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Molecular dynamics simulations of seismic discontinuities and phase transitions of $MgSiO_3$ from 4 to 6-coordinated silicate via a novel 5-coordinated phase

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ABSTRACT

This paper reports detailed molecular dynamics simulations over a large pressure-temperature range (0–140 GPa and 300–2000 K) in the Earth's mantle starting from the upper mantle phase enstatite $MgSiO_3$. The simulated seismic velocities show several discontinuities corresponding to the phase transitions of enstatite. With increasing pressure, enstatite $MgSiO_3$ transforms first to a new novel five-coordinated silicon phase, and then to the lower-mantle perovskite phase involving six-coordinated silicon atoms. The new intermediate phase is crystalline but orientationally disordered. The calculated seismic velocities and densities across the phase transitions for a pure $MgSiO_3$ mantle are consistent with previous estimates. These studies suggest that the major discontinuities between the upper mantle, transition zone, and the lower mantle could arise partially due to the changes in the silicon coordination.