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

Joseph Knight[1], Xiaopeng Wang[1], Lukas Gallandi[2], Olga Dolgounitcheva[3], Xinguo Ren[4], J. Vincent Ortiz[3], Patrick Rinke[5], Thomas Körzdörfer[2], Noa Marom*,[1]

1. Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70118, USA
2. Computational Chemistry, University of Potsdam, 14476 Potsdam, Germany
3. Department of Chemistry and Biochemistry, Auburn University, Auburn, Alabama 36849-5312, USA
4. Key Laboratory of Quantum Information, University of Science and Technology of China, Hefei, 230026, China
5. COMP/Department of Applied Physics, Aalto University School of Science, P.O. Box 11100, FI-00076 Aalto, Finland

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* (sc*GW*), partial self-consistency in the Green's function (scGW_0), non-self-consistent G_0W_0 based on several mean-field starting points, and a "beyond GW" second order screened exchange (SOSEX) correction to G_0W_0. The best performers overall are G_0W_0+SOSEX and G_0W_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.