Abstract Submitted
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Thermoelasticity of (Mg,Fe)SiO_3 perovskite[1] GAURAV SHUKLA, University of Minnesota Twin cities, ZHONGQING WU, University of Science and Technology of China, Hefei, Anhui, China, HAN HSU, National Central University, Jhongli City, Taoyuan 32001, Taiwan, MATTEO COCOCCIONI, Ecole Polytechnique Federale de Lausanne, Switzerland, RENATA WENTZCOVITCH, University of Minnesota Twin cities — We present LDA+U calculations of high temperature elastic properties of $(Mg_{(1-x)}Fe^{2+}_x)SiO_3$ bridgemanite ($0 \leq x \leq 0.125$), the most abundant constituent of Earth's lower mantle. Calculations of aggregate elastic moduli and acoustic velocities for the Mg-end member (x=0) are in excellent agreement with the latest high pressure and high temperature experimental measurements. In the iron bearing system, we particularly focus on the change in thermoelastic parameters across the state change that occurs in ferrous iron above ∼30 GPa, often attributed to a high-spin (HS) to intermediate spin (IS) crossover but explained by calculations as a lateral displacement of substitutional iron in the perovskite cage. We show that the measured effect on the equation of state of this change in the state of iron can be explained by the lateral displacement of substitutional iron, not by the HS to IS crossover. Calculated elastic properties of $(Mg_{0.875}Fe^{2+}_{0.125})SiO_3$ along an adiabatic mantle geotherm, somewhat overestimate longitudinal velocities but produce densities and shear velocities consistent with Preliminary Reference Earth Model data throughout most of the lower mantle.

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