Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Quantum Monte Carlo Computations for Equations of State, Phase Transitions, and Elasticity of Silica R.E. COHEN, Carnegie Instiution of Washington, B. MILITZER, Z. WU, University of California, Berkeley, K. DRIVER, Ohio State University, P.L. RIOS, M. TOWLER, R. NEEDS, University of Cambridge — We have performed Quantum Monte Carlo (QMC) computations for silica in the quartz, stishovite, and α-PbO_2 structures as functions of compression. In spite of the great success of DFT there is still need for improvement. The local density approximation (LDA) gives excellent results for individual silica phases, but LDA predicts stishovite to be the stable ground state rather than quartz. The Generalized Gradient Approximation (GGA) does give correct energy differences, but other properties, such as the bulk moduli, are worse with the GGA than the LDA. We included thermal contributions using density functional perturbation theory with the code ABINIT. We have also computed the shear elastic constant c_{11}-c_{12} in stishovite, which is associated with the phase transition to the $CaCl_2$ structure, with QMC. We find excellent agreement with experiments. We find that the main differences between QMC and DFT are crystalline phase dependent energy and pressure shifts. This work is supported by NSF grants EAR-0530282, EAR-0310139, and by DOE contract DE-FG02-99ER45795 to John Wilkins. Computations were performed on blueice at NCAR under a BTS grant, and on Tungsten and Abe at NCSA, and at the Carnegie Institution of Washington.

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Date submitted: 26 Nov 2007 Electronic form version 1.4