

TT 87: Low-Dimensional Systems: Molecular Conductors (jointly with CPP, HL, MA, O)

Time: Thursday 9:30–11:00

Location: H 3010

TT 87.1 Thu 9:30 H 3010

Nature of the empty electronic states of TCNQ and their thermal evolution due to the CDW instability of TTF-TCNQ revealed by NEXAFS — ●ALISA CHERNENKAYA¹, K. MEDJANIK^{1,2}, P. NAGEL³, M. MERZ³, S. SCHUPPLER³, E. CANADELL⁴, J.-P. POUGET⁵, and G. SCHÖNHENSE¹ — ¹JGU, Mainz, Germany — ²MAX-lab, Lund, Sweden — ³KIT, Karlsruhe, Germany — ⁴ICMAB, Bellaterra, Spain — ⁵Uni Paris-Sud, Orsay, France

The electronic structure of TTF-TCNQ was studied by near-edge x-ray absorption fine structure (NEXAFS) to detect a signature of the Peierls transition at 54 K [1]. All experimental unoccupied TCNQ orbitals predicted by first-principles calculations are clearly resolved, the $\sigma^*(\pi(a_g, b_{3u}))$ orbital was observed for the first time [2]. The temperature dependence of NEXAFS peak intensities gives evidence of a subtle modification of the electronic structure when the charge density wave (CDW) fluctuations develop as the Peierls transition of the TCNQ stacks is approached from higher temperatures. These changes are explained on the basis of the charge transfer, the shape of the lower empty TCNQ molecular orbitals and the deformation of TCNQ during the pre-transitional CDW fluctuations. Finally the data suggest that the internal stack deformation consisting in a substantial out of plane displacement of the central ring with respect to the cyano-groups allows to gain C-C bonding energy which helps the stabilization of the Peierls transition on the TCNQ stack.

[1] J.P. Pouget, Z. Kristallogr. 219, 711, 2004.

[2] A. Chernenkaya et al., EPJB, accepted.

TT 87.2 Thu 9:45 H 3010

Observation of charge localization and the charge ordering transition in (TMTTF)₂AsF₆ using NEXAFS — ●KATERINA MEDJANIK¹, ALISA CHERNENKAYA², SERGEJ NEPIJKO², GUNNAR ÖHRWALL¹, PASCALE FOURY-LEYLEKIAN³, PERE ALEMANY⁴, ENRIC CANADELL⁵, GERD SCHÖNHENSE², and JEAN-PAUL POUGET³ — ¹Lund University, MAX IV Laboratory, 22100 Lund, Sweden — ²Institut für Physik, JOGU, 55099 Mainz, Germany — ³Laboratoire de Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France — ⁴IQTCUB, Universitat de Barcelona, 08028 Barcelona, Spain — ⁵ICMAB-CSIC, 08193 Bellaterra, Spain

High-resolution near-edge X-ray absorption fine structure (NEXAFS) measurements at MAX II, Lund (beamline I1011 [1]) were performed on a (TMTTF)₂AsF₆ [2] single crystal upon cooling from room temperature to 90 K. Systematic shifts of different spectral features of the F 1s and S 2p signal by up to 0.8 eV to opposite sides on the photon-energy scale with respect to the spectra at room temperature have been detected. Most likely, the shift of the S 2p signal is connected with the breakdown of itinerant conductivity and loss of screening when entering the charge-localization regime. The appearance of a new F 1s pre-edge signal upon entry into the charge ordering (CO) phase at 90 K is a clear fingerprint of the reorganization of the anions in the layered material and changing in the dimerization of molecular orbitals with respect to room temperature. Project funded by DFG through SFB Transregio 49.

[1] I. A. Kowalik et al., J. Phys.: Conf. Ser. 211, 012030 (2010);

[2] M. de Souza et al., Physica B, 405, 92 (2010).

TT 87.3 Thu 10:00 H 3010

Low-Energy Excitations in the Quantum Spin Liquid κ -(BEDT-TTF)₂Cu₂(CN)₃ — ●ANDREJ PUSTOGOW¹, ELENA ZHUKOVA², BORIS GORSHUNOV², MARKO PINTERIC^{3,4}, SILVIA TOMIC⁴, JOHN SCHLUETER⁵, and MARTIN DRESSEL¹ — ¹Physikalisches Institut Universität Stuttgart — ²Moscow Institute of Physics and Technology, Russia — ³Faculty of Civil Engineering, Maribor, Slovenia — ⁴Institut za fiziku, Zagreb, Croatia — ⁵Argonne National Laboratory, USA

The suppression of long range magnetic order due to geometrical frustration gives rise to the quantum spin liquid state. Theoretical considerations predict enhanced absorption within the Mott gap caused by spinons, which results in a low-frequency power-law behaviour of the optical conductivity, i.e. for $\hbar\omega_c < J \approx 250K$. To verify this hypothesis, the optical conductivity of the spin liquid candidate κ -(BEDT-TTF)₂Cu₂(CN)₃ was measured, where the dimerized organic molecules are arranged on a triangular lattice. An ex-

remely wide energy range from radio frequencies up to the near infrared ($10^{-13}eV - 1eV$) was covered by dielectric spectroscopy, THz absorption and optical reflectivity measurements. We could indeed identify a power-law behaviour $\sigma(\omega) \propto \omega^\beta$ where two distinct exponents β change from 0.9 to 1.7 at low temperatures, with the corresponding crossover scaling with temperature: $\hbar\omega_c \approx k_B T$. While our results agree well with (ZnCu)₃(OD)₆(Cl)₂, another spin liquid candidate, theory predicts exponents of 2 and 3.33, respectively. Hence, these experimental findings may motivate a refinement of the theoretical framework.

TT 87.4 Thu 10:15 H 3010

Mott criticality in organic charge-transfer salts κ -(BEDT-TTF)₂X studied by thermal expansion under He-gas pressure — ●E. GATI¹, R. S. MANNA¹, U. TUTSCH¹, B. WOLF¹, L. BARTOSCH², T. SASAKI³, H. SCHUBERT¹, J. A. SCHLUETER⁴, and M. LANG¹ — ¹Physikalisches Institut, Goethe Uni, SFB/TR49, D-60438 Frankfurt — ²Inst. für Theoretische Physik, Goethe Uni, D-60438 FfM — ³IMR, Tohoku University, Sendai 980577, Japan — ⁴Materials Science Division, National Laboratory, Argonne, Illinois 60439, USA

The Mott transition and the underlying universality class have been intensively studied in the past. The proposal of a hitherto unknown *unconventional* universality class for the quasi 2D organic charge-transfer salt κ -(BEDT-TTF)₂Cu[N(CN)₂]Cl (κ -Cl) [1], based on resistivity measurements, has attracted particular interest. In this compound, the Mott transition can be accessed by chemical pressure or the application of very small hydrostatic pressures of 300 bar. We will present measurements of the thermal expansion of κ -Cl under ⁴He-gas pressure [2], a unique technique, which provides a very sensitive tool to investigate critical phenomena [3,4], including effects of coupling of electrons to the crystal lattice [5]. A comparison of our results with theoretical predictions of a scaling theory [4] shows that the critical properties are incompatible with the proposed unconventional universality class.

[1] F. Kagawa et al., Nature 436, 534 (2005).

[2] R. S. Manna et al., Rev. Sci. Instrum. 83, 085111 (2012).

[3] M. de Souza et al., PRL 99, 0370031 (2007).

[4] L. Bartosch et al., PRL 104, 245701 (2010).

[5] M. Zacharias et al., PRL 109, 176401 (2012).

TT 87.5 Thu 10:30 H 3010

Electronic structure and superconductivity of multi-layered organic charge transfer salts — ●HARALD O. JESCHKE, MICHAELA ALTMAYER, DANIEL GUTERDING, and ROSER VALENTI — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt

We examine the electronic properties of polymorphs of (BEDT-TTF)₂Ag(CF₃)₄(TCE) (1,1,2-trichloroethane) within density functional theory (DFT). While a phase with low superconducting transition temperature $T_c = 2.6$ K exhibits a κ packing motif, two high T_c phases are layered structures consisting of α' and κ packed layers. We determine the electronic structures and discuss the influence of the insulating α' layer on the conducting κ layer. In the κ - α'_1 dual-layered compound, we find that the stripes of high and low charge in the α' layer correspond to a stripe pattern of hopping parameters in the κ layer. Based on the different underlying Hamiltonians, we study the superconducting properties and try to explain the differences in T_c .

TT 87.6 Thu 10:45 H 3010

New Charge Transfer Systems based on PAHs — ●ANTONIA MORHERR¹, SEBASTIAN WITT¹, MARTIN BAUMGARTEN², HARALD O. JESCHKE³, and CORNELIUS KRELLNER¹ — ¹Physikalisches Institut, Goethe Universität Frankfurt, D-60438 Frankfurt am Main — ²MPI für Polymerforschung, D-55128 Mainz — ³Institut für Theoretische Physik, Goethe Universität Frankfurt, D-60438 Frankfurt am Main

The Polycyclic Aromatic Hydrocarbons (PAHs) Picene, Coronene and Phenanthrene attracted strong attention in the last years as first superconducting PAHs when intercalated with potassium [1]. K₃Picene shows a T_c of 18 K and the T_c of intercalated Coronene lies between 3.5 K and 15 K [2].

Here, we present charge transfer complexes with PAHs representing donor or acceptor molecules of these complexes. The knowledge of different crystallization modes of these systems, e.g. mixed stack or alternating stack configuration, are important for the physical proper-

ties. The complexes were grown by horizontal vapor growth technique or by growth from solution. Crystal structures, electrical transport measurements and spectroscopical investigations are presented in this contribution. In addition to the experimental data, we present band-structure calculations, which were performed by density functional

methods. The interpretation of both is one approach to understand growing conditions of different stack configurations and an important step towards the design of new charge transfer complexes.

[1] R. Mitsuhashi et al., *Nature* 464, 76 (2010)

[2] Y. Kubozono et al., *Phys. Chem. Chem. Phys.* 13, 16476, (2012)