**Benchmarking GW for quantum chemistry applications**

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For many years, computational limits have forced *GW* calculations to employ approximations without the possibility to systematically evaluate their validity. In such a situation, the search for accuracy and precision can become very challenging, up to the point where one risks sacrificing precision for the sake of accuracy. With increased computational resources, this situation is changing but performing fully converged none approximated GW for solids is still a big challenge. For finite size systems, however, calculations can be more tractable.
In this contribution I summarize the results of the *GW*100 project. The *GW*100 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. The quasi-particle energies of the HOMO and LUMO orbitals are calculated for the *GW*100 set at various levels of approximations. The use of different codes allows for a quantitative comparison of the type of basis set (plane wave or local orbital), 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.
At present 10 different codes have contributed to the project resulting in over 35 data sets. At *G*0*W*0@PBE level very tightly converged results obtained with very different codes, including fully analytic *GW*, answer the question on precision. A comparison of six different levels of self-consistency in *GW* to reference values calculated at CCSD(T) level of theory answers the question on accuracy.

**References**

https://gw100.wordpress.com/papers/