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Spin crossover in solid and liquid (Mg,Fe)O at extreme conditions[1] LARS STIXRUDE, Department of Earth Sciences, University College London, EERO HOLMSTROM, Department of Applied Physics, COMP Centre of Excellence, Aalto University, Finland — Ferropericlase, (Mg,Fe)O, is a major constituent of the Earth's lower mantle (24-136 GPa). Understanding the properties of this component is important not only in the solid state, but also in the molten state, as the planet almost certainly hosted an extensive magma ocean initially. With increasing pressure, the Fe ions in the material begin to collapse from a magnetic to a nonmagnetic spin state. This crossover affects thermodynamic, transport, and electrical properties. Using first-principles molecular dynamics simulations, thermodynamic integration, and adiabatic switching, we present a phase diagram of the spin crossover. In both solid and liquid, we find a broad pressure range of coexisting magnetic and non-magnetic ions due to the favorable enthalpy of mixing of the two. In the solid increasing temperature favors the high spin state, while in the liquid the opposite occurs, due to the higher electronic entropy of the low spin state. Because the physics of the crossover differ in solid and liquid, melting produces a large change in spin state that may affect the buoyancy of crystals freezing from the magma ocean in the earliest Earth.

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