TT 44: Focus Session: Superconducting Nickelates I

The discovery of superconductivity in hole-doped infinite-layer nickelates in 2019 has brought a breath of fresh air to the research on unconventional superconducting materials. These nickel oxides structurally closely resemble high-T_c cuprates and show a formally analogous nickel $d^{9-\delta}$ electronic configuration. Other striking similarities with cuprates have been recently reported, such as a dome-like doping dependence of the superconducting phase, sizeable antiferromagnetic exchange couplings, and a charge order instability in the underdoped region of the phase diagram. Likewise, a number of studies identified clear differences, e.g. concerning selected transport behavior as well as magnetic properties, and with regard to the relevance of oxygen-2p states. It is precisely this combination of strong similarities and specific differences that promises new, game-changing insights into the origin of high-temperature superconductivity. The goal of this focus seesion is to bring together the latest results for low-valence nickelates from studies of structure, electronic structure, magnetism, charge density waves and superconductivity, and thus setting the stage for a coherent picture of these complex quantum materials.

Organizers: Eva Benckiser (Max-Planck-Institute for Solid State Research, Stuttgart) and Frank Lechermann (Ruhr-Universität Bochum)

Time: Thursday 9:30–13:00 Location: HSZ 03

Invited Talk TT 44.1 Thu 9:30 HSZ 03

Atomic-scale insights to lattice and electronic structure in superconducting nickelates — •Berit Goodge — School of Applied and Engineering Physics, Cornell University — Kavli Institute at Cornell for Nanoscale Science, Cornell University — Max Planck Institute for Chemical Physics of Solids

Although the synthesis of superconducting nickelates [1,2] remains notoriously challenging [3,4], many materials realities including epitaxial strain, extended defects, impurities, and secondary phases are largely undiscussed in the context of understanding their measured properties. As direct probes of lattice and electronic structure down to the atomic scale, scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) offer unique insights to build a holistic understanding of both the intrinsic physical properties in these materials as well as more extrinsic features and their consequences, many of which arise from their multistep synthesis. Here, we discuss how quantitative lattice-scale measurements can disentangle many of these effects, revealing, for example, multi-band hole interactions [5], nontrivial interface reconstruction [6], and the impact of epitaxial strain [2, 7].

[1] Li et al., Nature 572, 624 (2019)
[2] Lee et al., arXiv:2203.02580 (2022)
[3] Lee et al., APL Mat. 8:4, 041107 (2020)
[4] Pan et al., Nat. Mat. 21, 160 (2022)
[5] Goodge et al., PNAS 118:2, (2021)
[6] Goodge et al., arXiv:2201.03613 (2022)
[7] Segedin et al., under review (2022)

Invited Talk TT 44.2 Thu 10:00 HSZ 03

Nickelate and cuprate superconductors: Similar yet different — •Vamshi Mohan Katukuri — Max Planck Institute for Solid State Research, Stuttgart, Germany

The discovery of superconductivity in hole-doped infinite-layer $NdNiO_2$ – a transition metal oxide that is both isostructural and isoelectronic to cuprate superconductors – has lead to renewed enthusiasm in the hope of understanding the origin of unconventional superconductivity. In this talk, I will present and discuss the similarities and differences in the electronic structure of nickelates and cuprates from the perspective of *ab initio* many body wavefunction analysis derived from state-of-the-art quantum chemistry calculations. After highlighting the main differences in the parent (undoped) infinite-layered $NdNiO_2$ and $CaCuO_2$ compounds, I will discuss the character of the doped hole by analyzing the electron-removal (which mimics hole-doping) states in the two compounds. In the end, I will discuss the evolution of the electronic structure of nickelates under pressure.

Invited Talk TT 44.3 Thu 10:30 HSZ 03

Superconducting instabilities in strongly-correlated infinite-layer nickelates — •Andreas Kreisel — Niels Bohr Institute, University of Copenhagen, Denmark

Unconventional superconductivity is often referred to as originating from a pairing mechanism different from electron-phonon interactions and connected to an anisotropic superconducting order parameter with sign change of the Cooper pair wavefunction. In this talk, I will start from a discussion of the mechanism of spin-fluctuation mediated pairing that can lead to d-wave states as evidenced in the cuprate superconductors, but also the sign-changing $s_\pm$ state that seems to be realized in Fe-based superconductors. The discovery of superconductivity in infinite-layer nickelates has immediately posed the question about the pairing mechanism and the pairing symmetry in this system and sparked proposals of analogs towards well studied families of materials in the class of unconventional superconductors. To connect to this open question, the leading superconducting instability is computed from magnetic fluctuations relevant for infinite-layer nickelates incorporating the strongly correlated multi-orbital nature of the low-energy electronic degrees of freedom. Observing the interplay between the Ni $d_{x^2-y^2}$ and d_{z^2} orbitals as well as the self-doping band, a transition from d-wave pairing symmetry to nodal $s_\pm$ superconductivity is uncovered. This is driven by strong fluctuations in the d_{z^2}-dominated orbital states. As probe of the detailed superconducting gap structure, we discuss the properties of the resulting superconducting condensate in light of tunneling and penetration depth experiments.

15 min. break

Invited Talk TT 44.4 Thu 11:15 HSZ 03

Infinite-layer nickelate thin films: From synthesis to spectroscopy — •Daniele Preziosi — Université de Strasbourg, CNRS, IPCMS UMR 7504, F-67034 Strasbourg, France

In the last three decades, special efforts were devoted to the realization of nickelates mimicking the electronic structure of cuprates. These efforts led to the realization of infinite-layer nickelates characterized by a stable $Ni-3d^9$ configuration and reduced dimensionality. A superconducting state below 15 K was reported for $Nd_{0.8}Sr_{0.2}NiO_2$ thin films deposited onto (001) $SrTiO_3$ (STO). Soon after this discovery, x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray scattering (RIXS) experiments on undoped ($LaNiO_2$, $NdNiO_2$) and doped ($Nd_{1-x}Sr_xNiO_2$) samples showed that infinite-layer nickelates show some important differences compared to layered cuprates, in particular a larger charge transfer energy and an important Nd 5d-Ni 3d hybridization. In this talk, after introducing our efforts to stabilize the infinite-layer phase, I will show that some of those aforementioned differences depend also on the presence/absence of a STO-capping-layer. A robust charge order is observed in undoped capping-free thin films, while strong magnetic excitations around 200 meV energy-loss characterize capped samples. Polarization-resolved RIXS measurements unambiguously demonstrated that also the low-energy excitations for uncapped samples are magnetic in nature, but largely damped. The 'altered' doping effect as observed from the enlarging of the XAS feature at the NiL_3-edge combined to a strong $Ni3d-Nd5d$ hybridization for uncapped samples, may speak in favor of this extra softening.

Invited Talk TT 44.5 Thu 11:45 HSZ 03

Superconducting layered square-planar nickelates: Synthesis, properties, and progress — •Grace Pan[1], Dan Ferenc Segedin[1], Harrison LaBollita[2], Qi Song[1], Berit Goodge[3], Lena Kourkoutis[3], Charles Brooks[1], Antia Botana[2], and Julia

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Since the discovery of high-T_c superconductivity in the cuprates, there have been sustained efforts to both understand the origins of this phase and discover new cuprate-like superconductors. One prime materials platform has been the rare-earth nickelates; indeed, superconductivity was discovered in the doped compound $Nd_{0.8}Sr_{0.2}NiO_2$ in 2019. Undoped $NdNiO_2$ belongs to a series of layered square-planar nickelates with chemical formula $Nd_{n+1}Ni_nO_{2n+2}$ and is known as the infinite-layer (n=∞) nickelate. Here, we describe the synthesis of the quintuple-layer (n=5) member, $Nd_6Ni_5O_{12}$, in which optimal cuprate-like electron filling ($d^{8.8}$) is achieved without chemical doping. We observe a superconducting transition beginning at ∼13 K. Electronic structure calculations fortified with experiments suggest that $Nd_6Ni_5O_{12}$ interpolates between cuprate-like and infinite-layer nickelate-like behaviour. By engineering a distinct superconducting nickelate, we identify the square-planar nickelates as a new family of superconductors that can be tuned via both doping and dimensionality. In this talk, I will further discuss ongoing experimental progress on the synthesis and characterization of these layered nickelates.

TT 44.6 Thu 12:15 HSZ 03

Nickelate superconductors: One-band Hubbard model plus decoupled *A* pocket picture — •Karsten Held[1], Motoharu Kitatani[2], Liang Si[1,3], and Paul Worm[1] — [1]Institute for Solid State Physics, TU Wien, Austria — [2]University of Hyogo , Japan — [3]Northwest University, Xi'an, China

At first glance, nickelate superconductors appear to be more complicated than their cuprate peers. Based on density functional theory (DFT) plus dynamical mean-field theory (DMFT) we however arrived at a picture that the physics of nickleate superconductors is dominated by the Ni $d_{x^2-y^2}$-band and the pockets are, in many respects, merely passive bystanders [1]. Other groups have argued instead for the importance of the Ni d_{z^2}-band based, e.g., on self-interaction corrected (sic)DFT+DMFT [2].

Taken the premise of a $d_{x^2-y^2}$-band Hubbard model description, we have predicted the phase diagram, superconducting critical temperature T_c vs. doping x [1]. Later experiments synthesizing high-quality films are in excellent qualitative and even quantitative agreement [3], as is the resonant inelastic x-ray (RIXS) spectrum. Also the pentalayer nickelate superconductor which has no pockets in DFT+DMFT and the increase T_c with pressure nicely match this picture [4].

[1] M. Kitatani *et al.*, npj Quantum Materials 5, 59 (2020)
[2] F. Lechermann, Phys. Rev. B 101, 081110 (2020);
A. Kreisel *et al.*, Phys. Rev. Lett. 129, 077002 (2022)
[3] K. Lee *et al.*, arXiv:2203.02580
[4] P. Worm *et al.*, Phys. Rev. Mater. 6, L091801 (2022)

TT 44.7 Thu 12:30 HSZ 03

Single-layer T' nickelates — Kerstin Wissel[1], Fabio Bernardini[2], Heesu Oh[2], Sami Vasala[3], Björn Blaschkowski[2], Pieter Glatzel[3], Matthias Bauer[4], Olivier Clemens[1], and •Andrés Cano[5] — [1]University of Stuttgart, Stuttgart, Germany — [2]University of Cagliari, Cagliari, Italy — [3]ESRF, Grenoble, France — [4]Padeborn University, Padeborn, Germany — [5]Institut NEEL, CNRS, Grenoble, France

The discovery of superconductivity in the infinite-layer nickelates has renewed the interest in these potential analogs of the high-Tc cuprates motivating the search for additional materials in this class [1]. In the talk, I will introduce the recently synthesised single-layer T' nickelates [2,3] and discuss their structural and electronic properties in relation to previous nickelates and cuprates.

[1] See e.g. A. Botana, F. Bernardini and A. Cano, JETP 159, 711 (2021) for a review.
[2] K. Wissel et al., Chem. Mater. 32, 3160 (2020)
[3] K. Wissel et al., Chem. Mater. 34, 7201 (2022)

TT 44.8 Thu 12:45 HSZ 03

Synthesis and physical properties of perovskite and infinite-layer nickelate crystals — •Pascal Puphal[1], Vignesh Sundaramurthy[1], Valentin Zimmermann[1], Björn Wehinger[2], Gaston Garbarino[2], Kathrin Küster[1], Ulrich Starke[1], Jürgen Nuss[1], Bernhard Keimer[1], Masahiko Isobe[1], and Matthias Hepting[1] — [1]Max Planck Institute for Solid State Research — [2]European Synchrotron Radiation Facility

Infinite-layer (IL) nickelates are an emerging family of superconductors whose synthesis in thin film form is an established process by now, whereas the growth of their bulk counterparts remains a formidable challenge. In a previous study, we achieved the reduction of perovskite La1-xCaxNiO3 single-crystals grown by a flux method under high external pressure to the IL phase $La_{1-x}Ca_xNiO_2$ [1]. The typical lateral dimension of these crystals was 150 μm. As an advanced approach, we recently accomplished the reduction of millimeter-sized $LaNiO_3$ crystals obtained by optical floating zone growth under high oxygen gas pressure to the IL phase $LaNiO_2$ [2]. We will present our characterization of the crystalline, magnetic, and electronic properties of the $LaNiO_2$ crystals, and give an outlook on the synthesis of millimeter-sized crystals of pure $LaNiO_3$ and $PrNiO_3$ as well as ones with hole- and electron doping.

[1] P. Puphal *et al.*, Sci. Adv. 7, eabl8091 (2021)
[2] P. Puphal *et al.*, arXiv:2209.12787 (2022)