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Electronic Spin State and Elasticity of (Mg, Fe)(Si, Al)O3-perovskite at high pressure LI LI, DONALD WEIDNER, Stony Brook University, JOHN BRODHOLT, STEPHEN STACKHOUSE, MARIA ALFREDSSON, DAVID PRICE, Universtiy College London — We investigate the effect of pressure on the electronic spin state of ferric iron in Al-bearing $MgSiO_3$-perovskite using first-principle computations (Density Functional Theory with the Generalized Gradient Approximation). We also calculate the single crystal elastic moduli (c_{ij}) for (Mg, Fe^{3+})(Si, Al)O_3 perovskite to understand the effect of chemical variations and spin state transitions of the Fe^{3+} ions on these properties. Ferric iron (6.25 mol%) and Al (6.25 mol%) substitute for Mg and Si respectively. Our results show that spin state transition from high spin (HS) to low spin (LS) occurs on the Fe^{3+} ions at high pressure, while there is no stability field for the intermediate spin state. Fe^{3+} alone can be responsible for the spin state transition. The models witness a transition pressure ranging from 97-126 GPa. Differential stress can change the pressure for the spin collapse. These results are one explanation to the reported experimental observations that the spin transition occurs over a wide pressure range. We find that ferric iron lowers the elastic moduli relative to the Al charge-coupled substitution. The spin state of the iron for this composition has a relatively small effect ($< 0.5\%$ variation) on both bulk modulus and shear modulus. Replace this text with your abstract body.

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