Abstract Submitted for the MAR05 Meeting of The American Physical Society

High-to-low spin transition in magnesium wustite under pressure¹ TAKU TSUCHIYA, RENATA WENTZCOVITCH, Chemical Eng and Materials Sci, Minnesota Supercomputing Institute, University of Minnesota, STEFANO DE GIRONCOLI, Scuola Internazionale Superiore di Studi Avanzati and DEM-OCRITOS National Simulation Center — Mg-Fe substitution is most commonly seen in natural solid solution minerals. High resolution X-ray spectroscopy has recently demonstrated that the major lower mantle (LM) minerals undergo a highto-low spin transition at LM pressures (23-135 GPa). Previous failures of standard DFT and "LDA+U" approaches to describe this phenomenon have hindered its investigation and consequences of fundamental importance to geophysics, such as heat transport in Earth?fs mantle. Here, using a rotationally invariant first principles formulation of LDA+U, where the Hubbard U parameter is computed in a internally consistent way, we report the first successful study of this transition in low solute concentration $(Mg_{1-x}Fe_x)O$, magnesiumwustite. This is believed to be the second most abundant phase of Earth's LM. This encouraging result appears to open for exploration a new class of problems of enormous significance to deep Earth geophysics.

 $^1\mathrm{Research}$ supported by JSPS, NSF/EAR 013533 (COMPRES), 0230319, and NSF/ITR 0428774.

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Date submitted: 02 Dec 2004 Electronic form version 1.4