Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Quantum Monte Carlo Calculation for the Equation of State of $MgSiO_3$ perovskite at high pressures[1] YANGZHENG LIN, Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road, NW, Washington DC 20015, USA, R.E. COHEN, Geophysical Lab, Carnegie Inst of Washington, 5251 Broad Branch Road NW, Washington, USA; Dept of Earth Science, University College London, London, UK, KEVIN P. DRIVER, BURKHARD MILITZER, Departments of Earth and Planetary Science and of Astronomy, University of California, Berkeley, CA 94720, USA, LUKE SHULENBURGER, Sandia National Laboratories, MS 1189, P.O. BOX 5800 Albuquerque, NM 87185-1189, USA, JEONGNIM KIM, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — Magnesium silicate ($MgSiO_3$) is among the most abundant minerals in the Earth's mantle. Its phase behavior under high pressure has important implications for the physical properties of deep Earth and the core-mantle boundary. A number of experiments and density functional theory calculations have studied perovskite and its transition to the post-perovskite phase. Here, we present our initial work on the equation of state of perovskite at pressures up to 200 GPa using quantum Monte Carlo (QMC), a benchmark ab initio method. Our QMC calculations optimize electron correlation by using a Slater-Jastrow type wave function with a single determinant comprised of single-particle orbitals extracted from fully converged DFT calculations. The equation of state obtained from QMC calculations agrees with experimental data.

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Date submitted: 15 Nov 2013 Electronic form version 1.4