## Abstract Submitted for the MAR06 Meeting of The American Physical Society

Dissociation of Ringwoodite investigated by first principles<sup>1</sup> YONGGANG YU, RENATA WENTZCOVITCH, TAKU TSUCHIYA, KOICHIRO UMEMOTO, JUN TSUCHIYA, Minnesota Supercomputing Institute and Department of Chemical Engineering and Materials Science, University of Minnesota, DONALD WEIDNER, Center for High Pressure Research and Department of Geosciences, State University of New York, Stony Brook, NY 11794, USA, RE-NATA WENTZCOVITCH'S GROUP AT UNIVERSITY OF MINNESOTA TEAM, DONALD WEIDNER'S GROUP AT STATE UNIVERSITY OF NEW YORK AT STONY BROOK COLLABORATION — The dissociation of Ringwoodite,  $Mg_2SiO_4$  gamma-spinel, into MgO and  $MgSiO_3$  perovskite is believed to be associated with the 660-km discontinuity in Earth's mantle. Details of this transition are important to clarify its effect on mantle convection: it is believed to inhibit flow across the "660" discontinuity. We have investigated the phase boundary using quasiharmonic free energy computations within the LDA and GGA. Once more the GGA transition pressure,  $P_{tr}$ , is higher and in much better agreement with the limited experiments available. The higher GGA  $P_{tr}$  can be rationalized by close inspection of the relationship between GGA and LDA functional forms. Our predictions of density, bulk modulus, and bulk velocity jumps across the transition are consistent with seismic observations.

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Yonggang Yu Minnesota Supercomputing Institute and Department of Chemical Engineering and Materials Science, University of Minnesota

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