TT 52: Nickelates II

Time: Wednesday 15:00–16:15 Location: H 3010

Invited Talk TT 52.1 Wed 15:00 H 3010

A tale of two kinds of superconducting nickelates — •Frank Lechermann — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Layered nickelates have been of interest since the early days of high-T_c superconducting (SC) cuprates as possible additional representants of unconventional superconductors. But only in 2019, a stable SC phase has been identified in thin-films of Sr-doped $NdNiO_2$ with a $T_c \sim 20$ K [1]. Further SC members from this class of low-valence nickelates have been spotted afterwards. And just when the debate about the similarity between SC cuprates and nickelates, both with akin $3d^{9-x}$ formal transition-metal valence, was at its zenith, a SC bilayer nickelate of formal $3d^{8-x}$ valence was detected at high pressure with $T_c \sim 80$ K in spring 2023 [2]. Interestingly, according to our theoretical investigations [3,4] all these SC nickelates have a multiorbital Ni-e_g flat-band scenario in common.

In this talk, it will be shown that an advanced combination of density functional theory (DFT) and dynamical mean-field theory (DMFT) provides unique access to this novel playground of high-T_c nickelate superconductivity. Albeit the whole field is still at its infancy, the multiorbital regime together with the SC properties at distinctly different $3d$ electron count renders obvious that many further surprises may be uncovered in the future.

[1] D. Li et al., Nature 572 (2019) 624
[2] H. Sun et al., Nature 621 (2023) 493
[3] F. Lechermann, Phys. Rev. X 10 (2020) 041002
[4] F. Lechermann et al., arXiv:2306.05121 (2023)

TT 52.2 Wed 15:30 H 3010

Tuning of the carrier localization, magnetic and thermoelectric properties in ultrathin $(LaNiO_{3-\delta})_1/(LaAlO_3)_1$(001) superlattices by oxygen vacancies — •Manish Verma and Rossitza Pentcheva — Department of Physics, Universität Duisburg-Essen

Understanding the role of defects on the complex behavior of transition metal oxides in bulk and the ultrathin limit is at the forefront of condensed matter physics. Using a combination of density functional theory calculations with an on-site Coulomb repulsion term (DFT+U) and Boltzmann transport theory within the constant relaxation time approximation, we explore the effect of oxygen vacancies on the electronic, magnetic, and thermoelectric properties in ultrathin $(LaNiO_{3-\delta})_1/(LaAlO_3)_1$(001) superlattices (SLs). For the pristine SL, an antiferromagnetic charge-disproportionated (AFM-CD) $(d^8\underline{L}^2)_{S=0}(d^8)_{S=1}$ phase is stabilized, irrespective of strain. At δ = 0.125 and 0.25, the localization of electrons released from the oxygen defects in the NiO_2 plane triggers a charge-disproportionation, leading to a ferrimagnetic insulator both at a_{STO} (tensile strain) and a_{LSAO} (compressive strain). At $\delta = 0.5$, an insulating phase emerges with alternating stripes of Ni^{2+} (high-spin) and Ni^{2+} (low-spin) and oxygen vacancies ordered along the [110] direction (S-AFM), irrespective of strain. This results in a robust n-type in-plane power factor of 24 μW/K^2 cm at a_{STO} and 14 μW/K^2 cm at a_{LSAO} at 300 K (assuming relaxation time τ = 4 fs). Additionally, the pristine and $\delta = 0.5$ SLs are shown to be dynamically stable.

TT 52.3 Wed 15:45 H 3010

influence of $SrTiO_3$ capping layer on infinite-layer nickelate thin films — •martando rath[1], yu chen[1], guillaume krieger[2], daniele preziosi[2], and marco salluzzo[1] — [1]CNR-SPIN, Napoli, Italy — [2]Université, de Strasbourg, CNRS, IPCMS UMR, France

By using core-level x-ray photoemission spectroscopy (XPS), we studied the electronic properties of epitaxial $NdNiO_2$ thin films. In particular, we compare the surface-interface electronic structure of $SrTiO_3$ (STO)-capped and uncapped $NdNiO_2$ samples by core-level Nd $3d$ and Ni $2p$ XPS spectra. Our preliminary results show the enhancement of $3d^94f^4\underline{L}$ ($\underline{L}$ stands for a hole on the oxygen ligands) compared to $3d^94f^3$ peak in Nd $3d_{5/2}$ of the nickelates sample capped with STO layer, which suggests the formation of a $Nd(Ti,Ni)O_3$ layer at the upper interface. The origin of this layer, recently found also at the bottom interface with the STO-single crystal, has been attributed to the polar discontinuity between neutral STO planes and charged $NdNiO_2$. A single $Nd(Ti,Ni)O_3$ layer indeed is able to solve the polar-catastrophe which would otherwise occur due to the alternating charged $(NiO_2)^{3-}$ and Nd^{3+} layers. Furthermore, we find substantial differences of the Ni $2p$ spectra, which indicates the sample with capping layer preserves the Ni^{1+} charge state with a fraction of Ni^{2+} in the final photo-excited state.

TT 52.4 Wed 16:00 H 3010

Gap Structure Evolution of Infinite-Layer Lanthanum Nickelates from Enhanced Correlations — •Fabian Jakubczyk[1,2], Armando Consiglio[2,3], Domenico Di Sante[4], Ronny Thomale[2,3], and Carsten Timm[1,2] — [1]Institute of Theoretical Physics, Technische Universität Dresden, 01069 Dresden — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [4]Department of Physics and Astronomy, University of Bologna, I-40127 Bologna, Italy

The newly discovered superconducting infinite-layer nickelates and in particular their gap symmetry pose challenges for the research community. For instance, controversial magnetotransport measurements point at either isotropic or anisotropic superconductivity, with possibly crucial impact of the rare-earth element. On the other hand, the existence of orbital-selective correlations, which are particularly strong for the Ni $3d_{x^2-y^2}$ orbital, seems to be generally accepted. In our work, we investigate potential spin-triplet superconductivity in lanthanum-based nickelates from the perspective of spin-fluctuation pairing and orbital selectivity. For this purpose, we construct a minimal model including Ni $3d$, as well as La $5d$ degrees of freedom. A gap structure with odd parity indeed becomes favored for a reasonable choice of interaction strength and quasiparticle renormalization. We therefore identify $LaNiO_2$ as a member of the nickelate family that is substantially different from isostructural d-wave cuprate superconductors.