Self-consistent *GW* in FHI-aims

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In recent years, the *GW* approximation emerged as a predominant approach to the calculation of electronic excitations in ab-initio electronic structure theory. Due to its numerical cost, *GW* is mostly introduced perturbatively following a density-functional theory or Hartree-Fock calculation (G_0W_0). At a higher computational cost, fully self-consistent *GW* (sc-*GW*) ameliorates several shortcomings of the G_0W_0 scheme, such as the violation of particle number conservation and the dependence on the starting point [1].

We present an implementation of sc-*GW* – and other partially self-consistent *GW* approaches – in the FHI-aims code [2] based on numeric atom-centered orbitals and the resolution of the identity technique for the computation of the Coulomb integrals [3]. Finally, we present an assessment of the sc-*GW* approach for excited- and ground-state properties of atoms, molecules and molecular interfaces. By applying this approach to organic charge-transfer compounds – exemplified by the tetrathiofulvalene tetracyanoquinodimethane dimer (TTF-TCNQ) – we show that sc-*GW* provides a promising framework to predict the ground-state properties of molecular interfaces, in particular when questions pertaining to charge transfer become important.

[1] F. Caruso *et al.*, arXiv:1202.3547v1
[2] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).
[2] X. Ren *et al.*, New J. Phys. **14**, 053020 (2012).