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Elastic and thermodynamic properties of post-perovskite $MgSiO_3$ from first-principles calculations LIU ZI-JIANG, CHEN QI-FENG, CAI LIN-CANG, Laboratory for Shock Wave and Detonation Physics Research, Institute of Fluid Physics, P. O. Box 919-102, China Academy of Engineering Physics, Mianya — The elastic and thermodynamic properties of post-perovskite MgSiO3 polymorph are investigated at high pressures and temperatures using the plane wave pseudopotential method within the local density approximation. This phase may be the most abundant mineral in the D" region. It is found that the post-perovskite phase has similar bulk modulus and larger shear modulus than perovskite at relevant pressures. The athermal elastic constant tensor of post-perovskite MgSiO3 are calculated as a function of pressure up to 200 GPa. The calculated results are in excellent agreement with other predictions over the pressure regime studied. The thermodynamic properties of post-perovskite MgSiO3 polymorph are predicted using the quasi-harmonic Debye model; the heat capacity and thermal expansion coefficient accord with the other calculations at high pressures and temperatures.

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