MA 55: Complex Oxides – Bulk Properties, Surfaces and Interfaces (joint session TT/MA/KFM)

Time: Friday 9:30–13:00 Location: H 0110

MA 55.1 Fri 9:30 H 0110

Superconductivity in strontium titanate within the dielectric function method — •Serghei Klimin[1], Jacques Tempere[1], Jozef Devreese[1], Cesare Franchini[2], and Georg Kresse[2] — [1]TQC, Universiteit Antwerpen, Antwerpen, Belgium — [2]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria

Strontium titanate exhibits unique features which are not encountered in conventional polar crystals at the same conditions. It becomes a superconductor at unusually low carrier densities. $SrTiO_3$ is probably the only substance where superconductivity and optical absorption can be convincingly attributed to the Fröhlich-like electron-phonon interaction and polarons. In the present talk, we report on our theoretical studies of superconductivity in strontium titanate with a comparative discussion of different theoretical interpretations of superconductivity in $SrTiO_3$. It is demonstrated that the dielectric function method used in our works [1] adequately describes the superconducting phase transition using only parameters available from experiments and microscopic calculatuions. We are particularly focused on unusual isotope effect in $SrTiO_3$. It is shown that renormalization of optical-phonon frequencies following from the isotope substitution leads to an increase of the critical temperature within the dielectric function method.
[1] S. N. Klimin, J. Tempere, J. T. Devreese, and D. van der Marel, Phys. Rev. B **89**, 184514 (2014); J. Sup. Nov. Magn. **30**, 757 (2017).

MA 55.2 Fri 9:45 H 0110

Anisotropic Rashba-type spin-orbit coupling of the two-dimensional electron system in (110) $SrTiO_3$-based heterostructures — •Karsten Wolff, Roland Schäfer, Robert Eder, Matthieu le Tacon, and Dirk Fuchs — Karlsruhe Institute of Technology, Institute for Solid State Physics

The two-dimensional electron system in (110) $Al_2O_{3-d}/SrTiO_3$ heterostructures displays anisotropic electronic transport. Structured microbridges allow to probe 4-point resistivity along different crystallographic orientations, i.e. [001] and [1-10]. The conductivity and electron mobility along the [001] direction is largest, while differences in sheet carrier concentration are only minor. The measurements show anisotropic normal magnetotransport for $T < 30\,K$ which is correlated to the anisotropic mobility. For temperatures below 5 K transport is dominated by Rashba-type spin orbit interaction (SOI) which displays anisotropic behavior, too. SOI is found largest along the [001] direction.

MA 55.3 Fri 10:00 H 0110

Thermoelectric properties of $(SrXO_3)_1(SrTiO_3)_m$(001) superlattices, X=V, Mn and Ru — •Manish Verma, Benjamin Geisler, Markus E. Gruner, and Rossitza Pentcheva — Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg

The thermoelectric properties of $SrTiO_3$ have been widely studied, primarily concerning the role of homogeneous bulk doping. However, the confinement realized in oxide superlattices may have a favorable effect on the thermoelectric properties. To this end we have investigated the electronic and thermoelectric properties of superlattices containing a monolayer of $SrXO_3$ (X=V, Mn and Ru) sandwiched between m=1,3 spacer layer(s) of $SrTiO_3$ (001) using a combination of density functional theory with an on-site Hubbard term and semi-classical Boltzmann theory. In all cases structural distortions containing octahedral tilts are energetically favored over tetragonal distortions and we explore their influence on the electronic and thermoelectric properties. Comparing the in-plane and out-of-plane transport properties we find no significant dependence on m for the in-plane transport properties. In turn on reduction of the $SrTiO_3$ thickness from m=3 to 1 enhances the dispersion along Γ-Z and thereby improves the out-of-plane thermoelectric properties. Funded by the DFG, CRC/TRR80 project G8.

MA 55.4 Fri 10:15 H 0110

Thermoelectricity close to a metal-insulator transition in ultrathin $LaNiO_3/LaAlO_3$(001) superlattices — •Benjamin Geisler and Rossitza Pentcheva — Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany

Transition metal oxides are a promising materials class for thermoelectric applications due to their chemical and thermal stability and environmental friendliness. Their thermoelectric response can be further improved by nanostructuring and reduced dimensionality. Here we explore the thermoelectric properties of $(LaNiO_3)_1/(LaAlO_3)_1$(001) superlattices near the confinement-induced metal-insulator transition by combining *ab initio* simulations including on-site Coulomb repulsion and Boltzmann theory. We find that the short-period vertical design strongly enhances the in-plane thermoelectricity owing to the Ni-site disproportionation, which is stabilized considerably by tensile epitaxial strain and octahedral tilting. The sensitivity of the system to epitaxial strain provides an additional parameter to optimize the thermoelectric performance. For a $SrTiO_3$(001) substrate, we predict room-temperature Seebeck coefficients and power factors that can compete with those of other oxide systems of current interest such as layered cobaltates. Comparison of the ultrathin superlattices with the metallic longer-period $(LaNiO_3)_3/(LaAlO_3)_3$(001) case establishes the metal-insulator transition as a crucial mechanism to obtain a high thermoelectric response.

Funding by the DFG within TRR 80 (G3 and G8) is acknowledged.

MA 55.5 Fri 10:30 H 0110

Confinement-driven electronic and topological phases in corundum-derived oxide honeycomb superlattices — •Okan Koeksal and Rossitza Pentcheva — Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg

On the basis of density functional theory calculations plus the Hubbard U interaction, we investigate electronic, magnetic and possibly topologically non-trivial phases in X_2O_3 honeycomb layers confined in the corundum structure α-Al_2O_3 (0001). Our results predict that the ground states for most of the systems of $X = 3d$ cations are trivial antiferromagnetic Mott insulators. If the symmetry of the two sublattices is imposed, the ferromagnetic phases of Ti, Mn, Co and Ni exhibit a characteristic set of four bands associated with the single occupation of e'_g (Ti) and e_g (Mn, Co, Ni) states. Moreover, the Dirac point can be tuned to the Fermi level by strain and a significant anomalous Hall conductivity arises when spin-orbit coupling (SOC) is switched on. A particularly strong SOC effect is identified for X = Ti at $a_{Al2O3} = 4.81$ Å accompanied by an unusually high orbital moment of -0.88 μ_B nearly quenching the spin moment of 1.01 μ_B. The emergence of this orbital magnetism makes the realization of Haldane's model of spinless fermions possible. The extension of this work to the 4d and 5d series led to the identification of cases of high orbital moment (Os) or candidates for Chern insulators (CI), i.e. X = Tc and Pt with C=-2 and -1, depending on the Coulomb repulsion strength. Support by the DFG within CRC/TRR80, project G3 is gratefully acknowledged.

MA 55.6 Fri 10:45 H 0110

Metal-Insulator Transition in Thin Films and Multilayers of Early Transition Metal Oxides from DFT+DMFT — •Sophie D. Beck and Claude Ederer — Materials Theory, ETH Zürich, Zurich, Switzerland

The wide variety of interesting phenomena and functionalities of complex oxide thin films and heterostructures is generally determined by a number of different factors, such as substrate-induced epitaxial strain, dimensional confinement, interface-related effects, or defects. Here, we systematically study the interplay between these effects in thin films and multilayers composed of materials such as correlated metals, Mott insulators and band insulators, using a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT). In particular, we investigate the evolution of octahedral rotations across interfaces between two materials with different rotation angles and/or tilt systems, and how this affects the range of electronic reconstruction in the interfacial region. We then show that these effecs can give rise to phenomena such as metallic interfaces in multilayers of two Mott insulators $LaVO_3$ and $LaTiO_3$ up to a metal-insulator transition in the correlated metal $CaVO_3$, for which we find that both tensile strain or reduced film thickness can lead to a strong quasiparticle renormalization.

MA 55.7 Fri 11:00 H 0110

Dimensionality-driven metal-insulator transition in spin-oribt coupled $SrIrO_3$ — •Philipp Schütz[1], Domenico Di Sante[1], Lenart Dudy[1], Judith Gabel[1], Martin Stübinger[1], Martin Kamp[1], Yingkai Huang[2], Massimo Capone[3], Marius-Adrian Husanu[4], Vladimir Strocov[4], Giorgio Sangiovanni[1], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Van der Waals - Zeeman Institute, University of Amsterdam, Netherlands — [3]CNR-IOM-Democritos National Simulation Center and International School for Advanced Studies (SISSA), Italy — [4]Swiss Light Source, Paul Scherrer Institut, Switzerland

Upon reduction of the film thickness we observe a metal-insulator transition in epitaxially stabilized, spin-orbit coupled $SrIrO_3$ ultra-thin films. By comparison of the experimental electronic dispersions with density functional theory at various levels of complexity we identify the leading microscopic mechanisms, i.e., a dimensionality-induced re-adjustment of octahedral rotations, magnetism, and electronic correlations. The astonishing resemblance of the band structure in the two-dimensional limit to that of bulk Sr_2IrO_4 opens new avenues to unconventional superconductivity by "clean" electron doping through electric field gating.

15 min. break.

MA 55.8 Fri 11:30 H 0110

Intrinsic defects effects to the electronic structure of Sr_2IrO_4 probed by scanning tunneling microscopy — •Zhixiang Sun[1], Jose M. Guevara[1], Ekaterina M. Pärschke[1], Steffen Sykora[1], Kaustuv Manna[1,2], Johannes Schoop[1], Andrey Malyuk[1], Sabine Wurmehl[1,3], Jeroen van den Brink[1], Bernd Büchner[1,3], and Christian Hess[1] — [1]IFW-Dresden, 01069 Dresden — [2]MPI-CPfS, 01187 Dresden — [3]Institute for Solid State Physics, TU Dresden

Due to its similarity to cuprates, there is tremendous interest on the possible superconducting ground-state in doped Sr_2IrO_4 (Ir214). Nevertheless, it has been found that doping of Ir214 is difficult. The mechanism of dopant induced insulator to metal transition (IMT) has not been fully clarified. We have carried out low temperature scanning tunneling microscopy/spectroscopy experiments on Ir214 crystals. Several different types of intrinsic defects have been identified and their effects to the local electronic structure have been probed. We noticed that for the apical oxygen site defects, their effects are spatially very localized (< 2 nm). Also on the spectra taken on top of these defects, in gap states with a charge transfer like behavior are observed. With a local defect model we simulated the spectra, which gives good a match with the results. Our results provide important observations on the effects of individual defects on the local electronic properties. This is crucial for further tailoring the electronic structure of Ir214. Furthermore, they can also facilitate the understanding of the general mechanism of IMT in Mott insulators.

MA 55.9 Fri 11:45 H 0110

Novel insights into the impurity-selective metal-insulator transition of paramagnetic V_2O_3 — •Frank Lechermann[1], Noam Bernstein[2], Igor Mazin[2], and Roser Valenti[3] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstr. 9, D-20355 Hamburg, Germany — [2]Code 6393, Naval Research Laboratory, Washington, DC 20375, USA — [3]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

The phase diagram of V_2O_3 with temperature and concentration of different dopants (e.g. Cr and Ti), still poses a formidable problem in condensed matter physics. By means of the charge self-consistent combination of density functional theory with dynamical mean-field theory, i.e. the DFT+DMFT approach, we provide new clues to the delicate interplay between electronic and lattice degrees of freedom. The impact of the defect chemistry is highlighted beyond the sole lattice expansion/contraction affect usually associated with impurity doping in this system. Local symmetry breakings are identified as one key feature to understand the tight competition between metal and insulator in vanadium sesquioxide.

MA 55.10 Fri 12:00 H 0110

Growth and characterization of *Pmnb*-Li_2FeSiO_4 single crystals — •Waldemar Hergett[1], Christoph Neef[1], Hubert Wadepohl[2], Hans-Peter Meyer[3], Mahmoud Abdel-Hafiez[4], and Rüdiger Klingeler[1,5] — [1]Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany — [2]Institute of Inorganic Chemistry, Heidelberg University, Heidelberg, Germany — [3]Institute of Earth Sciences, Heidelberg University, Heidelberg, Germany — [4]Institute of Physics, Goethe University, Frankfurt, Germany — [5]Center for Advanced Materials, Heidelberg University, Heidelberg, Germany.

Li_2FeSiO_4 single crystals featuring the high temperature *Pmnb* phase were grown by the high-pressure optical floating zone method. The resulting single crystals have been characterized by means of polarised-light and electron microscopy, EDX, powder and single crystal X-ray diffraction. The impact of the growth parameters and of the applied pressure on the crystal quality was investigated. The single crystal structure of the *Pmnb*-polymorph was solved for the first time. It exhibits layers of corner-sharing FeO_4- and SiO_4-tetrahedra in the crystallographic *ac*-planes which alternate with layers of LiO_4-tetrahedra. Magnetisation and specific heat studies confirm the high quality of the crystals and show a sharp λ-like anomaly associated with the onset of long-range antiferromagnetic order at $T_N = 17\,K$.

MA 55.11 Fri 12:15 H 0110

Excitonic dispersion of intermediate-spin state in $LaCoO_3$ revealed by resonant inelastic X-ray scattering — •Atsushi Hariki[1], Ru-Pan Wang[2], Andrii Sotnikov[1], Federica Frati[2], Jun Okamoto[3], Hsiao-Yu Huang[3], Amol Singh[3], Di-Jing Huang[3], Keisuke Tomiyasu[4], Chao-Hung Du[5], Frenk M. F de Groot[1], and Jan Kuneš[2] — [1]Institute for Solid State Physics, TU Wien, Austria — [2]Inorganic Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, The Netherlands — [3]Condensed Matter Physics Group, National Synchrotron Radiatiation Research Center, Taiwan, — [4]Department of Physics, Tohoku University, Sendai, Japan — [5]Department of Physics, Tamkang University, New Taipei City, Taiwan,

We perform Co *L*-edge resonant inelastic X-ray scattering of $LaCoO_3$ at 20 K. We observe a dispersive state with an energy shift from 480 to 290 meV as a function of momentum from $\boldsymbol{q} = (0, 0, 0.26\pi)$ to $\boldsymbol{q} = (0, 0, 0.90\pi)$. This dispersion is attributed to the mobility of the intermediate-spin (IS) state, which is viewed as an exciton. A theoretical calculation considering the excitonic dispersion of the IS state on the background of the low-spin (LS) state supports the interpretation. The present result suggests that the mobility pushes the IS state into play to the thermal spin-state transition of $LaCoO_3$ in addition to the (immobile) high-spin and LS states with lower atomic-multiplet energies, as suggested by recent theoretical studies [1].

[1] A. Sotnikov and J. Kuneš, Sci. Rep. 6, 30510 (2016).

MA 55.12 Fri 12:30 H 0110

Electronic signature of the vacancy ordering in NbO (Nb_3O_3) — Anna K. Efimenko[1], Nils Hollmann[1], Katharina Hoefer[1], Jonas Weinen[1], Daisuke Takegami[1], Klaus K. Wolff[1], Simone G. Altendorf[1], Zhiwei Hu[1], A. Diana Rata[1], Alexander C. Komarek[1], Agustinus Nugroho[2], Yen-Fa Liao[3], Ku-Ding Tsuei[3], H. H. Hsieh[4], H. -J. Lin[3], C. T. Chen[3], Liu Hao Tjeng[1], and •Deepa Kasinathan[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Insitiut Teknologi Bandung, Bandung, Indonesia — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]Chung Cheng Institute of Technology, Taoyuan, Taiwan

We investigated the electronic structure of the vacancy-ordered 4d-transition metal monoxide NbO (Nb_3O_3) using angle-integrated soft- and hard-x-ray photoelectron spectroscopies as well as ultra-violet angle resolved photoelectron spectroscopy. We found that density-functional-based band structure calculations can describe the spectral features accurately provided that self-interaction effects are taken into account. In the angle-resolved spectra we were able to identify the so-called vacancy band that characterizes the ordering of the vacancies. This together with the band structure results indicates the important role of the very large inter-Nb-4d hybridization for the formation of the ordered vacancies and the high thermal stability of the ordered structure of niobium monoxide.

MA 55.13 Fri 12:45 H 0110

Ultrahigh-resolution Resonant Inelastic X-ray Scattering from rare-earth nickelates: magnetic and dd-excitations — •Katrin Fürsich[1], Yi Lu[1], Davide Betto[2], Georg Christiani[1], Giniyat Khaliullin[1], Maurits W. Haverkort[3], Eva Benckiser[1],

Matteo Minola[1], and Bernhard Keimer[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]European Synchrotron Radiation Facility, Grenoble — [3]Institut für Theoretische Physik, Universität Heidelberg

Rare-earth nickelates ($RNiO_3$) have been subject to intense investigation, mostly because of the rich phase diagram comprising a sharp temperature-driven metal-to-insulator transition, an unusual antiferromagnetic ground state, and the prospect of mimicking the physics of high-T_c superconducting cuprates in orbitally engineered heterostructures. We have studied $RNiO_3$ thin-films and superlattices using ultrahigh-resolution resonant inelastic x-ray scattering (RIXS) at the Ni L_3 edge. Below the magnetic ordering temperature, we observe well-defined collective magnon excitations. Our experimental observation provides for the first time a solid basis for the theoretical description of the magnetism in $RNiO_3$. In addition to magnetic excitations, we investigated the electronic excitations of $RNiO_3$ as a function of temperature and tolerance factor, i.e. rare-earth radius. A sophisticated analysis based on an advanced double-cluster model gives intriguing insight into the microscopic and electronic structure of $RNiO_3$. Our study reveals that RIXS is an excellent technique to quantitatively characterize different ordering phenomena within one material.