

A first-principles study of nickelate superconductors

Hanghui Chen^{1, 2}

¹NYU-ECNU Institute of Physics, NYU Shanghai, Shanghai 200122, China

²Department of Physics, New York University, New York, New York 10012, USA

Email: hanghui.chen@nyu.edu

Abstract: The discovery of superconductivity in nickelates has drawn great attention. In this talk, I present our first-principles study on infinite-layer nickelates $RNiO_2$ (R is a rare earth element) and nickelate of Ruddlesden-Popper phase $La_3Ni_2O_7$. 1) We show that in $RNiO_2$, there is a substantial hybridization between Ni- d orbitals and conduction bands via an interstitial s orbital [1]. The consequences of this hybridization are i) an intrinsic charge order instability due to the charge transfer from Ni- d orbitals to conduction bands [2]; ii) a change in the Ni- d derived Fermi sheet from electron-like to hole-like along k_z direction; [3] and iii) a Van Hove singularity that enhances d -wave superconductivity. 2) We show that in $La_3Ni_2O_7$ under high pressure, the most favorable superconducting pairing symmetry is d_{xy} , if its DFT band structure is exactly reproduced by Wannier fitting [4]. More importantly, we find a strong sensitivity of pairing symmetry to the crystal field splitting between the two Ni e_g orbitals. A slight increase in Ni e_g crystal field splitting changes the pairing symmetry from d_{xy} to s_{\pm} [4]. Our work highlights the multi-orbital nature of nickelate superconductors, which leads to physical properties distinct from cuprate superconductors.

Reference:

- [1] Yuhao Gu, Sichen Zhu, Xiaoxuan Wang, Jiangping Hu, Hanghui Chen, “A substantial hybridization between correlated Ni- d orbital and itinerant electrons in infinite-layer nickelates”, *Communications Physics* **3**, 84 (2020).
- [2] Hanghui Chen, Yi-feng Yang, Guang-Ming Zhang and Hongquan Liu, “An electronic origin of charge order in infinite-layer nickelates”, *Nature Communications* **14**, 5477 (2023).
- [3] Wenjie Sun, Zhicheng Jiang, Chengliang Xia, Bo Hao, Yueying Li, Shengjun Yan, Maosen Wang, Hongquan Liu, Jianyang Ding, Jiayu Liu, Zhengtai Liu, Jishan Liu, Hanghui Chen, Dawei Shen, Yuefeng Nie, “Electronic Structure of Superconducting Infinite-Layer Lanthanum Nickelates”, arXiv:2403.07344 (2024).
- [4] Hongquan Liu, Chengliang Xia, Shengjie Zhou, Hanghui Chen, “Role of crystal-field-splitting and long-range-hoppings on superconducting pairing symmetry of $LaNiO$ ”, arXiv:2311.07316 (2023).