

Abstract Submitted
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Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules: A Benchmark of GW Methods NOA MAROM, JOSEPH KNIGHT, XIAOPENG WANG, Tulane University, LUKAS GALLANDI, University of Potsdam, Germany, OLGA DOLGOUNITCHEVA, Auburn University, XINGUO REN, USTC, VINCENT ORTIZ, Auburn University, PATRICK RINKE, Aalto University, Finland, THOMAS KORZDORFER, University of Potsdam, Germany — 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 (scGW₀), non-self-consistent G₀W₀ based on several mean-field starting points, and a “beyond GW” second order screened exchange (SOSEX) correction to G₀W₀. The best performers overall are G₀W₀+SOSEX and G₀W₀ 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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