# TT 3: Complex Oxides: Bulk Properties (joint session TT/MA/HL)

Time: Monday 9:30–13:00 Location: HSZ 201

TT 3.1 Mon 9:30 HSZ 201

**Single-crystal growth and magnetic phase diagram of $TbFeO_3$** — •Alexander Engelhardt[1], Georg Benka[1], Christian Oberleitner[1], Andreas Bauer[1], Andreas Erb[2], and Christian Pfleiderer[1] — [1]Physik Department E51, Technische Universität München, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Walther-Meißner-Str. 8, 85748 Garching, Germany

Single crystals of the multiferroic rare earth orthoferrite $TbFeO_3$ were synthesized by means of optical float-zoning. The magnetization, the longitudinal and the transverse ac susceptibility, as well as the specific heat were measured at low temperatures under large applied magnetic fields to determine the complex, anisotropic magnetic phase diagram of $TbFeO_3$ along the three major crystallographic axes. Taken together, our data are consistent with previous studies reported in the literature. As a new result we identify clear evidence in the bulk properties of the formation of a soliton lattice in a small temperature range, so far observed by means of neutron scattering only.

TT 3.2 Mon 9:45 HSZ 201

**Melting of excitonic dispersion in $LaCoO_3$: theory and experiment** — Atsushi Hariki[1], Ru-Pan Wang[2], Andrii Sotnikov[1,3], Keisuke Tomiyasu[4], Davide Betto[5], Nicholas B. Brookes[5], Yohei Uemura[2], Mahnaz Ghiasi[2], Frank M. F. de Groot[2], and •Jan Kuneš[1,6] — [1]Institute of Solid State Physics, TU Wien — [2]Debye Institute for Nanomaterials Science, Utrecht University — [3]Akhiezer Institute for Theoretical Physic, Kharkiv — [4]Department of Physics, Tohoku University — [5]European Synchrotron Radiation Facility, Grenoble — [6]Institute of Physics, Czech Academy of Sciences

We present Co $L_3$-edge resonant inelastic x-ray scattering (RIXS) on bulk $LaCoO_3$ across the thermally-induced spin-state crossover around 100 K. Owing to a high energy resolution of 20 meV, we observe unambiguously the dispersion of the intermediate-spin (IS) excitations in the low temperature regime. Approaching the intermediate temperature regime, the IS excitations are damped and the bandwidth reduced. The observed behavior can be well described by a model of mobile IS excitons with strong attractive interaction, which we solve using dynamical mean-field theory for hard-core bosons. Our results provide a detailed mechanism of how HS and IS excitations interact to establish the physical properties of cobaltite perovskites.

TT 3.3 Mon 10:00 HSZ 201

**Spin Selective Quasi-Particle Interference in $PdCoO_2$** — •Dibyashree Chakraborti[1,2], Chi Ming Yim[1], Luke Rhodes[1], Seunghyun Khim[2], Andrew Mackenzie[1,2], and Peter Wahl[1] — [1]School of Physics and Astronomy, St. Andrews, Scotland, United Kingdom, KY169SS — [2]Max Planck Institute of Chemical Physics of Solids, Noethnitzer Strasse, Dresden -01187

The metallic delafossite $PdCoO_2$, which is among the most conductive oxides currently known (at 295 K) [1], has risen to prominence due to interesting physical effects, such as unusually long mean free paths, leading to hydrodynamic effects being observed in electron flow [2]. Further, recent Angle Resolved Photoemission Spectroscopy (ARPES) studies have reported exciting surface-physics on the $CoO_2$-terminated surface. The $CoO_2$ surface shows evidence of large Rashba spin-splitting, arising from the interplay of energy scales due to strong spin orbit coupling and inversion symmetry breaking at the surface. [3]. In this study, we have identified and investigated the $CoO_2$ termination of $PdCoO_2$ with low temperature Scanning Tunneling Microscopy (STM). We present and discuss the quasi-particle interference imaging of the Rashba spin-split surface state, and the implications for possible spintronics applications.

[1] C.W. Hicks et al., Phys. Rev. Lett. 109, 116401 (2012)
[2] P.J.W. Moll et al., Science 351, 1061 (2016)
[3] V. Sunko et al., Nature 549, 492 (2017)

TT 3.4 Mon 10:15 HSZ 201

**Interplay of Electronic and Spin Degrees in Ferromagnetic $SrRuO_3$: Anomalous Softening of the Magnon Gap and Stiffness** — •Kevin Jenni[1], Stefan Kunkemöller[1], Daniel Brüning[1], Thomas Lorenz[1], Yvan Sidis[2], Astrid Schneidewind[3], Augustinus Agung Nugroho[4], Achim Rosch[5], Daniil Iljitsch Khomskii[1], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Deutschland — [2]Laboratoire Leon Brillouin, Grenoble, Frankreich — [3]JCNS, Forschungszentrum Jülich, Garching, Deutschland — [4]Institut Teknologi Bandung, Indonesien — [5]Institut für Theoretische Physik, Universität zu Köln, Deutschland

We succeeded to grow large single crystals of $SrRuO_3$ using the floating-zone technique [1,2]. The first inelastic neutron scattering study of the spin dynamics on single crystals yields the expected quadratic spin wave dispersion of a ferromagnet. However the magnon gap and stiffness considerably deviate from an earlier inelastic neutron scattering study on powders [3]. In addition we find a non-monotonous temperature dependence of the anisotropy gap and a softening of the magnon stiffness upon cooling. We discuss how Weyl points caused by SOC in $SrRuO_3$ couple electronic and spin degrees of freedom and how this interplay leads to the characteristic behavior in the spin dynamics [4].

[1] S. Kunkemöller et al., Chrys. Res Tec. 51, 299 (2016)
[2] S. Kunkemöller et al., PRB 96, 220406(R) (2017)
[3] S. Itoh et al., Nat. Commun. 7, 11788 (2016)
[4] K. Jenni et al., Phys. Rev. Lett. 123, 017202 (2019)

TT 3.5 Mon 10:30 HSZ 201

**$Ca_2RuO_4$: DFT + DMFT study of the magnetic order and dynamical susceptibility** — •Dominique Geffroy[1,2], Kyo-Hoon Ahn[1], Hoshin Gong[4], and Jan Kuneš[1,3] — [1]TU Wien, Vienna, Austria — [2]Masaryk University, Brno, Czech Republic — [3]Czech Academy of Science, Prague, Czech Republic — [4]Max Planck POSTECH/Korea Research Initiative, Pohang, Korea

Relativistic Mott insulators are complex compounds in which spin and orbital degrees of freedom become entangled due to a large spin-orbit coupling. Previous studies, both experimental and theoretical[1, 2], have shown that they are good candidates for novel forms of order, including excitonic magnetism[3]. We report results on the theoretical study of the prototypical relativistic Mott insulator $Ca_2RuO_4$. We use a realistic ab initio DFT + DMFT approach including SU(2) Coulomb interaction and spin-orbit coupling. The emergence of antiferromagnetic order at low temperature is correctly described. We present and discuss the spectra of the the collective modes in the ordered phase within the DMFT approximation.

[1] Jain et al., Nat. Physics 13, 633 (2017)
[2] G. Zhang and E. Pavarini, Phys. Rev. B 95, 075145 (2017)
[3] A. Akbari and G. Khaliullin, Phys. Rev. B 90, 035137 (2014)

TT 3.6 Mon 10:45 HSZ 201

**LDA+DMFT Approach to Resonant Inelastic X-Ray Scattering in Rare-Earth Nickelates** — •Mathias Winder[1], Atsushi Hariki[1], and Jan Kuneš[1,2] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Praha 8, Czechia

We present a computational study of *L*-edge resonant inelastic x-ray scattering (RIXS) across the metal-insulator transition (MIT) of $LuNiO_3$. We apply exact diagonalization to a material specific Anderson impurity model with a by DMFT obtained hybridization function. In contrast to other available methods, this approach enables us to describe simultaneously localized (*d*-*d*) and delocalized (unbound electron-hole pair) excitations in the RIXS spectra. We reproduce the experimentally observed behaviour of fluorescence-like and Raman-like features across the MIT and provide its material specific interpretation.

TT 3.7 Mon 11:00 HSZ 201

**Interplay of electronic correlations, charge disproportionation and lattice in $RNiO_3$ nickelates with R = Lu, Y, and Bi** — •Ivan Leonov — M. N. Mikheev Inst. of Metal Physics, Yekaterinburg, Russia — NUST 'MISiS', Moscow, Russia

In recent years, increasing attention has been drawn to the understanding of the rare-earth-element nickelate perovskites $RNiO_3$, which exhibit a sharp metal-insulator transition (MIT). The MIT is accompanied by a structural phase transformation, complicated by the appearance of unusual charge order and non-collinear magnetic phases in the Mott insulating regime. Here, I will focus on this particular problem and will discuss an application of the DFT+DMFT method to explore the electronic structure, magnetic and lattice properties of a series of $RNiO_3$ nickelates with R = Lu, Y, and Bi. I will discuss our

results for the pressure-induced Mott MIT in $RNiO_3$, which is found to be accompanied by a structural transformation. While the rare-earth and Bi $RNiO_3$ are closely related in their electronic state and crystal structure, these materials exhibit sufficiently different electronic properties. Our results for $BiNiO_3$ suggest the important role of the Bi 4*s* charge ordering (charge difference of ∼0.52 electrons), with a charge transfer between the Bi 4*s* and O 2*p* states and a stable $Ni^{2+}$ configuration, for understanding of the MIT in $BiNiO_3$ [1]. We find that electronic correlations are important to explain the electronic structure, magnetic state, and lattice stability of $RNiO_3$ (R = Lu, Y, and Bi).

[1] I. Leonov et al., Phys. Rev. B **100**, 161112(R) (2019).

**15 min. break.**

TT 3.8 Mon 11:30 HSZ 201

**Origin of orbital ordering in $LaTiO_3$ and $YTiO_3$** — •Xuejing Zhang and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

The origin of orbital ordering (OO) in correlated oxides is strongly debated. Two main mechanisms have been proposed as possible explanation for OO phenomena. The first is the classical Jahn-Teller effect and the second is the electronic super-exchange, introduced by Kugel-Khomskii. In the case of the paradigmatic $e_g$ systems $KCuF_3$ and $LaMnO_3$ it has been shown that the electronic Kugel-Khomskii mechanism is not sufficient to drive the OO transition alone, at the temperatures at which orbitally order is typically observed by the co-operative Jahn-Teller distortion.[1,2] In the case of $t_{2g}$ compounds, however, the problem remains open. In these systems both the electron-lattice coupling and the hopping integrals are typically smaller than those for $e_g$ compounds; on the other hand, orbital degeneracy is larger, which enhances the effects of super-exchange. Here we investigate representative $t^1_{2g}$ systems in which OO is observed, the Mott insulators $LaTiO_3$ and $YTiO_3$. We show that the Kugel-Khomskii transition temperature is about 390 K, comparable to the one of $KCuF_3$. This shows that static distortions are needed to explain the presence of OO at high temperature.

[1] E. Pavarini, E. Koch and A. I. Lichtenstein, Phys. Rev. Lett. 101, 266405 (2008).
[2] E. Pavarini and E. Koch, Phys. Rev. Lett. 104, 086402 (2010).

TT 3.9 Mon 11:45 HSZ 201

**Charge transport in oxygen-deficient $EuTiO_3$: The emerging picture of dilute metallicity in quantum-paraelectric perovskite oxides** — •Johannes Engelmayer[1], Xiao Lin[1], Christoph Grams[1], Raphael German[1], Tobias Fröhlich[1], Joachim Hemberger[1], Kamran Behnia[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Laboratoire Physique et Etude de Matériaux, PSL Research University, 75005 Paris, France

Quantum paraelectric $SrTiO_3$ is a large-gap band insulator that becomes metallic upon electron doping already at extremely small charge-carrier concentrations $\simeq 5 \times 10^{17}\mathrm{cm}^{-3}$. The observed $T^2$ resistivity in this material challenges conventional theories for electron–electron scattering. We report on a study of charge transport in the related compound $EuTiO_3$ where the carrier density is tuned via reduction. Because of a lower electric permittivity, the metal–insulator transition (MIT) in $EuTiO_{3-\delta}$ occurs at higher carrier densities compared to doped $SrTiO_3$. The critical carrier concentration $n_c$ for the MIT is discussed in the context of the so-called Mott criterion and compared with other doped perovskite compounds with a quantum-paraelectric parent. Similar to doped $SrTiO_3$, $EuTiO_{3-\delta}$ shows a distinct $AT^2$ resistivity, where the prefactor $A$ scales with $n$. Using a simple three-band model, the $A(n)$ behavior in doped perovskite titanates can be described over a large range of $n$.

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TT 3.10 Mon 12:00 HSZ 201

**Magnetic Phase diagram and thermal expansion studies of $NiTiO_3$** — •Kaustav Dey[1], Sven Sauerland[1], Johannes Werner[1], Rabindranath Bag[2], Surjeet Singh[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics , Heidelberg University, Germany — [2]IISER Pune, Maharashtra, India

We report the magnetic phase diagram of $S = 1$ magnetodielectric $NiTiO_3$ single crystals grown by the optical floating zone technique. The high-quality single crystals have been studied by specific heat, by magnetometry up to 60 T, and by thermal expansion and magnetostriction measurements up to 15 T, respectively. The compound evolves long-range antiferromagnetic order at $T_N = 22.5$ K with spins lying in the *ab*−plane. Pronounced anomalies in the thermal expansion coefficients $(\alpha_i, (i = a, b))$ at $T_N$ indicate strong magnetoelastic coupling in $NiTiO_3$. Magnetic length and entropy changes as detected by $\alpha$ and $c_p$ obey Grüneisen scaling which evidences one dominant (spin) degree of freedom driving the transitions. In addition, the magnetic phase diagram features a spin-reoriented phase below $B_c = 1.2$ T which suggests the presence of a small in-plane anisotropy. Notably, spin-reorientation is associated with a first-order-like anomaly in the magnetostriction. The high-field behavior of magnetization is linear and isotropic with saturation at 36 T thereby facilitating constructing the entire magnetic phase diagram.

TT 3.11 Mon 12:15 HSZ 201

**Low-Energy Excitations in $NiTiO_3$ and $Ni_{0.25}Mn_{0.75}TiO_3$ Probed by Antiferromagnetic Resonance** — •Martin Jonak, Kaustav Dey, Johannes Werner, Changhyun Koo, and Rüdiger Klingeler — Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany

We study magnetic excitations in $NiTiO_3$ and $Ni_{0.25}Mn_{0.75}TiO_3$ by means of X-band and high-frequency electron spin resonance spectroscopy. Our data for $NiTiO_3$ show that in the antiferromagnetically ordered and spin-reoriented phase, i.e. below $T_N$ and in external magnetic fields above the spin-reorientation field $B_C = 1.13(8)$ T, antiferromagnetic resonance (AFMR) modes are well described by a two-sublattice model with an easy *ab*-plane. Correspondingly, two zero-field excitation gaps are deduced at $\Delta_1 \approx 15$ GHz and $\Delta_2 = 185(2)$ GHz, respectively. At $B < B_C$, an additional magnon mode is observed, which rules out a simple two-sublattice model, thereby contradicting the presently established picture of the low-field ground state. The strongly Mn-doped $Ni_{0.25}Mn_{0.75}TiO_3$ exhibits at least two antiferromagnetically ordered phases. The low-temperature phase shows AFMR modes of a two-sublattice antiferromagnet with anisotropy gaps $\Delta_1 = 29(1)$ GHz and $\Delta_2 = 139(3)$ GHz.

TT 3.12 Mon 12:30 HSZ 201

**Electronic transformations in the semi-metallic transitional oxide $Mo_8O_{23}$** — •Venera Nasretdinova[1], Yaroslav Gerasimenko[1,2], Jernej Mravlje[2], Gianmarco Gatti[3], Petra Sutar[2], Damjan Svetin[1,2], Anton Meden[4], Viktor Kabanov[2], Alexander Kuntsevich[5,6], Marco Grioni[3], and Dragan Mihailovic[1,2] — [1]CENN Nanocenter, Ljubljana, Slovenia — [2]JSI, Ljubljana, Slovenia — [3]Institute of Physics, EPFL, Lausanne, Switzerland — [4]University of Ljubljana, Slovenia — [5]LPI of RAS, Moscow, Russia — [6]HSE, Moscow, Russia

$Mo_8O_{23}$ is a low-dimensional stoichiometric transitional metal oxide from $MoO_{3-x}$ family. Its room-temperature phase associated with charge density wave (CDW) is accompanied by non-monotonic resistivity at low temperatures well below structural transitions. Using tunneling and angle-resolved spectroscopy, transport measurements and density functional calculations we reveal electronic transformations leading to a multi-band correlated ground state [1, 2]. We observe the metal-to-insulator transition at 343 K in resistivity, consistent with CDW onset. At low temperatures, the picture with the only CDW order parameter is broken by the onset of the correlated ground state visible both in transport and spectroscopic probes. Spatially-resolved tunneling spectroscopy studies reveal the emergent electronic texture. We discuss the possible origins of the electronic order that emerge in the absence of any structural or magnetic transitions.

[1] V. Nasretdinova et al., Phys.Rev. B 99, 085101 (2019)
[2] V. Nasretdinova et al., Sci. Rep. 9, 15959 (2019)

TT 3.13 Mon 12:45 HSZ 201

**Cr and Ce magnetic ordering in $CeCrO_3$:revisited** — •Neetika Sharma[1], Reinhard K. Kremer[1], Clemens Ritter[2], and Fereidoon S. Razavi[3] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Institute Laue Langevin, Grenoble 38000, France — [3]Department of Physics, Brock University, St. Catharines, ON, L2S 3A1, Canada

We have investigated the magnetic structure of $CeCrO_3$ using neutron powder diffraction (NPD). $CeCrO_3$ crystallizes with the $GdFeO_3$ structure-type (Pbnm). Earlier neutron diffraction measurements on $CeCrO_3$ have proposed a G-type afm structure for the Cr and a C-type for the Ce sublattice. The analysis of the magnetic structure for

the Ce sublattice had been based on one magnetic peak (102) at d ∼ 3.152 Å. However, the proposed C-type coupling for Ce will generate primarily two magnetic Bragg peaks (100) at d ∼ 5.47 Å and (102) at d ∼ 3.152 Å. We have collected NPD patterns on a sample of $CeCrO_3$ using ILL's D20 high-intensity medium resolution diffractometer and did observe the previously reported magnetic Bragg peak at d ∼ 3.152 Å, however significantly less intense than reported before. Simulations indicate that only the presence of magnetic coupling of C-type on the Cr- and the Ce- sublattices can lead to a situation where the magnetic peak (102) at d ∼ 3.152 Å is a lot stronger than the (100) Bragg peak at d ∼ 5.47Å. Following this proposal we have analyzed our neutron diffraction data very carefully at low temperature (1.5K), and conclude a CyGz type magnetic ordering for the Cr sub-lattice with a very small Cy-component and Cy type coupling for Ce - sublattice.