

Role of nonlocal Coulomb correlations in pure and electron-doped Sr_2IrO_4

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The quasi-2D spin-orbit system Sr_2IrO_4 has raised tremendous interest recently, due to intriguing similarities to the high- T_c superconducting copper oxides. We study the evolution of the electronic structure of this material using a combination of ab initio density functional theory and many-body techniques. The effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions are included on a first-principles level. We calculate the momentum-resolved spectral function and compare to recent angle-resolved photoemission data, finding good agreement with experiment. Furthermore, we study the evolution of the electronic structure of Sr_2IrO_4 upon electron-doping. We show that short-range antiferromagnetic fluctuations are crucial to account for the electronic properties of the material even in the high-temperature paramagnetic phase. The emerging exotic metallic state exhibits pseudo-gap spectral features in good agreement with experiments on La-doped Sr_2IrO_4 , for which we propose a surprisingly simple theoretical mechanism.

- [1] C. Martins, B. Lenz, L. Perfetti, V. Brouet, F. Bertran, and S. Biermann, Nonlocal Coulomb correlations in pure and electron-doped Sr_2IrO_4 : Spectral functions, Fermi surface, and pseudo-gap-like spectral weight distributions from oriented cluster dynamical mean-field theory, *Phys. Rev. Materials* **2**, 032001 (2018)

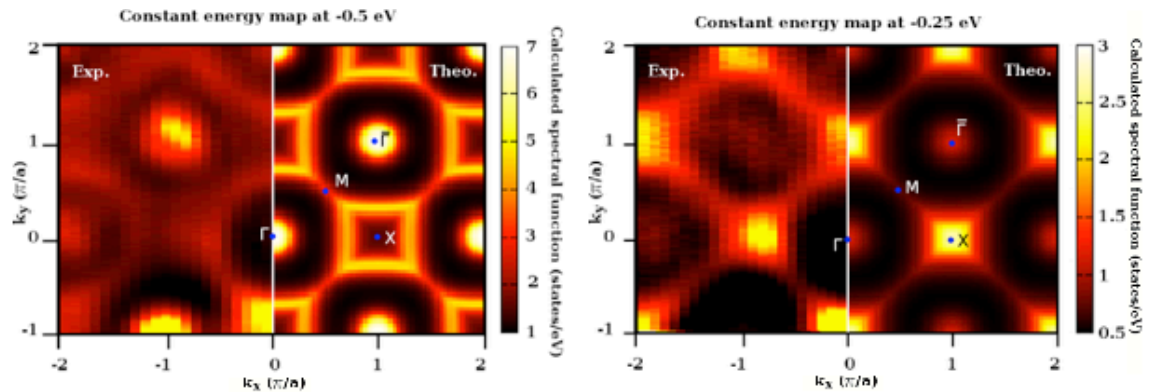


Figure 1: Constant energy maps of the spectral density at -0.5eV (left) and -0.25eV of undoped Sr_2IrO_4 . Experimental and theoretical spectral densities show good agreement.