# Spin crossover in $(Mg,Fe^{3+})(Si,Fe^{3+})O_3$ bridgmanite: effects of disorder, iron concentration, and temperature

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The spin crossover of iron in $Fe^{3+}$-bearing bridgmanite, the most abundant mineral of the Earths 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. The effect of concentration and disorder are addressed using complete statistical samplings of coupled substituted configurations in super-cells containing up to 80 atoms. Vibrational/thermal effects on the crossover are addressed within the quasiharmonic approximation. The effect of disorder seems quite small, while increasing iron concentration results in considerable increase in crossover pressure. Our calculated compression curves for iron-free, $Fe^{2+}$-, and $Fe^{3+}$-bearing bridgmanite compare well with the latest experimental measurements. The comparison also suggests that in a close 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. These effects reduce significantly with increasing temperature. 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.