TT 54: Correlated Electrons: Complex Oxides and Other Materials

Time: Thursday 9:30–13:00 Location: H22

TT 54.1 Thu 9:30 H22

Study of the correlation effects in single-crystal $TbFeO_3$ — •Alexander Engelhardt[1], Georg Benka[1], Christian Oberleitner[1], Andreas Bauer[1], Johanna Jochum[2], Andreas Erb[3] und Christian Pfleiderer[1] — [1]Physik Department E51, Technische Universität München, D-85748 Garching, Germany — [2]Technische Universität München, Heinz Maier-Leibnitz Zentrum, Lichtenbergstraße 1, 85748 Garching, Germany — [3]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meißner-Str. 8, D-85748 Garching, Germany

Single crystals of the multiferroic rare earth orthoferrite $TbFeO_3$ have been grown by means of the optical floating zone method. Using measurements of the magnetization, ac susceptibility and specific heat we have studied the complex, anisotropic magnetic phase diagram of $TbFeO_3$ for magnetic fields up to 9 T applied along all three major crystallographic axes. In particular, our findings may help to shed light on the nature and origin of the various magnetic phase transition and crossovers observed as a function of magnetic field and temperature.

TT 54.2 Thu 9:45 H22

Fluctuation regime based on dimer correlations in a novel $s = 1/2$ spin chain compound with $(IO_3)^-$ as stereochemically active lone pair group — Eleni Mitoudi-Vagourdi[1], Vladimir Gnezdilov[2,3], Dirk Wulferding[2,4], •Peter Lemmens[2,4], Karina V. Lamonova[5], Yurii Pashkevich[5], Reinhard Kremer[6], and Mats Johnsson[1] — [1]Dept. of Chem., Stockholm Univ., Stockholm, Sweden — [2]IPKM, TU-BS, Braunschweig, Germany — [3]ILTPE, Kharkov, Ukraine — [4]LENA, TU-BS, Braunschweig, Germany — [5]Galkin DonFTI, Kyiv, Ukraine — [6]MPI-FKF, Stuttgart, Germany

The novel iodate $KCu(IO_3)_3$ contains spin chains formed by $[CuO_6]$ octahedra, corner sharing with $[IO_3]$ groups. This leads to an oxygen plane around each Cu ion and two apical oxygens with larger Cu-O distances along chains. The resulting Cu binding potential is rather soft and allows pronounced fluctuations. Based on thermodynamic and Raman scattering data we give evidence for Cu dimer fluctuations, their commensurate lock-in, and long range ordering with a sequence of characteristic temperatures, $T_N = 1.3\text{K} < T_{JT} = 175\text{K} < T^* = 200\text{K}$.

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TT 54.3 Thu 10:00 H22

Percolation of frustrated polarons in the doped perovskite cobaltite $La_{1-x}Sr_xCoO_{3-\delta}$ — •Peter P. Orth[1], Daniel Phelan[2], Chris Leighton[3], and Rafael Fernandes[3] — [1]Iowa State University, USA — [2]Argonne National Laboratory, USA — [3]University of Minnesota, USA

Due to fascinating phenomena such as magneto-electronic phase separation and Co ion spin-state transitions, the archetypal cobaltite $La_{1-x}Sr_xCoO_{3-\delta}$ (LSCO) remains of high interest. Chemical substitution of La by Sr introduces both holes and magnetic moments into the diamagnetic parent compound. The tendency of Co to undergo spin-state transitions leads to the formation of 7-site spin polarons. Further doping results in a glassy magnetic state that transforms at x=0.18 into a ferromagnetic metal. As simple statistical considerations predict a percolation of polarons at much smaller values of x=0.05, this raises the question what suppresses the formation of ferromagnetism. Here, we address this question within a microscopic model capturing both competing magnetic interactions between the Co moments in different spin states as well the spatial inhomogeneity introduced by disorder. Large-scale parallel tempering classical Monte-Carlo simulations reveal that the origin of the delayed percolation transition lies in the frustration of ferromagnetic polarons via competing (anti-)ferromagnetic interactions. Our simulations explicitly show how frustrated polarons act as seeds of the observed magneto-electronic phase separated glassy state at intermediate doping $0.05 < x < 0.18$, providing a consistent microscopic understanding across the full doping range.

TT 54.4 Thu 10:15 H22

Tuning the electronic structure of $LaNiO_3$ heterostructures — •Jasmin Jandke[1], Muntaser Naamneh[1], Marco Caputo[1,2], Eduardo B. Guedes[1,2], Anna Zhakarova[1], Cinthia Piamonteze[1], Nicholas C. Plumb[1], Ming Shi[1], and Milan Radovic[1] — [1]Photon Science Department, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland — [2]Institute of Condensed Matter Physics, Ecole Polytechnique Fédrale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Since many years rare earth nickelates ($RNiO_3$) attract researchers interests due to their wide variety of fascinating physical properties which are tunable by the interplay of electron correlations and crystal structure [1]. It was suggested that the tunability of electron correlations could be used to induce a cupratelike Fermi surface in $RNiO_3$ thin films. Motivated by this, we are investigating the evolution of the electronic structure of $LaNiO_3$ (LNO) thin films in proximity to manganite layers (strontium and calcium doped lanthanum manganite - LSMO and LCMO) grown on STO and NGO substrates. The films were grown by pulsed laser deposition (PLD). The combined study of angle resolved photoemission spectroscopy (ARPES), transport properties and X-ray magnetic circular dichroism (XMCD) reveal an anomalies around T=50K and T=150K as well as a strong dependence on the substrate. Understanding these properties could be crucial for tuning the nickelates towards superconductivity.

[1] J. Chaloupka et al., Phys. Rev. Lett. 100, 016404 (2008)

TT 54.5 Thu 10:30 H22

High-pressure floating-zone growth of $LaNiO_3$ single crystals — •Kaustav Dey, Mahmoud M.Abdel-Hafiez, and Rüdiger Klingeler — Kirchhoff Institute for Physics, Heidelberg University, Germany

$LaNiO_3$ is known to be a correlated metal in the vicinity of a bandwidth controlled metal-insulator transition. A variety of experimental studies on polycrystalline $LaNiO_3$ have indicated it to be a Pauli paramagnetic metal. Recently, the successful growth of $LaNiO_3$ single crystals was published [1,2]. Suprisingly, Guo *et. al.* have reported that $LaNiO_3$ has an antiferromagnetic metallic ground state [2]. We discuss the successful growth and characterization of centimeter-sized single crystals of $LaNiO_3$ by means of the floating zone technique at oxygen pressures of up to 80 bar. Indeed, magnetisation and specific heat data on several $LaNiO_3$ single crystals grown at 40 bar show the presence of a anomaly in the range 150-160 K similar to what is reported in Ref. [2]. In contrast, no anomaly was observed in the crystals grown at 80 bar in agreement with Ref. [1]. We infer that higher pressure leads to better crystal quality in terms of phase purity and that the anomaly associated with antiferromagnetism reported in $LaNiO_3$ single crystals may not be of intrinsic nature.

[1] J. Zhang et al., Cryst. Growth Des. 17, 2730 (2017)
[2] H. Guo et al., Nat. Comm. 9:43 (2018).

TT 54.6 Thu 10:45 H22

Bond and magnetic order in rare-earth nickelates simultaniously probed by resonant inelastic x-ray scattering — •Katrin Fürsich[1], Yi Lu[1,2], Davide Betto[1], Georg Christiani[1], Eva Benckiser[1], Giniyat Khaliullin[1], Matteo Minola[1], and Bernhard Keimer[1] — [1]Max Planck Insitutte for Solid State Research, Stuttgart — [2]University of Heildelberg

We used high-resolution resonant inelastic x-ray scattering (RIXS) at the Ni L_3 edge to simultaneously investigate bond and magnetic order in the rare-earth nickelates $RNiO_3$. With the support of calculations based on a double-cluster model, we quantify bond order (BO) amplitudes for different thin flms and heterostructures, and discriminate short-range BO type fluctuations from long-range static order. Moreover we investigate the magnetic order in spatially confined nickelate layers following the method described in Ref. 1. While our study reveals a robust non-collinear spin spiral magnetic order, which is essentially unperturbed by bond order modulations and spatial confinement, we find a dramatically reduced magnon energy in systems with collinear magnetic order. These results give valuable insight into the interplay of different collective ordering phenomena in a prototypical 3d transition metal oxide and establish RIXS as tool of choice to quantitatively study several order parameters within one experiment.

[1] Lu, Betto, KF *et al.*, Phys. Rev. X **8**, 031014 (2018)

15 min. break.

TT 54.7 Thu 11:15 H22

Raman spectroscopy study of the lattice and spin dynamics in CrAs — •Yi Yao[1], Matthieu Le Tacon[1], Kaushik Sen[1], Michaela Souliou[1], Amir-Abbas Haghighirad[1], Michael Merz[1], Christoph Meingast[1], Frederic Hardy[1], Anahita Omoumi[2], Measson Marie-Aude[3], and Pawbake Amit[3] — [1]Karlsruhe Institute of Technology, Institute for Solid State Physics — [2]University Paris Sud — [3]Institut Néel, Magnetic and superconductivity group

We performed Raman measurements to probe the lattice and spin dynamics of high quality single crystals of CrAs, an antiferromagnetic (AFM) double-helical system that becomes superconducting under pressure[1]. The samples were grown using a flux method, and characterized using XRD and magnetic susceptibility measurements. At the AFM ordering temperature $T_N = 265$ K, below which helical AFM order sets in, the sample exhibits a strong first order structural transition, upon which the lattice parameter b expands by $\approx 3.39\%$. In the Raman experiments, four Raman active modes with A_g symmetry were observed, as predicted from group theory. All these modes exhibit pronounced anomalies in their frequencies and linewidths across T_N. In addition, we found a signature of magnon scattering, and signatures of spin-phonon coupling are discussed. Finally, our high-pressure Raman experiments show the suppression of T_N under hydrostatic compression, in agreement with previous studies[1,2].

[1] W. Wei. et al., Nature Comm. 5 (2014)
[2] Y. Shen. et al., Phys. Rev. B 93 (2016)

TT 54.8 Thu 11:30 H22

Structural and magnetic properties of vanadium trihalides VX_3 (X = Cl, Br) — •Neetika Neetika[1], Reinhard K Kremer[1], and Christina Drahten[2] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569, Stuttgart, Germany — [2]ESRF - the European Synchrotron, 71, Avenue des Martyrs, 38000 Grenoble, France

We have examined the structural and magnetic properties of the layered vanadium trihalides, VX_3 (X = Cl, Br). For both systems, specific heat measurements indicate two anomalies at $\sim$ 25K and $\sim$ 100K. Magnetization measurements prove antiferromagnetic ordering below $\sim$ 25K and negative Weiss temperatures indicating predominant antiferromagnetic interactions. Laboratory-based and synchrotron x-ray diffraction measurements show that anomaly at $\sim$ 100K is associated to a structural phase transition from the rhombohedral BiI_3 structure-type ($R\bar{3}$) at high temperature to either a monoclinic (C2/c) or triclinic ($P\bar{1}$) crystal structure at low temperature. First-principle calculations also indicate that the structural phase transition from rhombohedral to either monoclinic or triclinic is energetically favorable.

TT 54.9 Thu 11:45 H22

New insights into doped Sr_2IrO_4 — •Benjamin Lenz[1], Cyril Martins[2], and Silke Biermann[1,3] — [1]CPHT, Ecole Polytechnique, Palaiseau, France — [2]LCPQ, Université Paul Sabatier, Toulouse, France — [3]Collège de France, Paris, France

The spin-orbit system Sr_2IrO_4 has been in the spotlight in recent years due to its striking similarity to isostructural high-T_c superconducting copper oxides. Here, we present new insights into the spectral properties of Sr_2IrO_4 using a combination of ab-initio density functional theory and quantum cluster techniques. We find good agreement with available angular-resolved photoemission spectra in the antiferromagnetic low-temperature and high-temperature paramagnetic phases of pure Sr_2IrO_4, as well as for electron- and hole-doped compounds. Furthermore, we discuss an intriguing k-dependence in the composition of the spin-orbit entangled $j_{\text{eff}} = 1/2$ states.

TT 54.10 Thu 12:00 H22

Propagation of a single hole in Ca_2RuO_4 — •Adam Kłosiński[1], Jeroen van den Brink[2], Dmitri V. Efremov[2], and Krzysztof Wohlfeld[1] — [1]Faculty of Physics, University of Warsaw, Warsaw, Poland — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany

In recent years there has been a growing interest in the understanding of the correlated physics of Ca_2RuO_4, fuelled by the fundamental importance of the spin-orbit interaction in this compound on the one hand and by its close resemblance to the well-studied copper oxides on the other. In order to understand the latter, we focus here on the propagation of a single hole introduced into the Mott insulating ground state of Ca_2RuO_4 and verify its quantitative as well as qualitative differences w.r.t. the cuprates. To this end we introduce an effective multiorbital t-J-like model which we then solve using the linear spin wave theory and self-consistent Born approximation. We obtain the spectral function for fermionic spinless holes whose most striking feauture is its quasi-1D character.

TT 54.11 Thu 12:15 H22

Near-field optical probes of the current- and temperature-driven insulator-to-metal transition in the Mott insulator Ca_2RuO_4 — •Desislava Daskalova[1,2], Parmida Shabestari[1,2], Hao Chu[1,2], Maximilian Krautloher[1], Joel Bertinshaw[1], Bernhard Keimer[1], and Stefan Kaiser[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]4th Physics Institute, Stuttgart University, Germany

Many-body effects in correlated materials give rise to exciting quantum phenomena and phases of matter. Here we study calcium ruthenate (Ca_2RuO_4), a Mott insulator at room temperature, because it exhibits interesting magnetic, transport and structural properties. The delicate balance in its ground state is easily perturbed by temperature, pressure and small electric field (40 V/cm) which all induce an insulator-to-metal transition (IMT). However, distinctly different metallic phases in a temperature- or current-driven case are being stabilized. One goal is to distinguish the different mechanisms driving the transition, especially to understand the current-driven IMT which remains to be fully explained.

To this end we probe the changes in the optical properties of Ca_2RuO_4 during the current- and temperature-driven IMT using far-field infrared spectroscopy and scattering-type scanning near-field optical microscopy. Probing the nanoscale optical response throughout the transition allows us to identify the Mott insulating and metallic phases. We image the two different phases of Ca_2RuO_4 coexisting and evolving in a manner, characteristic to the driving mechanism.

TT 54.12 Thu 12:30 H22

Magnetic order and short-range correlations in γ_{II}-Li_2FeSiO_4 — •Martin Jonak[1], Christoph Neef[1], Waldemar Hergett[1], Sven Spachmann[1], Mahmoud Abdel-Hafiez[1,2], Johannes Werner[1], Changhyun Koo[1], Sven Sauerland[1], Clemens Ritter[3], Sergei Zvyagin[4], Alexey Ponomaryov[4], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany — [2]Physikalisches Institut, Goethe-Universität, Frankfurt am Main, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Multi-faceted magnetic characterisation of γ_{II}-Li_2FeSiO_4 single crystals (space group $Pmnb$) is presented. The system exhibits tetrahedrally coordinated Fe^{2+} ions in a high-spin $e_g^3 t_{2g}^3$ (i.e., $S = 2$) configuration. While static magnetic susceptibility shows a maximum at $T \approx 28$ K, long-range AFM order is found to evolve at $T_N = 17.0(5)$ K. Elastic neutron scattering on a powder sample reveals commensurate two-sublattice AFM order with a propagation vector (1/2, 0, 1/2). At $T = 4$ K, high-frequency electron-spin resonance (HF ESR) observes zero-field splitting of $\Delta = 700(20)$ GHz, and the closing of the AFM gap at $B = 16.2(2)$ T which is separated from a spin-flop-like phase emerging at $B = 18.0(5)$ T. Both transitions are confirmed by pulsed-field magnetisation. At high temperatures, magnetic anisotropy beyond the g-factor anisotropy extends up to $T \gtrsim 150$ K. The presence of short-range magnetic correlations at least up to $T \approx 110$ K is detected by specific heat and magnetostriction, as well as by HF ESR.

TT 54.13 Thu 12:45 H22

Multiferroicity in $Fe_4Ta_2O_9$ — Soumendra Panja[1], Jitender Kumar[1], Luminita Harnagea[1], Arun Nigam[2], Ramesh Nath[3], P . K Mukharjee[3], and •Sunil Nair[1] — [1]IISER Pune, India — [2]TIFR Mumbai, India — [3]IISER Tvm, India

We report on the observation of multiple coupled magnetic and ferroelectric states in the $Fe_4Ta_2O_9$ system, which appears to be the only genuine multiferroic in its material class. We suggest that the observed properties arise as a consequence of an effective reduction in the dimensionality of the magnetic lattice, with the magnetically active Fe^{2+} ions preferentially occupying a quasi 2D buckled honeycomb structure. A rich variety of coupled magnetic and ferroelectric states are seen which is similar to that observed in the distorted Kagome systems.