TT 31: Correlated Electrons: Low-Dimensional Systems -Materials 1

Time: Tuesday 9:30–12:15 Location: H41

TT 31.1 Tue 9:30 H41

Charge density waves and lattice dynamics in 1T-TaS_2 — •Tobias Ritschel[1,5], Jan Trinckauf[1], Gaston Garbarino[2], Alexei Bosak[2], Martin von Zimmermann[3], Helmuth Berger[4], Bernd Büchner[1,5], and Jochen Geck[1] — [1]IFW Dresden — [2]ESRF, Grenoble — [3]HASYLAB, Hamburg — [4]Ecole polytechnique Federale de Lausanne — [5]TU Dresden

The layered compound 1T-TaS_2 shows an interesting interplay of charge density wave (CDW) order and superconductivity. We studied the static CDW order by means of elastic X-ray diffraction as a function of temperature and external pressure, in order to shed light on the relation between these two collective electronic states. In addition, we investigated the pressure dependency of the lattice dynamics using inelastic X-ray scattering. The phonon dispersion around the CDW wave vector is strongly pressure dependent and a Kohn anomaly is observed well above the nearly commensurate to incommensurate phase transition temperature. We present the experimental data along with model calculations and discuss the results in relation to the pressure-induced superconductivity.

TT 31.2 Tue 9:45 H41

Phonon Softening in the CDW Systems $NbSe_2$ and $TiSe_2$ — •Roland Hott[1], Rolf Heid[1], Klaus-Peter Bohnen[1], Frank Weber[1,2], Stephan Rosenkranz[2], John-Paul Castellan[1,2], Raymond Osborn[2], Takeshi Egami[3], Ayman Said[4], and Dmitry Reznik[1,5] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, P. B. 3640, D-76021 Karlsruhe, Germany — [2]Materials Science Division, Argonne National Laboratory, Argonne, Illinois, 60439, USA — [3]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee, 37996, USA — [4]Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, 60439, USA — [5]Department of Physics, University of Colorado at Boulder, Boulder, Colorado, 80309, USA

We present new results on the soft-mode behaviour of phonons in the Charge Density Wave (CDW) systems $NbSe_2$ and $TiSe_2$. Our theoretical predictions from Density Functional Theory (DFT) based on ab-initio phonon calculations coincide with the CDW instability behaviour that we observed experimentally by means of high resolution Inelastic X-ray Scattering (IXS). While $TiSe_2$ shows a rather sharp phonon anomaly at T = 190 K, the anomaly in $NbSe_2$ at T = 33 K is much broader than expected for a Fermi surface nesting driven CDW instability. For $NbSe_2$, we exclude Fermi surface nesting as main origin of the phonon softening. For $TiSe_2$, the phonon softening seems to be well described within the framwork of DFT.

TT 31.3 Tue 10:00 H41

Charge Density Wave Transport Properties of the $(DCNQI\text{-}d_6)_2Cu$ radical anion salt — •Florian Hüwe[1], Matthias Schmiddunser[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius-Maximilians University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The class of organic metals provides intriguing examples of how the physical properties depend on the respective dimensionality of the underlying material system. The organic radical anion salt $(DCNQI\text{-}d_6)_2Cu$ undergoes a pronounced first-order phase transition upon cooling from a highly conducting quasi-3D metallic state with a conductivity of $\sigma_{RT} \approx 10^3 \frac{S}{cm}$ into a quasi-1D semiconducting, commensurate charge density wave (CDW) state.

Our contribution reports on the transport properties of electrocrystallized $(DCNQI)_2Cu$ single crystals in this CDW regime. Below the phase transition temperature of $T_c = 75K$ the resistance of the about $2cm$ long needle-like samples increases more than five orders of magnitude along the [001]-direction of preferred conductivity. In addition, features of non-linear conduction occur above threshold fields of $E_{th} \approx 10 - 100 \frac{V}{cm}$ which we examined with respect to heating and interference effects by (pulsed) current-voltage and noise measurements. Small μm-sized samples grown by microelectrolysis on a substrate with evaporated gold contacts allow for the investigation of electrical transport in the high-field limit. Finally, a connection between transport characteristics and charge carrier density is drawn.

Financial support by the DFG (project PF385/6-1) is gratefully acknowledged.

TT 31.4 Tue 10:15 H41

The Luttinger liquid theory of molybdenum purple bronze $Li_{0.9}Mo_6O_{19}$ — •Piotr Chudzinski[1,2], Thomas Jarlborg[1], and Thierry Giamarchi[1] — [1]DPMC-MaNEP, Universite de Geneve — [2]University of Regensburg

We study a quasi-1D material, the purple bronze $Li_{0.9}Mo_6O_{19}$ which becomes superconductor at 1.9K. Firstly, the band structure is calculated by use of ab-initio DFT-LMTO method. The unusual, very 1-dimensional band dispersion obtained in previous band calculations is confirmed and the overall band structure agrees reasonably with existing photoemission data. Dispersion perpendicular to the main dispersive direction is obtained and investigated in detail. Temperature and disorder effects are evaluated, in particular we check their influence on the band broadening. Based on this, in the second part of our work we derive an effective low energy theory within the Luttinger liquid framework. We estimate the strength of possible instabilities and values of charge modes compressibilities. Our aim is to understand experimental findings, in particular the ones which are certainly lying within 1D regime. We discuss the validity of our approach and further perspectives for the lower energy phases.

TT 31.5 Tue 10:30 H41

Competing soft phonon modes in $TbTe_3$ — •Michael Maschek[1], Rolf Heid[1], Stefan Rosenkranz[2], Ayman Said[2], Bogdan Leu[2], Paula Giraldo-Gallo[3], and Ian Fisher[3] — [1]Institute of Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Material Science Division, Argonne National Laboratory, Argonne, USA — [3]Geballe Laboratory for Advanced Materials, Stanford University, Stanford, USA

We report high energy resolution inelastic x-ray measurements of competing soft phonon modes in the vicinity of the charge-density-wave (CDW) phase transition in $TbTe_3$. We investigated two phonon modes having each a transverse polarization within the basal plane of the nearly tetragonal unit cell (a=4.308, b=25.57, c=4.314) but are dispersing along the reciprocal (100) and the (001) directions. Only the latter one is expected to go soft at $q_{\mathrm{CDW}} = (0, 0, 0.296)$ and $T_{\mathrm{CDW}} = 332K$. We found that both phonon modes go soft approaching T_{CDW} from high temperatures. The softenings are identical down to $T = 350K$, and only for $T < 350K$ we see a significantly stronger softening of the mode at q_{CDW}. Our results are corroborated by lattice dynamical calculations demonstrating the degeneracy between the two crystallographic axes with respect to the formation of CDW order.

15 min. break

TT 31.6 Tue 11:00 H41

High-mobility two-dimensional electron gas at a new oxide heterointerface — •Romain Giraud[1], Joseph Dufouleur[1], Yunzhong Chen[2], Nini Pryds[2], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01171 Dresden, Germany — [2]Department of Energy Conversion and Storage, Technical University of Denmark, RisØ Campus, 4000 Roskilde, Denmark

In oxides heterostructures, it is generally accepted that the formation of a two-dimensional electron gas (2DEG) occurs at the interface between two insulators with different band gaps, due to band bending. However, there is still an ongoing debate about the mechanisms that drive charge transfer at the interface.

In this work, we evidence the formation of a 2DEG at a new oxide heterointerface, which will be presented in detail. The universality of the overlayer critical thickness for the onset of metallicity will be discussed, as well as the origin of charge transfer. A thorough analysis of the Shubnikov-de Haas oscillations observed above 1 T at T = 22 mK will be presented. These reveal the enhanced mobility of electrons and the influence of magnetic interactions on the 2DEG band structure. Due to a long a phase coherence length, this heterointerface offers a unique opportunity to study quantum coherent transport in strongly-correlated d-electron systems.

TT 31.7 Tue 11:15 H41

High mobility of the strongly confined hole gas in $AgTaO_3$/ $SrTiO_3$ — •Udo Schwingenschlögl, Safdar Nazir, and Mousumi

Upadhyay-Kahaly — KAUST, PSE Division, Thuwal, Saudi Arabia

A theoretical study of the two-dimensional hole gas at the $(AgO)^-/(TiO_2)^0$ p-type interface in the $AgTaO_3/SrTiO_3$ (001) heterostructure is presented. The Ag 4d states strongly hybridize with the O 2p states and contribute to the hole gas. It is demonstrated that the holes are confined to an ultra thin layer (~ 4.9 Å) with a considerable carrier density of $\sim 10^{14}$ cm^{-2}. We estimate a hole mobility of 18.6 cm^{2}V^{-1}s^{-1}, which is high enough to enable device applications.

[1] Appl. Phys. Lett. **100**, 201607 (2012)

TT 31.8 Tue 11:30 H41

Electronic Reconstruction in (001) and (111) oriented $LaAlO_3/SrTiO_3$ interfaces — •David Doennig and Rossitza Pentcheva — Department of Earth and Environmental Sciences, Section Crystallography and Center of Nanoscience, University of Munich, Theresienstr. 41, DE-80333 Munich, Germany

The observation of a quasi two-dimensional electron gas (q2DEG), superconductivity and magnetism at the (001) interface between the band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) has opened possibilities for novel electronics applications. Based on density functional calculations, we explore if these multifunctional properties can be extended by changing the crystal orientation from (001) to (111). Despite the difference in stacking with AO and BO_2 planes of the perovskite ABO_3 structure in (001) oriented superlattices versus AO_3 and B layers in the (111) direction, analogous effects such as polar discontinuity arise when the A and B cations are varied across the interface. A further intriguing feature in (111) oriented interfaces is the formation of a buckled honeycomb lattice of the B-site cations. This lattice geometry, well known from graphene, promises to host even more exotic topological phases. The effect of interface termination, thickness of the substrate and strain will be discussed.

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TT 31.9 Tue 11:45 H41

Modelling random oxygen defects and magnetism at titanate interfaces — •Natalia Pavlenko[1,2], Thilo Kopp[1], G.A. Sawatzky[3], and J. Mannhart[2] — [1]EKM und Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada V6T1Z1

We analyze the magnetic state at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface within density unctional theory and provide evidence that it depends strongly on the oxidation state of the interfaces. We show that oxygen defects at titanate interfaces induce a complex multiorbital reconstruction which involves a lowering of the local symmetry and an inversion of t_{2g} and e_g orbitals resulting in the occupation of the eg orbitals of Ti atoms neighboring the O-defects. In contrast to stoichiometric nonmagnetic interfaces of $LaAlO_3$ and $SrTiO_3$, the defect-induced orbital reconstruction at LAO/STO interfaces generates a two-dimensional interface magnetic state not observed in bulk $SrTiO_3$. Using an effective two-band Hubbard model with disorder, we analyze the stability of the 2d-magnetic states at titanate interface for different concentrations of random defects.

TT 31.10 Tue 12:00 H41

Gating a two-dimensional electron gas using a multiferroic — •Christian Mix[1,2], Mathias Kläui[1], and Gerhard Jakob[1] — [1]Institute of Physics, Universität Mainz, Germany — [2]Graduate school of excellence MAINZ, Mainz, Germany

Recently, research on oxide interfaces has exposed a unexpected conducting state at the interface of lanthanum aluminate (LAO) and strontium titanate (STO), two bulk insulators [1]. Laser ablation enables to the deposition of a wide range of oxide multilayer systems with thickness control at atomic level. Many interesting applications can be introduced by the use of multilayered, epitaxial perovskite structures [2,3]. The sheet resistivity of the 2DEG at the STO/LAO interface possesses a strong dependence on an out-of-plane electrical field. Thus the use of a ferroelectric layer on top of the STO/LAO interface system can lead to a remanent control of the conductivity of the 2DEG. Here, results on the growth and characterization of the multiferroic $BiFeO_3$ on the STO/LAO interface system containing a 2DEG are shown. On the other hand, piezo force microscopy (PFM) is utilized as a tool to observe the ferroelectric domain structure of the BFO thin film with the 2DEG as a back electrode.

[1] J. Mannhart, D.H.A. Blank, H.Y. Hwang, A.J. Millis, J.-M. Triscone, MRS Bullentin **33** (2008) 1027
[2] N.A. Spaldin, M. Fiebig, Science **309** (2005) 391
[3] C. Chen, S. Thiel, J. Mannhart, J. Levy, Science **323** (2009) 1026