INSTITUT NEEL Grenoble

Proposition de stage Master 2 - Année universitaire 2024-2025

General Scope

The discovery of superconductivity in the nickelates has led to one of the most active topics of research in condensed matter physics in the last two years (see e.g. [1]). These systems open new exciting perspectives to eventually understand the fundamentals ofunconventional superconductivity in oxides [2]. Recently, high-temperature superconductivity of up to ~80 K was discovered in the double-layer ruddelsden-popper Nickelate La3Ni2O7 under pressure [3]. The hypothesis is that emergence of superconductivity under pressure is directly linked to the octahedral tilts present in these materials and their influence on the electronic properties of the materials respectively such as the crystal field (see fFg 1).

In this project, we aim to use electronic structure calculations using density functional theory in combination with machine learning methods in order to construct from first-principles theory the structural phase diagram as a function of pressure and temperature and its relationship to the electronic structure of the materials.

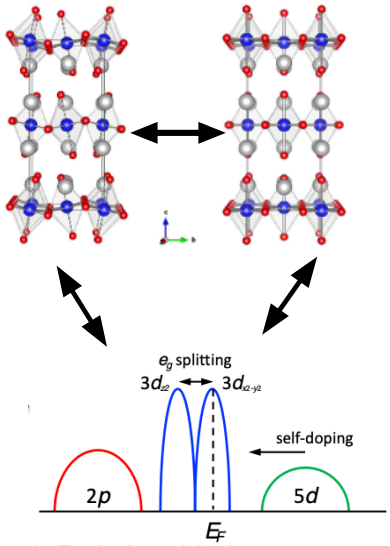

Fig 1: Relationship between crystal structure and electronic structure

This will allow us to unveal the intricate relationship between the structural and electronic properties and the superconductivity, which will bring us a step closer to understand the unconventional superconductivity in the novel Nickelate superconductors.

[1] Nickelate superconductors: an ongoing dialog between theory and experiments, A. S. Botana, F. Bernardini, and A. Cano, JETP 159, 711 (2021); arXiv:2012.02764

[2] Preempted phonon-mediated superconductivity in the infinite-layer nickelates, Q.N. Meier, JB de-Vaulx et al,Phys. Rev. B 109, 184505 (2024)

[3[Signatures of superconductivity near 80 K in a nickelate under high pressure, Hualei Sun, Mengwu Huo, et al Nature 621, 493 (2023)

Research topic and facilities available

The internship will be carried out at the Condensed Matter Theory (TMC) group at Institut NEEL. The available facilities include a HPC local cluster for the numerical calculations.

Possible collaboration and networking

The internship will be carried out in the framework of an ongoing national and international collaboration that includes theoreticians from U. Cagliari (Italy) and U. Arizona (USA) and experimentalists (Institut NEEL & ICMCB, CNRS Bordeaux).

Possible extension as a PhD

Yes

Required skills

Theory. Solid state physics. Numerical calculations. Machine learning

Starting date 01/09/2023 (tentative)

Contact

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