SCIENCES SORBONNE UNIVERSITÉ

2020-2021

Master thesis proposal

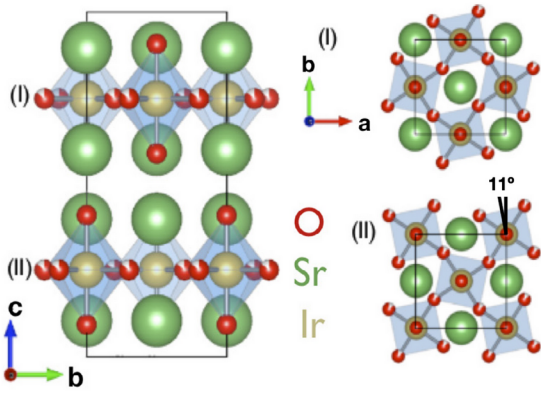
Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
Tower 23 - 4th floor -23-22
Director: Guillaume Fiquet

Title: Interplay of spin-orbit coupling and electron correlations in Sr_2IrO_4

Keywords: Iridates, dynamical mean-field theory, first-principles calculations, strongly correlated electron systems

Scientific description:
The iridate Sr_2IrO_4 has attracted a lot of interest in recent years due to its unique quantum entangled groundstate, which is caused by the interplay of spin-orbit coupling, structural distortions and Coulomb correlations. A realistic description of electronic and magnetic properties of Sr_2IrO_4 can be obtained from combining first-principles density functional theory calculations with many-body methods that can account for the strong electron-electron interactions inherent to the Ir 5d shell.
The technique of choice for the present internship will be a cluster extension of dynamical mean-field theory that we introduced recently[1]. Although the qualitative behaviour of many electronic and magnetic properties could already be correctly reproduced by considering a model which is based on a single quantum entangled band, experiments using angle-resolved photoemission spectroscopy[2] and polarized neutron diffraction[3] casted parts of this interpretation into doubt.
In this project, we aim at investigating a more complete description in terms of a multi-band model. Our goal will finally be to determine more precisely the role that orbital degrees of freedom play in the description of electronic and magnetic properties of Sr_2IrO_4.



[1] B Lenz *et al* 2019 *J. Phys.: Condens. Matter* **31** 293001
[2] A Louat *et al* 2019 *Phys. Rev. B* **100** 2015135 (→preprint)
[3] J Jeong *et al* 2020 *Phys. Rev. Lett.* **125** 097202 (→preprint)

Techniques/methods in use: Dynamical mean-field theory; density functional theory
Applicant skills: Background in solid-state or material physics; strong interest in theory and simulations; basic programming skills; basic skills in density functional theory useful, but not required
Industrial partnership: No

Internship supervisors:Benjamin LENZ (✉: benjamin.lenz@upmc.fr, ☎: 01 44 27 98 19, 🖳: www.impmc.upmc.fr/~lenz/), Michele CASULA
Internship location: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, Campus Jussieu

Possibility for a Doctoral thesis: Yes, to be discussed with the applicant