GW100 benchmarking *GW* for molecules

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The GW100 set is a benchmark set of the ionization potentials and electron affinities of 100 molecules computed using the *GW* method using different independent *GW* codes and different *GW* methodologies [1]. The quasiparticle energies of the highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) are calculated for the GW100 set at the G0W0@PBE level. The use of different codes allows for a quantitative comparison of the type of basis set (plane wave or local orbital) and handling of unoccupied states, the treatment of core and valence electrons (all electron or pseudopotentials), the treatment of the frequency dependence of the self-energy (full frequency or more approximate plasmon-pole models), and the algorithm for solving the quasi-particle equation.

The current data includes reference data at CCSD(T) level [2] and 7 different flavors of *GW* self-consistency [3]. In the mean while 8 different codes ran GW100 resulting in over 23 data sets.

References

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