TT 34: Correlated Electrons: Metal-Insulator Transition 2

Time: Thursday 14:00–19:00 Location: H 2053

TT 34.1 Thu 14:00 H 2053

Phase transitions and orbital fluctuations in 3d^2 vanadates — •Eva Pavarini[1], Molly De Raychaudhury[2], and Ole K. Andersen[3] — [1]Institut für Festkörperforschung, Forschungzentrum Jülich, Jülich, Germany — [2]S.N. Bose National Centre for Basic Sciences, Kolkata, India — [3]Max-Planck Institut für Festkörperforschung, Stuttgart, Germany

We investigate [1] the importance of quantum orbital fluctuations in the orthorhombic and monoclinic phases of the Mott insulators $LaVO_3$ and YVO_3. First, we construct *ab-initio* material-specific t_{2g} Hubbard models. Then, by using dynamical mean-field theory, we calculate the spectral matrix as a function of temperature. Our Hubbard bands and Mott gaps are in very good agreement with spectroscopy. We show that in orthorhombic $LaVO_3$, quantum orbital fluctuations are strong and that they are suppressed *only* in the monoclinic 140 K phase. In YVO_3 the suppression happens already at 300 K. We show that Jahn-Teller *and* $GdFeO_3$-type distortions are both crucial in determining the type of orbital and magnetic order in the low temperature phases.

[1] M. De Raychahudhury, E. Pavarini, O.K. Andersen, Phys. Rev. Lett. **99**, 126402 (2007).

TT 34.2 Thu 14:15 H 2053

Magnetic Moment Collapse-Driven Mott Transition in MnO — •Jan Kunes[1], Alexey V. Lukoyanov[2], Vladimir I. Anisimov[3], Richard T. Scalettar[4], and Warren E. Pickett[4] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg 86135 — [2]Ural State Technical University-UPI, 620002 Yekaterinburg, Russia — [3]Insitute of Metal Physics, Russian Academy of Sciences, 620041 Yekaterinburg, Russia — [4]Department of Physics, University of California, Davis 95616, U.S.A.

We employ a combination of numerical density-functional bandstructure and dynamical mean-field theory to study the evolution of electronic properties of MnO under pressure. Motivated by recent high-pressure experiments we investigate the relationship between high-spin to low-spin transition (moment collapse), insulator-to-metal (Mott) transition and isostructural volume collapse. Our results, which closely resemble the experimental observations, demonstrate that the moment collapse and Mott transition happen simultaneously and that the crystal-field splitting, not the band broadening, is the driving force behind the transition. The Mott transition turns out to be essentially a consequence of local atomic states, high-spin or low-spin, placing different constraints on the electron propagation resulting in insulating or metallic ground states respectively. Energy vs volume curve shows that the specific volume changes discontinuously at the transition. The study represents a significant progress over previous theories which did not provide a reliable picture of the Mott transition.

TT 34.3 Thu 14:30 H 2053

Birth and Death of Quasiparticles in the Mott-Hubbard Prototype V_2O_3 — Leonetta Baldassarre[1], Andrea Perucchi[1,2], Daniele Nicoletti[1], Alessandro Toschi[3], •Giorgio Sangiovanni[3], Karsten Held[3], Massimo Capone[4], and Stefano Lupi[1] — [1]CNR-INFM COHERENTIA and Dipartimento di Fisica, Università di Roma "La Sapienza" — [2]Sincrotrone Trieste S.C.p.A., in Area Science Park, Trieste — [3]Max-Planck Institut für Festkörperforschung, Stuttgart — [4]SMC, CNR-INFM and Dipartimento di Fisica, Università di Roma "La Sapienza" and ISC-CNR, Roma

The infrared conductivity of V_2O_3 is measured in the whole phase diagram to study the behavior of quasiparticles which appear above the Néel temperature T_N, and eventually disappear further enhancing the temperature. We present theoretical calculations demonstrating that this loss of coherence in the vicinity of the Mott transition is enhanced by small changes of the lattice parameters. This leads to a downturn in the optical conductivity at small frequencies, as our experimental data show above 450 K.

TT 34.4 Thu 14:45 H 2053

Interplay of electron-electron and electron-phonon interaction in the metal to insulator transition in vanadium oxides. — •Leonetta Baldassarre[1,2], Emanuele Arcangeletti[1], Andrea Perucchi[1], Daniele Nicoletti[1], Daniele Di Castro[1], Carlo Marini[1], Paolo Postorino[1], and Stefano Lupi[1] — [1]CNR-INFM COHERENTIA and Department of Physics, University of Rome "La Sapienza" , Rome, Italy — [2]Experimentalphysik II, Universität Augsburg, D-86135 Augsburg, Germany

Several families of vanadium oxides display metal to insulator transitions (MIT) often driven by both temperature (T) and pressure (P) with jumps of conductivity up to 7 orders of magnitude. While the transition in V_2O_3 is considered as induced mainly by electronic correlation (Mott-Hubbard transition), the MIT mechanism that drives the electronic transition in VO_2 is still unclear, probably determined by an interplay between electronic and lattice degrees of freedom.

Here we present a complete investigation of MIT as a function of T and P of V_2O_3 and VO_2. Infrared measurements have been performed in a wide range of T (10-600 K) and P (0-15 GPa) in order to cover the rich phase diagrams of those materials. P-dependent Raman measurements have also been performed on VO_2 so to follow also the lattice dynamics. Moreover, the high temperature incoherent phase is discussed in V_2O_3, the ideal playground to study the correlation effects on the low-energy electrodynamics.

TT 34.5 Thu 15:00 H 2053

Pressure-induced phase transitions in the oxyhalides TiOX — •Christine Kuntscher[1], Simone Frank[1], Alexej Pashkin[1], Helge Hoffmann[1], Matthias Klemm[1], Siegfried Horn[1], Andreas Schönleber[2], Sander van Smaalen[2], Sebastian Glawion[3], Michael Sing[3], and Ralph Claessen[3] — [1]Experimentalphysik 2, Universität Augsburg, D-86135 Augsburg, Germany — [2]Laboratory of Crystallography, Universität Bayreuth, 95440 Bayreuth, Germany — [3]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany

The titanium oxyhalides TiOX (X=Cl,Br) are spin-Peierls compounds with exotic properties. With the electronic configuration $3d^1$ they are Mott-Hubbard insulators with a charge gap of ≈2 eV. They were discussed to exhibit a resonating valence bond state and high-temperature superconductivity upon doping. However, up to now a metallization upon doping was not successful. Our recent pressure-dependent infrared spectroscopic investigations on TiOCl suggest that the application of external pressure is an alternative way to induce an insulator-to-metal transition in TiOX [1]. We have extended our spectroscopic investigations on TiOX to the far-infrared range, in order to verify the pressure-induced metallization. X-ray powder diffraction measurements under pressure show that the insulator-to-metal transition coincides with a structural phase transition.

We acknowledge the ANKA Angströmquelle Karlsruhe and the ESRF for the provision of beamtime and the DFG for financial support.

[1] C. A. Kuntscher et al., Phys. Rev. B **74**, 184402 (2006).

TT 34.6 Thu 15:15 H 2053

Spectral weight transfer upon doping in the low-dimensional Mott-Hubbard systems TiOCl and TiOBr — •Sebastian Glawion, Karin Goss, Markus Scholz, Michael Sing, and Ralph Claessen — Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg

Transition metal oxyhalides have seen increasing interest in the past few years due to their non-canonical phase transitions into incommensurate and commensurate spin-Peierls phases and their potential as prototypical $3d^1$ Mott insulators. For pristine TiOCl and TiOBr, a transition into a metallic phase under pressure has been reported which, however, seems to be structurally driven. Using XPS and ARPES we investigated the possibility of band-filling controlled metal-insulator transitions using n- and p-type doping. The layered crystal structure allows for easy intercalation of different dopant species into the van-der-Waals gaps between the Cl-separated Ti-O double layers. Indeed, XPS shows that the Ti valency is reduced through charge transfer from the dopant. While the new spectral weight in the charge gap, as observed by ARPES, nicely follows the expected behaviour for the correlated bands of a Mott insulator, no quasiparticle peak can be found at the chemical potential. The seeming abscence of a metallic QP can be reconciled in a picture where its coherent weight is transferred to higher binding energies due to coupling to polaronic or other degrees of freedom.

15 min. break

TT 34.7 Thu 15:45 H 2053

Spectral weight distribution of d^1 Mott insulators $LaTiO_3$ and $YTiO_3$ — H. Roth[1], •T.C. Koethe[1], Hua Wu[1], Z. Hu[1], A. Hendricks[1], J. Gegner[1], M.W. Haverkort[1], T. Lorenz[1], J.C. Cezar[2], N.B. Brookes[2], I.S. Elfimov[3], G.A. Sawatzky[3], and L.H. Tjeng[1] — [1]II.Physikalisches Institut Universität zu Köln — [2]European Synchrotron Radiation Facility (ESRF), BP 220, 38043 Grenoble Cedex, France — [3]Department of Physics and Astronomy, University of British Columbia, 6224 Agricultural Road, Vancouver, British Columbia, Canada, V6T 1Z1

We have utilized bulk-sensitive photoelectron spectroscopy to study the valence band spectral weight distribution of d^1 Mott insulators $LaTiO_3$ and $YTiO_3$. We observed appreciable differences in the spectra, reflecting the difference in the one-electron band width. We also found that the Ti 3*d* spectra of both materials are much broader than the occupied 3*d* bands calculated by band theories. The mean-field inclusion of the Hubbard U explains the band gap but produces even narrower bands, indicating the complete breakdown of standard mean-field theories in describing excitation spectra. We associate the observed spectra with the propagation of a hole in a system with surprisingly well suppressed charge fluctuations thereby showing characteristics of a t-J model.

TT 34.8 Thu 16:00 H 2053

Charge ordering in perovskite rare-earth titanate compounds — •A. C. Komarek[1], M. Reuther[1], N. Hollmann[1], A. Cousson[2], F. Bouree[2], M. Hölzel[3,4], A. Senyshyn[3,4], P. Link[3], D. Trots[5,4], C. Baehts[5,4], T. Lorenz[1], and M. Braden[1] — [1]Institute of Physics II, University of Cologne, Cologne — [2]LLB, CEA/CNRS, Saclay — [3]TU Munich, FRM-II, Garching — [4]Institute for Materials Science, TU Darmstadt, Darmstadt — [5]Hasylab/DESY, Hamburg

Having a single electron in the 3d shell, the rare-earth (RE) titanates $RETiO_3$ have attracted strong interest to study the complex interplay of charge, orbital and magnetic degrees of freedom. Substituting divalent earth-alkali for the RE, a metal-insulator transition is induced, which in case of $Y_{1-x}Ca_xTiO_3$ occurs only at rather high doping. We have studied the hole-doped system $(Y,Er,Lu)_{1-x}Ca_xTiO_3$ by various diffraction techniques, by resistivity and by magnetic susceptibility measurements. This system shows a complex phase diagram of structural distortions accompanied by a metal-insulator transition. We ascribe the complex behavior to the coexistence of an insulating monoclinic phase with a metallic low-temperature orthorhombic phase. Our neutron diffraction data show that charge ordering occurs in the monoclinic phase. Even away from half-doping, we find two distinct Ti sites in a checkerboard arrangement, with significantly different TiO_6 coordination.

TT 34.9 Thu 16:15 H 2053

Dynamic scaling at MIT in yttrium hydride switchable mirrors — •A. V. Pronin[1], I. G. Romijn[2], H. B. Brom[2], A. F. Th. Hoekstra[2], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD), FZD, 01314 Dresden, Germany — [2]Kamerlingh Onnes Laboratory, Leiden University, 2300 RA Leiden, The Netherlands

Yttrium hydride demonstrates a remarkable transition of its electronic and optical properties upon change of hydrogen concentration: a thin YH_x film can be continuously and reversibly brought from a shiny metal at $x = 2$ to a transparent dielectric at $x = 3$, by changing pressure of the surrounding hydrogen gas [1]. It has been showed that the metal-insulator transition (MIT) could be neatly passed under constant hydrogen pressure by changing the carrier doping via ultraviolet illumination at low temperatures [2]. Pronounced electron-electron interactions are posited to lead to the opening of a large optical gap. The established scaling laws of the conductivity with temperature and doping [2] are strong indications for the quantum nature of the metal-insulator transition in YH_x. To shed more light on the quantum nature of the MIT, the frequency dependence of conductivity is very informative. In an extensive frequency range, frequency ω and temperature T will influence the conductivity in a similar way, which will lead to a so-called ω/T-scaling behaviour. In this talk results on the optical conductivity in the sub-terahertz regime will be presented.

[1] J. N. Huiberts, *et al.*, Nature (London) **380**, 231 (1996).
[2] A. F. Th. Hoekstra, *et al.*, Phys. Rev. Lett. **86**, 5349 (2001).

TT 34.10 Thu 16:30 H 2053

Bulk electronic structure of the layered cobaltate $La_{2-x}Sr_xCoO_4$ — •A. Hendricks, T.C. Koethe, Z. Hu, N. Hollmann, M. Benomar, M. Cwik, T. Lorenz, and L.H. Tjeng — II. Physikalisches Institut Universität zuKöln

The electronic and magnetic properties of the perovskite system $La_{1-x}Sr_xCoO_3$ has been investigated for many decades now and still is subject of active research. In the undoped compound $LaCoO_3$, the correlated nature of the cobalt 3+ ions leads to a temperature driven spin state transition from a $S = 0$ low spin (LS) ground state to a higher spin state, the nature of which has been discussed controversially as either $S = 1$ intermediate or $S = 2$ high spin (HS) state. Upon introducing Co^{2+} by doping with Sr, a metal insulator transition and long range ferromagnetic ordering have been observed. Very recently, the related system $La_{2-x}Sr_xCoO_4$ has been synthesized in order to investigate properties of Co 2+/3+ ions in a environment, which leads in the case of cuprates and nickelates to interesting charge and spin ordering phenomena. While the magnetism of the cobaltates appears to be dominated by Co^{2+} ions in HS, exhibiting short range magnetic order at low temperatures, the spin state of the Co^{3+} is still under debate. Using bulk sensitive soft-x-ray photoelectron spectroscopy, we investigated the valence band electronic structure of $La_{2-x}Sr_xCoO_4$, $0.3 \leq x \leq 0.8$, and its temperature dependence. Our results demonstrate a strong Co^{3+} LS contribution.

TT 34.11 Thu 16:45 H 2053

The spin state issue in the $RBaCo_2O_{5.5}$ cobaltates — •Hua Wu, Zhiwei Hu, Tobias Burnus, Daniel Khomskii, and Liu Hao Tjeng — II. Physikalisches Institut, Universität zu Köln

The double perovskites $RBaCo_2O_{5+\delta}$ (R=rare earth, $0 \leq \delta \leq 1$) display intriguing phenomena such as charge and orbital ordering, as well as antiferromagnetic to ferromagnetic transition, depending on the oxygen concentration. In particular, the δ=0.5 system shows a giant magnetoresistance effect, and its metal-insulator transition has been often interpreted in terms of a spin-state transition [1,2], which, however, is fiercely debated [3,4]. To address the spin-state issue, we performed density-functional theory calculations which include a mean-field correction for the correlation effects caused by the Co 3*d* electrons. We have investigated various scenarios with different combinations of the low-, intermediate- and high-spin (LS, IS, and HS) states. Our results show that the pyramidally coordinated Co^{3+} ions are exclusively in the HS state since [3], in disagreement with [1,2]. The octahedrally coordinated Co^{3+} can be stabilized into a LS-HS ordered state if we take into account the superstructure recently reported [4]. Our results put limits as to how much spin-state transition could accompany the metal-insulator transition.

[1] C. Frontera *et al.*, Phys. Rev. B **65**, 180405(R) (2002).
[2] A. A. Taskin *et al.*, Phys. Rev. Lett. **90**, 227201 (2003).
[3] Z. Hu *et al.*, Phys. Rev. Lett. **92**, 207402 (2004).
[4] D. D. Khalyavin *et al.*, Phys. Rev. B **75**, 134407 (2007).

TT 34.12 Thu 17:00 H 2053

X-ray absorption and x-ray magnetic dichroism study on Ca_3CoRhO_6 and Ca_3FeRhO_6 — •Tobias Burnus[1], Zhiwei Hu[1], Júlio C. Cezar[2], Seiji Niitaka[3], Hua Wu[1], Hidenori Takagi[3,4], Chun Fu Chang[1], Nicholas B. Brookes[2], Ling-Yun Jang[5], Keng S. Liang[5], and L. Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]RIKEN and CREST, Saitama, Japan — [4]University of Tokyo, Japan — [5]National Synchrotron Research Center, Hsinchu, Taiwan

The valence-state of the transition-metal ions in the chain-like compounds Ca_3CoRhO_6 and Ca_3FeRhO_6 is currently an issue under debate. Using numerical simulations and x-ray absorption spectroscopy at the Rh-$L_{2,3}$, the Co-$L_{2,3}$, and the Fe-$L_{2,3}$ edges we reveal a Co^{2+}/Rh^{4+} configuration in Ca_3CoRhO_6 and Fe^{3+}/Rh^{3+} in Ca_3FeRhO_6. X-ray magnetic circular dichroism at the Co-$L_{2,3}$ edge shows that the Co^{2+} ions carry a giant orbital moment of about $1.7\mu_B$. We attribute this to a $d^1_0 d^1_2$ ground state for the high-spin Co $3d^7$ configuration in trigonal prismatic coordination. The intrachain-ferromagnetic coupling of two neighboring Co ions is mediated by a low-spin Rh^{4+} ion ($S = 1/2$) in between.

15 min. break

TT 34.13 Thu 17:30 H 2053

Crystal Structure of layered manganites — •Olaf Schumann[1], Stephen Price[1], Hua Wu[1], Theresa Fernandez-Diaz[2], Pascal

Reutler[3], Alexandre Revcolevschi[3], and Markus Braden[1] — [1]II. Phys. Institut; Universität zu Köln, Zülpicher Straße 77, 50937 Köln — [2]ILL, Grenoble, France — [3]LPCES, Paris Orsay, France

Manganites in a perowskite structure have attracted strong attention during the past years, mainly because of the discovery of the colossal magneto resistivity effect (CMR) and complex charge, orbital and magnetic ordering phenomena. Because of the twining in the perowskites, precise structural investigations to determine the ordering pattern are hampered. Therefore we investigated the single-layer manganites, which show similar ordering phenomena but only small magneto-resistivity effects. Since these materials are not intrinsically twinned, structure determination can be performed with much higher precision. For the ordered phase of half-doped manganites, two models were proposed, the Zener polaron model with bond-centered charge ordering and the so called CE-type model with size centered charge and orbital order, leading to two different Mn-sites. We present the results of powder and single crystal diffraction studies on $La_{0.5}Sr_{1.5}MnO_4$. From a neutron diffraction study on the D10 diffractometer and several x-ray diffraction experiment on our home diffractometer we can unambigously distinct between the two proposed models. The Zener-polaron model does not yield a satisfying description of the observed intensities. Details of the the ordered structure in the CE-Type model will be discussed.

TT 34.14 Thu 17:45 H 2053

Nanometer-scale phase separation in colossal magnetoresistive manganite — •Sahana Roessler[1], Stefan Ernst[1], Steffen Wirth[1], Frank Steglich[1], B. Padmanabhan[2], Suja Elizabeth[2], and H. L. Bhat[2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany — [2]Department of Physics, Indian Institute of Science, Bangalore 560012, India

In strongly correlated electron systems an intrinsic instability of the electronic state and competing long-range interactions may result in the formation of nanometer-sized regions of different phases. We have carried out scanning tunneling microscopy/spectroscopy on single crystals of a colossal magnetoresistive manganite $Pr_{0.68}Pb_{0.32}MnO_3$ at different temperatures in order to probe their spatial homogeneity across the metal-insulator transition temperature T_{M-I}. In this compound, the Curie temperature T_C is lower than T_{M-I} [1]. Spectroscopic studies revealed inhomogeneous maps of the zero-bias conductance with small patches of metallic clusters on a length scale of 2-3 nm only within a narrow temperature range close to the metal-insulator transition. A detailed analysis of conductance histograms based on these maps gave direct evidence for phase separation into insulating and metallic regions in the paramagnetic metallic state, i.e. for $T_C \lesssim T \lesssim T_{M-I}$, and homogeneous states otherwise, i.e. for $T < T_C$ as well as $T > T_{M-I}$ [2].

[1] B. Padmanabhan *et al.* J. Magn. Magn. Mat. **307** 288 (2006).
[2] S. Rößler *et al.* IEEE Trans. Magn. **43** 3064 (2007).

TT 34.15 Thu 18:00 H 2053

Scanning tunneling microscopy and spectroscopy study of charge and orbital ordering transition in $La_{0.5}Sr_{1.5}MnO_4$ — •Grzegorz Urbanik[1,2], Paul Sass[1], Christian Hess[1], Torben Hänke[1], Bernd Büchner[1], Antoni Ciszewski[2], Pascal Reutler[3], and Alexandre Revcolevschi[3] — [1]Institute for Solid State Research, IFW-Dresden, 01171 Dresden, Germany — [2]Institute of Experimental Physics, University of Wroclaw, 50-204 Wroclaw, Poland — [3]Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris Sud, Bâtiment 414, 91405 Orsay, France

The charge and orbital ordering compound $La_{0.5}Sr_{1.5}MnO_4$ has been studied by Scanning Tunneling Microscopy (STM) and Spectroscopy (STS). Cleaving of the crystal exposes flat surfaces on which atomically resolved topographic images are routinely achieved above the charge ordering temperature $T_{CO} \approx 225$ K and below (down to $T \approx 205$ K). We have studied the temperature dependence of the electronic structure both for $T > T_{CO}$ and $T < T_{CO}$. The temperature dependent STS clearly reveals finite DOS at the Fermi level for $T > T_{CO}$ and the opening of a gap $\Delta \approx 0.5$ eV just below T_{CO}. In the topographic studies we find nanometer scale modulations with various periodicity and orientations. We compare these modulations with the inherent charge and orbital ordered state of this material.

TT 34.16 Thu 18:15 H 2053

$Hg_2Ru_2O_7$, a New Magnetic Pyrochlore Showing a Metal-Insulator Transition — •Reinhard K. Kremer, Jun Sung Kim, Wilhelm Klein, and Martin Jansen — Max Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

The new pyrochlore compound $Hg_2Ru_2O_7$ was prepared under elevated oxygen pressure and characterized by x-ray diffraction, magnetic susceptibility, heat capacity, electrical resistivity and Hall effect measurements. $Hg_2Ru_2O_7$ undergoes a simultaneous metal-insulator and antiferromagnetic ordering transition at ∼108 K with the critical temperature decreasing under hydrostatic pressure.[1] $Hg_2Ru_2O_7$ is compared with other p-block metal oxoruthenates with pyrochlore structure which qualitatively show a very similar behavior. General trends are discussed.

[1] W. Klein, R. K. Kremer and M. Jansen, J. Mater. Chem. **17**, 1356 (2007).

TT 34.17 Thu 18:30 H 2053

Frustrated metallicity in the quasi-one-dimensional metal $PrBa_2Cu_4O_8$ — •Alessandro Narduzzo[1,2], Araz Enayati-Rad[1], Florence Rullier-Albenque[3], Shigeru Horii[4], and Nigel E. Hussey[1] — [1]University of Bristol, UK; — [2]IFW Dresden, Germany; — [3]Saclay, Paris, France; — [4]University of Tokyo, Japan.

We have investigated the metallic ground state of the extremely anisotropic quasi-one-dimensional metal $PrBa_2Cu_4O_8$ ($t_b^2 : t_a^2 : t_c^2 \sim 4000 : 2 : 1$), the non-superconducting analogue of the high-T_c cuprate $YBa_2Cu_4O_8$, as a function of disorder content, introduced either through atomic-site substitution or electron irradiation [1, 2]. A common single disorder threshold is found to drive interchain and inchain resistivities into a low temperature regime where they display $d\rho/dT < 0$. The survival of a large magnetoresistance of orbital origin reveals the itinerancy of the electronic system not to be suppressed by the presence of disorder [3]. We propose an interpretative scenario based on a microscopic electronic fragmentation of the metallic chains, though in contrast to many previous theoretical proposals, coherent hopping between chains appears to remain a relevant perturbation within the disordered system.

[1] New J. Phys. 8 (2006) 172-183; [2] Phys. Rev. Lett. vol. 99, 136402 (2007); [3] Phys. Rev. Lett. vol. 98, 146601 (2007).

TT 34.18 Thu 18:45 H 2053

Dynamics of correlated charge carriers in the close proximity to the Mott-Hubbard transition — •Michael Dumm[1], D. Faltermeier[1], S. Yasin[1], N. Drichko[1], M. Dressel[1], and J. Merino[2] — [1]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid 28049, Spain

We explored the dynamics of correlated charge carriers in close proximity to the Mott-Hubbard transition experimentally and theoretically in the quasi two-dimensional organic conductor κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br$_x$Cl$_{1-x}$ ($x = 0.73$ and 0.85). In the dc and optical conductivity data, we observe typical signatures of Fermi liquid behavior below the characteristic temperature $T^* \approx 30$ K and frequency $\nu^* \approx 400$ cm^{-1}: a T^2 and ν^2 dependence in resistivity and scattering rate, respectively and a substantial enhancement of the effective mass of the correlated carriers once we approach the metal-to-insulator transition by increasing U/t, i. e. by decreasing the Br content. The experimental results obtained by infrared spectroscopy agree well with DMFT calculations of a Hubbard model on a frustrated square lattice. Both, temperature and frequency dependence of optical conductivity and effective charge carrier number are successfully described by the theoretical model. If the temperature is increased above T^*, the Drude peak observed in the optical data at $T < T^*$ and $\nu < \nu^*$ vanishes and the optical spectral weight of the correlated carriers decreases indicating a gradual destruction of the quasiparticles.