Physics of (Nd,Sr)NiO_2 phases by theoretical and experimental approaches

Transition metal oxides exhibit a wide range of properties such as magnetism, ferroelectricity or superconductivity, coexisting within in a reduced number of structural families. In particular, ABO_3 perovskite oxides have attracted widespread interest from the community due to its great structural flexibility, but also because it is relatively simple to develop as thin films or heterostructures combining several materials exhibiting strong couplings between them and unprecedented properties at interfaces.

Beyond perovskites in which transition metal ions are surrounded by an oxygen cage octahedra within a three dimensional network, several oxides exhibit a two-dimensional organization of cations and anions, and this is the case of the "infinite-layer" compounds of ABO_2 chemical formula. These materials are the building blocks of the high critical temperature superconducting cuprates ($SrCuO_2$) [Nature **351**, 549 (1991)] once properly doped. However, they remain less studied than the classical ABO_3 oxide perovskites.

Very recently, a new phase of the "infinite-layer" family has been identified as a new superconductor [Nature **572**, 624 (2019)] : the Sr doped $NdNiO_2$ material. This discovery crowns ten years of research of superconductivity in Ni-based oxides [PRL **100**, 016404 (2008)] and paves the way toward the identification of new oxide superconductors.

The proposed thesis subject aims to understand the physics of (Nd, Sr)NiO_2 compounds and the origin of the superconducting phase. According to the results obtained, other perovskites, involving materials similar to the rare earth nickelates $RNiO_3$ (R = Lu-La, Y) could be explored in their "infinite layer" phase. The thesis will be organized in two parts. The first part will be theoretical and mainly carried out at the Laboratoire de Cristallographie et Sciences des Matériaux (CRISMAT, W. Prellier, J. Varignon, http://www-crismat.ensicaen.fr). This main part will be based on electronic structure *first-principles* calculations carried out within the framework of the density functional theory (DFT) allowing to identify structural, magnetic and electronic properties of $NdNiO_2$ in bulk and under strontium doping. The second part will be experimental and mainly conducted at Unité Mixte de Physique CNRS/Thales (UMPHy, M. Bibes, http://oxitronics.cnrs.fr). This part will be devoted to the development of "infinite layer" phases in the form of thin layers using pulsed laser deposition, followed by an *ex situ* annealing in a hydrogen-rich atmosphere by CaH_2 decomposition. The samples will be characterized by X-ray diffraction, magnetotransport measurements and X-ray spectroscopy at UMPHy.

The candidate should have a strong background in condensed matter physics and be familiar with numerical simulations (notably on DFT). In addition, some knowledge in the development of thin layers and their structural characterization would be *a plus*.

Contacts :

- Wilfrid Prellier, CRISMAT, CNRS Research Director, Lab director wilfrid.prellier@cnrs.fr
- Julien Varignon, CRISMAT, Assistant Professor ENSICAEN, julien.varignon@ensicaen.fr
- Manuel Bibes, Unité Mixte de Physique CNRS/Thales, CNRS Research Director, manuel.bibes@cnrs-thales.fr