PhD position

Theoretical modelling of superconducting nickelates:

Effects of doping from atomic substitution, disorder and dimensionality effects, computation of physical observables, Fermi surface reconstructions and instabilities.

Keywords: *condensed-matter, theoretical modelling, superconductivity, electronic correlations, disorder, dimensionality.*

Scientific context:

Superconductivity is a macroscopic quantum state of matter with fascinating signatures including zero resistance and expulsion of magnetic flux. After the revolutionary discovery of superconductivity with high critical temperature (Tc) in cuprates, few decades ago, the possibility of replacing copper by nickel has rapidly emerged. Indeed, both elements are neighbors in the periodic table. This aim of realizing cuprate analogue superconductors remained unsuccessful for a long time, but the situation started to change recently when superconductivity was first reported in a $LaNiO_3/La_{0.7}Sr_{0.3}MnO_3$ superlattice. Then a breakthrough came in 2019 with the report of superconductivity up to Tc=15K in a film $Nd_{0.8}Sr_{0.2}NiO_2$. These pioneering results have now been reproduced and enlarged to other systems, opening a new era in the research on superconductivity, with more than one hundred published articles [1].

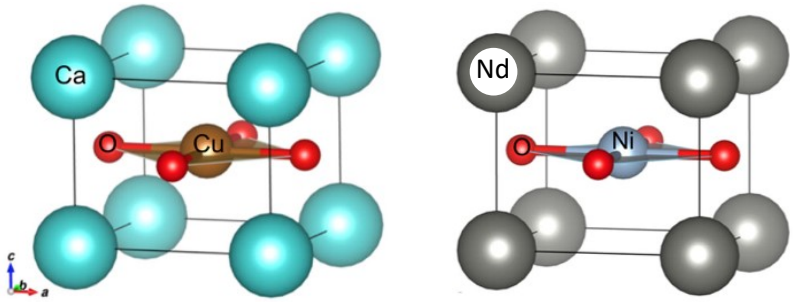
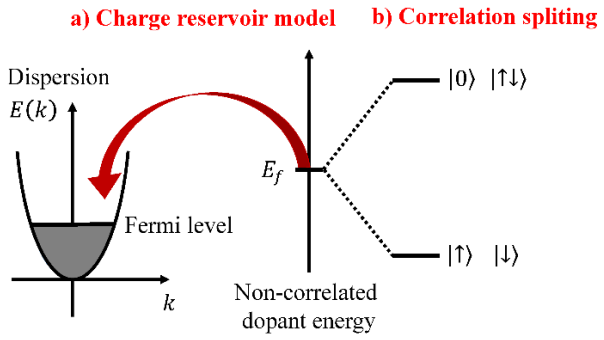


Figure 1:
Crystal structure of the cuprate $CaCuO_2$ (left) and the nickelate $NdCuO_2$ (right). In both cases superconductivity can be realized by doping.

Similar to CuO_2 layers in cuprates, NiO_2 layers in nickelates form a square lattice with Ni^+ ions in a d^9 electronic configuration (see Fig.1). In both cases superconductivity is achieved by doping a parent compound, here $NdNiO_2$, showing strong electronic correlations. But nickelates present also specificities, such as the possible absence of magnetic order in the undoped parent, and different Fermi surface and correlation strengths. Furthermore, since doping is realized by atomic substitution of rare-earth (Nd substitution), new effects may emerge, resulting from disorder and electronic correlations from the rare-earth (see fig.2).

Figure 2:



a) Schematic description of a «charge reservoir» doping of a metallic system by inserting impurities with an electronic level energy E_f. The Fermi level energy is tuned phenomenologically in order to incorporate the impurity holes or electrons in the Fermi surface.

b) Schematic description of the local energy splitting on a strongly correlated impurity that behaves like a Kondo impurity : the local charge is locked to 1 due to Coulomb repulsion, but a Kondo resonance may occur at low temperature, entangling the impurity with conduction electrons.

Project:
Since the discovery of superconductivity in nickelates, various *ab initio* calculations have been published, providing relevant information on the electronic band structure and the stability of crystal structures and interfaces. In most of these theoretical studies, doping is modelled as a static charge reservoir effect, by simply shifting the Fermi energy level.
In this Phd project, atomic substitution will be modelled using a complementary approach which takes into account effects of disorder and strong electronic correlations. For this purpose, we will study phenomenological model Hamiltonians (Kondo and Hubbard) focusing on an appropriate description of microscopic interactions between d electrons from Nickel and f electrons from the rare-earth.
The theoretical method will adapt and generalize the Dynamical Mean Field Theory (DMFT) approach that we have developed previously for studying substitution effects in Kondo alloys [2]. One of the goals is to predict rich temperature-pressure-doping phase diagrams for nickelates, and to analyze non-linear and disorder effects induced by substitution, like Fermi surface reconstructions. We also expect to discover exceptional points (Fermi arcs, pseudogaps, etc…) as well as quantum phase transitions including superconducting instabilities. The model parameters will be first chosen phenomenologically, then more quantitative calculations will be implemented using *ab initio* parameters computed by our collaborators.

Collaborations:
This theoretical PhD work is part of the project SUPERNICKEL which is granted by the French national research agency (ANR). It will be performed in tight and regular collaboration with the french experimental teams expert in the field, which synthesize and characterize nickelates, especially in the following laboratories: ICMCB (Bordeaux), Institut Néel (Grenoble), CRISMAT (Caen), ISMO (Orsay), GEMAC (Versailles).

Profile:
We are looking for a very motivated student, with a Master in Physics, a solid background in condensed-matter, and interests in theoretical modelling.
With this PhD project, the student will acquire expertise in the field of unconventional superconducting materials, and more generally on quantum materials with strongly correlated electrons. In an international research environment, this project will also provide an opportunity for discovering and using methods of calculations that are developed for modelling quantum and disordered materials. Depending on the profile and wishes of the PhD student, the project can be oriented either to mainly analytical developments with relatively light numerics, or to more numerical developments.

Practical aspects:
The PhD thesis can start **from October 1st 2021**, at the Laboratory **LOMA, Bordeaux University and CNRS**. Income: CNRS Phd-student salary

To apply, please send us an email with your CV, a letter of motivation and the transcript of marks of your Master. **Applications will be reviewed as received, with the position remaining open untill filled**:
Advisor **:** Sébastien Burdin (LOMA, Bordeaux) - sebastien.burdin@u-bordeaux.fr
Collaboration with Claudine Lacroix (Institut Néel, Grenoble) - claudine.lacroix@neel.cnrs.fr

References:
[1] https://gdr-meeticc.cnrs.fr/2019/11/09/bibliographie-supraconductivite-dans-les-nickelates/
[2] Burdin S and Fulde P, Phys. Rev. B 76, p104425 (2007); Burdin S and Lacroix C, Phys. Rev. Lett. 110, p226403 (2013); Burdin S and Lacroix C, J. Phys.: Condens. Matter 31, p395601 (2019); Poudel B, Zwicknagl G, Lacroix C and Burdin S, J. Magn. Magn. Mater. 520, p167405 (2021) ; Poudel B, Lacroix C., Zwicknagl G and Burdin S, New J. Phys. 23, p 063073 (2021).