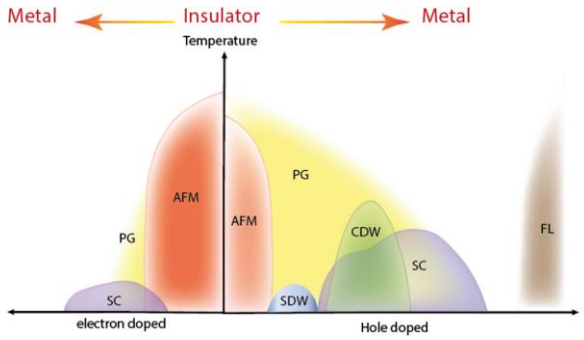
NÉEL INSTITUTE Grenoble

Topic for Master 2 internship – Academic year 2024-2025

High temperature superconducting oxychlorides: a model for the electronic structure of cuprates

General Scope: High-Tc superconductivity in cuprates is one of the most challenging topics in modern physics. Despite extensive research, their underlying mechanisms remain poorly understood. These quantum materials not only demonstrate high critical temperatures at ambient pressure but also feature some of the most complex phase diagrams (Figure 1).



In this context, the discovery of Na- and vacancy-doped $Ca_2CuO_2Cl_2$ oxychloride is highly promising to bridge the gap between theory and experiment. This is primarily due to its exceptionally simple crystal structure, which remains stable across all doping levels and temperatures, and its strong two-dimensional character, stemming from the replacement of apical oxygen by chlorine. As a result, advanced calculations that incorporate correlation effects, such as quantum Dynamical Mean Field Theory (DMFT), become more accessible and effective.

So far, there has been only a limited experimental investigation of $Ca_2CuO_2Cl_2$, focusing on a narrow range of doping levels [1]. In this project, we aim to examine how the electronic structure evolves across different phases, including superconductivity, the pseudogap, and the strange metal phase.

Research topic and facilities available: During this internship, we will further investigate the fermiology of these materials using static Angle-Resolved Photoemission Spectroscopy (ARPES) at the Laboratoire Physique des Solides, in close collaboration with the PULS group. This follows up on our previous experiment conducted at the CASSIOPEE synchrotron source (SOLEIL, Saint Aubin), which was incomplete due to time constraints but yielded promising preliminary results [2].

As part of the PhD project, we will expand our investigation into out-of-equilibrium dynamics using time-resolved ARPES (trARPES) at LPS (Orsay) to monitor the ultrafast behavior of quasiparticles. Additionally, we aim to manipulate the electronic properties with ultrafast pulses, exploring potential light-induced phase transitions.

Preparing for these experiments will require special attention, as the materials are sensitive to air. We will utilize a specialized glove box at the Néel Institute for handling them. Additionally, we will conduct crystalline characterization through X-ray diffraction and superconducting characterization using magnetometry. Transport measurements will be performed at LPS (Orsay).

Possible collaboration and networking: Interpretation of the results could be made in collaboration with group performing *ab-initio* electronic structure calculation including correlation effects in Paris (S. Biermann, Ecole Polytechnique). Sample synthesis will be made in collaboration with the group of Prof. H. Yamamoto (Tohoku University, Sendai, Japan) and Prof. M. Azuma (Tokyo Inst. of Technology), as well as collaborators at Inst. Néel.

Possible extension as a PhD: Yes, this project is part of a PhD program, of which this Master Internship could be a first approach.

Required skills: A good background in electronic properties of material, with the will to have a global approach, from material synthesis and characterization to advanced spectroscopic properties. Teamwork will be an essential part of the project's success.

Starting date: from Winter 2025

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Bibliography:

[1] A. Damascelli, Z. Hussain, Z.-X. Shen, *Rev. Mod. Phys.* **75**, 473 (2003)
[2] B. Bacq-Labreuil, *et al. hal-04362638* (2024)