TT 47: Correlated Electrons: Other Materials

Time: Wednesday 10:30–13:00 Location: H21

TT 47.1 Wed 10:30 H21

Phonon renormalization in $LaCoO_3$ by inelastic neutron and x-ray scattering — •Maximilian Kauth[1], Frank Weber[1], and John-Paul Castellan[1,2] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie — [2]Laboratoire Léon Brillouin, CEA Saclay

$LaCoO_3$ exhibits two broad magnetic-electric transitions, a diamagnetic to paramagnetic spin-state transition at $T_{SS} \approx 100\,K$ and a metal-insulator transition at $T_{MI} \approx 500\,K$. The spin transitions on heating are proposed to be as follows [1]: from a homogeneous LS state to a mixed Low-Spin/High-Spin (LS/HS) state with strong spin-charge fluctuations at T=T_{SS} and, subsequently, into a homogeneous HS state at T=T_{MI}. The lattice participates in the state mixture by expansion of CoO_6 octahedra around the HS sites, while the ones around LS sites have a reduced size [2]. The originally proposed static order [2] has not been observed experimentally and, hence, the ordering is expected to be dynamic and short-ranged. We investigated the lattice dynamical properties of $LaCoO_3$ using inelastic neutron scattering. Based on detailed ab-initio lattice dynamical calculations (performed in our institute), we aim for a comprehensive understanding of lattice dynamics in $LaCoO_3$. The above discussed crossovers and spin state order should be reflected in the lattice degrees of freedom via quasi elastic scattering and phonon renormalization effects.

[1] M. Karolak et al., PRL **115**, 046401 (2015)
[2] J. B. Goodenough, J. Phys. Chem. Solids **6**, 287 (1958)

TT 47.2 Wed 10:45 H21

Excitonic transition in (Pr,Ca)CoO_3 family — •Jan Kuneš and Pavel Augustinský — Insitute of Physics, AS CR, Prague

The members of $(Pr_{1-y}Y_y)_{1-x}Ca_xCoO_3$ family exhibit a continuous phase transition accompanied by disappearance of the fluctuating moment of Co and increase of resistivity by several decades. Most intriguing feature of the low temperature phase is breaking of the time reversal symmetry without presence of ordered atomic moments. We will argue that the experimental observations are explained by condensation of atomic size excitons, which gives rise to ordered magnetic multipoles. We will present model calculations performed with dynamical-mean field theory, which demonstrate general features of the excitonic condensation. In addition, we will present results of material specific LDA+U calculations which uncover the excitonic order in $Pr_{0.5}YCa_{0.5}CoO_3$ and explain its low temperature behavior.

[1] J. Kuneš, P. Augustinský, PRB **90**, 235112 (2014).

TT 47.3 Wed 11:00 H21

Theoretical study of spin-state transition in $LaCoO_3$ using LDA+MLFT — •Evgeny Gorelov[1], Igor Krivenko[2], Michael Karolak[3], and Alexander Lichtenstein[1,2] — [1]European XFEL GmbH Albert-Einstein-Ring 19, 22761 Hamburg, Germany — [2]University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany — [3]University of Würzburg, Sanderring 2, 97070 Würzburg, Germany

$LaCoO_3$ demonstrates variety of phase transitions due to competing interactions governing it's electronic structure, including metal-to-insulator transition around T≈500 K and gradual spin-state transition around T≈80-120 K. In this work we focus on spin-state transition, and use theoretical approach of M. Haverkort, taking into account transition metal ion and it's octahedral oxygen surrounding [1]. This approach allow us to calculate the resonant Co $L_{2,3}$ X-ray absorption spectra (XAS), using ab-initio calculated model parameters, i.e. nearest neighbors hopping matrix. The calculations are performed for experimental crystal structures for different temperatures in the range of 5-600 K [2]. In our calculations we include Co 3*d* orbitals with full Coulomb vertex, and five ligand orbitals, constructed from 2*p* orbitals of O atoms, forming the octahedra around Co ion. We discuss changes in the XAS spectra induced by thermal expansion of the lattice, as well as caused by change of electron temperature.

[1] M. W. Haverkort, M. Zwierzycki, and O. K. Andersen, PRB **85**, 165113 (2012)
[2] P. G. Radaelli and S.-W Cheong, PRB **66**, 094408 (2002)

TT 47.4 Wed 11:15 H21

Construction of effective low-energy interactions for three-orbital cuprate models with electronic correlation — •Cornelia Hille[1], Xiaodong Cao[2], Carsten Honerkamp[3], Philipp Hansmann[2], and Sabine Andergassen[1] — [1]Institut für Theoretische Physik, Universität Tübingen, Tübingen, Germany — [2]Max Planck Institute for Solid State research, Stuttgart, Germany — [3]Institute for Solid State Theory, RWTH Aachen, Aachen, Germany

Real materials typically have involved bandstructures and a many-body solution of the full Hamiltonian is not feasible. To identify the most relevant degrees of freedom we often start from ab initio single particle (e.g. DFT, Hartree Fock, GW) calculations and integrate out states of high energy remaining with a low-energy effective Hamiltonian. For basically all transition metal oxides this procedure leads to the question if and how to include oxygen 2p states explicitly. We present effective low-energy interactions for three-orbital cuprate models calculated in a cRPA framework. We find effective copper d-state interactions which are strongly dynamically screened by transitions involving the oxygen 2p states.

TT 47.5 Wed 11:30 H21

Self-consistent GW+EDMFT simulation of $SrVO_3$ - Hubbard vs. plasmon physics — •Lewin Boehnke[1], Fredrik Nilsson[2], Ferdi Aryasetiawan[2], and Philipp Werner[1] — [1]University of Fribourg, Switzerland — [2]Lund University, Sweden

$SrVO_3$ has been considered a prototypical strongly correlated metal for more than a decade Its (inverse) photoemission spectra [1] show a characteristic three peak structure close to the Fermi level.

We develop a multi-orbital GW+extended dynamical mean-field theory [2,3] framework, applying approximations of increasing rigor to orbital subsets of increasing degree of correlation with the goal of unbiased finite temperature ab-initio calculations of materials classes with relevant local and non-local many-body correlations.

We use a suitable continuous time quantum Monte Carlo impurity solver (CT-Hyb) [4] to deal with the frequency dependence of the effective impurity interaction and a tailored Matsubara frequency implementation of the GW-algorithm to solve self consistency cycle.

For $SrVO_3$ we find that the screening from nonlocal Coulomb interactions substantially reduces the effective local interaction, suppressing the Hubbard bands. At the same time, plasmon satellites are formed that are consistent with experimental observations. [1]

[1] K. Morikawa, T. Mizokawa, K. Kobayashi, A. Fujimori, H. Eisaki, S. Uchida, F. Iga, and Y. Nishihara, PRB **52**, 13711 (1995)
[2] S. Biermann, F. Aryasetiawan, and A. Georges, PRL **90**, 086402 (2003)
[3] T. Ayral, S. Biermann, and P. Werner, PRB **87**, 125149 (2013)
[4] E. Gull, *et al.* RMP **83**, 349 (2011)

15 min. break

TT 47.6 Wed 12:00 H21

The electronic structure of palladium in the presence of many-body effects — •Andreas Östlin[1,2], Wilhelm Appelt[3,1], Igor di Marco[4], Weiwei Sun[4], Milos Radonjic[1], Michael Sekania[1], Levente Vitos[2,4,5], and Liviu Chioncel[3,1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Materials Science and Engineering, Applied Materials Physics, KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden — [3]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [4]Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [5]Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O. Box 49, H-1525 Budapest, Hungary

Including on-site electronic interactions described by the multi-orbital Hubbard model we study the correlation effects in the electronic structure of bulk palladium within the framework of combined density functional and dynamical mean field theory, DFT+DMFT, using the fluctuation exchange approximation. The agreement between the experimentally determined and the theoretical lattice constant and bulk modulus is improved when correlation effects are included. At the same time we discuss the possibility of satellite formation in the high energy binding region. Investigation of non-local correlation effects

within the *GW* method is also performed.

TT 47.7 Wed 12:15 H21

Phase separation in $Y_{0.63}Ca_{0.37}TiO_3$ — •Thomas Koethe[1], Bernhard Zimmer[1], Raphael German[1], Alexei Barinov[2], Alexander Komarek[1,3], Fulvio Parmigiani[2], Markus Braden[1], and Paul van Loosdrecht[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Elettra Sincrotrone, Trieste (Italy) — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

We have investigated the domain structure and Raman response of $Y_{0.63}Ca_{0.37}TiO_3$ single crystals which show a clear metal-to-insulator transition at ca. 170 K, with a wide hysteresis in the resistivity ranging down to ca. 50 K. We observe by use of a conventional optical microscope the appearance of two distinct regions at temperatures below ca. 200 K, with a characteristic length scale of order of 10 μm. By means of Raman spectroscopy we can identify the regions to correspond to the metallic and insulating domains, and follow the evolution of the domains as function of temperature down to 5 K. Preliminary results of spacially resolved PES confirm the presence of electronically distinct regions on the μm scale at low temperature.

TT 47.8 Wed 12:30 H21

Breathing Mode Distortion and Magnetic Order in Rare-Earth Nickelates RNiO$_3$ — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Rare-earth nickelate perovskites display a rich and not yet fully understood phase diagram, where all RNiO$_3$ compounds with R from Sm to Lu undergo a non-magnetic metal-insulator transition (MIT). This transition is connected to a lattice distortion, which can be described as breathing mode of the oxygen octahedra surrounding the Ni cations. Between 100-250 K the RNiO$_3$ compounds undergo a magnetic transition to an antiferromagnetic (AFM) state, with a wave-vector $k = \left[\frac{1}{4}\frac{1}{4}\frac{1}{4}\right]$ relative to the underlying simple cubic perovskite structure.

Here, we use density functional theory and its extensions (DFT+U, DFT+DMFT) together with distortion mode analysis to explore the interplay between lattice distortions, magnetic order, and the strength of the local Coulomb interaction U in rare earth nickelates. Our results show a strong dependency of the breathing mode amplitude on the magnetic order, with a much larger breathing mode obtained for the AFM state compared to the ferromagnetic case. Furthermore, we demonstrate that DFT+U is able to capture the correct trends of the lattice distortions across the nickelate series.

TT 47.9 Wed 12:45 H21

Metal-insulator transition in 2D antiferromagnet $FePS_3$ upon applied pressure — •Matthew John Coak[1], Charles Robert Sebastian Haines[1,2], and Siddarth Shankar Saxena[1] — [1]Cavendish Laboratory, University of Cambridge — [2]CamCool Research Ltd, UK

$FePS_3$ belongs to a rich family of structurally and magnetically quasi-two-dimensional compounds, with a magnetic ground state in which spins are ordered as ferromagnetic chains coupled antiferromagnetically. At ambient pressure, it is an insulator with a direct gap of approximately 0.5 eV and a room temperature resistivity of approximately 104 Ωcm.

We present the results of resistivity measurements under pressures up to 110 kbar for this material. The insulating phase is suppressed at a pressure in the range 40-70 kbar giving way to a new metallic phase. Interesting intermediate behaviour is seen at pressures around the transition as the gap closes. At high pressure, the resistivity develops linear temperature dependence with an upturn in resistivity which may indicate a low temperature phase transition or impurity scattering.