O.2 DFT+DMFT implementation in ABINIT: Update on implementations and applications

Bernard Amadon¹

¹ CEA, DAM, DIF, F-91297 Arpajon, France, and Université Paris-Saclay, CEA, Laboratoire Matière en Conditions Extrêmes, 91680 Bruyères-le-Châtel, France.

We present here some recent update on the DFT+DMFT implementation in ABINIT regarding (1) the definition of Projected local orbitals Wannier functions, (2) the calculation of Green's function in Continuous time Quantum Monte Carlo (CTQMC) using Legendre Polynomial and (3) the calculation of the distributions of correlated orbitals configurations as computed in DFT+DMFT. We briefly present some applications of these features.

