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

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Résumé

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. 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-O in NiO).
This new implementation is based on the extension of Projected Localized Orbital Wannier functions to several atoms and orbitals, previously implemented in ABINIT.

The role of those inter-shell interactions has rarely been discussed in the literature, but has been proved to be non-negligible (1.8 eV in Ce). 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.

Mots-Clés: corrélations, DMFT, Wannier, cRPA

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