

Algorithmic inversion and dynamical functionals to address correlations in materials

T. Chiarotti
Caltech (USA)

Energy functionals of the Green's function (GF) provide a suitable alternative to density-functional theory (DFT), offering the flexibility to accurately predict both spectral and ground state quantities. Functionals of the GF are dynamical, i.e., they are stationary for the solution of the Dyson equation featuring a self-energy; as opposed to the static Kohn-Sham equations of DFT they are much more difficult to treat. In this talk I address the challenges of frequency-dependent formulations by introducing the algorithmic-inversion method on sum-over-poles (AIM-SOP), showing a link between the Dyson equation and non-linear eigenvalue problems and solving it via embedding theory [1,2]. Furthermore, I discuss a generalization of the DFT+Hubbard functional to host a frequency-dependent screening, resulting in an energy functional of the local Green's function, termed dynamical Hubbard [2]. This allows to perform charge or full self-consistent calculations, that I showcase on the paradigmatic example of SrVO₃, calculating its spectrum, equation of state, and phonons at Gamma, obtaining results comparable to state-of-the art DMFT methods [2]. In addition, the case of the four monoxides MnO, NiO, FeO, and CoO is discussed, obtaining again state-of-the art agreement to the experiments [3]. Last, I present the generalization of AIM-SOP to many-body problems, linking it to DMFT and quantum embedding, and providing a framework to address strong correlations in defects and solids [4].

[1] T. Chiarotti, N. Marzari, and A. Ferretti, PRR 4, 013242 (2022)

[2] T. Chiarotti, A. Ferretti, and N. Marzari, PRR 6, L032023 (2024)

[3] M. Caserta, T. Chiarotti, and N. Marzari (in preparation)

[4] A. Carbone, T. Chiarotti, M. Capone, and N. Marzari (in preparation)