Molecular dynamics simulation of the density jump at the 660 km seismic discontinuity

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MD simulation is used to predict the structure and elasticity of Mg2SiO4 spinel, MgO, and MgSiO3 perovskite at high temperatures and high pressures. We further apply MD simulation to predict the densities of these three phases at the high T and P conditions corresponding to the 660 km discontinuity, and compare the simulated results with seismologically observed density jumps at the 660 km discontinuity, in order to give constraint on the chemical and physical properties of this discontinuity.