GW0 for > 10K electrons: Stochastic GW

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Stochastic Quantum Chemistry (SQC) is a new paradigm we developed for electronic structure and dynamics, which rewrites traditional quantum chemistry as stochastic averages, avoiding the steep power law scaling of traditional methods. As an example I will discuss Stochastic GW (SGW). The GW technique is known to achieve high accuracy, with only a 0.1-0.3 eV experiment-theory deviation for affinities and ionization energies. SGW reproduces the results of traditional deterministic GW for small systems, but also handles very large systems; as an example, we easily calculated affinities, charging energies, and photoelectron spectroscopy for Si clusters and Si and P platelets with up to 11000 valence electrons, for polymers with thousands of atoms, and for periodic systems with very large supercells. These systems are significantly bigger than any calculable in existing approaches, so that SGW makes a quantum jump in the ability to calculate accurate electronic affinities and potential energies for large molecules. We will specifically discuss recent improvements in the algorithm and implementation which makes SGW superior to traditional techniques already for tetracene, and reduces experiment-theory deviations to $\sim$0.1 eV. These include a post-processing G0W0 –> GW0 partial-self consistency, as well as a new stochastic-compression approach for efficiently representing giant sets of data, as appear in stochastic GW.