# TT 52: Nickelates and Other Complex Oxides

Time: Friday 9:30–11:15 Location: H31

TT 52.1 Fri 9:30 H31

**High-temperature superconductivity and polymorph structures in $La_3Ni_2O_7$** — •Matthias Hepting[1], Pascal Puphal[1], Pascal Reiss[1], Niklas Enderlein[2], Yu-Mi Wu[1], Vignesh Sundaramurthy[1], Peter A. van Aken[1], Hidenori Takagi[1], Bernhard Keimer[1], Y. Eren Suyolcu[1], Björn Wehinger[3], and Philipp Hansmann[2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]University of Erlangen-Nürnberg, Erlangen, Germany — [3]ESRF, Grenoble, France

The recent discovery of high-temperature superconductivity in $La_3Ni_2O_7$ under high pressure has drawn considerable interest [1]. Using high-resolution synchrotron x-ray diffraction and scanning transmission electron microscopy, we observed that $La_3Ni_2O_7$ single crystals which show signs of filamentary superconductivity exhibit a crystal structure composed of alternating monolayer (ML) and trilayer (TL) units [2]. This lattice architecture diverges significantly from the previously assumed bilayer configuration [1]. In addition, we employed density functional theory to examine the distinct contributions of the ML and TL structural units to the electronic structure of the $La_3Ni_2O_7$ polymorph. In combination with recent angle resolved photoemission spectroscopy experiments [3], our findings set the stage for future investigations into unique properties of the ML-TL polymorph and the possibility of bulk high-temperature superconductivity.

[1] H. Sun et al., Nature 621, 493 (2023);
[2] P. Puphal et al., Phys. Rev. Lett 133, 146002 (2024);
[3] S. Abadi et al., arXiv:2402.07143

TT 52.2 Fri 9:45 H31

**Theory of potential impurity scattering in pressurized superconducting $La_3Ni_2O_7$** — •Steffen Bötzel[1], Frank Lechermann[1], Takasada Shibauchi[2], and Ilya Eremin[1] — [1]Theoretische Physik III, Fakultät für Physik und Astronomie, Ruhr-Universität Bochum — [2]Department of Advanced Materials Science, The University of Tokyo, Kashiwa, Chiba 277-8561, Japan

We study the effect of the point-like non-magnetic impurities on the superconducting state of La-327 and show that the interlayer $s_{\pm}$-wave and $d$-wave symmetries show a very different behavior as a function of impurity concentration, which can be studied experimentally by irradiating the La-327 samples by electrons prior applying the pressure. While $d-$wave superconducting state will be conventionally suppressed, the $s_{\pm}$-wave state shows more subtle behavior, depending on the asymmetry between bonding and antibonding subspaces. For the electronic structure, predicted to realize in La-327, the $s_{\pm}-$wave state will be robust against complete suppression and the transition temperature, $T_c$ demonstrates a transition from convex to concave behavior, indicating a crossover from $s_{\pm}$-wave to $s_{++}$-wave symmetry as a function of impurity concentration. We further analyze the sensitivity of the obtained results with respect to the potential electronic structure modification.

TT 52.3 Fri 10:00 H31

**Surface effects in infinite layer nickelates** — •Leonard M. Verhoff[1], Liang Si[1,2], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, Vienna, Austria — [2]School of Physics, Northwest University, Xi'an, China

Nickelates have emerged as a compelling platform for studying high-temperature superconductivity, drawing comparisons to cuprates. Infinite layer rare-earth (R) nickelates, $RNiO_2$, consist of an alternating stacking of $NiO_2$ layers and rare-earth spacing layers along the crystallographic $z$-axis. While their bulk structure has been extensively studied computationally, the samples that exhibit superconductivity in experiments are thin nickelate films. They are synthesized through a chemical reduction process that removes apical oxygen from perovskite $RNiO_3$, often grown on substrates such as $SrTiO_3$ (001).

We explore emerging surface effects by studying the formation of various surfaces within the framework of DFT. While perfect stoichiometry favors a $NiO_2$-terminated surface, the presence of excess apical oxygen in the surface region – possibly a remnant of the chemical reduction process – might favor an RO-terminated surface. The atomic structures of the studied surfaces strongly influence the local electronic structure in the surface region. These surface effects indicate the absence of an electron pocket around the $\Gamma$ point – even for $NdNiO_2$ surfaces, in contrast to DFT and *dynamical mean field theory* bulk calculations.

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TT 52.4 Fri 10:15 H31

**Uniaxial pressure dependencies of the metal-to-metal transition in $P2_1/a$ and $Bmab$ $La_4Ni_3O_{10}$ single crystals** — •Lukas Gries, Jan Arneth, Ning Yuan, Ahmed Elghandour, and Rüdiger Klingeler — Kirchhoff Institut for Physics, Heidelberg, Germany

The $n = 3$ Ruddlesden-Popper nickelate $La_4Ni_3O_{10}$ exhibits an intriguing metal-to-metal transition (MMT) accompanied by the evolution of intertwined charge and spin order [1]. We report report high-resolution capacitance dilatometry and magnetisation data on phase-pure single crystals of $P2_1/a$ and $Bmab$ $La_4Ni_3O_{10}$ grown by the high-pressure floating-zone method [2]. Our data show pronounced magnetoelastic coupling at the MMT for both phases. The extracted uniaxial pressure dependencies are negative for the $ab$ plane and positive along the $c$ axis. The uniaxial pressure dependencies are quantified and the relevant energy scales are investigated via Grüneisen scaling and Ehrenfest analysis.

[1] J. Zhang et al., Nat. Commun. 11, 6003 (2020)
[2] N. Yuan, et al., J Cryst. Growth 627, 127511 (2024)

TT 52.5 Fri 10:30 H31

**A versatile microscope for simultaneous optical and thermodynamic investigation of $Ca_3Ru_2O_7$** — •Simli Mishra[1], Elena Gati[1], Fei Sun[1], Hilary Noad[1], Dmitry Sokolov[1], Andrew Mackenzie[1,2], and Veronika Sunko[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]School of Physics and Astronomy, University of St. Andrews, St. Andrews, UK — [3]Department of Physics, University of California, Berkeley, California, USA

Ruddlesden-Popper-type ruthenates are well-known for hosting intriguing phenomena, including unconventional superconductivity, metal-insulator transitions, spin-orbit coupling, and strange metal behavior. Among these, the bilayer ruthenate $Ca_3Ru_2O_7$ is a polar metal that exhibits strong electronic correlations. It undergoes an antiferromagnetic transition at 56 K and a first-order structural phase transition at 48 K at ambient pressure.

In our experiments, we utilize a versatile, optics-based microscope with high spatial resolution, to investigate quantum materials. The setup has been integrated with a uniaxial pressure cell that enables pressure to be used as both a tuning parameter and a thermodynamic probe. Using this technique, we simultaneously measure the optical reflectivity and the elastocaloric effect to understand the behavior of $Ca_3Ru_2O_7$ as a function of temperature and uniaxial pressure.

TT 52.6 Fri 10:45 H31

**Designed cleaving planes in ruthenium dioxide for ARPES experiments** — •Marieke Visscher[1,2], Lea Richter[1], Sebastian Buchberger[2], Bruno Saika[2], Andy Mackenzie[1,2], and Phil King[2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, UK

Ruthenium dioxide has a complex band structure, underpinning a variety of phenomena including superconductivity under strain and a Dirac nodal line network. It has also been proposed as a candidate altermagnet, and although recent studies suggest it lacks the requisite magnetic order, it has been shown to host unusual spin-polarised states in its band structure. These phenomena motivate the need for more detailed studies into its electronic structure. Angle-resolved photoemission spectroscopy (ARPES) would be an ideal probe for this, but the three-dimensional structure of ruthenium dioxide makes it difficult to prepare atomically clean and flat surfaces with conventional methods. We have therefore investigated a fabrication method based on Focused Ion Beam (FIB) structuring to stimulate sample cleavage along desired crystallographic planes. With this method, we were able to obtain high quality surfaces, on which we performed ARPES measurements. With this new capability to tailor the sample cleavage, we

significantly improve the quality of ARPES data from this compound, opening new perspectives for studying its low-energy electronic structure.

TT 52.7 Fri 11:00 H31

**Localized Ti-4s molecular orbitals and correlated 3d states in the bad metal $TiO_x$** — •Daisuke Takegami[1,2], Anna Melendez-Sans[2], Takashi Miyoshino[1], Ryo Nakamura[1], Miguel Ferreira-Carvalho[3,2], Georg Poelchen[2], Chun-Fu Chang[2], Masato Yoshimura[4], Ku-Ding Tsuei[4], Haruka Matsumoto[5], Asuka Yanagida[5], Takuro Katsufuji[5], Liu Hao Tjeng[2], and Takashi Mizokawa[1] — [1]Department of Applied Physics, Waseda University, Japan — [2]Max Planck Institute for Chemical Physics of Solids, Germany — [3]Institute of Physics II, University of Cologne, Germany — [4]National Synchrotron Radiation Research Center, Taiwan — [5]Department of Physics, Waseda University, Japan

We have investigated the electronic structure of the rocksalt $TiO_x$ system using polarizationdependent hard x-ray photoelectron spectroscopy. The spectra showed a vanishingly small intensity at the Fermi level, classifying $TiO_x$ as a bad metal. With the main spectral features attributed to the $Ti^{2+}$ 3d2 configuration, we were able to detect spectroscopically also the co-existence of both Ti and O vacancies. The presence of $Ti^{3+}$ states were identified. It was a surprise not to find signs for Ti1+ entities. Instead a sharp occupied state of Ti 4s origin was unveiled in the valence band, which gave evidence that localized Ti-4s-based molecular orbitals are formed around the O vacancies. Our findings suggest that a defect free and stoichiometric TiO would have been a strongly correlated a Mott-Hubbard insulator, and that the 4s is an important degree of freedom for low-valent 3d materials.