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Spin-orbital polarization in paramagnetic transition metal oxides: Sr_2IrO_4 versus Sr_2RhO_4

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We discuss the notions of spin-orbital polarisation and ordering, and adress their consequences in transition metal oxides. Extending the combined density functional and dynamical mean field theory (DMFT) scheme as implemented in [1] to the case of materials where spin-orbit interactions are important, we investigate the electronic excitations of the paramagnetic phases of Sr_2IrO_4 and Sr_2RhO_4. We show that the interplay of spin-orbit interactions and structural distortions suppresses spin-orbital fluctuations to the extent, that the resulting state in Sr_2IrO_4 is a paramagnetic spin-orbital ordered Mott insulator. In Sr_2RhO_4, they lead to a reduced effective band degeneracy, but still keep the material in a (spin-orbitally polarized) metallic state. Studying these two compounds with time-resolved X-ray diffraction and time-resolved photo-emission would be of great interest to understand spin-orbital polarisation and ordering even better.

Références

[1] M. Aichhorn, L. Pourovskii, V. Vildosola, M. Ferrero, O. Parcollet, T. Miyake, A. Georges, and S. Biermann, "Dynamical mean-field theory within an augmented plane-wave framework: Assessing electronic correlations in the iron pnictide LaFeAsO", Phys. Rev. B **80**, p. 0.85101 (2009).