DS 15: Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II (joint session TT/DS/MA)

Time: Thursday 9:30–12:30 Location: HSZ/0003

DS 15.1 Thu 9:30 HSZ/0003

Bulk High-Temperature Superconductivity and Density Waves in Layered Nickelates — •Jun Luo[1,2], Jie Dou[1,2], Shuo Li[1], Qin Xin Shen[1,2], Xu Yang Feng[1,2], De Min Chai[1,2], Ran Sheng Jia[1,2], Jie Yang[1,2], and Rui Zhou[1,2] — [1]Institute of Physics, Chinese Academy of Sciences, and Beijing National Laboratory for Condensed Matter Physics, Beijing 100190, China — [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China

The recent advances in bilayer nickelates $La_3Ni_2O_7$ have revealed fascinating high-temperature superconductivity (HTSC) under high-pressure conditions, offering a promising platform to explore unconventional superconducting mechanisms. In this talk, I will first discuss the discovery of bulk HTSC in Pr-doped $La_2PrNi_2O_7$, where Pr substitution effectively suppresses intergrowth phases, resulting in nearly pure bilayer structures. Superconducting onset temperature reaches 82.5 K at 16 GPa. Clear diamagnetic signals confirm the bulk nature of HTSC. I will also present microscopic evidence of charge and spin density wave (CDW/SDW) orders in $La_3Ni_2O_7$, revealed through 139La nuclear quadrupole resonance (NQR). Below the density wave transition temperature, we observe distinct line splitting and magnetic broadening, indicating unidirectional CDW order coupled with SDW order. By integrating insights from high-pressure and NQR studies, this work provides a comprehensive understanding of the structural and electronic mechanisms underlying HTSC in bilayer nickelates, paving the way for future experimental and theoretical investigations.

DS 15.2 Thu 9:45 HSZ/0003

ARPES spectra and the role of interstitial-s orbital in infinite-layer nickelates calculated by DFT+DMFT — •Leonard Verhoff[1], Liang Si[1,2], and Karsten Held[1] — [1]Institut für Festkörperphysik, Technische Universität Wien, Wien, Austria — [2]School of Physics, Northwest University, Xi'an, China

Infinite-layer nickelates, such as $NdNiO_2$, are a compelling platform to explore the microscopic origin of unconventional high-temperature superconductivity, from both theoretical and experimental perspectives.

Experimentally, infinite-layer nickelates are reduced from the stable perovskite phase, leaving an empty apical oxygen site. *Density functional theory* (DFT) calculations show that the resulting interstitial vacancy hosts localized, s-like states about 2 eV above the fermi level, while recent *angle-resolved photoemission spectroscopy* (ARPES) measurements of superconducting $NdNiO_2$ thin films conjectured Fermi surfaces with major s-like orbital character, highlighting a possible role of interstitial-s states in superconductivity.

We present DFT and *dynamical mean field theory* calculations of Fermi surfaces and band structures for both bulk and slab geometries, directly comparable to ARPES spectra. Our ARPES simulations explicitly include first-principles photoemission matrix elements, capturing the impact of orbital shapes on the measured intensity. We show how the correlated band structure reproduces low-energy ARPES spectra and identify the features dominated by interstitial-s character.

We acknowledge support through a joint German and Austrian Science Funds (DFG and FWF) project; FWF project ID I5398.

DS 15.3 Thu 10:00 HSZ/0003

A photoinduced two-dimensional electron gas (2DEG) at infinite-layer nickelate/strontium titanate interfaces — •D. Sanchez-Manzano[1], G. Krieger[2], A. Raji[3], B. Geisler[4], V. Humbert[1], H. Jaffres[1], J. Santamaria[5], R. Pentcheva[4], A. Glotter[3], D. Preziosi[2], and Javier E. Villegas[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, France. — [2]Institute of Physics and Chemistry of Materials of Strasbourg, CNRS, University of Strasbourg, France. — [3]Laboratoire de Physique de Solides, CNRS, Université Paris-Saclay, France. — [4]Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany — [5]6Departamento de Física de Materiales, Universidad Complutense de Madrid, Spain

We demonstrate, through experiments (transport, electron microscopy & spectroscopy) and density functional theory (DFT), that a high-mobility 2DEG can be optically switched on and off at an oxide interface where such a state does not naturally exist [1]. We show that near-ultraviolet light instantly creates a volatile 2DEG at the interface between $SrTiO_3$ (a band insulator) and infinite-layer $NdNiO_2$ (a poor metal), resulting in a conductivity increase of up to five orders of magnitude. This stems from structural and electronic reconstructions that, along with a built-in interfacial electric field, facilitate the Ti-3d band occupation by photogenerated carriers. These findings open venues for engineering photoconductance in strongly correlated systems.

[1] Sanchez-Manzano et al., Nat. Mater. (2025).
https://doi.org/10.1038/s41563-025-02363-y

DS 15.4 Thu 10:15 HSZ/0003

Democratizing nickelates superconductors: Topotactic reduction induced by aluminum sputter deposition — •Lucía Iglesias[1], Dongxin Zhang[1], Aravind Raji[2,3], Luis M. Vicente-Arche[1], Alexandre Gloter[2], and Manuel Bibes[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay — [2]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay — [3]Synchrotron SOLEIL

Superconductivity in infinite-layer (IL) nickelates (ABO_2) was discovery in 2019, opening a new research frontier. However, progress remains limited by the challenging topotactic reduction needed to remove all apical oxygens from the perovskite precursor, typically achieved through a complex ex situ CaH_2 method. Although recent in situ approaches, such as metal overlayer deposition via molecular beam epitaxy and atomic hydrogen bombardment, have improved control and reproducibility, their restricted accessibility highlights the need for simpler synthesis routes. Here, we demonstrate a broadly accessible method to fabricate superconducting IL $Pr_{0.8}Sr_{0.2}NiO_2$ films via aluminum deposition using direct-current magnetron sputtering. The sputtered Al drives the reduction through a redox reaction, converting the precursor perovskite into the superconducting IL phase. Systematic optimization of Al-induced reduction yields high-quality films with a maximum transition temperatures of 17 K, consistent with the best reported values. This accessible and highly reproducible approach provides an effective alternative to existing techniques and lowers barriers to the exploration of nickelate superconductors.

DS 15.5 Thu 10:30 HSZ/0003

Two-dimensional vortex matter in infinite-layer nickelates — •David Sanchez-Manzano[1], Vincent Humbert[1], Araceli Gutiérrez-Llorente[1,2], Dongxin Zhang[1], Jacobo Santamaría[3], Manuel Bibes[1], Lucia Iglesias[1], and Javier E. Villegas[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Univerisité Paris-Saclay, 91767 Palaiseau, France — [2]Escuela Superior de Ciencias Experimentales y Tecnología, Universidad Rey Juan Carlos, 28933 Madrid, Spain — [3]GFMC, Dpto. de Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, 28040 Madrid, Spain

Characterizing the dimensionality of the superconducting state in the infinite-layer (IL) nickelates is crucial to understanding its nature. Most studies have addressed the problem by studying the anisotropy of the upper critical fields. Yet, the dominance of Pauli-paramagnetism effects over orbital ones makes it challenging to interpret the experiments in terms of dimensionality. Here we address the question from a different perspective, by investigating the vortex phase diagram in the mixed-state. We demonstrate that superconducting $Pr_{0.8}Sr_{0.2}NiO_2$ thin films present a vortex liquid-to-glass transition of a two-dimensional nature. The obtained results suggest that bidimensionality is an intrinsic property, and that superconductivity resides in fully-decoupled NiO_2 planes. In this scenario, the coherence length along the c-axis must be shorter than the distance between those planes, while Josephson and magnetostatic coupling between them must be negligible. We believe that these conclusions are relevant for theories on the origin of superconductivity in the IL-nickelates.

DS 15.6 Thu 10:45 HSZ/0003

Systematically Controlled Disorder to Probe Pairing Symmetry in Infinite-Layer Nickelates — •A. Ranna[1], R. Grasset[2], M. Gonzalez[3], K. Lee[3], B. Y. Wang[3], D. Zhang[4], W. Sun[5], C. Parzyck[6], Y. Wu[6], M. Konczykowski[2], M. Bibes[4], K. M. Shen[6], Y. F. Nie[5], L. Iglesias[4], H. Y. Hwang[3], A. P. Mackenzie[1], and B. H. Goodge[1] — [1]MPI CPfS, Germany — [2]LSI, Ecole Polytechnique, France — [3]Stanford University, USA — [4]CNRS Thales, France — [5]Nanjing University, China — [6]Cornell University, USA

Superconductivity in infinite-layer nickelates has expanded rapidly with advances in thin-film synthesis and reduction techniques. A central question is the symmetry of the superconducting gap in these materials. Because superconducting samples can only be stabilized as thin films and suffer surface degradation during the post-growth reduction process, some conventional probes to determine the gap symmetry remain challenging to perform and interpret. Here, we leverage high-energy electron irradiation to controllably introduce point-like defects without altering film stoichiometry or crystallinity. Tracking superconductivity with systematically increasing disorder shows a steady suppression of transition temperature and rising normal state resistivity, indicative of an unconventional, sign-changing gap [1] . Additionally, this method offers a unique way to study the effect of point defects on superconducting and electronic properties in nickelates across rare-earth compositions, doping, and strain to disentangle intrinsic behavior from synthesis-related variability.

[1] Ranna et al., *PRL* **135**, 126501 (2025).

15 min. break

DS 15.7 Thu 11:15 HSZ/0003

Correlated electronic structure of $La_3Ni_2O_6$ and $La_3Ni_2O_{6.5}$

— •Frank Lechermann, Steffen Bötzel, and Ilya M. Eremin — Theoretische Physik III, Fakultät für Physik und Astronomie, Ruhr-Universität Bochum, Bochum, Germany

There are two known superconducting nickelate families, i.e. low-valence Ni($3d^{9-\delta}$) compounds and Ruddelsden-Popper (RP) compounds with Ni($3d^{8\pm\delta}$) valence. While both families host NiO_2 square planes, key difference is given by the missing apical oxygen atoms in the low-valence nickelates. A possible route to connect both nickelate families might be given by the reduction of the $La_3Ni_2O_7$ RP bilayer compound, i.e. by removing it's apical oxygens. Complete removal results in the $La_3Ni_2O_6$ compound, while taking out only half of the apical oxygens results in the $La_3Ni_2O_{6.5}$ compound. Both reduced materials are so far only scarcely characterized experimentally, but display quite intriguing correlation physics from theory. We will discuss the results of advanced first-principles many body calculations for these two nickelates, highlighting different mechanisms of Mott criticality as well as challenging low-temperature physics.

DS 15.8 Thu 11:30 HSZ/0003

Superconductivity governed by Janus-faced fermiology in strained bilayer nickelates

— •Siheon Ryee[1], Niklas Witt[2], Giorgio Sangiovanni[2], and Tim Wehling[1] — [1]University of Hamburg, Hamburg, Germany — [2]University of Würzburg, Würzburg, Germany

High-temperature superconductivity in pressurized and strained bilayer nickelates has emerged as a new frontier. One of the key unresolved issues concerns the fermiology that underlies superconductivity. On both theoretical and experimental sides, no general consensus has been reached, and conflicting results exist regarding whether the relevant Fermi surface involves a γ pocket—a hole pocket with d_{z^2}-orbital character centered at the Brillouin zone corner. Here, we address this issue by unveiling a Janus-faced role of the γ pocket in spin-fluctuation-mediated superconductivity. We show that this pocket simultaneously induces dominant pair-breaking and pair-forming channels for the leading $s_\pm$-wave pairing. Consequently, an optimal superconducting transition temperature T_c is achieved when the γ pocket surfaces at the Fermi level, placing the system near a Lifshitz transition. This suggests that superconductivity can emerge, provided the maximum energy level of the γ pocket lies sufficiently close to the Fermi level, either from below or above. Our finding not only reconciles two opposing viewpoints on the fermiology, but also naturally explains recent experiments on $(La,Pr)_3Ni_2O_7$ thin films, including the superconductivity under compressive strain, two conflicting measurements on the Fermi surface, and the dome shape of T_c as a function of hole doping.

DS 15.9 Thu 11:45 HSZ/0003

Bonding-antibonding $s_\pm$ superconductivity in bilayer nickelates: potential experimental signatures

— •Steffen Bötzel, Frank Lechermann, and Ilya Eremin — Ruhr-Universität Bochum, Bochum, Germnay

The discovery of high-T_c superconductivity in Ruddelsden-Popper bilayer nickelates under applied high pressure and/or compressive strain provides a promising platform to study the interplay of multiorbital intralayer and interlayer Cooper-pairing in bilayer systems. In particular, dominant interlayer pairing may naturally lead to a bonding-antibonding $s_\pm$-gap structure, which directly reflects the bilayer geometry. Such a scenario would produce characteristic experimental signatures that differ from *d*-wave type gap symmetries. In this contribution, we theoretically address the possible gap structures in bilayer nickelates and discuss how a interlayer-dominated bonding-antibonding $s_\pm$-gap structure can be potentially distinguished from a *d*-wave type pairing using experimentally observables.

DS 15.10 Thu 12:00 HSZ/0003

Interlayer interaction-driven $s^\pm$-to-d_{xy}-wave superconductivity in $La_3Ni_2O_7$ under pressure

— •Lauro B. Braz[1], George B. Martins[2], and Luis G. G. de V. D. Da Silva[1] — [1]Instituto de Física, Universidade de São Paulo, Rua do Matão 1371, São Paulo, São Paulo 05508-090, Brazil — [2]Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Minas Gerais 38400-902, Brazil

Experimental and theoretical progress on the normal-state properties of the high-temperature superconductor $La_3Ni_2O_7$ has provided evidence of strong interlayer interactions. To better understand the effects of interlayer interactions in $La_3Ni_2O_7$ under high pressure, we investigate a two-layer, two-orbital electron model that includes both intra- and interlayer Coulomb interaction terms within the framework of the matrix random-phase approximation. Our analysis reveals that interlayer interactions play a crucial role in determining the preferred superconducting pairing symmetry. Specifically, when interlayer interactions are included, a d_{xy}-wave pairing symmetry is favored over the $s^\pm$-wave symmetry, which was previously found to dominate in their absence. Furthermore, we find that interlayer interactions enhance interorbital pairing by incorporating contributions from all three electron pockets, which originate from both $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbital characters. This results in the emergence of nodes in the superconducting gap function - features absent in the $s^\pm$-wave state - ultimately stabilizing the d_{xy}-wave pairing symmetry.

DS 15.11 Thu 12:15 HSZ/0003

Incommensurate spin-fluctuations and competing pairing symmetries in $La_3Ni_2O_7$

— •Han-Xiang Xu[1] and Daniel Guterding[2] — [1]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing, China — [2]Technische Hochschule Brandenburg, Brandenburg an der Havel, Germany

The discovery of superconductivity in the bilayer nickelate $La_3Ni_2O_7$ under high pressure raises key questions about the pairing symmetry and microscopic mechanism. Using a three-dimensional multi-orbital Hubbard model including all Ni 3d and O 2p states, we analyze the superconducting instability within the random phase approximation. Spin fluctuations with incommensurate wave vectors $(\pi/2, \pi/2)$ and $(7\pi/10, 7\pi/10)$ coexist and compete, leading to nearly degenerate sign-changing $s_\pm$- and $d_{x^2-y^2}$-wave pairing channels. The leading symmetry depends sensitively on pressure and the ratio of Hund's rule to Coulomb interactions. Cooperative incommensurate fluctuations stabilize a $d_{x^2-y^2}$-wave state for realistic parameters, while their competition may explain the absence of magnetic order. These findings reconcile previous contradictory results and highlight the importance of careful model construction for bilayer nickelates.

[1] H.-X. Xu and D. Guterding, arXiv:2501.05254