

*Séminaire AXE 1 - Sciences et Matériaux Quantiques*



**Mardi 14 Avril 2026 | 11:00 | Auditorium de l'IPCMS**

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***Iridates in the light of dynamic mean-field theory: from low-energy models and the Mott transition to the spectroscopic signatures of spin polarons***

In the quest for exotic phases of matter, iridates hosting a spin-orbit entangled  $j_{\text{eff}}=1/2$  ground state have been in the spotlight for several years. In particular the parallels between their low-energy physics and that of high-temperature superconducting cuprates have led to an increased interest both from experiment and theory. For the latter, the interplay of spin-orbit coupling, Coulomb interactions and crystal-field terms renders the simulation of electronic properties of these systems a challenging endeavor, necessitating methods that go beyond density functional theory.

In this talk, I will first introduce two prototypical iridates,  $(\text{Ba,Sr})_2\text{IrO}_4$ , and discuss the validity of single- or few-band models which were proposed to capture their low-energy physics. A particular focus will be set on the Mott metal-insulator transition in these models as studied via a combination of different *ab initio* techniques with dynamical mean-field theory. In a second part, we will have a look at the antiferromagnetic low-temperature phase of the material and revisit the question of its nature – are  $(\text{Ba,Sr})_2\text{IrO}_4$  actually Slater or Mott insulators? Finally, I will discuss the consequence of coherent low-energy quasiparticles, so-called spin-polarons, on the optical conductivity and shed new light on the characteristic two-peak structure measured for iridates.

F. Cassol et al., Phys. Rev. B **109**, 155120 (2024)

F. Cassol et al., arXiv: **2509.20337** (2025)

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