

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Thermoelastic Properties of Olivine and its High Pressure Polymorphs at High Pressures and Temperatures: A First-Principles Study¹

MARIBEL NÚÑEZ VALDEZ, School of Physics and Astronomy, University of Minnesota, ZHONGQIN WU, School of Earth and Space Sciences, University of Science and Technology of China, YOUNGGANG YU, Department of Chemical Engineering and Materials Science, University of Minnesota, RENATA WENTZ-COVITCH, Department of Chemical Engineering and Materials Science, Minnesota Supercomputing Institute (MSI), University of Minnesota — We combine density functional theory (DFT) within the local density approximation (LDA), the quasi-harmonic approximation (QHA), and a model of vibrational density of states (VDoS) to calculate aggregate elastic moduli and sound velocities of olivine (α -phase) $(\text{Fe}_x, \text{Mg}_{1-x})_2\text{SiO}_4$, and its high pressure polymorphs, wadsleyite (β -phase) and ringwoodite (γ -phase), the most abundant minerals of the Earth's upper mantle (UM) and transition zone (TZ). Comparison of results with high-pressure and room-temperature data and ambient-pressure and high-temperature data shows very good agreement. Using our findings, we investigate the discontinuities in elastic moduli and velocities associated with the α to β and β to γ transformations at pressures and temperatures relevant to seismic discontinuities near 410 km and 520 km depth. This information offers clearly defined reference values to advance understanding of the role that chemical composition and temperature play in these mantle boundary layers.

¹Research supported by NSF/EAR-1019853 and EAR-0810272. Computations used the VLab cyberinfrastructure at the MSI

Maribel Nunez Valdez
University of Minnesota

Date submitted: 11 Nov 2011

Electronic form version 1.4