TT 46: Low-Dimensional Systems: Molecular Conductors

Time: Tuesday 14:00–16:00 Location: HSZ 204

TT 46.1 Tue 14:00 HSZ 204

Tuning the hole injection barrier in the intermolecular charge-transfer compound DTBDT-F_4TCNQ at metal interfaces — Dennis Bayer[1], Sandra Diehl[1,2,4], Martin Baumgarten[3,4], Klaus Müllen[3,4], •Torsten Methfessel[1,4], and Hans-Joachim Elmers[1,4] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, 55128 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [4]SFB/TR49

The codeposition of the organic molecules dithienobenzodithiophene (DTBDT)[1] and tetrafluorotetracyanoquinodimethane (F_4TCNQ) on metal surfaces in ultrahigh vacuum leads to the formation of a novel organic charge-transfer (CT) salt. By scanning tunneling spectroscopy at room-temperature we determined the energetic positions of the highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals of acceptor (F_4TCNQ) and donor (DTBDT) in the pure and in the mixed phase. The mixed phase exhibits a new HOMO close to the Fermi energy depicting a charge-transfer of less than one elementary charge in agreement with earlier results of the CT-salt TMP-TCNQ[2]. The binding energy of this new orbital varies in dependency on the underlying metal substrate, i.e. 0.4 eV on C(R15 × 3)/W(110) , 0.25 eV on a monolayer Co/W(110) and 0.16 eV on hcp Co(0001), thus revealing the possibility of tuning the hole injection barrier.

[1] P. Gao et al., Advanced Materials 21, 213 (2009)
[2] K. Medjanik et al., Physical Review B 82, 245419 (2010)

TT 46.2 Tue 14:15 HSZ 204

The Search for Massless Dirac Fermions — •Rebecca Beyer[1], Armin Dengl[1], Tomislav Ivek[1,2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Institut za fiziku, P.O. Box 304, HR-10001 Zagreb, Croatia

The quasi-two dimensional organic conductor α-(BEDT-TTF)$_2$I$_3$ is a semimetal at high temperature and low pressure. At $T_{MI} = 136$ K (ambient pressure) it undergoes a metal-insulator transition and becomes charge ordered. Pressure is known to reduce the transition temperature and theory predicts a Zero-Gap-Semiconducting (ZGS) state once the transition is fully suppressed. This ZGS state was thoroughly investigated in terms of Landau Levels: many different experiments prove the existence of a zero-energy Landau-Level at high pressures ($p > 15$ kbar) and low temperatures ($T < 10$ K). Only few studies comment on the evolution of the ZGS and the linear dispersion relation in the band structure with pressure or temperature. For example first principle band structure calculations predict a Dirac cone even at room temperature and ambient pressure but with a finite chemical potential.

We present infrared reflectivity measurements under intermediate hydrostatic pressures ($0 < p < 10$ kbar) on α-(BEDT-TTF)$_2$I$_3$ between room temperature and 10 K. We show the evolution of the insulating gap and investigate the possible coexistence of massless and normal charge carriers in one of the few bulk materials with a ZGS state.

TT 46.3 Tue 14:30 HSZ 204

Charge-carrier dynamics at the Mott transition in κ-(BEDT-TTF)$_2$X-Salts — •Benedikt Hartmann[1], David Zielke[1], Jana Polzin[1], Robert Rommel[1], John A. Schlueter[2], Takahiko Sasaki[3], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL, USA — [3]Institute for Materials Research, Tohoku University, Sendai, Japan

The nature of criticality at the Mott transition recently has been in the focus of intense experimental and theoretical research. The quasi-2D organic charge-transfer salts κ-(ET)$_2$X are considered as model systems for studying the Mott metal-insulator transition (MIT) in reduced dimensions. We investigated partially deuterated κ-[(H$_8$-ET)$_{0.2}$(D$_8$-ET)$_{0.8}$]$_2$Cu[N(CN)$_2$]Br, which is located very close to the critical pressure p_0 and further utilized the possibility to reversibly tune the 'chemical pressure' by employing different cooling rates shifting the system to the critical region of the generalized phase diagram. By means of fluctuation (noise) spectroscopy as a powerful new tool for studying charge-carrier dynamics without injecting additional electrons, we observe a pronounced and sudden slowing down of the dynamics near the finite-temperature critical endpoint (p_0, T_0) of the Mott transition. A striking divergence of the low-frequency resistance fluctuations at T_0 for certain cooling rates is accompanied by a signature in higher-order statistical moments (second spectrum) being a hint to spatial correlations. We dicuss this in terms of glassiness of the electronic system which may be an universal feature of MITs.

TT 46.4 Tue 14:45 HSZ 204

STM investigations of κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br — •Sandra Diehl[1,2,3], Torsten Methfessel[1,3], Jens Müller[3,4], Michael Lang[3,4], and Hans-Joachim Elmers[1,2,3] — [1]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, 55128 Mainz — [3]SFB/TR 49 — [4]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main

We investigate the organic charge-transfer salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br as an example for an organic superconductor. The superconducting properties strongly deviate from BCS theory but resemble the properties of high-T_c cuprates which has been attributed to their two dimensional structure leading to electronic correlation effects [1]. In order to understand their electronic properties we measured temperature dependent differential conductivity spectra using scanning tunneling spectroscopy. With this method the shape of the superconducting gap can be determined. In addition to the superconducting gap of the expected size we observe a second, much wider gap indicating a surprisingly large correlation effect. Furthermore, we present STM images showing the alternating structure of conducting and insulating layers. All investigations were done under UHV-conditions ($5 \cdot 10^{-11}$ mbar) using a low temperature scanning tunneling microscope. The surface of the crystals was prepared by in-situ cleaving.

[1] R. H. McKenzie, Science **278**, 820 (1997)

TT 46.5 Tue 15:00 HSZ 204

Low temperature phase diagram of κ-(BETS)$_2$FeCl$_4$ — •Michael Kunz[1], Werner Biberacher[1], Karl Neumaier[1], Natasha D. Kushch[2], and Mark V. Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Institute of Problems of Chemical Physics, Chernogolovka, Russia

The organic charge transfer salts of the (BETS)$_2$FeX$_4$ (X = Cl or Br) family are a subject of intensive research due to interesting correlation effects and magnetic ordering coexisting with superconductivity. κ-(BETS)$_2$FeCl$_4$ is an antiferromagnetic (AFM) metal with a Néel temperature $T_N \approx 0.45$ K. Interlayer resistance measurements were used to track the behavior of the phase boundaries with a magnetic field applied in different directions. Thus the low temperature phase diagram of κ-(BETS)$_2$FeCl$_4$ under applied magnetic field, which shows some remarkable features, was obtained. Shubnikov-de Haas oscillations below the Néel temperature reveal a significant impact of antiferromagnetism on the Fermi surface.

TT 46.6 Tue 15:15 HSZ 204

Studying the Mott criticality via thermal expansion under ^{4}He-gas pressure — •Rudra Sekhar Manna[1], Elena Gati[1], Ulrich Tutsch[1], Takahiko Sasaki[2], and Michael Lang[1] — [1]Physics Institute, Goethe University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany — [2]Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

Quasi-2D organic charge-transfer salts κ-(ET)$_2$X show a variety of ground state properties accessible upon either changing the anion X or by applying hydrostatic pressure. The T-P phase diagram includes a first-order Mott transition line which terminates at a second-order critical end point. Interestingly, deuterated κ-(d8-ET)$_2$Cu[N(CN)$_2$]Br (κ-d8 in short) lies on the verge of the Mott transition line at ambient pressure. Thus, for this material temperature sweeps are sufficient to experimentally access the critical end point and thereby to study the controversy surrounding the Mott criticality. Recent scaling theory [1] applied to previous thermal expansion data on κ-d8 crystals [2] speaks in favor of a 2D Ising universality class. Here we present thermal expansion measurements performed under ^{4}He-gas pressure [3] on κ-d8 crystals along the in-plane a-axis. The aim of this work is to pressure-

tune the system in the vicinity of the Mott critical end point and to compare the results with theoretical predictions [1, 4].

[1] L. Bartosch *et al.*, Phys. Rev. Lett. **104**, 245701 (2010).
[2] M. de Souza *et al.* Phys. Rev. Lett. **99**, 037003 (2007).
[3] R. S. Manna *et al.*, Rev. Sci. Instrum. **83**, 085111 (2012).
[4] M. Zacharias *et al.*, Phys. Rev. Lett. **109**, 176401 (2012).

TT 46.7 Tue 15:30 HSZ 204

Photo-induced phase transition in TTF-CA — •Patricia Haremski, Tobias Peterseim, Tomislav Ivek, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Germany

30 years ago, the first experiments on photo-induced phase transitions on the quasi 1D organic mixed-stacked TTF-CA salt paved the way for numerous experimental and theoretical studies on nonequilibrium states. TTF-CA shows a neutral (N) to ionic (I) phase transition at $T_{NI} = 81.5\,\mathrm{K}$ with a change of ionicity from 0.2 (N) to 0.6 (I) and a dimerization of TTF and CA molecules along the stacking direction. Step-Scan FTIR spectroscopy was used to investigate the photo-induced transitions in TTF-CA by pulsed laser excitation. For different temperatures below T_{NI} and different laser intensities, temporal changes of the infrared reflection spectrum with polarization parallel and perpendicular to the stacking direction were recorded. The reduction of the a_g-modes intensity indicates that the dimerization is dissolved and metastable domains are created. The temporal evolution of the changes in reflectivity can be described by a non-exponential decay function and exhibits similarities to the decay process observed in 1D random-walk annihilation process in photo-excited polyacetylen. Due to the multi-instability in the vicinity of T_{NI}, large domains are formed with an extended lifetime in the microsecond range.

TT 46.8 Tue 15:45 HSZ 204

Electronic transport through defective carbon nanotubes — •Fabian Teichert[1], Andreas Zienert[1], and Jörg Schuster[2] — [1]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Continuing the miniaturization, microelectronics will ultimately approach the atomic scale. One prominent example are carbon nanotubes (CNT), which could be used for transistors and interconnects. So far CNTs cannot be grown or deposited in an ideal and reproducible way inside a device. As one consequence they contain defects.

The present work aims to describe the transport properties of defective armchair CNTs. The focus is set on monovacancies and divacancies. The calculation of the transmission spectrum and the conductivity is done by a fast recursive equilibrium Green's function formalism, which scales linearly with the length of the tube, allowing to treat large systems. The electronic structure is described by the density functional based tight binding model. Single defects, double defects and the behavior of single configurations with many defects are studied. Furthermore, the mean influence of certain defect densities and the diameter of the CNT is investigated within a statistical analysis. It is shown that in the limit of small transmission the system is in the regime of strong localization, where the conductivity scales exponentially with the number of defects. Consequently, a localization length can be extracted, which depends on the defect density and on the CNT diameter.