Spin-orbit Coupling within Dynamical Mean-Field Theory: Coulomb Correlations in 4d and 5d Transition Metal Oxides

C. Martins,[1,2,*] M. Aichhorn,[3] and S. Biermann[1,2]

[1] *Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France.*
[2] *Japan Science and Technology Agency, CREST, Kawaguchi 332-0012, Japan.*
[3] *Institute of Theoretical and Computational Physics, TU Graz, Graz, Austria.*
[*] *New address: CEA, DAM, DIF, F-91297, Arpajon, France.*

We present an approach that extends the combined local-density approximation (LDA) and dynamical mean-field theory (DMFT) scheme to the case of materials with large spin-orbit (SO) interactions. The LDA+DMFT implementation developed in the framework of the full-potential linear augmented plane-wave method by Aichhorn *et al.* [1] can now be applied to systems where the correlated Wannier orbitals must be built out of local orbitals defined in the strong spin-orbit coupling limit. The screened Coulomb interaction and Hund's coupling are evaluated consistently from a first-principles constrained random-phase approximation scheme [2].

Using this LDA+SO+DMFT implementation, in conjunction with a continuous-time quantum Monte Carlo algorithm, we investigate the electronic excitations in the paramagnetic phases of strontium iridate (Sr_2IrO_4) and strontium rhodate (Sr_2RhO_4). We show that the interplay of spin-orbit interactions, structural distortions and Coulomb interactions suppresses spin-orbital fluctuations. As a result, the room temperature phase of Sr_2IrO_4 is a paramagnetic spin-orbitally ordered Mott insulator. In Sr_2RhO_4, the effective spin-orbital degeneracy is reduced, but the material remains metallic, due to both, smaller spin-orbit and smaller Coulomb interactions. Our *ab initio* calculations for both compounds are in excellent agreement with photoemission data [3].

[1] M. Aichhorn, L. Pourovskii, V. Vildosola, M. Ferrero, O. Parcollet, T. Miyake, A. Georges, and S. Biermann, Phys. Rev. B **80**, 085 101 (2009).

[2] L. Vaugier, H. Jiang, and S. Biermann (to be published).

[3] C. Martins, M. Aichhorn, L. Vaugier, and S. Biermann, Phys. Rev. Lett. **107**, 266 404 (2011).

Contact: cyril.martins@cea.fr