TT 50: Focus Session: Superconducting Nickelates II

Time: Thursday 15:00–17:00 Location: HSZ 03

TT 50.1 Thu 15:00 HSZ 03

Fermi liquid on the verge of antiferromagnetism: Nonlocal correlations in bulk $LaNiO_3$ as seen by SX-ARPES — •Johannes Falke[1], Cheng-En Liu[1,2,3], Keng-Yung Lin[1,4], Chang-Yang Kuo[1,2,3], Hanjie Guo[1], Alexander Komarek[1], Chun-Fu Chang[1], Philipp Hansmann[5], and Liu Hao Tjeng[1] — [1]MPI CPfS, Dresden, Germany — [2]NYCU, Hsinchu, Taiwan — [3]NSRRC, Hsinchu, Taiwan — [4]NTU, Taipei, Taiwan — [5]FAU, Erlangen, Germany

Soft X-ray ARPES measurements were performed on large single crystals of the metallic oxide $LaNiO_3$ along high symmetry directions, revealing the bulk electronic structure of the full valence band. The experimental Fermi surface is accurately reproduced by conventional band theories, whereas the nonzero frequency part of the spectra shows k-dependent renormalizations that cannot be explained by DFT even accounting for octahedral rotations and require true many-body methods to accurately explain.

TT 50.2 Thu 15:15 HSZ 03

Insights into the electronic structure of oxygen reduced and doped nickelates from core-level spectroscopy — •Rebecca Pons — Max-Planck Institut für Festkörperforschung, Stuttgart, Germany — Stewart Blusson Quantum Matter Institute, UBC Vancouver, Canada

With the observation of superconductivity in Sr-doped infinite-layer nickelate $Nd_{0.8}Sr_{0.2}NiO_2$ research interest in this material class intensified. We used ozone assisted molecular beam epitaxy to grow RNiO$_3$ thin films (R=La,Pr) and investigated the subsequent topotactic soft-chemistry reaction, needed to synthesize the square-planar phase, at different stages of reduction by x-ray absorption spectroscopy. We observe the evolution of the Ni oxidation state and that the process is laterally homogeneous down to length scales of 50 nm. To reach the superconducting phase hole doping of the infinite-layer nickelates is required with an optimal doping level around x=0.2. This can be achieved by self-doping in quintuple-layer Ruddlesden-Popper nickelates or alkaline-earth doping, Ca or Sr, in infinite-layer films. Using angle-resolved photoemission spectroscopy (ARPES) we studied changes in the Fermi surface upon alkaline-earth doping in (La,Ca)NiO$_3$.

TT 50.3 Thu 15:30 HSZ 03

Thickness-dependent interface polarity in infinite-layer nickelate superlattices — •Chao Yang[1], Roberto A. Ortiz[1], Yi Wang[2], Wilfried Sigle[1], Hongguang Wang[1], Eva Benckiser[1], Bernhard Keimer[1], and Peter A. van Aken[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, 70569, Germany — [2]Center for Microscopy and Analysis, Nanjing University of Aeronautics and Astronautics, Nanjing, 210016, P.R. China

The interface polarity plays a vital role in the physical properties of oxide hetero-interfaces, since it can enforce a reconstruction of the electronic and atomic structure. In the recently discovered superconducting nickelate thin films, interfacial effects could play an important role. This motivated our investigation of the electronic and atomic structure at the atomic scale at interfaces of infinite-layer nickelate thin films. Using four-dimensional scanning transmission electron microscopy (4D-STEM) and electron energy-loss spectroscopy (EELS), we systematically studied the effects of oxygen distribution and site occupancy, polyhedral distortion, elemental intermixing, as well as dimensionality on interface properties of infinite-layer NdNiO2/SrTiO3 superlattices. The oxygen intensity and distribution maps show the local symmetry change from octahedral to square planar induced by the reduction process and a gradual change of the oxygen content in the nickelate layers. Remarkably, we demonstrate spatially controlled interface polarity with accompanying interface reconstructions. Our results provide insights to understand the effects of polarity and dimensionality on the interface properties of infinite-layer nickelates.

TT 50.4 Thu 15:45 HSZ 03

GW+EDMFT investigation of $Pr_{1-x}Sr_xNiO_2$ under pressure — •Viktor Christiansson, Francesco Petocchi, and Philipp Werner — University of Fribourg, Fribourg, Switzerland

The recent experimental observation of a large pressure effect on T_c in $Pr_{1-x}Sr_xNiO_2$ opens up an interesting prospect for reaching even higher values of T_c in the nickelates. On the theoretical side, systematic changes with pressure also provides a new possibility for probing the single- versus multi-orbital nature of these systems. In this talk, we discuss the electronic structure of this system as a function of pressure and doping, based on numerical calculations using self-consistent GW+EDMFT. We show that the normal state properties demonstrate a non-trivial interplay between physical pressure and chemical doping, and we find small but systematic changes with increasing pressure. The proper treatment of correlation effects, beyond density functional theory, is shown to play an important role in revealing these trends. While the pressure dependent changes of the undoped compound suggest a more single-orbital-like behavior towards the high-pressure regime, a qualitatively different behavior is observed for the doped system with a multi-orbital nature manifesting itself also at high pressures.

TT 50.5 Thu 16:00 HSZ 03

Nature of magnetic coupling in bulk infinite-layer nickelates versus cuprates — •Armin Sahinovic, Benjamin Geisler, and Rossitza Pentcheva — Fakultät für Physik, Universität Duisburg-Essen

In contrast to cuprates, where the proximity of antiferromagnetism (AFM) and superconductivity is well established, first indications for AFM interactions in superconducting infinite-layer nickelates [1] were only recently obtained [2,3]. Here, we explore, based on first-principles simulations, the nature of the magnetic coupling in $NdNiO_2$ as a function of the on-site Coulomb and exchange interaction, varying the explicit hole doping and the treatment of the Nd $4f$ electrons. The U-J phase diagrams for undoped nickelates and cuprates indicate G-type ordering, yet show different U dependency. By either Sr hole doping or explicit treatment of the Nd $4f$ electrons, we find a transition to a Ni C-type AFM ground state. We trace this back to a distinct response of the Ni vs. Cu e_g orbitals to the hole doping. The interaction between Nd $4f$ and Ni $3d$ spin stabilizes C-type AFM order on both sublattices. Though spin-orbit interactions induce a band splitting near the Fermi energy, the bad-metal state is retained under epitaxial strain. The magnetocrystalline anisotropy features an in-plane easy axis, related to the planar NiO_2 coordination. These results establish the nickelates as a unique platform to study unconventional superconductivity.

[1] D. Li et al., Nature 572, 624 (2019)
[2] J. Fowlie et al., Nature Physics 18, 1043 (2022)
[3] H. Lu et al., Science 373, 213 (2021)

TT 50.6 Thu 16:15 HSZ 03

Magnetic interactions in $InNiO_3$ compared to RNiO$_3$ — •Alexander Yaresko, Graham McNally, Minu Kim, and Hidenori Takagi — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

RNiO$_3$ nikelates undergo with lowering temperature a metal-to-insulator (MIT) transition, accompanied by orthorhombic-to-monoclinic distortion of their crystal structure, and another transition at T_N to a magnetically ordered state with the ordering vector $\mathbf{q}$=(1/2, 0, 1/2). Two Ni sites in the monoclinic unit cell are nonequivalent, with the average Ni_1–O distance being significantly larger than Ni_2–O. In compounds with the large radius of a R^{3+} ion the two transitions occur simultaneously. As the R size decreases, the crystal structure becomes more distorted. As a consequence, the MIT temperature increases while T_N decreases. Recently, a new $InNiO_3$ compound, in which an In^{3+} ion is even smaller than the smallest rare-earth Lu^{3+}, has been synthesized. We performed DFT(+U) calculations for $InNiO_3$ and compare the results to other nikelates. In order to quantify the effect of structural distortions on the magnetic properties we estimated exchange interactions between magnetic Ni_1 ions by mapping the energies of spin-spirals with different wave vectors $\mathbf{q}$ to an effective Heisenberg model. We found that the strongest interactions are those along Ni_1-O-Ni_2-O-Ni_1 bonds but their strength decreases with increasing lattice distortions. The experimental $\mathbf{q}$=(1/2, 0, 1/2) order can only be reproduced if a sufficiently small value of Coulomb repulsion U is used for more covalent Ni_2 ion.

TT 50.7 Thu 16:30 HSZ 03

Transport properties of $Nd_{1-x}Sr_xNiO_2$ based on a realistic 3-band model — •Steffen Bötzel, Ilya Eremin, and Frank

Lechermann — Institut für theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany

Here, we consider theoretically the quasiparticle transport in the superconducting nickelate $Nd_{1-x}Sr_xNiO_2$ based on a realistic 3-band low-energy model derived from a first-principle approach [1]. The transport properties are obtained from the standard Kubo formalism. They depend on the band structure near the Fermi surface and are consequently a probe of the hitherto poorly understood low-energy electronic structure. We find significant contributions from different orbitals and bands depending on temperature and doping. Their interplay gives rise to multi-band characteristics, which are in accordance to available experimental data. This observation is important for the ongoing debate whether the low-energy physics is single- or multi-band like and points towards multi-band physics in these compounds.

[1] F. Lechermann, Phys. Rev. X. 10, 041002 (2020)

TT 50.8 Thu 16:45 HSZ 03

High-pressure crystal growth and physical properties of Ruddlesden-Popper trilayer nickelates $La_4Ni_3O_{10}$ — •Ning Yuan, Kaustav Dey, Jan Arneth, Ahmed Elghandour, and Rüdiger Klingeler — Kirchhoff Institute for Physics, Heidelberg University, Germany

Single crystals of $La_4Ni_3O_{10}$ were successfully grown by the high-pressure optical floating-zone method under 20 bar oxygen pressure. We investigate the different growth and post-annealing processes leading to two different polymorphs, namely $P2_1/a$ (No.14) and *Bmab* (No.64), respectively, and report high-resolution thermal expansion, specific heat and magnetometry data on both of them. Our thermodynamic studies show sharp anomalies associated with the reported Metal-to-Metal Transition (MMT) in $La_4Ni_3O_{10}$ and distinct anisotropy. For the $P2_1/a$ phase, the MMT transition is found at 134 K while it appears at 152 K for *Bmab*. Our thermal expansion data in particular confirm that the MMT transition is associated with strong lattice changes (cf. [1]) but is also reveals clear contradictions to the published XRD data [2].

[1] D. Rout *et al.*, Phys. Rev. B 102, 195144 (2020)
[2] J. Zhang *et al.*, Phys. Rev. M 4, 083402 (2020)