

## MgSiO<sub>3</sub> post-perovskite at D'' conditions

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The thermoelastic properties of the new polymorph of MgSiO<sub>3</sub> with the CaIrO<sub>3</sub> structure and more stable than the Pbnm-perovskite phase at conditions close to those expected in the D'' region has been investigated by first-principles computations and contrasted with those of the perovskite phase. Although we investigate only single and pure phases, the elasticity of aggregates containing predominantly these phases is expected to differ similarly, although in smaller magnitude. We therefore predict the major trends in seismic properties expected to occur in the presence of such phase change, such as velocity discontinuities, ratios of velocities and density anomalies, and anisotropy in aggregates with preferred orientation. Consequences of this model mineralogy for the D'' region will be discussed.

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## Development of transferable interatomic potentials for oxides and silicates using DFT calculations

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Atomistic modeling of physical properties of minerals and melts under extreme conditions of pressure and temperature requires a reliable and transferable representation of the interaction potential. Electronic structure calculations from first principles have proven the most accurate techniques, but their computational cost is still too high for systems that require a large number of atoms and long simulation times. It is, therefore, highly desirable to obtain interatomic potentials that include the essential interactions and that are transferable in a wide range of p/T and between different compositions.

Here we present an ionic interaction model that includes explicitly ionic polarization effects up to the quadrupolar level, and size and shape deformations of the ions that depend on the ionic environment of the individual ions. In the spirit of Born-Oppenheimer dynamics the energy due to these terms has to be minimized before the forces on the ions are calculated. The potential parameters are optimized by fitting forces and multipoles of individual ions and the stress tensor of different reference configurations to corresponding properties obtained by planewave-DFT calculations.

The resulting interaction potentials are shown to be transferable between different coordination environments and in a wide range of p/T. This is demonstrated for simple oxides, like MgO or Al<sub>2</sub>O<sub>3</sub>. Examples include phase stability of crystal polymorphs, thermoelastic properties, solid-melt interfaces, melt structure and transport properties. Finally, first results of new potentials for silica and silicates will be presented and discussed.

### References

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