

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

Sorting Category: 17.5 (C)

**Auxiliary-Field Quantum Monte Carlo Studies of  
Pressure-Induced Phase Transitions in Silicon and MnO<sup>1</sup>**

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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 transi-  
tions: in Si, from the diamond to metallic  $\beta$ -tin transition at  $\sim 11$  GPa;  
and in MnO, the volume and magnetic moment collapse at  $\sim 100$  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 agree-  
ment with the experiment. Applications to the MnO phase transition  
will then be presented.

<sup>1</sup>Supported by DOE (CMSN and QMC EndStation), ONR, NSF, and  
ARO. Calculations were performed at NCCS Jaguar

Prefer Oral Session  
 Prefer Poster Session

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Date submitted: 20 Nov 2008

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