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EINLADUNG zum IFP-SEMINAR

Nickelate superconductors - a renaissance of the one-band Hubbard model

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Ort: Für TU-Mitarbeiter:
Freihausgebäude der TU Wien
Wiedner Hauptstrasse 8-10
Seminarraum DB gelb 09
9. OG, gelbe Leitfarbe
Für Externe und Studierende:
via ZOOM,
https://tuwien.zoom.us/j/96297500262

Abstract:

The discovery of superconductivity in nickelates by the group of Harold Hwang in 2019 [1] marked the beginning of a new age of superconductivity, the nickel age. These novel (Sr-doped) $NdNiO_2$ superconductors are not only isostructural to the well known cuprate superconductor $CaCuO_2$ but also both, Ni and Cu, are formally $3d^9$ in the respective parent compound. In stark contrast to the cuprates, it proved difficult for other groups to reproduce superconductivity in nickelates. With density functional theory (DFT) and dynamical mean-field theory calculations we were able to show [2] that the novel nickelates are prone to the intercalation of hydrogen, and that this topotactic hydrogen turns the electronic structure upside down - making it disfavorable for superconductivity. Carefully removing the excess hydrogen then indeed turned out to be the key for other groups to synthesize superconducting nickelates as well [3].

At first glance, the nickelates appear to be more complicated than their cuprate peers. Besides the Ni $d_{\{x2 -y2\}}$ band that crosses the Fermi level, there are additional pockets around the *A* and at low doping possibly γ-moment that are of predominant Nd character. However, calculations including [2,4,5] indicate that these are merely passive bystanders and electron (hole) reservoirs, while the actual physics is governed by the Ni $d_{\{x2 -y2\}}$ band. This suggests, the most intensively studied model for superconductivity, the one-band Hubbard mode to be at the heart superconductivity in the nickelates, albeit with a properly adjusted doping because of the *A* -pocket. This is even more true than for the cuprates, where the close vicinity of the oxygen band indicates a charge transfer insulator and hence the Emery model as the basic model. On this presumption, with ab initio determined parameters and adjustment of the doping, we were able to predict the superconducting phase diagram in nickelates [5] even prior to experiments [4,6] to good accuracy. This gives us some hope that we are on a good way toward a more thorough understanding and reliable prediction of unconventional superconductors.

[1] D. Li et al., Nature 572, 624 (2019).
[2] L. Si et al., Phys. Rev. Lett. 124, 166402 (2020).
[3] S. Zeng et al., Phys. Rev. Lett. 125, 147003 (2020).
[4] J. Karp et al., Phys. Rev. X 10, 021061 (2020).
[5] M. Kitatani et al., npj Quantum Materials 5, 59 (2020)
[6] D. Li et al., Phys. Rev. Lett. 125, 027001 (2020).