TT 3: CE: Charge Density Wave & Peierls Instability

Time: Monday 10:30–13:15 Location: HSZ 304

TT 3.1 Mon 10:30 HSZ 304

Infrared study of the blue bronze $K_{0.3}MoO_3$ — •Rebecca Beyer, Neven Barišić, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart, Germany

The blue bronzes $A_{0.3}MoO_3$ (A = Rb, K, Tl) are well known quasi-one-dimensional materials. They exhibit a Peierls-type metal-insulator phase transition around 180 K which is connected to the formation of a charge density wave (CDW) in the conducting direction. While temperature dependent dc-resistivity indicates the CDW in all three directions, so far most measurements concentrated on the conducting b- and a^*-direction and no thorough investigations of the physical properties of the insulating c^*-direction have been carried out.
We report first optical conductivity measurements on the potassium blue bronze $K_{0.3}MoO_3$ along the b- and the c^*-direction in order to evaluate the influence of the long range order of the CDW on the perpendicular direction. Measurements were performed with polarized light in a wide frequency range from 30 cm^{-1} up to 11000 cm^{-1} for several selected temperatures between 300 K and 50 K. At high frequencies we have carefully analyzed the changes in the strong interband transition related to the gap opening. In addition two phonon lines are observed around 900 cm^{-1} and attributed to stretching vibrations of terminal O- with Mo-atoms. Degenerated at high temperatures, those lines split and shift in frequency once the CDW develops.

TT 3.2 Mon 10:45 HSZ 304

A band structure study of $BaNi_2P_4$ - Dimorphism from a Peierls instability? — •Eugen Wolf, Andreas Leithe-Jasper, Christoph Geibel, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The recent discovery of high temperature superconductivity in iron pnictide compounds stimulated a rebirth of interest in transition metal pnictides in general. In particular, a focus of attention is devoted to compounds that exhibit structural phase transitions caused by the interplay of electronic and lattice degrees of freedom. Here, we present a density functional based (LDA and GGA) computational study of the compound $BaNi_2P_4$ that shows a tetragonal to orthorhombic phase transition at about 370 K. In our calculations, we can reproduce the orthorhombic ground state which is non magnetic since the electronic density of states at the Fermi level is rather low in both phases with a sizably reduced value for the orthorhombic structure. However, the calculated energy difference between the tetragonal and the orthorhombic lattice is far to small to account for the high transition temperature. Possible scenarios for the transition are discussed, especially in the light of a Peierls instability that has been debated controversially in the literature [1,2].
[1] Keimes V, Johrendt D, Mewis A, ZAAC **621**, 925, (1995).
[2] Palacios AA, Alemany P, Alvarez S, et al. Annales de quimica - international edition **93**, 385-393, (1997).

TT 3.3 Mon 11:00 HSZ 304

Dynamic Charge Correlations Near the Peierls Transition — •Martin Hohenadler[1], Holger Fehske[2], and Fakher Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, GER — [2]Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, 17489 Greifswald, GER

The quantum phase transition between a repulsive Luttinger liquid and an insulating Peierls state is studied in the framework of the one-dimensional spinless Holstein model. We focus on the adiabatic regime but include the full quantum dynamics of the phonons. Using continuous-time quantum Monte Carlo simulations, we track in particular the dynamic charge structure factor and the single-particle spectrum across the transition. With increasing electron-phonon coupling, the dynamic charge structure factor reveals the emergence of a charge gap, and a clear signature of phonon softening at the zone boundary. The single-particle spectral function evolves continuously across the transition. Hybridization of the charge and phonon modes of the Luttinger liquid description leads to two modes, one of which corresponds to the coherent polaron band. This band acquires a gap upon entering the Peierls phase, whereas the other mode constitutes the incoherent, high-energy spectrum with backfolded shadow bands. Coherent polaronic motion is a direct consequence of quantum lattice fluctuations. In the strong-coupling regime, the spectrum is described by the static, mean-field limit. Importantly, whereas finite electron density in general leads to screening of polaron effects, the latter reappear at half filling due to charge ordering and lattice dimerization.

TT 3.4 Mon 11:15 HSZ 304

The role of charge order in the layered superconducter $NbSe_2$ — •Dirk Rahn[1], Stefan Hellmann[1], Christian Sohrt[1], Matthias Kalläne[1], Timur Kim[2], Bernd Büchner[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, Germany — [2]IFW Dresden, Germany

The layered compound $2H$-$NbSe_2$ has emerged from a prototype BCS like superconductor to a material with a coexistence of charge-density waves (CDW) and superconductivity (SC) at low temperatures. These two phenomena have led to strong controversity about the symmetry of the gap function [1] and the nature of the interplay between them. Due to the analogy with the high-T_c cuprates, recent ARPES studies of the near-E_F electronic structure [2,3] tried to unveil the gap symmetry as well as the role of the CDW in SC. These studies end up with a contradiction between CDW enhanced and CDW weakened SC and with an uncertainty in the gap symmetry because the measurements were done at $T > T_c/2$. We present a comprehensive ARPES study of the momentum-resolved near-E_F electronic sturcture at $T \approx 1$ K. This allows us to determine the parts of the Fermi surface that stabilize the CDW as well as those parts that are gapped by SC. Furthermore, we see clear fingerprints of different phonon modes in the spectra, which enables us to reveal the correlation between SC, CDW, and the different parts of the phonon spectrum.
[1] Huang *et al.*, Phys. Rev. B **76**, 212504 (2007)
[2] Kiss *et al.*, Nat. Phys. **3**, 720 (2007)
[3] Borisenko *et al.*, Phys. Rev. Lett. **102**, 166402 (2009).

15 min. break

TT 3.5 Mon 11:45 HSZ 304

Extended Phonon Collapse in the Charge-Density-Wave Compound $NbSe_2$ — •Frank Weber[1,2], Stephan Rosenkranz[2], John-Paul Castellan[2], Raymond Osborn[2], Roland Hott[1], Rolf Heid[1], Klaus-Peter Bohnen[1], Takeshi Egami[3], Ayman Said[4], and Dmitry Reznik[1,5] — [1]Karlsruhe Institute of Technology, Institute of Solid State Physics, P. O. Box 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 investigated the phonon softening in the charge density wave compound $NbSe_2$ using the high-resolution hard inelastic x-ray scattering beamline 30-ID-C at the Advanced Photon Source, Argonne National Laboratory. The acoustic Σ_1 phonon branch was measured from the zone center Γ to the M point at temperatures between 250 K and 8 K across the CDW transition at $T_{CDW} = 33$ K. Density functional theory calculations for the lattice dynamical properties which predict an extended phonon breakdown are used to analyze the detailed nature of the softening phonon branch. Work supported by US DOE BES-DMS DE-AC02-06CH11357.

TT 3.6 Mon 12:00 HSZ 304

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[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. O. Box. 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 investigated the soft-mode behaviour of phonons in the Charge Density Wave (CDW) systems $NbSe_2$ and $TiSe_2$ both theoretically in

Density Functional Theory (DFT) based on ab-initio phonon calculations and experimentally by means of high resolution Inelastic X-ray Scattering (IXS). For both materials, the theoretical predictions for the phonon softening using the experimental lattice parameters coincide with the experimentally observed CDW instability behaviour. 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 $TiSe_2$, there is no need to go beyond DFT in order to describe the phonon softening.

TT 3.7 Mon 12:15 HSZ 304

The influence of conduction band population on the charge density wave phase of $TiSe_2$ — •Matthias M. May[1,2], Isaak Unger[1], Christoph Janowitz[1], and Recardo Manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The origin of the charge density wave (CDW) phase transition of the transition-metal dichalcogenide $TiSe_2$ has been subject of research for more than 30 years now with a recent tendency towards an excitonic model [1]. This view was probed by investigating the influence of an additional population of the Ti 3*d* conduction band. The population was realised by means of band bending due to H_2O adsorption [2] and band gap engineering via ternary compounds, monitored with ARPES at BESSY as well as conductivity measurements. Results indicate the existence of an optimal size for the band gap.

[1] C. Monney, C. Battaglia, E.F. Schwier, C. Didiot, M.G. Garnier, H. Beck, P. Aebi and H. Berger, Physica B 404, 3172 (2009)
[2] J. Rasch, T. Stemmler, B. Mueller, L. Dudy and R. Manzke, Phys. Rev. Letters 101, 237602 (2008)

TT 3.8 Mon 12:30 HSZ 304

Electron Energy-Loss Spectroscopy on the Transition-Metal Dichalchogenide 2*H*-$TaSe_2$ — •Andreas König[1], Roman Schuster[2], Helmuth Berger[3], Martin Knupfer[1], and Bernd Büchner[1] — [1]IFW Dresden, Institute for Solid State Research, P. O. Box 270116, D-01171 Dresden, Germany — [2]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [3]Insitut de Physique de la Matière Complexe, EPFL, CH-1051 Lausanne, Switzerland

2*H*-$TaSe_2$ is one of the various polytypes of the transition-metal dichalchogenide (TMDC) $TaSe_2$. It consists of hexagonal layers with weak interlayer van-der-Waals bonding. It shows phase transitions to a charge-density wave (CDW) and to a superconducting state. Although there is strong evidence for the competition of these two ordering effects as well as for a Peierls transition scenario for the origin of the CDW, a theoretical understanding of the mechanism leading to the phase transitions is still subject of discussions. What is already proved for 2*H*-$TaSe_2$ and a few other TMDCs is a negative dispersion of the bulk plasmon in the normal state and an even larger bandwidth of this negative dispersion in the CDW state, which is altogether not a behavior of a common metal. Furthermore, the slope of the plasmon dispersion is doping dependent. We performed Electron Energy-Loss Spectroscopy in transmission on thin films of 2*H*-$TaSe_2$ for different potassium contents as well as for different temperatures above and below the CDW transition temperature to investigate the connection of the CDW phase transition to the plasmon dispersion.

TT 3.9 Mon 12:45 HSZ 304

Raman study of the charge density wave system $ErTe_3$ — •Hans-Martin Eiter[1], Michela Lavagnini[1], Reinhard Rossner[1], Jiun-Haw Chu[3], Ian R. Fisher[3], Leonardo Degiorgi[2], and Rudi Hackl[1] — [1]Walther-Meissner Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [2]Laboratorium für Festkörperphysik, ETH - Zürich, CH-8093 Zürich, Switzerland — [3]GLAM, Stanford University, CA 94304, USA

We present results of Raman scattering experiments on $ErTe_3$ as a function of temperature and photon polarization. At high energy, electron-hole excitations across the charge density wave (CDW) gap are observed. Below 100 cm^{-1} strongly temperature dependent collective excitations dominate the spectra. With both light polarizations along the *c*-axis of the single domain crystal a large gap $2\Delta_0$ in the range of 0.4 eV opens below the first CDW transition at 265 K. The gap of the second transition at 155 K is only present for *aa* polarizations. The related amplitude modes do not exactly mirror the anisotropy of the electronic gaps but rather show components of the the higher tetragonal symmetry highlighting the intimate coupling of the electrons to the quasi-tetragonal lattice. The high gap ratios $2\Delta_0/k_BT_c$ in the range above 10 compare well to results of photoemission experiments and indicate that fluctuations substantially suppress the mean-field transition temperature.

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TT 3.10 Mon 13:00 HSZ 304

Collective excitations and low temperature transport properties of bismuth — •Piotr Chudzinski and Thierry Giamarchi — DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet CH-1211 Geneva, Switzerland

We examine the influence of collective excitations on several transport coefficients (conductivitiy, magneto-optical conductivity, Nernst effect) for semimetal, bismuth. A longstanding problem of the transport coefficients in this material is the fact that their amplitude and temperature dependences do not obey naive Fermi liquid expectations. For the conductivity, we show that at high temperatures Baber scattering is able to explain quantitatively the DC resistivity experiments, while at low temperatures many-body effects need to be introduced to explain qualitative deviations from the standard T^2 behavior. An atypical feature in magneto-optical conductivity is predicted. The Nernst effect in bismuth was recently the subject of several contradictory theoretical studies. We show that a plasmon physics allows to get a coherent picture and leads to very large values of the Nernst signal. We use two complementary methods- Feynmann diagrams and field theory (Hubbard-Stratonovich transformation). These methods, which go beyond the standard RPA study, allow to set a limit to the validity of our model and to make contact with the other family of semimetals, $1T-TiSe_2$, also subject of recent experimental interest. To complete the discussion of semimetals, we also study the case of graphite.