

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Composition Dependence of Pressure-Induced Spin Transitions in the (Mg,Fe)SiO₃ Perovskite and (Mg,Fe)O Rocksalt System AMELIA BERTA, University of Wisconsin-Madison, KRISTIN PERSSON, Massachusetts Institute of Technology, GERBRAND CEDER, Massachusetts Institute of Technology, DANE MORGAN, University of Wisconsin-Madison — Recent experimental results suggest that Fe undergoes a high-spin to low-spin transition in both the rocksalt and perovskite phases at lower mantle pressures. These spin transitions may have a profound impact on the properties of lower mantle phases. In this work the critical spin-transition pressures for Fe in perovskite (Mg,Fe)SiO₃ and rocksalt (Mg,Fe)O are calculated using *ab initio* methods. We focus in particular on the alloy nature of the material, studying the spin-transition pressure for varying concentrations of Fe. The results show that as the concentration of Fe increases, the transition pressure decreases in the perovskite. This is directly opposite the trend observed for spin transition pressures found in rocksalt (Mg,Fe)O. The difference in trends in spin-transition pressure is explained by the difference in physics between the two structures.

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Date submitted: 30 Nov 2005

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