TT 80: Low-Dimensional Systems - Poster Session

Time: Wednesday 15:00–19:00 Location: P2

TT 80.1 Wed 15:00 P2

Engineering of low-energy models for topological insulators with d-electrons — •Martin Edelmann, Michael Karolak, and Giorgio Sangiovanni — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg

We present ab-initio calculations performed on Nickel-based bulk materials and heterostructures via density-functional-theory (DFT). We explore different geometries and heterostructures, focussing on cases with e_g-orbitals. This constitutes the first step for upcoming many-body calculations to possibly realize a topological state with d-orbitals.

In our first DFT-calculations, the in-plane lattice parameters were changed in order to match different substrates and explore the possibility of realizing a band-insulator. Another road to this goal is the introduction of one (or multiple) insulating planes in between the bulk material to create a heterostructure and suppress inter-orbital hopping.

We discuss the Wannier projection procedure to obtain the minimal low-energy one-body Hamiltonian which will serve as an input for the many-body calculations.

TT 80.2 Wed 15:00 P2

Symmetry protection in topological insulators: fundamentals and applications — •Stephan Rachel — Institut für Theoretische Physik, TU Dresden

We consider two-dimensional topological insulators as prototypes of symmetry protected topological phases where spin-orbit coupling gives rise to the topological insulator phase. The appearance of additional non-topological terms might cause quantum phase transitions into trivial phases when this topologically trivial term overweights the spin-orbit coupling. Usually such a phase transition is associated with closing of the bulk gap. In contrast, time-reversal symmetry breaking terms immediately destroy the topological phase without closing of the bulk gap unless the axial spin symmetry remains preserved. These findings pave the way for interesting applications in topological nano-ribbons.

TT 80.3 Wed 15:00 P2

Polaritons in a Quantum Spin Hall Insulator — •Alexander Janot[1], Bernd Rosenow[1], and Gil Refael[2] — [1]Institut für Theoretische Physik, Universität Leipzig, 04009 Leipzig, Germany — [2]Department of Physics, California Institute of Technology, Pasadena, CA 91125, USA

We study the topological properties of mixed matter-light particles, so called polaritons, in a quantum spin hall insulator coupled to photonic cavity modes. Taking into account the spin and polarization structure of electrons and photons, respectively, we find that the electron-photon coupling matrix can be characterized by a non-trivial pseudo-spin vector. For a topological quantum spin hall system this vector wraps around the Bloch sphere twice as the wave vector covers the entire Brillouin zone, while the winding number is zero in the topologically trivial case. We find that the Hilbert space spanned by the two lower polariton branches is no longer degenerate as in the absence of spin-orbit coupling, and exhibits a pseudo-spin vector which is constraint to the x-y plane. This picture changes for the case of a chiral cavity supporting only one polarization. Focusing on the lower polariton branch, the excitonic components of the polaritons are characterized by a non-trivial pseudo-spin vector. This findings suggest a possible variety of new topological phenomena in coupled light-matter systems.

TT 80.4 Wed 15:00 P2

Electronic reconstruction at the isopolar $LaTiO_3$/$LaFeO_3$ interface — •Judith Gabel[1], Josée E. Kleibeuker[1,2], Zhicheng Zhong[3], Hiroaki Nishikawa[4], Andreas Müller[1], Florian Pfaff[1], Dave H.A. Blank[2], Michael Sing[1], Gertjan Koster[2], Karsten Held[3], Ralph Claessen[1], and Guus Rijnders[2] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg — [2]Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente — [3]Institute of Solid State Physics, Vienna University of Technology — [4]B.O.S.T., Kinki University

We report the formation of a new non-magnetic Mott insulating phase (U =0.5 eV) at the isopolar interface between two insulating antiferromagnets, $LaTiO_3$ and $LaFeO_3$. The formation is driven by the combination of electrochemical energy, which can be described by O band alignment, and crystal field splitting energy of the t_{2g} and e_g bands. As a result of these two driving forces, the Fe 3d bands rearrange and electrons are transferred from Ti to Fe. Using X-ray photoelectron spectroscopy, we find a strong electron transfer of almost $1\,e^-$/interface unit cell. The shown route for interfacial electronic reconstruction opens possibilities to design new functional oxide heterointerfaces.

TT 80.5 Wed 15:00 P2

Probing the eletronic structure of γ-Al_2O_3/$SrTiO_3$ oxide heterostructures by hard x-ray photoelectron spectroscopy — •Philipp Schütz[1], Florian Pfaff[1], Philipp Scheiderer[1], Götz Berner[1], Mihaela Gorgoi[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Materials Systems (RCCM), Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie (HZB-BESSY II), Albert-Einstein-Strasse 15, 12489 Berlin, Germany

The heterointerface between the band insulators γ-Al_2O_3 and $SrTiO_3$ hosts a two-dimensional electron system (2DES) with exceptionally high electron mobility. The promising spinel/perovskite complex oxide heterostructure has been studied by hard x-ray photoelectron spectroscopy with high interface sensitivity. A detailed core level and valence band analysis yields information about the electronic structure, including band bending and band alignment at the interface. Evidence for the two-dimensional nature of the conducting interface is obtained from the angle dependent chemically shifted Ti^{3+} 2p core level signal, which is generally attributed to Ti ions with electrons hosted in the Ti 3d shell. The 2DES is found to be strongly confined within several unit cells of $SrTiO_3$ in proximity to the interface, with sheet carrier densities in the range of $10^{-14}\,cm^{-2}$.

TT 80.6 Wed 15:00 P2

Magnetization of two-dimensional electron systems in MgZnO/ZnO heterostructures — •Schorsch Michael Sauther[1], Matthias Brasse[1], Stephan Albert[1], Yusuke Kozuka[2], Joseph Falson[2], Atsushi Tsukazaki[2], Christian Heyn[3], Fauzia Jabeen[4], Marc Andreas Wilde[1], Anna Fontcuberta i Morral[4], Masashi Kawasaki[2], and Dirk Grundler[1] — [1]Phys.-Dep. E10, TU München — [2]Dep. of App. Phys. and QPEC, University of Tokyo — [3]Inst. f. Angew. Phys., Universität Hamburg — [4]LMSC, EPF Lausanne

Two-dimensional electron systems (2DESs) in oxide heterostructures have created great interest in the last few years. We study the magnetization M of MgZnO/ZnO heterostructures with 2DESs of small carrier density and high mobility at low temperatures and in high magnetic fields B. We report a sawtooth-like oscillating signal $M(B)$, i.e. the de Haas-van Alphen-effect, from which we extract thermodynamic energy gaps. Furthermore we observe non-equilibrium currents and unexpected overshoots in $M(B)$ that we analyze in terms of the residual disorder. The work is supported by the DFG via TRR 80.

TT 80.7 Wed 15:00 P2

Interface properties of NiMnSb/MgO and NiMnSi/MgO heterostructures — •Rui-Jing Zhang[1], Ulrich Eckern[1], and Udo Schwingenschlögl[2] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

The electronic and magnetic properties of the interfaces between the half-metallic Heusler alloys NiMnSb, NiMnSi and MgO have been investigated using first-principles density-functional calculations with projector augmented wave potentials generated in the generalized gradient approximation. In the case of the NiMnSb/MgO (100) interface the half-metallicity is lost, whereas the MnSb/MgO contact in the NiMnSb/MgO (100) interface maintains a substantial degree of spin polarization at the Fermi level ($\sim$ 60%). Remarkably, the NiMnSi/MgO (111) interface shows 100% spin polarization at the Fermi level, despite considerable distortions at the interface, as well as rather short Si/O bonds after full structural optimization. This behavior markedly distinguishes NiMnSi/MgO (111) from the corresponding NiMnSb/CdS and NiMnSb/InP interfaces.

TT 80.8 Wed 15:00 P2

MBE-growth of $LaNiO_3$ based heterostructures - From empirical growth to designing new materials — •Friederike Wrobel, Gennady Logvenov, Georg Christiani, Eva Benckiser, and Bernhard Keimer — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

Motivated by predictions of model calculations, which showed that heterostructured nickelates provide the essential ingredients for the occurrence of high T_c-superconductivity [1], we started to investigate these materials. Confinement and strain influence the structure, orbital occupation and electronic as well as magnetic properties [2,3]. Superlattices with 2 unit-cell thick layers of $LaAlO_3$ (LAO) and 2 layers of $LaNiO_3$ (counted in pseudo-cubic unit cells) show a transition to an antiferromagnetically ordered state at low temperatures. In contrast, samples with a periodicity of 4 layers of $LaNiO_3$ remain paramagnetic/metallic at all temperatures. Here, we present first results on how to extend our study on nickelate superlattices. Our goal is to modify the electronic and magnetic structure by charge carrier doping, either via oxygen reduction or chemical doping. Oxide molecular beam epitaxy (oxide MBE) is used to realize new superlattice systems and to improve the sample quality.

[1] J. Chaloupka, G. Khaliullin, Phys. Rev. Lett. **100**, 016404 (2008)
[2] M. Wu *et al.*, Phys. Rev. B **88**, 125124 (2013)
[3] A. Frano *et al.*, Phys. Rev. Lett. **111**, 106804 (2013)

TT 80.9 Wed 15:00 P2

Phase Transitions in Nickelate Thin Films and Superlattices Studied by Raman Light Scattering — •Matthias Hepting, Mathieu Le Tacon, Eva Benckiser, Matteo Minola, Friederike Wrobel, Dmitry Kukuruznyak, Georg Christiani, Gennady Logvenov, and Bernhard Keimer — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Recent work on heterostructures based on rare-earth nickelates revealed that it is possible to control their magnetic and electronic properties by epitaxial strain and spatial confinement [1,2]. To gain a deeper understanding of the correlation between the electronic and the structural phase transitions, we have developed an advanced method of Raman spectroscopy which enables the study of heterostructures as thin as ∼10nm.

Here we present temperature-dependent Raman spectra of $PrNiO_3$ based thin films and superlattices in different strain states and with different periodicities. We will discuss how signatures of a charge ordered ground state are mirrored in the Raman spectrum of tensile strained $PrNiO_3$ and how this observation can give deeper insights on the character of the ground state of rare-earth nickelates [3].

[1] A. Boris *et al.*, Science **332**, 937 (2011)
[2] A. Frano *et al.*, Phys. Rev. Lett. **111**, 106804 (2013)
[3] S. Lee, *et al.*, Phys. Rev. Lett., **106** 016405 (2011)

TT 80.10 Wed 15:00 P2

Under-pressure measurements of resistivity and magnetic susceptibility and the pressure-temperature phase diagram of $(DOEO)_4[HgBr_4]$TCE organic charge-transfer crystals — •Alisa Chernenkaya[1,2], S. Köhler[3], E. Gati[3], V. Ksenofontov[4], K. Medjanik[2], A. Kotov[5], R. Morgunov[5], E. Yagubskii[5], H.-J. Elmers[2], M. Lang[3], and G. Schönhense[2] — [1]Graduate School Materials Science in Mainz, 55128, Mainz, Germany — [2]Inst. für Physik, JGU, 55128, Mainz, Germany — [3]Phys. Inst., J.W. GUF, 60438, Frankfurt am Main, Germany — [4]Inst. für Anorg. und Analyt. Chem., JGU, 55128, Mainz, Germany — [5]Inst. of Probl. of Chem. Phys., RAS, 142432 Chernogolovka, Russia

The asymmetrical molecule DOEO (1,4-(dioxandiil-2,3-dithio) ethylenedithiotetrathiafulvalene)is the essential building block of the cation-radical salt $(DOEO)_4[HgBr_4]$TCE (TCE is 1,1,2-trichloroethane) [1].

It was shown before that the temperature dependence of resistivity of $(DOEO)_4[HgBr_4]$TCE at ambient pressure is non-trivial [1]. There is a maximum at $T = 120$ K and a minimum at $T = 70$ K in resistivity. We found evidence of an antiferromagnetic phase existing below 40 K. $(DOEO)_4[HgBr_4]$TCE is a possible candidate for a superconducting state below 7 K due to the comparability to BEDT-TTF salts. We performed characterization of phases and phase transitions and present a tentative pressure-temperature phase diagram.

Funded by DFG (Transregio TR49).

[1] A. Bardin et. al., Coord. Chem., 32, 88 (2006).

TT 80.11 Wed 15:00 P2

In-plane dependence of the FFLO state in the quasi-2D organic superconductor β''-$(ET)_2SF_5CH_2CF_2SO_3$ — •R. Beyer[1], E. Green[1], J.A. Schlueter[2], R. Zahn[1], S. Jahns[3], G. Zwicknagl[3], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor (HLD), Helmholtz-Zentrum Dresden- Rossendorf (HZDR), Germany — [2]Materials Science Division, Argonne National Laboratory, USA — [3]Institute for Mathematical Physics, TU Braunschweig, Germany

In recent years, clear thermodynamic evidence for FFLO superconductivity in the organic superconductor κ-$(ET)_2Cu(NCS)_2$, where ET stands for bisethylenedithio-tetrathiafulvalene, was found [1]. Performing high-resolution specific-heat measurements, we found as well evidence for the FFLO state in β''-$(ET)_2SF_5CH_2CF_2SO_3$, when the magnetic field is applied parallel to the superconducting ET layers [2]. Theoretical studies predict a strong in-plane critical field anisotropy of the FFLO phase. As a consequence of the low-dimensional character of the electronic structure, the calculations predict pronounced fluctuation effects which are reflected in substantial broadening of the superconducting transition. Therefore, we carried out specific-heat measurements with three different in-plane field orientations. The phase diagram with the pronounced upturn around 9.5 Tesla is independent of the in-plane field orientation. This points to an FFLO wave vector, that is fixed to a certain in-plane direction.

[1] R. Lortz *et al.*, Phys. Rev. Lett. **99**, 187002 (2007)
[2] R. Beyer *et al.*, Phys. Rev. Lett. **109**, 027003 (2012)

TT 80.12 Wed 15:00 P2

Unconventional thermal conductivity of the organic superconductor κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br$ — S. Kühlmorgen[1], J. Wosnitza[1], J. Müller[2], T. Herrmannsdörfer[1], and •R. Schönemann[1] — [1]Hochfeld-Magnetlabor (HLD), Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [2]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt, Germany

We have investigated the organic superconductor κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br$ by means of high-resolution thermal-conductivity measurements. The thermal conductivity was measured in a wide temperature range between 0.15 and 17 K. Data were taken at fields up to 14 T in the super- and normal-conducting state of κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br$. In the superconducting state, a strong increase of the thermal conductivity below the transition temperature is observed, passes through a maximum and decreases with further decreasing the temperature. This maximum disappears when higher magnetic fields are applied. From our measurements we can conclude that the phonons are the dominant carriers for thermal transport. In the investigated temperature range the thermal conductivity in the superconducting state is higher than in the normal state. Down to lowest temperatures, this is due to quasi-particle scattering which affects the mean free path of the phonons.

TT 80.13 Wed 15:00 P2

Multiferroicity in the Mott insulating charge-transfer salt κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$ — •E. Gati[1], P. Lunkenheimer[2], J. Müller[1], A. Loidl[2], B. Hartmann[1], N.H. Hoang[1], H. Schubert[1], J.A. Schlueter[3], and M. Lang[1] — [1]Institute of Physics, Goethe University Frankfurt(M), SFB/TR49, Germany — [2]Experimental Physics V, University of Augsburg, Germany — [3]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

Multiferroics are materials which show a coincident electric and magnetic order and have been extensively studied throughout the last years. In a recent work [1], multiferroicity has been found in κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$, a two-dimensional organic charge-transfer salt. In contrast to well-known spin-driven ferroelectricity in helical magnets, a charge-order-driven mechanism has been proposed in this case. To get more insight into this issue, in particular to check for sample-to-sample variations, we performed measurements of the dielectric constant and magnetic susceptibility [2] on the same single crystals. We confirm that magnetic and electric order appear nearly simultaneously. Furthermore, we discuss results on various other, differently prepared single crystals. The results verify an order-disorder-type ferroelectric state and are incompatible with an inhomogenous, short-range-ordered state which has been proposed recently [3].

[1] P. Lunkenheimer et al., Nature Mater. 11, 755 (2012)
[2] M. Lang et al., arXiv: 1311.2715
[3] S. Tomić et al., J. Phys.: Cond. Mat. 25, 436004 (2013)

TT 80.14 Wed 15:00 P2

Dilatometric investigations on the quasi-2D organic charge-

transfer salt κ-(ET)$_2$Cu[N(CN)$_2$]I — •Carola Dietrich[1], Rudra Sekhar Manna[1], John A. Schlueter[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, SFB/TR 49, D-60438, Frankfurt (M), Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

High-resolution thermal expansion measurements have been performed on the quasi-two-dimensional organic charge-transfer salt κ-(ET)$_2$Cu[N(CN)$_2$]I along the in-plane c-axis and the out-of-plane b-axis for temperatures 1.4 K $\leq T \leq$ 200 K. In accordance with previous studies [1], we find a highly anomalous expansivity at high temperatures followed by a pronounced glass-like transition for both axes. The glass-like transition at $\sim$ 84 K is similar to that observed for the related κ-(ET)$_2$X salts with X = Cu[N(CN)$_2$]Br and Cu[N(CN)$_2$]Cl [2], and can be assigned to a freezing of orientational degrees of freedom of the terminal ethylene groups. The expansivity along the c-axis shows a hump-like anomaly at around 20 K, where a pronounced minimum was also observed in thermopower measurements [3]. We attribute the thermal expansion anomaly, which remains unaffected upon applying magnetic fields $B \leq 8$ T, to short-range magnetic correlations. Upon further cooling, a rather small anisotropic anomaly is observed at around 5 K of unknown origin.

[1] M. Kund *et al.*, Synth. Met. **70**, 951 (1995)
[2] J. Müller *et al.*, Phys. Rev. B **65**, 144521 (2002)
[3] M. A. Tanatar *et al.*, Phys. Rev. B **62**, 15561 (2000)

TT 80.15 Wed 15:00 P2

Resistivity measurements on the quasi-two-dimensional organic conductor κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl — •Sebastian Köhler[1], John Schlueter[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt(M), SFB/TR49, D-60438 Frankfurt(M), Germany — [2]Material Science Division, Argonne National Laboratory, Argonne, IL 60439-4831, USA

The organic charge-transfer salt κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl is a member of the family of (BEDT-TTF) or short - (ET)-based organic conductors in which conducting layers formed by ET molecules alternate with insulating anion layers. Notably the κ-type configuration is of high interest as these compounds exhibit a rich phase diagram containing metallic, (Mott-)insulating and even superconducting behaviour which can be easily accessed either by chemical pressure or by applying hydrostatic physical pressure. In contrast to the extensively studied copper-based salts, the monoclinic κ-(ET)$_2$Hg(SCN)$_{3-n}$X$_n$ (X=Cl,Br; n=1,2) compounds use mercury as metallic ion in the anion layer. At ambient pressure and high temperatures κ-(ET)$_2$Hg(SCN)$_2$Cl exhibits metallic behaviour with a metal-to-insulator transition at T_{MI}=34K and an AFM transition at T_{AFM}=27K [1].We present resistivity measurements of κ-(ET)$_2$Hg(SCN)$_2$Cl at various hydrostatic pressure values provided by using ^{4}He as pressure-transmitting medium.We find a significant shift of the metal-to-insulator transition to lower temperatures with a rate $\partial T_{MI}/\partial p \approx$ 0.3K/MPa and an increase in metallicity at lower temperatures similar to the behaviour observed for κ-(ET)$_2$Cu[N(CN)$_2$]Cl.

[1]Yasin et al., Physica B **407** (2012) 1689

TT 80.16 Wed 15:00 P2

Statistical properties of the charge-carrier dynamics at the Mott critical endpoint in κ-(BEDT-TTF)$_2$X-Salts — •David Zielke[1], Benedikt Hartmann[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 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 can be reversibly tuned through the critical region in the generalized phase diagram by employing different cooling rates which has a crucial effect on the ratio of bandwith W to on-site Coulomb repulsion U. On this poster, we describe our statistical analysis of the resistance fluctuations by means of time-resolved transport measurements in the vicinity of the finite-T critical endpoint (p_0, T_0). Utilizing a fast data acquisition card in combination with a self-written software we derive the resistance noise power spectral density and higher-order statistical moments (second spectrum). At T_0, we observe a drastic enhancement and slowing down of the low-frequency resistance fluctuations for certain cooling rates together with a frequency dependent signature in the second spectrum. We interpret our observations in terms of a glassy electronic system possibly being universal for MITs.

TT 80.17 Wed 15:00 P2

Antiferromagnetism, superconductivity and quantum oscillations in the bifunctional organic conductor κ-(BETS)$_2$FeBr$_4$ — •Ludwig Scheidhammer[1], Michael Kunz[1], Werner Biberacher[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 layered organic metal κ-(BETS)$_2$FeBr$_4$ is a bifunctional material that consists of organic layers containing a metallic π electron system and inorganic layers that carry localized magnetic moments. It shows an antiferromagnetic (AFM) transition with the Néel temperature $T_N \approx 2.5$ K and a superconducting (SC) transition at the critical temperature $T_c \approx 1.1$ K. Shubnikov-de Haas oscillations have been studied in both the normal metallic and AFM states at different magnetic field orientations. From the angle dependence of the oscillation amplitude the exchange field can be obtained. The comparison of the oscillations in AFM and normal metallic state yields information on the Fermi surface reconstruction in the AFM state. We also present the angle dependence of the metamagnetic transition and discuss its influence on superconductivity.

TT 80.18 Wed 15:00 P2

Vibrational infrared spectroscopy of a charge-ordered κ-phase under pressure — Sarika Singh[1], Rebecca Beyer[1], •Tomislav Ivek[1,2], Matija Čulo[2], Rimma N. Lyubovskaya[3], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Institut za fiziku, Zagreb, Croatia — [3]Institute of Problems of Chemical Physics, Chernogolovka, Russia

Dimerized organic conductors from the κ-(BEDT-TTF)$_2X$ family are regarded as prime examples of Mott physics in two dimensions. Due to highly frustrated electron-electron interactions within the half-filled band, their ground states vary from superconducting X = Cu[N(CN)$_2$]Br, over spin liquid insulator of X = Cu$_2$(CN)$_3$, to canted antiferromagnetic insulator X = Cu[N(CN)$_2$]Cl. The related phase diagrams are generally well-described by the Hubbard model with only on-site repulsion U. On the other hand, the recent addition to the family, the X = Hg(SCN)$_2$Cl, undergoes a phase transition into a charge order at 30 K and ambient pressure. This particular ground state is completely unexpected within the Hubbard model.

In order to examine the exotic charge-ordered phase of κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl, we performed vibrational reflectance infrared measurements under hydrostatic pressure up to 11 kbar and at temperatures from 300 down to 10 K. By tracking the charge-sensitive ν_{27}(B$_{1u}$) molecular vibration we are able to map the molecular charges present in the p–T phase diagram. We discuss the effects of pressure on the charge order by taking into account the nearest-neighbor electron repulsion within the paired-electron crystal model.

TT 80.19 Wed 15:00 P2

Photo-induced phase transition in α-(BEDT-TTF)$_2$I$_3$ probed by FTIR and photoconductivity measurements — •Tobias Peterseim, Patricia Haremski, Tomislav Ivek, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Germany

In recent years, the study of nonequilibrium states generated by external stimuli, for instance photo-induced phase transition (PIPT), gained a lot of attention as they shed new light on the physics of the equilibrium state in various materials classes. Furthermore, the observed PIPT show potential routes to build new electronic devices for the application, i.e. optical switches or volatile memories.

The 2D organic salt α-(BEDT-TTF)$_2$I$_3$ is such a candidate in the class of molecular conductors revealing a metal-insulator phase transition at 136 K. It is accompanied by a charge disproportionation between the different molecular sites. We investigated the photoresponse of α-(BEDT-TTF)$_2$I$_3$ in the charged-ordered state. The observed photocurrent shows a non-exponential decay with a residual conductivity. Furthermore, it exhibits a distinct dependency on the laser intensity and the applied electric field including a delayed switching into a high conducting state. Additionally, we performed time-dependent FTIR measurements where traces of a photo-induced metallic phase could be observed. Its decay is in accordance with the photocurrent measurements. However, no indication for the residual conductivity could be found in the time-dependent infrared spectra. We will suggest a possible model which explains the observations.

TT 80.20 Wed 15:00 P2

Ab-initio Hubbard parameters for molecular crystals by a symmetry decomposed Ewald method — •Michael M.E. Baumgärtel and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich, and RWTH Aachen University, 52425 Jülich, Germany

For strongly correlated molecular crystals we determine realistic Hubbard parameters ab-initio. Restricting to electrons in the partially filled bands, screening by the other electrons renormalizes the Hubbard parameters. The intra-molecular screening is treated within DFT, while inter-molecular Coulomb interaction is modeled by a lattice of distributed polarizabilities. Charging of a molecular orbital breaks the periodic symmetry of dipole interactions. By separating the linear response, we obtain a periodic dipole-dipole interaction operator that is independent of the actual polarization pattern. Inverting this operator gives the self-consistent linear screening. In reciprocal space the interaction matrix is low-dimensional, but long-range. However, we obtain rapidly converging matrix elements through an optimized Ewald-summation.

We present eigen-spectra of Fourier transformed dipole interaction matrices. For the sampling of the electric field of the charged molecular orbital on the lattice of polarizabilities we derived an Ewald summation. Employed on a Brillouin zone grid our fast diagonalization method yields the Hubbard parameters, both on-site and long-ranged, for any charging of molecular orbitals. We demonstrate our method for Fullerenes as well as TTF-TCNQ crystals.

TT 80.21 Wed 15:00 P2

Leaf-to-leaf distances and their moments in finite and infinite m-ary acyclic graphs — •Andrew M. Goldsborough, S. Alex Rautu, and Rudolf A. Römer — University of Warwick, Coventry, UK

It has recently been shown [1] that two-point correlation functions in tensor network wavefunctions are related to the length of the path through the network that connects the two lattice sites. In reference to a binary tree tensor network (TTN) [2], we analyse the geometry of a complete regular binary tree where the leaves represent the points on a 1-D lattice. We find an analytic expression for the average path length for a given separation in a tree with n levels. This expression is then generalised to give any raw statistical moment for m-ary trees with open and periodic boundary conditions. We also present first results for random binary trees.

[1] G. Evenbly and G. Vidal, J. Stat. Phys. 145, 891 (2011)
[2] Y. Shi, L. Duan, and G. Vidal, Phys. Rev. A 74, 022320 (2006)

TT 80.22 Wed 15:00 P2

Incommensurate insulator and pairing in an asymmetric ladder system — •Anas Abdelwahab[1], Eric Jeckelmann[1], and Martin Hohenadler[2] — [1]Leibniz Universität Hannover — [2]Universität Würzburg

We investigate a ladder system made of two inequivalent legs, a Hubbard chain and a free electron gas. Analytical approximations, density-matrix renormalization group, and continuous-time quantum Monte Carlo are used to determine ground-state properties such as correlation functions, gaps, and spectral functions of this system. At half filling and intermediate Hubbard on-site interaction we observe three different phases as a function of the inter-chain hopping. The system is a Luttinger liquid and a correlated band insulator at weak and strong inter-chain hopping, respectively. For intermediate inter-chain hopping we find an insulating phase with gap minima at incommensurate wave numbers. In this parameter regime and close to half filling doped particles have a significant binding energy but pairing correlations decay rapidly.