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Ab Initio Studies of $MgSiO_3$ Post-Perovskite[1] FEIWU ZHANG[2], ARTEM OGANOV[3], ETH Zurich — Recent discovery of a post-perovsike phase of $MgSiO_3$ was considered as a new era in the studies of the Earth's deepest mantle. This discovery provides some explanations for many puzzling problems of the Earth's D" layer (pressures ∼120-136 GPa, temperature ∼2000-4000 K), such as the large seismic anisotropy, heterogeneity, variable depth, strong shear wave velocity discontinuity at the top, and anticorrelation between shear and bulk sound velocities. High pressures and temperatures existing in planetary interiors dramatically alter the structure and properties of materials, but are difficult to reproduce in the laboratory. Present-day quantum-mechanical simulations often give accuracy sufficient for geophysical or planetological purposes. The key roles of the $MgSiO_3$ post-perovsike phase transition will be addressed by further theoretical studies, including elasticity and anelasticity, electrical conductivity, radiative conductivity, energetics of stacking faults, effects of impurities on stability and properties of post-perovskite.

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