

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First principles elasticity of olivine¹ MARIBEL NÚÑEZVALDEZ, School of Physics and Astronomy, University of Minnesota, RENATA WENTZ-COVITCH, Dept. of Chemical Engineering and Material Sciences, University of Minnesota, KOICHIRO UMEMOTO, Geology and Geophysics, University of Minnesota — We examine by first principles the static elasticity of olivine, $\text{Mg}_{2-x}\text{Fe}_x\text{SiO}_4$ ($x = 0.125$), a major constituent of the Earth's upper mantle. We investigate the effect of atomic arrangement and composition on single crystal and poly-crystalline elastic moduli. Wave propagation anisotropy in single crystals and polarization anisotropy in aggregates with preferred orientation are also investigated and compared with those of forsterite for a thorough understanding of the effect of iron on these properties.

¹Research supported by NSF/ATM 0428774 and EAR 0810272. Computations were performed at the Minnesota Supercomputing Institute

Maribel NúñezValdez
School of Physics and Astronomy, University of Minnesota

Date submitted: 19 Nov 2009

Electronic form version 1.4