A unified description of ground and excited state properties of finite systems: the self-consistent GW approach

Fabio Caruso, Patrick Rinke, Xinguo Ren, Angel Rubio,[(*)] and Matthias Scheffler

Fully self-consistent GW (sc-GW) – based on the iterative solution of Dyson's equation – incorporates many-body correlation effects in the electronic ground-state, providing a recipe to consistently describe ground- and excited-states on an equal footing. We have implemented sc-GW in the localized basis all-electron code FHI-aims [1]. We show that, for finite systems, the ground-state properties as well as the excitation spectrum of the sc-GW Green's function are unique and are not affected by different initialization of the sc-GW loop, curing the pathological dependence on the starting point of one-shot GW (G_0W_0). In addition, self-consistency systematically improves ionization energies and Galitskii-Migdal total energies of closed shell systems compared to G_0W_0 based on Hartree-Fock and density-functional theory in local and semilocal approximations. Since our implementation is based on interacting Green's functions (unlike all G_0W_0 implementations) it is also a first step towards going beyond the GW approach.

(*) also at: Dep. de Fisica de Materiales, Univ. del Pais Vasco, San Sebastian, Spain

[1] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).