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Computing observables and correlation functions of molecular systems with auxiliary-field quantum Monte Carlo[1] MARIO MOTTA, SHIWEI 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 [2] for auxiliary-field quantum Monte Carlo [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 atmoshpere and medium-sized organic molecules. Accurate estimates for electronic density and dipole moment of molecular systems are obtained.

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[2]S. Zhang, J. Carlson and J. E. Gubernatis, *Phys. Rev. B* **55**, 7464 (1997);
[3]S. Zhang and H. Krakauer, *Phys. Rev. Lett.* **90**, 136401 (2003)

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