Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Spin states and hyperfine interactions of iron incorporated in $\mathbf{MgSiO_3}$ post-perovskite[1] YONGGANG YU, HAN HSU, MATTEO COCOCCIONI, RENATA WENTZCOVITCH, University of Minnesota — Using density functional theory + Hubbard U (DFT+U) calculations, we investigate the spin states and nuclear hyperfine interactions of iron incorporated in magnesium silicate ($MgSiO_3$) post-perovskite (Ppv), a major mineral phase in the Earth's D" layer, where the pressure ranges from about 120 to 135 GPa. In this pressure range, ferrous iron (Fe^{2+}) substituting for magnesium at the dodecahedral (A) site remains in the high-spin (HS) state; intermediate-spin (IS) and low-spin (LS) states are highly unfavorable. As to ferric iron (Fe^{3+}), which substitutes magnesium at the A site and silicon at the octahedral (B) site to form (Mg,Fe)(Si,Fe)O_3 Ppv, we find the combination of HS Fe^{3+} at the A site and LS Fe^{3+} at the B site the most favorable. Neither A-site nor B-site Fe^{3+} undergoes a spin-state crossover in the D" pressure range. The computed iron quadrupole splittings are consistent with those observed in Mössbauer spectra. The effects of Fe^{2+} and Fe^{3+} on the equation of state of Ppv are found nearly identical, expanding the unit cell volume while barely affecting the bulk modulus.

[1]This work was supported by EAR-081272, EAR-1047629, and by.the MRSEC Program of NSF grants DMR 0212302 and DMR-0819885. Calculations were performed at the Minnesota Supercomputing Institute (MSI).

Han Hsu
University of Minnesota

Date submitted: 11 Nov 2011 Electronic form version 1.4