

Abstract Submitted
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Spin state of ferrous iron in perovskite RYAN REQUIST, Stony Brook University, KOICHIRO UMEMOTO, University of Minnesota, RENATA WENTZCOVITCH, University of Minnesota — Diamond anvil cell experiments at pressures up to 145 GPa have shown evidence for a high spin to low spin transition in iron in magnesium silicate perovskite (MgSiO_3 .) The spin transition will influence the optical absorption spectrum and elastic properties of this mineral. We present density functional calculations of $(\text{Mg,Fe})\text{SiO}_3$ with ferrous iron substituting for magnesium at a concentration of 12.5%. The calculations use the local density approximation with Hubbard term (LDA+U) and supercells containing up to 160 atoms. We describe the pressure dependence of the iron spin state. Research supported by NSF/EAR 0230319, NSF/ITR 0428774 and 0426757, VLab, NSF/ITR 0325218, ITAMIT.

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