TT 20: Focus Session: The Nickel Age of Superconductivity: Cuprates Reloaded or Something New?

Time: Tuesday 9:30–12:45 Location: HSZ 03

Invited Talk TT 20.1 Tue 9:30 HSZ 03
Superconductivity in infinite layer nickelates — •Harold Hwang — Stanford University and SLAC National Accelerator Laboratory

Ever since their discovery, superconductivity in cuprates has motivated the search for materials with analogous electronic or atomic structure. Here we present how soft chemistry approaches can be used to synthesize superconducting infinite layer nickelates from their perovskite precursor phase [1], using topotactic reactions. We will discuss our preliminary understanding of aspects that are similar and different from the cuprates, as well as initial exploration of the doping dependence of the phase diagram.

[1] D. F. Li, K. Lee, B. Y. Wang, M. Osada, S. Crossley, H. R. Lee, Y. Cui, Y. Hikita, and H. Y. Hwang, Nature 572, 624 (2019).

Invited Talk TT 20.2 Tue 10:00 HSZ 03
Materials design of dynamically stable d^9 layered nickelates — •Ryotaro Arita — Department of Applied Physics, University of Tokyo, Tokyo, Japan — RIKEN Center for Emergent Matter Science, Saitama, Japan

The recent discovery of superconductivity in the doped nickelate $Nd_{0.8}Sr_{0.2}NiO_2$ has stimulated renewed interest in unconventional superconductivity in layered correlated materials. Recently, we perform a systematic computational materials design of layered nickelates that are dynamically stable and whose electronic structure better mimics the electronic structure of high-T_c cuprates. While the Ni $3d$ orbitals are self-doped from the d^9 configuration in $NdNiO_2$ and the Nd-layer states form Fermi pockets, we find more than 10 promising compounds for which the self-doping is almost or even completely suppressed. We derive an effective single-band model for those materials and find that the system is in a strongly-correlated regime. We also investigate the possibility of palladate analogues of high-T_c cuprates. Once synthesized, these nickelates and palladates will provide a firm ground for studying superconductivity in the Mott-Hubbard regime of the Zaanen-Sawatzky-Allen classification, which will also help the understanding of the superconductivity in high-T_c cuprates realized in the charge-transfer regime.

Invited Talk TT 20.3 Tue 10:30 HSZ 03
Superconductivity in Nickelates: Similarities and Differences from Cuprates — •Michael Norman — Materials Science Division, Argonne National Laboratory, USA

The recent discovery of superconductivity in Sr-doped NdNiO2 has refocused attention on the relation of nickelates to cuprates. First, I review the experimental situation, including earlier work on trilayer nickelates, as well as the new work on infinite-layer nickelates. Next, I comment on various proposed models, including charge-transfer, Mott, and Kondo. Then, I relate these models to the electronic structure of nickelates, contrasting this with cuprates. Finally, I comment on relevant parameters in regards to the observation of superconductivity.

15 min. break.

Invited Talk TT 20.4 Tue 11:15 HSZ 03
Comparing the electronic structure and magnetism of hole doped Nickelate and Cuprate superconductorslate and Cuprate superconductors — •George Sawatzky, Mi Liang, Mona Berciu, Kateryna Foyevtsova, and Ilya Elfimov — Stuart Blusson Quantum Matter Institute Institute University of British Columbia Vancouver BC V6T1Z4,

Using the same theoretical methods used for the cuprates we investigate the electronic and magnetic structure and excitations of the new infinite layer $NdNiO_2$. We show that the nickelates are expected to be Mott Hubbard rather than charge transfer gap insulators provided that there are no other bands crossing the Fermi energy. In this case the much larger charge transfer energy will result in a strongly reduced superexchange interaction and also reduces the crystal field splittings of the d levels. This results in a near degeneracy of the triplet and singlet states for the hole doped nickelate . All these effects make the Nick=elates very different from the cuprates.

Invited Talk TT 20.5 Tue 11:45 HSZ 03
Doping infinite-layer nickelates: A superlattice approach — •Eva Benckiser — Max Planck Institute for Solid State Research, Stuttgart, Germany

Recently, the observation of superconductivity in strontium-doped $NdNiO_2$ thin films has attracted a lot of attention [1]. We have been working on a different approach to dope the infinite-layer nickelates, where we considered layer-selective, topotactically reduced rare-earth nickelate layer stacks in a superlattice structure with the aim to control the doping level by the stack thickness. In my talk I will present our results from x-ray spectroscopy together with *ab-initio* calculations of the layer-resolved, local nickel electronic configuration in these artificial superlattices and discuss similarities and differences to the electronic structure of copper in high-temperature superconductors.

[1] D. Li, K. Lee, B. Y. Wang, M. Osada, S. Crossley, H. R. Lee, Y. Cui, Y. Hikita, and H. Y. Hwang, Nature 572 (2019) 624

TT 20.6 Tue 12:15 HSZ 03
Topotactic hydrogen in nickelate superconductors and akin infinite-layer oxides $AB\mathbf{O}_2$ — •Karsten Held[1], Liang Si[1,2], Wen Xiao[2], Josef Kaufmann[1], Yi Lu[3], Jan M. Tomczak[1], and Zhicheng Zhong[2] — [1]Institute for Solid State Physics, TU Wien, Austria — [2]Chinese Academy of Science NIMTE, Ningbo, China — [3]Institute for Theoretical Physics, Heidelberg University, Germany

The seminal work by Li et al. [1] opens the door wide to the nickelate age of superconductivity. But it appears to be most difficult to reproduce. Since the chemical reduction of ABO_3 (A: rare earth; B transition metal) with CaH_2 may result in both, ABO_2 and ABO_2H, we calculate [2] the topotactic H binding energy by density functional theory (DFT). We find intercalating H to be energetically favorable for $LaNiO_2$ and $NdNiO_2$ but not for Sr-doped $NdNiO_2$.

This topotactical hydrogen turns the electronic structure upside down. Our DFT+dynamical mean field theory calculations show [2] that $3d^9$ $LaNiO_2$ is similar to (doped) cuprates, whereas $3d^8$ $LaNiO_2H$ is a two-orbital Mott insulator, similar to $LaNiO_3|LaAlO_3$ heterostructures prior to engineering their bandstructure to a cuprate-like one [3]. Topotactic H might hence explain why some nickelates are superconducting and others are not.

[1] D. Li et al., Nature 572, 624 (2019).
[2] L. Si, W. Xiao, J. Kaufmann, J.M. Tomczak, Y. Lu, Z. Zhong, K. Held, arXiv:1911.06917.
[3] P. Hansmann, X. Yang, A. Toschi, G. Khaliullin, O. K. Andersen, and K. Held, Phys. Rev. Lett. 103, 016401 (2009).

TT 20.7 Tue 12:30 HSZ 03
Role of interface polarity in the electronic reconstruction of infinite-layer vs. perovskite nickelate films on $\mathbf{SrTiO_3(001)}$ — •Benjamin Geisler and Rossitza Pentcheva — Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg

Motivated by the recent observation of superconductivity in the infinite-layer nickelate $NdNiO_2$ on $SrTiO_3(001)$ by Li *et al.* [1], we explore the effect of interface polarity on the electronic properties of $NdNiO_n/SrTiO_3(001)$ and $LaNiO_n/SrTiO_3(001)$ thin films ($n = 2, 3$) by performing first-principles calculations including a Coulomb repulsion term. For infinite-layer nickelate films ($n = 2$), electronic reconstruction drives the emergence of a two-dimensional electron gas (2DEG) at the interface due to a strong occupation of the Ti $3d$ states. This effect is more pronounced than in the paradigmatic $LaAlO_3/SrTiO_3(001)$ system and accompanied by a substantial reconstruction of the Fermi surface. We contrast our findings with results for the perovskite compounds ($n = 3$). Moreover, we analyze the topotactic reaction from a perovskite to an infinite-layer heterostructure and show why the reduction is confined to the nickelate film, whereas the $SrTiO_3$ substrate remains intact.

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[1] D. Li *et al.*, Nature **572**, 624 (2019)