Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Quantum Monte Carlo simulations of a single iron impurity in MgO[1] KEVIN DRIVER, SHUAI ZHANG, BURKHARD MILITZER, University of California, Berkeley, R.E. COHEN, Carnegie Institution of Washington, Geophysical Laboratory — Ferropericlase [(Mg,Fe)O] is the second most abundant mineral in Earth's lower mantle. A high-spin to low-spin transition in Fe2+ that occurs in the middle of the lower mantle has been observed in diamond anvil experiments and confirmed within density functional theory (DFT). The spin transition has significant influence on the physical properties and behavior of the lower mantle. However, details on the mechanism of spin transition are still being understood in both experiment and DFT [1]. Here, we aim to benchmark the high-spin to low-spin transition of a single iron atom impurity in MgO using quantum Monte Carlo (QMC). High-spin and low-spin equations of state are initially computed using density functional theory within the LDA+U approximation, which provide trial Slater-Jastrow wave functions for QMC. Equations of state are then computed with variational and diffusion Monte Carlo in 8- and 64-atom cells using the QMCPACK code.[2]. QMC results are in general agreement with experiment and DFT studies.

[1] J.-F. Lin, S. Speziale, Z. Mao, and H. Marquardt, Rev. Geophys., 51, 244 (2013).
[2] http://qmcpack.cmscc.org/

[1]Grants: Funding provided by the NSF (DMS-1025370, DMS-1025392). Computational resources provided by the NCAR and LBL.

Kevin Driver
University of California, Berkeley

Date submitted: 15 Nov 2013 Electronic form version 1.4