Calculation of effective interaction among different electronic shell using cRPA in ABINIT

R. Outerovitch and B. Amadon

CEA, DAM, DIF, F-91297 Arpajon, France

The calculation of the Hubbard $U$ and Hund $J$ parameters used in DFT+U or DFT+DMFT has been implemented in ABINIT using the constrained Random Phase Approximation in 2014 [1]. This implementation only considers intra-shell correlation ($f-f$ in Ce for example).

We present here a work on the generalization of this implementation that allows us to perform inter-shell interaction calculation. In general, inter-shell interactions can be computed on a single atom (e.g. $f-d$ in Ce), or on different atom site (e.g. Ni$d$-Op in NiO)[2]. This new implementation is based on the extension of Projected Localized Orbital Wannier functions to several atoms and orbitals, previously implemented in ABINIT[3].

The role of those inter-shell interactions has rarely been discussed in the literature, but has been proved to be non-negligible ($U^{fd} = 1.8$ eV in Ce)[2]. We hope that the ability to calculate those terms from first principle will allow us to quantitatively explain the difficulties that DFT+U or DFT+DMFT face when treating some correlated materials.

References

