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Spin crossover in (Mg,Fe^{3+})(Si,Fe^{3+})O_3 bridgmanite: effects of disorder, iron concentration, and temperature[1] GAURAV SHUKLA, RENATA WENTZCOVITCH, Univ of Minnesota - Twin Cities — The spin crossover of iron in Fe^{3+}-bearing bridgmanite, the most abundant mineral of the Earth's lower mantle, is by now a well-established phenomenon, though several aspects of this crossover remain unclear. Here we investigate effects of disorder, iron concentration, and temperature on this crossover using ab initio LDA + U_{SC} calculations. Disorder and concentration effects are addressed using complete statistical samplings of coupled substituted configurations up to 80 atoms supercells, while the vibrational effects using the quasiharmonic approximation. Our calculated compression curves for iron-free and iron-bearing bridgmanite compare well with the latest experimental measurements. The comparison also suggests that in a closed system, Fe^{2+} present in the sample may transform into Fe^{3+} by introduction of Mg and O vacancies with increasing pressure. As in the spin crossover in ferropericlase, this crossover in bridgmanite is accompanied by a clear volume reduction and an anomalous softening of the bulk modulus throughout the crossover pressure range. Though the concentration of $[Fe^{3+}]_{Si}$ in bridgmanite may be small, related elastic anomalies may impact the interpretation of radial and lateral velocity structures of the Earth's lower mantle.

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