Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules: A Benchmark of GW Methods

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The performance of different GW methods is assessed for a set of 24 organic acceptors. Errors are evaluated with respect to coupled cluster singles, doubles, perturbative triples [CCSD(T)] reference data for the vertical ionization potentials (IPs) and electron affinities (EAs), extrapolated to the complete basis set limit. Additional comparisons are made to experimental data, where available. We consider fully self-consistent GW (scGW), partial self-consistency in the Green’s function (scGW$_0$), non-self-consistent G$_0$W$_0$ based on several mean-field starting points, and a “beyond GW” second order screened exchange (SOSEX) correction to G$_0$W$_0$. The best performers overall are G$_0$W$_0$+SOSEX and G$_0$W$_0$ based on an IP-tuned long range corrected hybrid functional with the former being more accurate for EAs and the latter for IPs. Both provide a balanced treatment of localized vs. delocalized states and valence spectra in good agreement with photoemission spectroscopy (PES) experiments.

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