# High Accuracy Auxiliary-Field Quantum Monte Carlo for Molecules and Solids

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As computers continue to grow increasingly more powerful, it is becoming increasingly more realistic to consider post-Density Functional Theory (DFT) methods - electronic structure methods that are slightly more costly, yet significantly more accurate than DFT. One class of methods particularly well-suited for the post-DFT era owing to their modest scaling with system size are quantum Monte Carlo methods. In this work, we demonstrate how Auxiliary-Field Quantum Monte Carlo (AFQMC), a quantum Monte Carlo technique most commonly used to study lattice models, may be used to determine the ground state properties of molecules and solids with an accuracy comparable to that of CCSD(T) for a substantially lower computational cost. In specific, we illustrate that, by combining AFQMC with approaches rooted in the quantum chemistry community, including the use of multideterminant trial wave functions, explicit correlation, and tensor hypercontractions, we can obtain the total energies of the majority of the G1 test set with only milliHartree errors. Going forward, we hope to extend our techniques to strongly correlated solids, which are both beyond the reach of standard quantum chemistry techniques and inaccurately modeled by DFT.