TT 19: Correlated Electrons: Metal-Insulator Transition 3

Time: Tuesday 14:00–15:15 Location: HSZ 301

TT 19.1 Tue 14:00 HSZ 301

On the spin-state and metal-insulator transition in $R\mathbf{BaCo_2O_{5.5}}$ — •T.C. Koethe[1], Z. Hu[1], Hua Wu[1], C. Schüssler-Langeheine[1], J.C. Cezar[2], F. Venturini[2], N.B. Brookes[2], H.H. Hsieh[3], H.-J. Lin[3], C.T. Chen[3], S.N. Barilo[4], S.V. Shiryaev[4], G.L. Bychkov[4], and L.H. Tjeng[1] — [1]II.PhysikalischesInstitut Universität zu Köln — [2]ESRF, Grenoble, France — [3]NSRRC, Hsinchu, Taiwan — [4]Belarus Academy of Sciences,Minsk, Belarus

The novel layered perovskite $R\mathrm{BaCo_2O_{5.5}}$ (R = rare earth) has attracted considerable interest in the last decade. It shows an intriguing mix of properties, including giant magneto-resistance, metal-insulator and antiferro-ferromagnetic transitions, and a sign change of the thermoelectric power across these transitions. Explanation of these properties is subject of on-going debate. The so-called spin-blockade mechanism together with the occurrence of a spin-state transition of the octahedral Co^{3+} ions was proposed [Maignan *et al.*, PRL **93** 026401 (2004)]. Other scenarios invoke, for example, order-disorder effects, involving essentially all possible spin state configurations for the octahedral and pyramidal Co^{3+} ions. Using high quality single crystals and bulk sensitive photoelectron and x-ray absorption spectroscopy, we were able to identify the spin-state of the Co ions, thereby arriving at a very different scenario than proposed so far in the literature. We also find that the transfer of spectral weight near the Fermi level across the metal-insulator transition is very modest, in contrast to existing assumptions but in agreement with our observation on the evolution of the spin-state as a function of temperature.

TT 19.2 Tue 14:15 HSZ 301

Spin blockade, orbital occupation and charge ordering in $\mathbf{La_{1.5}Sr_{0.5}CoO_4}$ — •Chun Fu Chang[1], Zhiwei Hu[1], Hua Wu[1], Tobias Burnus[1], Nils Hollmann[1], Mohammed Benomar[1], Thomas Lorenz[1], Arata Tanaka[2], Hong-Ji Lin[3], Hui-Huang Hsieh[4], Chien-Te Chen[3], and Liu Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan — [3]National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30077, Taiwan — [4]ChungCheng Institute of Technology, National Defense University, Taoyuan 335, Taiwan

Using Co-$L_{2,3}$ and O-K x-ray absorption spectroscopy, we reveal that the charge ordering in $La_{1.5}Sr_{0.5}CoO_4$ involves high spin (S=3/2) Co^{2+} and low spin (S=0) Co^{3+} ions. This provides evidence for the spin blockade phenomenon as a source for the extremely insulating nature of the $La_{2-x}Sr_xCoO_4$ series. The associated e_g^2 and e_g^0 orbital occupation accounts for the large contrast in the Co-O bond lengths, and in turn, the high charge ordering temperature. Yet, the low magnetic ordering temperature is naturally explained by the presence of the non-magnetic (S=0) Co^{3+} ions. From the identification of the bands we infer that $La_{1.5}Sr_{0.5}CoO_4$ is a narrow band material.

TT 19.3 Tue 14:30 HSZ 301

Application of Sum Rules to Resonant Magnetic Diffraction — •Marcel Buchholz[1], Christian Schüssler-Langeheine[1], Maurits W. Haverkort[1,2], Hsueh-Hung Wu[1,3], Chun-Fu Chang[1], Matthias Cwik[1], Mohammed Benomar[1], Enrico Schierle[4], Arata Tanaka[5], Markus Braden[1], and Liu Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Max Planck Institut für Festkörperforschung, Stuttgart — [3]NSRRC, Hsinchu, Taiwan — [4]Helmholtz-Zentrum Berlin — [5]ADSM, Hiroshima University, Japan

Sum rules relating the spin and orbital moment to integrals over the x-ray magnetic circular dichroism (XMCD) signal are well established and widely used to determine fundamental quantum numbers for ferromagnetic systems.

Resonant magnetic diffraction is closely related to the XMCD effect and can be used to apply sum rules also to magnetically ordered systems without net magnetic moment like antiferromagnets or magnetically ordered systems with multiple sublattices. We tested this approach using holmium metal as a model system. The determination of the proper phase turns out to be a crucial point in the analysis.

We applied the sum-rule analysis to Sr- and Ca-doped La_2CoO_4 and compare the results to microscopic model calculations.

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TT 19.4 Tue 14:45 HSZ 301

Pressure-induced superconductivity in the Mott insulator $\mathbf{GaNb_4S_8}$ — Xin Wang[1], •Martin K. Forthaus[2], Karl Syassen[1], Mathias Kraken[3], Jochen Litterst[3], Hubertus Luetkens[4], Dirk Johrendt[5], and Mohsen M. Abd-Elmeguid[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germnay — [2]II. Physikalisches Institut, Iniversität zu Köln, Köln, Germany — [3]Institut für Physik der kondensierten Materie, TU Braunschweig, Braunschweig, Germany — [4]Paul Scherrer Institut, Villigen, Switzerland — [5]Department Chemie und Biochemie, LMU München, München, Germany

$GaNb_4S_8$ (cubic fcc $GaMo_4S_8$ type structure) belongs to a new class of Mott insulators in which the electronic conduction originates from hopping of localized electrons (S = 1/2) among widely separated tetrahedral Nb_4 metal clusters. The magnetic susceptibility ($\chi(T)$) of $GaNb_4S_8$ shows Curie-Weiss behavior ($100 \leq T \leq 300$ K) and reveals a sudden drop around 30 K but no long range magnetic order has been detected down to 1.6 K. Recent strutural investigation shows that the drop of $\chi(T)$ is associated with a tetragonal distortion. We find pressure-induced superconductivity in $GaNb_4S_8$ with $T_C = 2.1$ K at $p = 10$ GPa which increases with pressure up to 4 K at 23 GPa. As our μSR experiments at ambient pressure clearly shows that the tetragonal distortion in $GaNb_4S_8$ is associated with the onset of short range magnetic order, we discuss the possibility of a nonconventional pressure-induced superconducting state.

TT 19.5 Tue 15:00 HSZ 301

The local/non-local duality of 5f electrons in actinide compounds: A mean-field study — •Duc-Anh Le[1], Sebastien Burdin[2], Peter Fulde[1], and Gertrud Zwicknagl[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Institute of Theoretical Physics, University of Cologne, Germany — [3]Institute for Mathematical and Theoretcal Physics, TU Braunschweig, Germany

The local/non-local duality of 5f electrons in actinide compounds has been observed in a great variety of experiments including photoemission spectroscopy, inelastic neutron scattering, muon spin relaxation measurements, and x-ray inelastic scattering. A general microscopic mechanism leading to the partial localization of 5f orbitals has been proposed within the so-called 'dual model' (D. V. Efremov, et al., Phys. Rev. B 69, 115114 (2004)). It is a generalized multi-orbital Hubbard model which includes the direct Coulomb interaction as well as the Hund's rule correlations. Using a generalized slave boson method (F. Lechermann, et al., Phys. Rev. B 76, 155102 (2007)), we study this model for an electronic filling corresponding to the prototype compound UPt3. We then analyse the calculated phase diagram and discuss the local/non-local and magnetic/non-magnetic phases in terms of orbitally dependent quasi-particle residues and partial electronic occupations.