

Electronic Structure of Iridates: a combined Density Functional Theory Dynamical Mean Field Theory Point of View

Silke Biermann

CPHT, Ecole Polytechnique

In recent years, the field of electronic structure calculations for correlated electron materials has seen great progress due to the advent of combinations of many-body theory such as dynamical mean field theory (DMFT) and density functional theory (DFT). Specifically, for iridates, combined DFT+DMFT has allowed to give a quantitative meaning to the effective single-orbital problem [1] arising in some compounds, and to obtain estimates for spectral or optical properties. In this talk, we will give an introduction to DMFT and its use in electronic structure calculations. We will focus on strategies for modelling complex oxides and discuss the notion of an effective orbital degeneracy. Current topics, such as the calculation of the effective local Coulomb interactions ("Hubbard U") will be explained [2].

[1] C. Martins, M. Aichhorn, L. Vaugier, S. Biermann, Phys. Rev. Lett. 107, 266404 (2011)

[2] L. Vaugier, H. Jiang, S. Biermann, Phys. Rev. B 86, 165105 (2012)