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

R. Outerovitch[1] and B. Amadon [1]

[1] 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*-O*p* 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

[1] B. Amadon, T. Applencourt, F. Bruneval, Phys. Rev. B **89**, 125110 (2014).

[2] P. Seth, P. Hansmann, A. van Roekeghem, L. Vaugier, and S.Biermann, Phys. Rev. Lett. **119**, 056401 (2017).

[3] B. Amadon, A. Gerossier, Phys. Rev. B **91**, 161103(R) (2015).