Spin states and hyperfine interactions of iron incorporated in MgSiO₃ post-perovskite

YONGGANG YU, HAN HSU, MATTEO COCCOCIONI, 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 (MgSiO₃) 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 (Fe²⁺) 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 (Fe³⁺), which substitutes magnesium at the A site and silicon at the octahedral (B) site to form (Mg,Fe)(Si,Fe)O₃ Ppv, we find the combination of HS Fe³⁺ at the A site and LS Fe³⁺ at the B site the most favorable. Neither A-site nor B-site Fe³⁺ 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 Fe²⁺ and Fe³⁺ on the equation of state of Ppv are found nearly identical, expanding the unit cell volume while barely affecting the bulk modulus.

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Han Hsu
University of Minnesota

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