Computing observables and correlation functions of molecular systems with auxiliary-field quantum Monte Carlo\textsuperscript{1} MARIO MOTTA, SHI-WEI ZHANG, The College of William and Mary — The quantitative study of correlated materials requires accurate and efficient calculations of electronic density, forces and correlation functions. To achieve this goal, we formulated and implemented a back-propagation scheme\textsuperscript{2} for auxiliary-field quantum Monte Carlo\textsuperscript{3} electronic structure calculations. We discuss the numerical stability and computational complexity of the technique, and assess its performance computing ground-state properties for a broad set of molecules, including constituents of the primordial terrestrial atmosphere and medium-sized organic molecules. Accurate estimates for electronic density and dipole moment of molecular systems are obtained.

\textsuperscript{1}This work is supported by NSF and the Simons Foundation