Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Quantum Monte Carlo Computations of the $(Mg_{1-X}Fe_X)SiO_3$ Perovskite to Post-perovskite Phase Boundary[1] YANGZHENG LIN, Extreme Materials Initiative, Geophysical Lab, Carnegie Institution, R.E. COHEN, EMI, Geophysical Lab, Carnegie Inst; Dept. für Geo- und Umweltwissenschaften, Ludwig-Maximilians-Universitaet, ANDREA FLORIS, Dept Physics, King's College, LUKE SHULENBURGER, Sandia National Labs, KEVIN P. DRIVER, Dept Earth Planet Sci, Univ of California, Berkeley — We have computed total energies of $FeSiO_3$ and $MgSiO_3$[1] perovskite and post-perovskite using diffusion Monte Carlo with the qmcpack GPU code. In conjunction with DFT+U computations for intermediate compositions $(Mg_{1-X}Fe_X)SiO_3$ and phonons computed using density functional perturbation theory (DFPT) with the pwscf code, we have derived the chemical potentials of perovskite (Pv) and post-perovskite (PPv) $(Mg_{1-X}Fe_X)SiO_3$ and computed the binary phase diagram versus P, T, and X using a non-ideal solid solution model. The finite temperature effects were considered within quasi-harmonic approximation (QHA). Our results show that ferrous iron stabilizes PPv and lowers the Pv-PPv transition pressure, which is consistent with previous theoretical and some experimental studies. We will discuss the correlation between the Earth's D layer and the Pv to PPv phase boundary. Computations were performed on XSEDE machines, and on the Oak Ridge Leadership Computing Facility (OLCF) machine Titan under project CPH103geo of INCITE program. [1] Lin *et al.*. Phys. Rev. B 90(18), 184103 (2014)

[1]E-mail: rcohen@carnegiescience.edu; This work is supported by NSF.

Yangzheng Lin
Carnegie Institution of Washington

Date submitted: 04 Nov 2015 Electronic form version 1.4