Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Auxiliary-Field Quantum Monte Carlo Studies of Pressure-Induced Phase Transitions in Silicon and MnO[1] WIRAWAN PURWANTO, HENRY KRAKAUER, ERIC WALTER, SHIWEI ZHANG, College of William and Mary — Accurate theoretical predictions across structural phase transitions are challenging, as they typically involve different electronic structures on the two sides of the transition. We use the phaseless auxiliary-field quantum Monte Carlo (AFQMC) method—which yields accurate many-body wave functions by means of importance sampled random walks in the space of Slater determinants—to calculate the equation of state near two phase transitions: in Si, from the diamond to metallic β-tin transition at ~ 11 GPa; and in MnO, the volume and magnetic moment collapse at ~ 100 GPa. The Si phase transition serves as a test case to study the accuracy of the AFQMC method; the calculated transition pressure is in good agreement with the experiment. Applications to the MnO phase transition will then be presented.

[1]Supported by DOE (CMSN and QMC EndStation), ONR, NSF, and ARO. Calculations were performed at NCCS Jaguar

Wirawan Purwanto
College of William and Mary

Date submitted: 20 Nov 2008 Electronic form version 1.4