

TT 22: Low-Dimensional Systems: Charge Order

Time: Monday 15:00–16:30

Location: BEY 81

TT 22.1 Mon 15:00 BEY 81

Competing soft phonon modes in charge-density-wave rare-earth tritellurides — ●MICHAEL MASCHKE¹, SVEN KRANNICH¹, FRANK WEBER¹, ROLF HEID¹, STEPHAN ROSENKRANZ², AYMAN SAID², IAN FISHER³, PAULA GIRALDO-GALLO³, and AHMET ALATAS² — ¹Karlsruhe Institute of Technology, Karlsruhe, Germany — ²Material Science Division, Argonne National Laboratory, Argonne, USA — ³Geballe Laboratory for Advanced Materials, Stanford University, Stanford, USA

We report competing soft phonon modes close to the charge-density-wave (CDW) transition in the rare-earth tritelluride DyTe₃ obtained by high energy resolution inelastic x-ray measurements. We investigated transverse polarized modes dispersing along the reciprocal (100) and (001) directions corresponding the two CDW orders lying in the basal plane of the nearly tetragonal unit cell. DyTe₃ has two CDW-transitions ($T_{CDW,1} = 50K$, $T_{CDW,2} = 310K$), but for technical reasons we could only investigate the transition at $T_{CDW,2}$. We found a full softening at $q_{CDW,2} = (0, 0, 0.3)$ and a strong but not complete softening of the orthogonal mode at $q_{CDW,1} = (0.3, 0, 0)$ at the same temperature which is reminiscent of previous measurements on TbTe₃. Our results are corroborated by lattice dynamical calculations demonstrating the near degeneracy between the two crystallographic axes with respect to the formation of CDW order.

TT 22.2 Mon 15:15 BEY 81

Electronic band structure of 1T-TaS₂ and new implications for the Mott-phase — ●TOBIAS RITSCHEL^{1,5}, JAN TRINCKAUF¹, GASTON GARBARINO², ALEXEI BOSAK², MARTIN VON ZIMMERMANN³, KLAUS KOEPERNIK¹, HELMUTH BERGER⁴, BERND BÜCHNER^{1,5}, and JOCHEN GECK¹ — ¹IFW, Dresden — ²ESRF, Grenoble — ³HASYLAB, Hamburg — ⁴Ecole polytechnique Federale de Lausanne — ⁵TU Dresden

The layered compound 1T-TaS₂ exhibits a multitude of distinct charge density wave (CDW) phases as a function of temperature and pressure. A unique feature of 1T-TaS₂ among the CDW systems is the occurrence of a commensurate (C)-CDW phase which is commonly described as a Mott-phase due to electron-electron interactions and which is extremely sensitive upon applying external pressure. We studied the electronic band structure of the C-CDW phase in terms of density functional theory (DFT) as a function of the amplitude of the lattice modulation. Surprisingly we found that the experimental electronic band structure of the so-called Mott-phase, can already be very well described by conventional DFT calculations in the local density approximation (LDA). Moreover slight changes of the amplitude of the lattice modulation have dramatic effects on the calculated band structure, which agrees very well with the strong pressure dependence of the C-CDW phase. We will discuss our results with respect to Mott-physics associated with the C-CDW phase and its pronounced sensitivity to pressure.

TT 22.3 Mon 15:30 BEY 81

Influence of Doping on the Phonon Softening in the CDW Systems NbSe₂ and TiSe₂ — ●ROLAND HOTT¹, ROLF HEID¹, KLAUS-PETER BOHNEN¹, FRANK WEBER^{1,2}, STEPHAN ROSENKRANZ², JOHN-PAUL CASTELLAN^{1,2}, and DMITRY REZNIK^{1,3} — ¹Karlsruhe Institute of Technology, Institute of Solid State Physics, P. B. 3640, D-76021 Karlsruhe, Germany — ²Materials Science Division, Argonne National Laboratory, Argonne, Illinois, 60439, USA — ³Department of Physics, University of Colorado at Boulder, Boulder, Colorado, 80309, USA

We studied the influence of doping on the soft-mode behaviour of phonons in the Charge Density Wave (CDW) systems NbSe₂ and TiSe₂ both experimentally by means of high resolution Inelastic X-ray Scattering (IXS) and theoretically in Density Functional Theory (DFT) based ab-initio phonon calculations. In agreement with our experiments on Cu-doped TiSe₂ and Co-doped NbSe₂ our calculations show that doping weakens the tendency towards the CDW instability.

[1] F. Weber et al., Phys. Rev. B 87 (2013) 245111

[2] F. Weber et al., Phys. Rev. Lett. 107 (2011) 266401.

TT 22.4 Mon 15:45 BEY 81

Interplay of covalency and correlations in the edge shared spin 1/2 A₃T₂O₄ chain compounds (A = Na, K; T = Cu, Ni) — ●DEEPA KASINATHAN¹, KLAUS KOEPERNIK², and HELGE ROSNER¹ — ¹MPI CPFS, Dresden, Germany — ²IFW Dresden, Germany

Na₃Cu₂O₄, K₃Cu₂O₄ and K₃Ni₂O₄ belong to a new class of quasi-1D insulating cuprates which feature strongly buckled, one-dimensional $\frac{1}{\infty}$ CuO₂ ribbon-like chains consisting of edge-sharing CuO₄ plaquettes. Structural analysis of the metal-oxygen bond lengths and thermodynamic measurements [1,2,3] imply that these systems are intrinsically charge ordered (... (Ni/Cu)²⁺-(Ni/Cu)³⁺-(Ni/Cu)²⁺-(Ni/Cu)³⁺...) and show dominant antiferromagnetic interactions. No electronic structure analysis of these systems exist to date. Using density functional theory based calculations (LDA, Wannier functions, LDA+U), we analyze the microscopic origin of the magnetic interactions in these systems. The main interaction along the chains are the second neighbor superexchanges. Nonetheless, a careful analysis of the first neighbor interaction between the magnetic (Cu²⁺/Ni³⁺) cation and the non-magnetic cation (Cu³⁺/Ni²⁺) is necessary. We report on the interplay of covalency, crystal field splitting and correlations in these systems.

[1] H. Zentgraf, K. Claes, and R. Hoppe, Z. Anorg. Allg.Chem. 462, 92 (1980)

[2] M. Sofin, Eva-Maria Peters, and M. Jansen, J. Solid State Chem. 178, 3708 (2005)

[3] K. Duris, R. K. Kremer, and M. Jansen, Z. Anorg. Allg. Chem. 637, 1101 (2011)

TT 22.5 Mon 16:00 BEY 81

Doping dependence of charge order in single-layered manganites R_{1-x}A_{1+x}MnO₄ — ●JOHANNES ENGELMAYER, HOLGER ULBRICH, MARKUS BRADEN, and THOMAS LORENZ — II. Physikalisches Institut, Universität zu Köln, Germany

Single-layered manganites show a complex interplay between charge, orbital, and magnetic degrees of freedom. For half-doped ($x = 0.5$) La_{1-x}Sr_{1+x}MnO₄ and Pr_{1-x}Ca_{1+x}MnO₄ the so-called Goodenough model is well established. This model proposes a site-centered charge order with a checkerboard pattern of Mn³⁺ and Mn⁴⁺ ions that is accompanied by an orbital order. This charge and orbital order induces a magnetic order with ferromagnetic three-spin zig-zag chains and antiferromagnetic interchain coupling. For $x > 0.5$ zig-zag chains with larger step size have been reported in Pr_{1-x}Ca_{1+x}MnO₄ and Nd_{1-x}Sr_{1+x}MnO₄, e.g. four-spin zig-zag chains arise for $x = 2/3$ due to a 2:1 ratio of Mn⁴⁺ and Mn³⁺ [1]. In order to study the effect of different dopants on the ordering temperature, single crystals of Pr_{1-x}Sr_{1+x}MnO₄, Nd_{1-x}Ca_{1+x}MnO₄ and Nd_{1-x}Sr_{1+x}MnO₄ with $0.5 \leq x \leq 0.75$ were grown and their structural parameters were determined. We present measurements of resistivity, magnetization, and specific heat that show features associated with charge order. The dependence of the ordering temperature on the dopants and the doping level is discussed.

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[1] H. Ulbrich, M. Braden, Physica C 481, 31 (2012)

TT 22.6 Mon 16:15 BEY 81

Charge ordered metals on the triangular extended Hubbard model — ●LUCA FAUSTO TOCCHIO^{1,2}, CLAUDIUS GROS¹, XUE-FENG ZHANG³, and SEBASTIAN EGGERT³ — ¹University of Frankfurt, Germany — ²SISSA, Trieste, Italy — ³University of Kaiserslautern, Germany

We study the extended Hubbard model on the triangular lattice as a function of filling and interaction strength. The complex interplay of kinetic frustration and strong interactions on the triangular lattice leads to exotic phases where long range charge order and a finite metallic conductivity coexist. Variational Monte Carlo simulations show that two kinds of ordered metallic states are stable as function of nearest neighbor interaction and filling; in one of the two phases we observe separation into two classes of particles: one of them contributes to stable order, while the other one forms a partially filled band on the remaining substructure. The relation to charge ordering in charge transfer salts is discussed.