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A hell of a problem (or a problem from hell): Spin crossover in iron in lower mantle minerals

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Iron in minerals of the Earth's lower mantle (LM) undergoes a high spin (HS) to low spin (LS) transition at high pressures. Using DFT + U_{sc} we have successfully investigated this phenomenon in low iron concentration ferropericlase (B1-type $Mg_{(1-x)}Fe_xO$), and bridgmanite (perovskite-type $Mg_{(1-x)}Fe_xSiO_3$ and $Mg_{(1-x)}Fe_xSi_{(1-x)}Fe_xO_3$ with $x < 0.2$), the most abundant LM phases [e.g., 1-8]. We have developed a thermodynamics formalism based on an ideal solid solution model that describes the HS to LS state change as a continuous crossover passing through an insulating intermediate mixed spins (MS) state, as suggested by compressibility measurements. Major elastic anomalies accompany the iron spin state change. Such anomalies affect propagation of acoustic/seismic waves that have important consequences for understanding Earth's internal state. This understanding of the spin crossover phenomenon based on equilibrium thermodynamics is general and applicable other insulators at the onset of the spin state transition.

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