Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Effects of aluminum on spin-state crossover of iron in the Earth's lower mantle[1] RENATA WENTZCOVITCH, HAN HSU, YONGGANG YU, University of Minnesota — Using density functional theory + Hubbard U (DFT+U) calculations, we investigate how aluminum affects the spin-state crossover of iron in $MgSiO_3$ perovskite and post-perovskite, the major mineral phases in and at the bottom of the Earth's lower mantle. We find that aluminum does not change the response of iron spin state to the increasing pressure, namely, only the ferric iron (Fe^{3+}) residing the octahedral (B) site undergoes a crossover from high-spin to low-spin state, same as aluminum-free iron-bearing $MgSiO_3$. The presence of aluminum, however, does affect the population of B-site ferric iron significantly – the majority of Fe^{3+} reside the dodecahedral (A) site at lower pressures, and the population of B-site Fe^{3+} increases with pressure at higher pressure range. Therefore, in the Earth's lower mantle, the amount of B-site Fe^{3+} and the degree of elastic anomalies (and thus the possible seismic anomalies) associated with spin-state crossover is directly affected by the concentration and configuration of aluminum.

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

Han Hsu
University of Minnesota

Date submitted: 11 Nov 2011 Electronic form version 1.4