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Ab Initio Study of Thermodynamics of Fe and Spin Transitions in the Lower Mantle DANE MORGAN, AMELIA BERTA, University of Wisconsin - Madison, KRISTIN PERSSON, GERBRAND CEDER, Massachusetts Institute of Technology — Recent experiments have demonstrated spin transitions in Fe in both the rocksalt ferropericlase (Mg,Fe)O and perovskite (Mg,Fe)SiO_3 phases at lower mantle pressures. The spin transitions have potentially profound implications for the materials properties of the lower mantle. However, the coupling of thermodynamic temperature effects and the spin transition is still poorly understood. In this talk we present an ab initio based thermodynamic model for Fe spin transitions in lower mantle phases. We build a free energy model which includes configurational, vibrational, magnetic, and electronic contributions. The resulting free energy expressions are used to construct a phase diagram for the lower mantle ferropericlase which includes the impact of Fe spin transitions.

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