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Study of Atoms and Molecules with Auxiliary-Field Quantum Monte Carlo[1] WIRAWAN PURWANTO, MALLIGA SUEWATTANA[2], HENRY KRAKAUER, SHIWEI ZHANG, ERIC J. WALTER, College of William and Mary, VA — We study the ground-state properties of second-row atoms and molecules using the phaseless auxiliary-field quantum Monte Carlo (AF QMC) method.[3] This method projects the many-body ground state from a trial wave function by means of random walks in the Slater-determinant space. We use a single Slater-determinant trial wave function obtained from density-functional theory (DFT) or Hartree-Fock (HF) calculations. The calculations were done with a plane-wave basis and supercells with periodic boundary condition. We investigate the finite-size effects and the accuracy of pseudopotentials within DFT, HF, and AF QMC frameworks. Pseudopotentials generated from both LDA (OPIUM[4]) and HF[5] are employed. We find that the many-body QMC calculations show a greater sensitivity to the accuracy of the pseudopotentials. With reliable pseudopotentials, the ionization potentials and dissociation energies obtained using AF QMC are in excellent agreement with the experimental results.

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