. Rev. Lett. **95**, 097203 (2005)

TT 19.5 Tue 15:00 HSZ 301

A possible dimerized ground state in the spin-1/2 cuprate $Na_3Cu_2SbO_6$ — •Miriam Schmitt[1] and Helge Rosner[2] — [1]TU Dresden — [2]MPI CPfS Dresden

Simulated by the resent discovery of helical ground states in spin-1/2 chain cuprates, we present an electronic structure study of the newly synthesized compound $Na_3Cu_2SbO_6$. This compound contains Cu_2O_6 sub-units build from edge shared CuO_2 plaquettes. The Cu_2O_6 sub-units are arranged in chains along the y-direction, interrupted by SbO_6 octahedra. The Cu-O-Cu bond angle in the Cu_2O_6 units is about 95°, therefore a competition of ferromagnetic and antiferromagnetic interactions can be expected. We investigate the electronic and magnetic structure of $Na_3Cu_2SbO_6$ starting from LDA band structure calculations that are mapped to an effective one-band tight-binding model and subsequently to an extended Heisenberg model. A variety of possible ground states is compared with respect to their total energy including the strong correlation using the LDA+U scheme. Furthermore, we discuss frustration of the magnetic exchange interaction along the chains due to next-nearest neighbor coupling and the influence of inter-chain interaction.

supported by the DFG (Emmy-Noether-program)

TT 19.6 Tue 15:15 HSZ 301

Magneto–elastic effects in Azurite — •Andreas Brühl[1], Katarina Removic–Langer[1], Yeekin Tsui[1], Bernd Wolf[1], Michael Lang[1], and Jürgen Schreuer[2] — [1]Physikalisches Institut, J.W.Goethe–Universität Frankfurt — [2]Institut für Mineralogie, J.W.Goethe–Universität Frankfurt, Frankfurt am Main

Quantum spin systems with frustration exhibit comprehensive phase diagrams with a variety of possible ground states. One of the simplest one-dimensional frustrated quantum systems is the $S = 1/2$ diamond chain. According to recent theoretical calculations for the distorted diamond chain the ground state is either a ferrimagnetic phase, a dimerized phase or a spin liquid phase. So far, experimental work has been hampered by lacking appropriate compounds until recently, when Kikuchi et al. found that the natural mineral azurite ($Cu_3(CO_3)_2(OH)_2$) is a model substance for the distorted diamond chain. In this contribution we present results of magnetic susceptibility, thermal expansion and pulse field ultrasonic measurements on a high quality azurite single crystal. From the pronounced anomalies in the coefficient of thermal expansion as a function of temperature and the elastic constant as a function of magnetic field around the saturation field of 32 T, we infer an extraordinarily strong magneto–elastic coupling constant. We discuss our results in light of the different possible ground states that have been proposed for this material.

TT 19.7 Tue 15:30 HSZ 301

Electronic structure and magnetic properties of the spin-$\frac{1}{2}$ system Bi_2CuO_4 — •Oleg Janson[1,2] and Helge Rosner[1] — [1]MPI CPfS Dresden — [2]SPbSU St. Petersburg, Russia

Bi_2CuO_4 crystallizes in the tetragonal system, with isolated CuO_4 plaquettes arranged parallel to the xy plane and staggered in chains along the z axis. Initially, Bi_2CuO_4 was treated as 1D compound, but low temperature data, especially the magnetic moment of 0.93 μ_B, show that quantum fluctuations are strongly suppressed and exclude a 1D model. Neutron scattering data reveal FM-ordered chains along z, that are AFM ordered with respect to each other [1]. To elucidate the origin of the surprisingly FM-ordered chains, we performed DFT calculations to evaluate the relevant orbitals and couplings. Total energy calculations yield a magnetic groundstate coinciding with the experimental data. From a tight-binding fit of the LDA band structure we obtained the exchange integrals. The most important result is that the main coupling is between the chains and the in-chain interaction is relatively small. Thus, the FM arrangement of chains is due to strong AFM exchange of neighbouring plaquettes that belong to the different chains. Therefore, Bi_2CuO_4 has to be described as a compound with 3D coupling.

This investigation was supported by the DFG, Emmy Noether-program

[1] J. L. García-Muñoz, J. Rodríguez-Carvajal et al. J. Phys.: Condens. Matter, **2** (1990) 2205–2214

TT 19.8 Tue 15:45 HSZ 301

High Field Magnetization and ESR on a S = 1 Spin Ladder — •C. Mennerich[1], C. Golze[1,2], V. Kataev[2], A. Alfonsov[2], R. Klingeler[2,3], B. Büchner[2], D.J. Price[4], M. Goiran[3], H. Rakoto[3], J.-M. Broto[3], O. Kataeva[5], M. Broekelmann[1], S. Grossjohann[6], W. Brenig[6], and H.-H. Klauss[1] — [1]IPKM,TU Braunschweig, Germany — [2]IfW Dresden, Germany — [3]LNCMP Toulouse, France — [4]U Glasgow, United Kingdom — [5]Arbuzov Institute, RAS, Kazan, Russia — [6]IThP, TU Braunschweig, Germany

The compound $Na_2Ni_2(ox)_2(H_2O)_2$ (ox =C_2O_4) forms a S=1 spin ladder. SQUID measurements show a pronouced maxima at temperatures between 39 K and 47 K along different crystallographic axes. This behaviour results from antiferromagnetic interactions and a single ion anisotropy D in the distorted octahedral surrounding of the Ni(II) ions. To determine the anisotropy D and the g-factor we performed high frequency (up to 740 GHz) high field (up to 30 T) ESR measurements on a powder sample resulting in D = 11.5 K and g = 2.2. Using these results we analysed the susceptibility and magnetization measurements. High field magnetization measurements up to 55 Tesla on a powder sample show typical magnetization steps in very good agreement with our simulations. These results prove that the system is close to the decoupled dimer limit. Further support for this conclusion stems from quantum monte carlo simulations performed for different ratios of intra-dimer to inter-dimer coupling taking into account the single ion anisotropy D.

This work is supported by the DFG within SPP1137 under contract KL1086/6-1.

TT 19.9 Tue 16:00 HSZ 301

Mössbauer Study of the Fe(II) S=2 Spin Chain System $K_2Fe(C_2O_4)_2$ — •H.-H. Klauss[1], F. Gouider[1], F.J. Litterst[1], S. Grossjohann[2], A. Honecker[2], W. Brenig[2], and D.J. Price[3] — [1]IPKM, TU Braunschweig, Germany — [2]IThP, TU Braunschweig, Germany — [3]Department of Chemistry, U Glasgow, United Kingdom

Fe(II) in $K_2Fe(C_2O_4)_2$ is arranged in zig-zag chains in which the magnetic exchange is primarily mediated by the oxalate $(C_2O_4)2$- anions [1]. Mössbauer spectroscopy proves a well isolated orbital singlet ground state of the Fe in a very unusual trigonal prismatic local symmetry. Magnetic susceptibility measurements reveal a Curie-Weiss like behaviour at high temperatures and a broad cusp at 20 K consistent with dominant 1-D antiferromagnetic interactions. 3-D magnetic order is found below 7 K by Mössbauer spectroscopy. In the magnetic susceptibility an upturn is found below 7 K indicating a weak ferromagnetic component in the dominantly antiferromagnetically ordered state. Using Quantum Monte Carlo the magnetic susceptibility for a S=2 spin chain is calculated and compared with the experimental data. This results in an intrachain magnetic exchange constant of $J||/k_B \approx 6$ K. From an RPA analysis of the 3-D ordering temperature the interchain magnetic exchange constant is estimated to be one order of magnitude smaller consistent with a dominant 1-D character of the magnetic interaction in this system.

[1] M.B. Hursthouse, M.E. Light, and D.J. Price, Angew. Chem. Int. Ed. 43 (2004) 472.

TT 19.10 Tue 16:15 HSZ 301

From weakly coupled tetrahedra to molecular like host guest magnets — •R. Takagi[1], R. Becker[1], M. Johnsson[1], R. K. Kremer[2], R. Valenti[3], and P. Lemmens[4] — [1]Dept. Inorg. Chem., Stockholm Univ., Sweden — [2]MPI-FKF, Stuttgart, Germany — [3]Univ. Frankfurt, Germany — [4]IPKM, TU Braunschweig, Germany

The search for novel weakly coupled or molecular like magnets in the range of lone pair oxohalogenides based on Cu^{2+}, Ni^{2+}, and Mo^{2+} has been very fruitful in recent years. We give an overview on their structural, electronic and magnetic properties. Established magnetic structures have dimers, chains, tetrahedra, 5- and 13-spin centers. The latter are realized as guests in cages of high symmetry host structures.

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— 15 min. break —

TT 19.11 Tue 16:45 HSZ 301

Magnetic properties of Vanadium Oxide Nanotubes — •I. Hellmann[1], R. Klingeler[1], E. Vavilova[1,2], Y. Arango[1], A. Popa[1], V. Kataev[1], Ch. Täschner[1], and B. Büchner[1] — [1]Leibniz-Institute for Solid State and Materials Research IFW Dresden, Germany — [2]Kazan Physical Technical Institute, RAS, Kazan, Russia

A new class of nanoscale low-dimensional magnets, mixed valent vanadium-oxide multiwall nanotubes (VO_x-NTs), shows up diverse properties ranging from spin frustration and semiconductivity to ferromagnetism by doping with either electrons or holes [1]. To obtain insights into the magnetic properties of these novel nanosize magnets we have studied the static magnetisation M of undoped VO_x-NTs in the temperature range from 2 K to 600 K in magnetic fields up to 14 T. The data provide evidence for the occurrence of two magnetically nonequivalent vanadium sites in the structure. These sites can be presumably attributed to $V^{4+}(d^1, S=1/2)$ ions in the octahedral and tetrahedral oxygen coordination, respectively. The former are strongly antiferromagnetically correlated and exhibit some signatures of a spin-liquid behaviour. The latter are much weaker magnetically coupled and dominate the low-temperature static magnetic response. In addition to $M(H,T)$ measurements we present also ESR and NMR results obtained on the same samples and discuss possible models of spin coupling and low-energy spin dynamics in VO_x-NTs.

[1] L. Krusin-Elbaum *et al.*, Nature **431**, 672 (2004)

TT 19.12 Tue 17:00 HSZ 301

Stripe Correlations in $Na_{0.75}CoO_2$ — •Jochen Geck[1], Martin von Zimmermann[2], Helmuth Berger[3], Sergey Borisenko[1], Helmut Eschrig[1], Klaus Koepernik[1], Martin Knupfer[1], and Bernd Büchner[1] — [1]IFW Dresden, Germany — [2]HASYLAB at DESY, Germany — [3]EPF Lausanne, Switzerland

Spin and charge stripes in correlated two-dimensional electron systems are one of the hot spots of today's condensed matter research. So far, stripes have been observed in materials based on square lattices like the nickelates and the high-temperature superconducting cuprates. Here we show, based on high-energy x-ray diffraction data and LDA calculations, that sodium-density stripes are formed in $Na_{0.75}CoO_2$; a material based on a triangular lattice. The LDA calculations show that the sodium order results in a sizeable dip of the density of states at the Fermi level, pointing to band structure effects as a driving force for the ordering. This indicates that the stripe order is an intrinsic feature of the two-dimensional CoO_2-layers. Similarities regarding the pinning of stripe correlations in the high-temperature superconducting cuprates and the Na_xCoO_2-materials will also be discussed.

TT 19.13 Tue 17:15 HSZ 301

Density Functional Calculations of the Total Energy and Electronic Structure of Na_xCoO_2 Using the LDA — •Klaus Koepernik, Helmut Eschrig, Jochen Geck, and Bernd Buechner — IFW Dresden, Germany

We analyze the low temperature electronic structure of $Na_{0.75}CoO_2$. Full potential all-electron density functional calculations within the local density approximation (LDA) have been performed. A number of low symmetry superstructures in the Sodium planes have been compared with respect to the LDA total energy. Our findings support the symmetry recently found in diffraction experiments. The superstructure favoured by LDA calculations shows a Sodium charge density wave (CDW) in aggree-

ment with the experimental results. Besides Coulomb energy arguments in favour of the CDW the density of states indicates a band energy gain due to the CDW. The band energy favorization of the CDW is further supported by a small Sodium offset from its symmetry position, increasing the amplitude of the wave. Comparision with the cuprates shows rather big differences in the doping mechanism and therefore in the low energy physics.

TT 19.14 Tue 17:30 HSZ 301

Magnetically driven microwave absorption in $La_1Sr_1MnO_4$: Pulsed magnetic fieldstudies — •R. Klingeler[1,2], V. Kataev[1], U. Schaufuss[1], B. Büchner[1], P. Reutler[1,3], A. Revcolevschi[3], M. Goiran[2], H. Rakoto[2], J.M. Broto[2], and B. Raquet[2] — [1]IFW Dresden, Germany — [2]LNCMP Toulouse, France — [3]UniversitéParis-Sud, France

Spin degrees of freedom are expected to dominate the magnetism in layered hole-free $La_1Sr_1MnO_4$ as the orbital momentum of the Mn ions is quenched by the anisotropic crystal field. Surprisingly, our thermal expansion and NEXAFS data indicate that orbitals are still relevant. There is a temperature driven reorientation of the orbital states. Recent inelastic neutron scattering (INS) data reveal a large spin gap of ∼2.2 THz and two in-gap excitations at 0.8 THz and 1.7 THz in the antiferromagnetically (AF) ordered ground state. The origin of the large anisotropy and the in-gap excitations is unclear. Here we report high frequency electron spin resonance, magnetization and electrical conductivity measurements in magnetic fields up to 60 T. In the AF ordered state we observe a surprisingly strong absorption of sub-Terahertz electromagnetic radiation in fields above 15 T. In the DC limit conductivity measurements yield a significant negative magnetoresistance $R(H)$ as well. However, there are no anomalies in $R(H)$ as well as in the magnetization $M(H)$ in the field range where strong microwave absorption is observed. At still larger fields $M(H)$ reveals the anomaly which can be associated with the lower in-gap spin excitation found in the INS. We discuss our results in terms of an unusual interplay between structure, orbitals and spins.

TT 19.15 Tue 17:45 HSZ 301

Phase transition of β-$MoTe_2$ studied by transport measurements and soft x-ray photoemission spectroscopy — •Thorsten Zandt, Robert Heimburger, Lenart Dudy, Beate Müller, Alica Krapf, Helmut Dwelk, Christoph Janowitz, and Recardo Manzke — Inst.f.Physik, Humboldt-Universität zu Berlin

$MoTe_2$ undergoes a phase transition at about 1125 K from a low-temperature semiconducting β-phase (hexagonal) to a high-temperature metallic β-phase (monoclinic). Upon cooling, for monoclinic β-$MoTe_2$ an additional phase transition is observed at 250 K. This transition is accompanied by a discontinuous structural change, i.e. the monoclinic angel β of 93°55′ changes to 90° [1] resulting in an orthorhombic Td-$MoTe_2$ structure. In this contribution we present a detailed temperature dependent study of the transport and electronic properties of the 250K-phase transition of the $MoTe_2$ single crystals. The in-plane resistivity as well as the magnetic susceptibility reveal a distinct hysteretic behavior at the phase transition. In addition, temperature dependent soft x-ray photoemission of Te 4d core levels show a large splitting, which could indicate the occurrence of charge density wave (CDW) formation in β-$MoTe_2$, although there is no direct evidence yet like superlattice spots in the electron diffraction pattern. This will be discussed within a model in which the competition between Coulomb and elastic interactions may drive the first-order lock-in transition to Td-$MoTe_2$ at 250 K.
[1] Clarke, R, Marseglia E and Hughes H P 1978 Phil. Mag. 38 121

TT 19.16 Tue 18:00 HSZ 301

Two-Dimensional Electron-Electron Scattering in the Inherent Conducting Polymer $\{(CH_3)_{0.92}ReO_3\}_\infty$ — •R. Miller[1], E.–W. Scheidt[1], G. Eickerling[1], Ch. Helbig[1], R. Herrmann[1], W. Scherer[1], and P. Schwab[2] — [1]Chemische Physik und Materialwissenschaften, Universität Augsburg, 86159 Augsburg, Germany — [2]Theoretische Physik II, Universität Augsburg,

The metal-oxide system polymeric methyltrioxorhenium $\{(CH_3)_{0.92}ReO_3\}_\infty$ (*poly*-MTO) is a unique representative of an inherent conductive organometallic polymer. In particular the $\{ReO_2\}_\infty$ planes characterize *poly*-MTO as a prototype for a purely two-dimensional system. The resistivity data of pure *poly*-MTO exhibit a crossover from metallic ($d\rho/dT > 0$) to insulating ($d\rho/dT < 0$) behavior at a characteristic temperature $T_{min} \cong 38$ K. Above T_{min} the resistivity $\rho(T)$ is remarkably well described by a two-dimensional electron system. Below T_{min} an unusual resistivity behavior, similar to that found in doped cuprates, is observed. The resistivity increases as $\rho \sim \ln(1/T)$ before it follows a $\sqrt{T}$ temperature dependence below 2 K. We suggest a crossover from purely two-dimensional charge-carrier diffusion within the $\{ReO_2\}_\infty$ planes to three-dimensional diffusion at low temperatures in a disorder-enhanced electron-electron interaction scenario (Altshuler-Aronov correction).

TT 19.17 Tue 18:15 HSZ 301

Sample-dependent resistivity profiles in κ-$(ET)_2Cu[N(CN)_2]Br$ organic superconductors - interrelations with other normal- and superconducting-state properties — •C. Strack[1], C. Akinci[1], V. Paschenko[1], B. Wolf[1], E. Uhrig[1], W. Assmus[1], M. Lang[1], J. Schreuer[2], L. Wiehl[2], J. Schlueter[3], J. Wosnitza[4], D. Schweitzer[5], and J. Wyckhoff[6] — [1]Physikalisches Institut, J.W. Goethe-Universität Frankfurt, FOR 412 — [2]Institut für Mineralogie, J.W. Goethe-Universität Frankfurt, FOR 412 — [3]Materials Science Division, Argonne NL, Illinois, USA — [4]Institut für Festkörperphysik, TU Dresden — [5]3. Physikalisches Institut, Universität Stuttgart — [6]Max Planck Institut für Chemische Physik fester Stoffe, Dresden

The organic superconductor κ-$(ET)_2Cu[N(CN)_2]Br$ shows striking sample-to-sample variations in the electrical resistivity [1]: While most of the crystals reveal a ρ(T) maximum around 90 K with a semiconducting behaviour above, some remain metallic for $T < 300$ K. In the absence of significant differences in the crystals' structural parameters, chemical composition and ESR spectra, these results indicate that real structure phenomena, i.e. disorder and/or defects, strongly affect the inelastic scattering [1]. Here we report on a comparative resistivity study on a variety of crystals with quite different ρ(T) profiles. The work aims at seeking out interrelations between the anomalous scattering contributions at intermediate temperatures and features of the normal- and superconducting-state, such as the glass transition at $T_g \approx 77$ K, the temperature $T^* \approx 40$ K [1], as well as the superconducting transition temperature. [1] C. Strack et al., Phys. Rev. B 72, 054511 (2005)

TT 19.18 Tue 18:30 HSZ 301

Coulomb parameters and spectral function for TTF-TCNQ — •Erik Koch — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich

The key ingredient for a realistic description of strongly correlated materials by a model Hamiltonian is the reliable determination of the Coulomb repulsion parameters. For molecular crystals this is possible. For the example of the quasi one-dimensional organic conductor TTF-TCNQ we show how to calculate the Coulomb repulsion energies between charges in the HOMO/LUMO orbitals. As these molecules, like most π-systems, are planar, we find that a description by a standard Hubbard model with only on-site interaction U is not sufficient. Instead, interactions between charges on different molecules have to be taken into account. Including these longer range interactions has a strong effect on the spectral function, giving results consistent with the photoemission data, without having to assume unrealistically large band-width, as is necessary when when neglecting the Coulomb terms between neighboring molecules.

TT 19.19 Tue 18:45 HSZ 301

Infrared and Raman studies of the competition between spin and charge order in quasi-1D conductors — •Michael Dumm[1], Matteo Masino[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Dipartimento di Chimica and INSTM-UdR, Università di Parma, Parma, Italy

Charge order (CO) phenomena and their competition with spin order are one focus of recent research on low-dimensional highly correlated materials like organic conductors or transition-metal oxides. In the quasi-1D $(TMTTF)_2X$ charge-transfer salts charge disproportionation (CD) on the $(TMTTF)_2$-dimers leads to a ferroelectric CO state. Subsequently, at lower T a transition into a spin-Peierls ground state is observed. Up to now, issues like the charge-order patterns and the coexistence of charge- and spin-ordered ground states in this class of materials remain unclear. We address these issues with T-dependent polarized infrared and Raman spectroscopy on single crystals of $(TMTTF)_2X$.

In the mid-IR spectra, we observed a splitting of several vibronic modes below the charge-order transition which can be directly linked to the CD on the molecules. At far-IR frequencies below 100 cm^{-1}, new intradimer vibrations get IR active along all three crystal axes in the CO state due to the unequal charge distribution on the TMTTF molecules. Above the CO transition, these modes are Raman active. We performed a detailed

analysis of the temperature dependence of these modes. We find for the first time clear evidence that the charge order coexists with the spin-Peierls ground state at low temperatures despite the fact that both are competing ground states.