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Elasticity of iron-bearing olivine polymorphs investigated by first principles MARIBEL NÚÑEZ VALDEZ, School of Physics and Astronomy, University of Minnesota, YONGGANG YU, Dept. of Chemical Engineering and Material Sciences, University of Minnesota, RENATA WENTZCOVITCH, Dept. of Chemical Engineering and Material Sciences and Minnesota Supercomputing Institute, University of Minnesota — We calculate by first principles the effect of iron on the high pressure-temperature elasticity of olivine polymorphs: α-phase (olivine), β-phase (wadsleyite) and γ-phase (ringwoodite), the major constituents of the Earth's upper mantle and transition zone (TZ). We combine the LDA, the quasiharmonic approximation, and a model vibrational density of states for the solid solution to calculate the full elastic tensor C_{ij}, bulk (K) and shear (G) moduli of $(Mg_{0.875}Fe_{0.125})_2SiO_4$. Comparison with experimental data at ambient conditions validates our results. In the pressure and temperature range of the upper mantle and TZ we study single crystal wave propagation anisotropy and polarization anisotropy in aggregates with preferred orientation.

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