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Phase equilibria and velocity discontinuities across the post-perovskite transition in (Mg,Fe)SiO_3[1] RENATA WENTZCOVITCH, GAURAV SHUKLA, KANCHAN SARKAR, Univ of Minnesota - Twin Cities — The enigmatic nature of the region above the Earth's core-mantle boundary known as the D" region, is often characterized by a significant contrast in seismic wave velocities. The perovskite (Pv) to post-perovskite (PPv) transition in bridgmanite ((Mg,Fe)SiO_3 perovskite) is one of the keys for understanding this region. In this study, we present DFT + U_{SC} calculations of phase equilibria in bridgmanite across the post-perovskite transition. Thermal effects are addressed within the quasi-harmonic approximation. By computing high-pressure and high-temperatures elastic/acoustic properties of Pv and PPv phases, we also investigate seismic signature of the PPv-transition, believed to cause the D" discontinuity. Aggregate elastic moduli and sound velocities for the Mg-end member are successfully compared with limited experimental data available. Predicted velocity discontinuities across the PPv transition are consistent with seismic observations in some places of the global D" discontinuity. Our robust estimates of the phase boundary and elastic properties of the perovskite and post-perovskite phases will help to clarify the origin of lateral velocity variations in the deep lower mantle region and constrain its composition and thermal structure.

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