

## TT 33: CE: Metal-Insulator Transition 1

Time: Wednesday 10:30–13:00

Location: HSZ 105

TT 33.1 Wed 10:30 HSZ 105

**A Microscopic View on the Mott transition in Cr-doped  $V_2O_3$**  — ●NICOLAUS PARRAGH<sup>1</sup>, STEFANO LUPI<sup>2</sup>, LEONETTA BALDASSARE<sup>3</sup>, DANIELE NICOLETTI<sup>4</sup>, MARINO MARSÌ<sup>5</sup>, PHILIPP HANSMANN<sup>1</sup>, ALESSANDRO TOSCHI<sup>1</sup>, TANUSRI SAHA-DASGUPTA<sup>6</sup>, OLE-KROGH ANDERSEN<sup>7</sup>, GIORGIO SANGIOVANNI<sup>1</sup>, and KARSTEN HELD<sup>1</sup> — <sup>1</sup>Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — <sup>2</sup>CNR-IOM and Università di Roma "La Sapienza", Italy — <sup>3</sup>Sincrotrone Trieste, Italy — <sup>4</sup>Università di Roma "La Sapienza" Italy — <sup>5</sup>Laboratoire de Physique des Solides, CNRS-UMR 8502, Orsay, France — <sup>6</sup>S.N.Bose Center for Basic Sciences, Kolkata, India — <sup>7</sup>Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The metal-insulator transition in Chromium-doped Vanadium Sesquioxide has received much attention since its discovery in 1969. After several attempts for describing it in the framework of single-band Hubbard models some key experiments revealed the intimate multi-band nature of this material. Here I will present the results of a recent experiment combining Infrared (IR), Scanning Photoemission Microscopy (SPEM) and X-ray Diffraction (XRD) and local density approximation + dynamical mean field theory (LDA+DMFT) calculations showing for the first time that microscopic islands characterized by bad metallic behaviour form close to the first-order transition. The bad metallicity is only partially reduced by applying pressure, pointing to a non-trivial interplay between the orbital degrees of freedom [1].

[1] Nature Communications 1, 105 (2010)

TT 33.2 Wed 10:45 HSZ 105

**Symmetry of magnetite in the low-temperature phase** — ●CHUN-FU CHANG<sup>1</sup>, ARATA TANAKA<sup>2</sup>, MARCEL BUCHHOLZ<sup>1</sup>, CHRISTOPH TRABANT<sup>1,3</sup>, ENRICO SCHIERLE<sup>3</sup>, JUSTINA SCHLAPPA<sup>3</sup>, DETLEF SCHMITZ<sup>3</sup>, MARITA DÖHLER<sup>1</sup>, PASCAL VOGT<sup>1</sup>, LIU HAO TJENG<sup>1,4</sup>, and CHRISTIAN SCHÜSSLER-LANGEHEINE<sup>1,3</sup> — <sup>1</sup>II. Physikalisches Institut, Universität zu Köln, Germany — <sup>2</sup>Department of Quantum Matter, ADSM, Hiroshima University, Japan — <sup>3</sup>Helmholtz-Zentrum Berlin, Germany — <sup>4</sup>Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Magnetite ( $Fe_3O_4$ ) undergoes upon cooling below 123 K a first order phase transition, which is accompanied by a rise of the resistivity by two orders of magnitude: the Verwey transition. Below the transition, magnetite exhibits a complex crystal structure; structural studies so far assume a pseudo orthorhombic symmetry. We have carried out a combined experimental and theoretical analysis of the local symmetry of the divalent iron ions in octahedral environment in magnetite. Our results clearly show that the local symmetry of these iron ions cannot be described as pseudo-orthorhombic. A monoclinic distortion is not a small correction but dominant. This has important consequences for the kind of orbital order that can form in magnetite. The orbital-order models based on the pseudo-orthorhombic symmetry are hence challenged. On the other hand a model assuming a complex orbital order matches the experimental data very well. Supported by the DFG through SFB 608, by the BMBF through projects 05 S3XBA/5 and 05 KS7PK1, and by the HZB.

TT 33.3 Wed 11:00 HSZ 105

**The Verwey transition ultrafast: lattice and charge/orbital order go head-to-head** — ●N. PONTIUS<sup>1</sup>, C.-F. CHANG<sup>2</sup>, T. KACHEL<sup>1</sup>, C. TRABANT<sup>1,3</sup>, M. BEYE<sup>1</sup>, W. SCHLOTTER<sup>3</sup>, S. DE JONG<sup>3</sup>, F. SORGENFREI<sup>4</sup>, R. KUKREJA<sup>3</sup>, B. BRÄUER<sup>3</sup>, M. DÖHLER<sup>2</sup>, S. HOSSAIN<sup>3</sup>, C. BACK<sup>3</sup>, A. SCHERZ<sup>3</sup>, D. ZHU<sup>3</sup>, J. TURNER<sup>3</sup>, W.-S. LEE<sup>3</sup>, Y.-D. CHUANG<sup>3</sup>, O. KRUPIN<sup>3</sup>, M. BUCHHOLZ<sup>2</sup>, P. VOGT<sup>2</sup>, W. WURTH<sup>4</sup>, A. FÖHLISCH<sup>1</sup>, H. A. DÜRR<sup>3</sup>, and C. SCHÜSSLER-LANGEHEINE<sup>1,3</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — <sup>2</sup>II. Physikalisches Institut, Universität zu Köln — <sup>3</sup>SLAC National Accelerator Laboratory, USA — <sup>4</sup>Institut für Experimentalphysik, Universität Hamburg

At 120K magnetite ( $Fe_3O_4$ ) undergoes a metal-to-insulator transition, the Verwey transition. It is accompanied by a transition from a charge/orbital ordered state with a monoclinic symmetry to a high temperature cubic phase without electronic order. Until today the question whether this transition is mainly driven by the lattice or by electronic degrees of freedom remains unanswered.

Here we report on a time-resolved resonant soft x-ray diffraction experiment performed at the LCLS in Stanford, USA. We studied the structural and electronic response when the insulator-to-metal transition is induced by a fs laser pulse which selectively excites the electronic subsystem. Surprisingly, the data show that both, a change of lattice symmetry and the quenching of charge/orbital order occur on a sub 200fs timescale. Moreover, the measurements suggest the formation of a new transient phase, which has not been observed in equilibrium.

TT 33.4 Wed 11:15 HSZ 105

**Magnetic order in  $Pr_{1-x}Ca_{1+x}MnO_4$  with  $x=2/3$**  — ●H. ULBRICH<sup>1</sup>, P. STEFFENS<sup>2</sup>, O.J. SCHUMANN<sup>1</sup>, D. LAMAGO<sup>3</sup>, Y. SIDIS<sup>3</sup>, and M. BRADEN<sup>1</sup> — <sup>1</sup>II. Phys. Institut, Universität zu Köln — <sup>2</sup>ILL, Grenoble (France) — <sup>3</sup>LLB, Saclay (France)

Stripe and checkerboard ordering of charges in several metal oxide compounds are thought to be linked to exotic behaviour such as high-temperature superconductivity and colossal magnetoresistivity (CMR). The coupling of charges, orbitals and spins (COS) are essential for the understanding of the CMR in the manganites. When the doping level deviates away from half-doping ( $x>0.5$ ), significant controversies have arisen regarding the COS ordered structure [1,2]. Two different models have been proposed: The Bi-stripe model and the Wigner-crystal model. Investigations in  $La_{0.42}Sr_{1.58}MnO_4$  exhibit an incommensurate stripe-like coupling of four order parameters: charges, orbitals and magnetic ordering of  $Mn^{3+}$  and  $Mn^{4+}$  spins [3]. In order to decide between the Wigner-crystal model and the Bi-stripe model, we studied  $Pr_{0.33}Ca_{1.67}MnO_4$  by elastic and inelastic neutron scattering. Our observations are in agreement with the Wigner-crystal model [4]. First studies of the magnon dispersion around the incommensurable magnetic satellites exhibit an 'hour-glass' like behaviour similar to the spin dispersion in  $La_{2-x}Ba_xCuO_4$  at low doping [5].

[1] S. Mori et al., Phys. Rev. Lett. 81, 3972 (1998).

[2] P.G. Radaelli et al., Phys. Rev. B 59, 14440 (1999).

[3] H. Ulbrich et al., submitted to Phys. Rev. Lett.; arXiv: 1008.4496.

[4] H. Ulbrich et al., manuscript in preparation.

[5] J.M. Tranquada et al., Nature (London) 429, 534 (2004).

TT 33.5 Wed 11:30 HSZ 105

**Charge-dynamics in Pr-doped La,Sr-bilayer manganites with 40% hole doping** — ●JAN THÖNE, TORBEN HÄNKE, VOLODYMYR ZABOLOTNYI, MIRCAE APOSTU, KLAUS KOEPERNIK, SERGEI BORISENKO, BERND BÜCHNER, and JOCHEN GECK — Leibniz Institute for Solid State and Materials Research Dresden

To analyse the charge dynamics of La,Sr-bilayer manganites we performed angle resolved photoemission measurements on  $(La_{1-x}Pr_x)_{1.2}Sr_{1.8}Mn_2O_7$  single crystals. The spectra are compared to a tight-binding Wannier model. The measured bilayer splitting is much smaller than the calculated one, indicating a strongly reduced hybridization between the bilayer-planes in the real material. Further the spectral function exhibits fingerprints of a periodic perturbation with an interaction strength of around 400 meV. A possible origin of such a perturbation are CE-type charge-order fluctuations.

15 min. break

TT 33.6 Wed 12:00 HSZ 105

**Total Energy Study of Orbital Ordering Phenomena with LDA+DMFT** — ●ANDREAS FLESCHE<sup>1</sup>, ERIK KOCH<sup>2</sup>, and EVA PAVARINI<sup>1</sup> — <sup>1</sup>Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich — <sup>2</sup>German Research School for Simulation Sciences, 52425 Jülich

Orbital and magnetic ordering phenomena play a crucial role in the physics of strongly correlated transition-metal oxides.  $LaMnO_3$ , the parent compound of the colossal magnetoresistance manganites, is considered a textbook example of an orbitally ordered material. To determine the orbital and spin order in this system, we perform low temperature total energy [1,2] calculations based on the LDA+DMFT approach. Consequences for the origin of the cooperative Jahn-Teller distortions [3] will be discussed.

[1] B. Amadon et al., PRL 96, 066402 (2006)

[2] I. Leonov et al., PRL 101, 096405 (2008)

[3] E. Pavarini and E. Koch, PRL 104, 086402 (2010)

TT 33.7 Wed 12:15 HSZ 105

**LDA+DMFT study of (Sr, Ca)<sub>n+1</sub>Ru<sub>n</sub>O<sub>3n+1</sub> ruthenates**  
— ●EVGENY GORELOV and EVA PAVARINI — IFF and IAS, Forschungszentrum Jülich, 52425 Jülich

The ruthenates of the Ruddelsen-Popper series (Sr, Ca)<sub>n+1</sub>Ru<sub>n</sub>O<sub>3n+1</sub> are unique among transition-metal oxides: changes in the number of RuO<sub>2</sub> layers, Sr/Ca content and temperature lead to a variety of different properties, ranging from Mott insulating behavior and orbital order to metallic ferro- and meta- magnetism.

In order to understand how structural changes affect the properties, we perform LDA+DMFT calculations for material-specific Hubbard models describing the partially filled *Ru* 4*d*<sup>4</sup> shells. Since the *e<sub>g</sub>* *Ru* bands are well above the Fermi level, we consider only the *t<sub>2g</sub>* bands. For *n* = 3 the unit cell contains two inequivalent *Ru* atoms, thus for this system we perform six-orbital LDA+cDMFT calculations.

The LDA+cDMFT scheme used is based on the ab-initio NMTO downfolding procedure and a weak-coupling CT-QMC impurity solver with full rotationally-invariant Coulomb interaction. We use a self-energy matrix in orbital space -  $\Sigma_{ij}$ .

We identify the main difference among the materials in a substantial rearrangement of *Ru* *t<sub>2g</sub>* occupations, controlled by the interplay between Coulomb repulsion, number of RuO<sub>2</sub> layers *n*, which reflects effective dimensionality, and changes in the *t<sub>2g</sub>* crystal field.

TT 33.8 Wed 12:30 HSZ 105

**Evidence for a temperature-induced spin-state transition of Co<sup>3+</sup> in La<sub>2-x</sub>Sr<sub>x</sub>CoO<sub>4</sub>** — ●NILS HOLLMANN<sup>1</sup>, MAURITS HAVERKORT<sup>2</sup>, MOHAMMED BENOMAR<sup>1</sup>, MATTHIAS CWIK<sup>1</sup>, MARKUS BRADEN<sup>1</sup>, and THOMAS LORENZ<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln, Germany — <sup>2</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany

The magnetic susceptibility of mixed-valent La<sub>2-x</sub>Sr<sub>x</sub>CoO<sub>4</sub> single crystals in a doping range of 0.5 ≤ *x* ≤ 0.8 and in a temperature range up to 1000 K is studied with the focus on the spin-state of the Co ions. The materials bear close resemblance to LaCoO<sub>3</sub>, a compound well-known for a spin-state transition of its Co<sup>3+</sup> ions. In La<sub>2-x</sub>Sr<sub>x</sub>CoO<sub>4</sub>,

the magnetism below room temperature can be described by paramagnetic Co<sup>2+</sup> in the high-spin state and Co<sup>3+</sup> in the non-magnetic low-spin state [1]. Above room temperature, however, an increase in susceptibility compared to the behavior expected from Co<sup>2+</sup> is seen. We attribute this rise in moment to a thermally-induced spin-state transition of Co<sup>3+</sup>, and analyze the experimental data by comparison to full-multiplet calculations for the thermal population of a higher-spin state of Co<sup>3+</sup>. We find the energy gap between the spin states being in the order of 2000 K, which hardly changes with doping. *This work is supported by the SFB through SFB 608.*

[1] N. Hollmann *et al.*, New Journal of Physics **10**, 023018 (2008).

TT 33.9 Wed 12:45 HSZ 105

**Two Pressure-induced structural phase transitions in TiOCl** — ●JIHAAN EBAD-ALLAH<sup>1</sup>, ANDREAS SCHOENLEBER<sup>2</sup>, SANDER VAN SMAALEN<sup>2</sup>, MICHAEL HAFLAND<sup>3</sup>, MATTHIAS KLEMM<sup>1</sup>, SIEGFRIED HORN<sup>1</sup>, SEBASTIAN GLAWION<sup>4</sup>, MICHAEL SING<sup>4</sup>, RALPH CLAESSEN<sup>4</sup>, and CHRISTINE KUNTSCHER<sup>1</sup> — <sup>1</sup>Experimentalphysik II, Universität Augsburg, 86159 Augsburg, Germany — <sup>2</sup>Laboratory of Crystallography, Universität Bayreuth, 95440 Bayreuth, Germany — <sup>3</sup>European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France — <sup>4</sup>Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany

The titanium oxyhalides TiOX (with X=Cl or Br) are low-dimensional materials which undergo an unconventional transition to a spin-Peierls state via a structural incommensurate state. With the electronic configuration 3*d*<sup>1</sup> these compounds are Mott-Hubbard insulators with a charge gap of ≈2 eV. As a follow-up to our recent investigations on TiOX [1], we studied the crystal structure of TiOCl by powder X-ray diffraction measurements at room temperature up to high pressures of p≈25 GPa. Besides a phase transition at p<sub>c1</sub>≈15 GPa from the orthorhombic Pmmn to the monoclinic P2<sub>1</sub>/m crystal structure with a 2a×2b×c superstructure, we find a pressure-induced isostructural phase transition p<sub>c2</sub>≈22 GPa for the monoclinic phase with anomalies in the lattice parameters [2].

[1] C. A. Kuntscher *et al.*, Eur. Phys. J. Special Topics **180**,29 (2010).

[2] J. Ebad-Allah *et al.*, Phys. Rev. B **82**, 134117 (2010).