INTERNSHIP PROPOSAL

Laboratory name: Institut de minéralogie, de physique des matériaux et de cosmochimie (IMPMC), Sorbonne Université – CNRS – MNHN
CNRS identification code: UMR 7590
Internship director's name: Benjamin Lenz
e-mail: benjamin.lenz@upmc.fr Phone number: 01 44 27 98 19
Co-supervisor: Léo Gaspard (leo.gaspard@sorbonne-universite.fr)
Web page: https://impmc.sorbonne-universite.fr/en/research_teams/quantum-theory-of-matter.html
Internship location: Sorbonne Université, 4 place Jussieu, 75005 Paris

Thesis possibility after internship: YES
Funding: NO

Simulating the current-driven insulator to metal transition of Ca_2RuO_4

Ca_2RuO_4 is a quasi two-dimensional layered perovskite, which has a Mott insulating ground state at ambient conditions. Upon heating, it undergoes an insulator to metal transition at T_{IMT} ~ 360 K, which coincides with a structural transition from short to long **c**-axis and involves orbital ordering[1]. Recent experiments have revealed a **current-induced transition** leading to a metallic phase (denoted L*) that is electronically and structurally distinct from the thermally driven metallic phase[2]. In this phase, the insulating (metallic) state exhibits a slightly larger (smaller) **c**-axis compared to the zero-current counterparts, entailing modifications of its electronic structure. However, despite detailed experimental investigations and first theoretical studies, a comprehensive understanding of the material's electronic properties in the L* phase is still lacking. In particular, the nematic Fermi surface measured experimentally remains puzzling (see Figure).

The objective of this Master thesis is the application of state-of-the art numerical techniques to describe the L* phase of Ca_2RuO_4, focussing on the aspect of nematicity that has been observed experimentally. The **first principle theoretical study of Ca_2RuO_4** will involve density functional theory (DFT) calculations, in order to derive and parametrize an effective low-energy model using a combination of Wannier functions and constrained Random Phase Approximation (cRPA). The model will then be solved using **dynamical mean-field theory** (DMFT) to describe the evolution of the correlated electronic states across the transition. Results of the simulations will be confronted with angle-resolved photoemission spectra (ARPES) that have been measured experimentally.

[1] Gorelev, E. et al. *Phys. Rev. Lett.* **104**, 226401 (2010) ; [2] Suen, C. T. et al. *Nat. Phys.* **20**, 1757–1763 (2024).

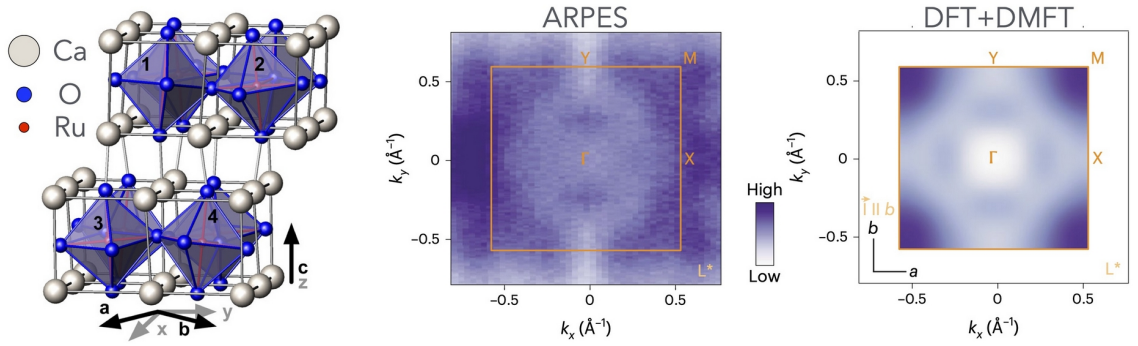

Figure: (Left) Crystal structure of Ca_2RuO_4 featuring rotated, distorted RuO_6 octahedra; (Centre) angle-resolved photoemission spectrum of the Fermi surface in the L phase showing a clear x-y asymmetry ; (Right) first DFT+DMFT calculation of the Fermi surface in the L* phase, not capturing this asymmetry. Figures taken from Refs. 1&2.*

Condensed Matter Physics:	YES	Soft Matter and Biological Physics:	NO
Quantum Physics:	MAYBE	Theoretical Physics:	YES