Abstract Submitted
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Lattice dynamics and thermal equation of state of cubic $CaSiO_3$ perovskite[1] TAO SUN, Key Laboratory for Geodynamics, University of the Chinese Academy of Sciences, Beijing, China, RENATA WENTZCOVITCH, University of Minnesota, Twin Cities, MN 55455 — $CaSiO_3$ perovskite (CaPv) is believed to be the third most abundant mineral in the Earth's lower mantle and is a major component of mid-ocean ridge basalt (MORB). A well constrained thermal equation of state for CaPv is key to several geophysical problems, e.g., lower mantle composition, density contrast between mantle and plates, nature of D" region, etc. Its experimental and theoretical determination have been very challenging because the cubic structure that CaPv adopts at lower mantle conditions is unstable at low temperatures and some of its harmonic phonons have imaginary frequencies. We have used a recently developed hybrid method combining ab initio molecular dynamics with vibrational normal mode analysis to compute its free energy and thermal equation of state at lower mantle conditions. These results are essential to understand the fate of subducted MORB in the mantle.

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