

INTERNSHIP PROPOSAL

Laboratory name: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie
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Internship location: Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie
(IMPMC), Sorbonne Université, Campus Jussieu, Paris
Thesis possibility after internship: YES
Funding: NO, see with doctoral school

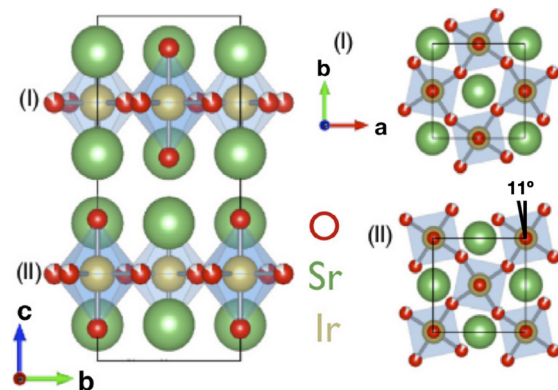
Interplay of spin-orbit coupling and electron correlations in Sr₂IrO₄

The iridate Sr₂IrO₄ 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 Sr₂IrO₄ 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 Sr₂IrO₄.

- [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)



Condensed Matter Physics: <u>YES</u>	Soft Matter and Biological Physics: NO
Quantum Physics: YES	Theoretical Physics: <u>YES</u>