

Abstract Submitted  
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**Quantum Monte Carlo Equations of State of  $\alpha$ - and  $\beta$ -Magnesium Silicate**<sup>1</sup> KEVIN P. DRIVER, JOHN W. WILKINS, The Ohio State University — The 410 km seismic discontinuity in Earth's mantle is ascribed to the  $\alpha$  to  $\beta$ -(Mg,Fe)<sub>2</sub>SiO<sub>4</sub> phase transformation. Considering Mg-endmembers, density functional theory (DFT) predictions within LDA and GGA disagree on the phase boundary by 50% [1]. Quantum Monte Carlo (QMC) offers a route to avoid the approximation of the exchange-correlation potential in DFT and provide a benchmark for the phase boundary, elastic moduli, and thermodynamic properties. Zero point and thermal contributions are included by using DFT linear response within the quasi-harmonic approximation. Preliminary results indicate the QMC phase relations and bulk moduli are in reasonable agreement with experiment.

[1] Y. Yu, Z. Wu., R. M. Wentzcovitch, *Earth Planet. Sci. Lett.* 273, 115 (2008).

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