Efficient G_0W_0 using localized basis sets: a benchmark for molecules

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Electronic structure calculations within Hedin's *GW* approximation are becoming increasingly accessible to the community. In particular, as it has been shown earlier and we confirm by calculations using our **MBPT_LCAO** package [1], the computational cost of the so-called G_0W_0 can be made comparable to the cost of a regular Hartree-Fock calculation. In this work, we study the performance of our new G_0W_0 implementation (based on a contour deformation technique) to reproduce the ionization potentials of all 117 closed-shell molecules belonging to the G2/97 test set (see figure below), using a pseudo-potential starting point provided by the popular density-functional package **SIESTA** [2]. Moreover, the ionization potentials and electron affinities of a set of 24 acceptor molecules [3] are compared to experiment and to reference all-electron calculations.

References

[1] http://mbpt-domiprod.wikidot.com
[2] Soler J. M. *etal* J. Phys.: Condens. Matter, **14** (2002) 2745.
[3] Knight J. W. *etal* J. Chem. Theory Comput., **12** (2016) 615.

Figures

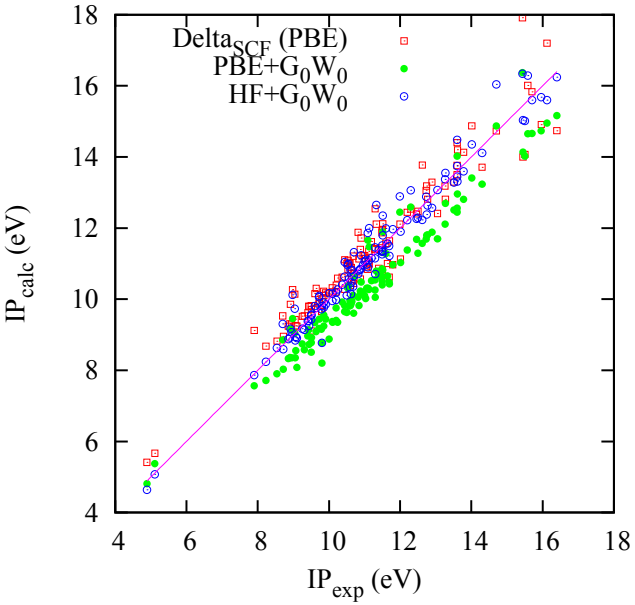

Figure 1: Ionization potentials of G2/97 test set computed with Delta SCF, and PBE+G_0W_0, and HF+G_0W_0. HF+G_0W_0 shows a least deviation from experimental data.