Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Geometry optimization with a noisy potential energy surface JEFFREY GROSSMAN, LUCAS WAGNER, University of California, Berkeley — Molecular and solid systems in the excited state and in the weak-binding regime (for example) are often not described well by current density functional(DFT) methods, often leading to inaccurate minimum energy structures. Quantum Monte Carlo(QMC) is a tempting method to improve on these deficiencies, since it offers a highly accurate fully correlated first principles description. However, QMC suffers from two major deficiencies: 1) forces are not easily calculated and 2) the energy is obtained with stochastic uncertainty, which makes optimization a challenging task. We examine several ways of compensating for this uncertainty while only using the reliable total energies obtained in QMC.

Lucas Wagner
University of California, Berkeley

Date submitted: 27 Nov 2007 Electronic form version 1.4