Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Auxiliary Field Quantum Monte Carlo Study of Ground State Properties of Atoms and Molecules[1] MALLIGA SUEWATTANA, College of William and Mary, SHIWEI ZHANG, College of William and Mary, HENRY KRAKAUER, College of William and Mary, ERIC WALTER, College of William and Mary — We apply a recently developed quantum Monte Carlo (QMC) method [2] to calculate the ground state properties of several atoms and molecules. The QMC method projects the many-body ground state from a trial state by random walks in the space of Slater determants. The Hubbard-Stratonovich transformation is employed to decouple the Coulomb interaction between electrons. A trial wave function $|\Psi_T\rangle$ is used in the approximation to control the phase problem in QMC. We also carry out Hartree-Fock (HF) and density functional theory (with the local density approximation (LDA)) calculations. The generated single Slater determinant wave functions are used as $|\Psi_T\rangle$ in QMC. The dissociation and ionization energies are calculated for Aluminum, Silicon, Phosphorous, Sulfur, Chlorine and Arsenic atoms and molecules. The results are in good agreement with experimental values.

[1]Supported by NSF and ONR
[2]Shiwei Zhang, Henry Krakauer, Phys. Rev. Lett. **90**. 136401 (2003).

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Date submitted: 01 Dec 2004 Electronic form version 1.4