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***Ab initio* Study of the Composition Dependence of the Pressure-Induced Spin Transition in Perovskite (Mg,Fe)SiO_3** AMELIA BENGTSON, University of Wisconsin - Madison, KRISTIN PERSSON, MIT, DANE MORGAN, University of Wisconsin - Madison — We present *ab initio* calculations of the zero-temperature compositional dependent spin transition in (Mg,Fe)SiO_3 perovskite at pressures relevant to Earth's lower mantle. Equations of state are fit for a range of compositions and used to predict the Fe^{2+} high- to low-spin transition pressure and associated changes in volume and bulk modulus. We predict a relatively constant transition pressure for $x < 0.25$, but a significant decrease for higher Fe concentrations, contrary to the trend for rocksalt (Mg,Fe)O, suggesting the mechanism for spin transition is highly dependent on the structural environment of Fe. The spin transition is dominated by both the spin flip energy and the change in volume from high- to low-spin. Furthermore, volume trends show that high-spin Fe^{2+} is larger than Mg^{2+} even under pressure, but low-spin Fe^{2+} is smaller at ambient conditions and approximately the same size as Mg^{2+} under pressure, which has implications for correctly calculating Fe partitioning coefficients in the lower mantle. We also find the spin transition pressure differs between Fe^{2+} and Fe^{3+}; therefore the coupling behavior of these two species must be examined closely.

Amelia Bengtson
University of Wisconsin - Madison

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