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Phase stability and elasticity of CaSiO3 perovskite FAWEI ZHENG, Department of Chemical Engineering and Materials Science, U of MN -Twin cities, MN, USA, TAO SUN, Key Laboratory of Computational Geodynamics, University of the Chinese Academy of Sciences, Beijing, China, RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, and Minnesota Supercomputing Institute,, U of MN -Twin cities, MN, USA — CaSiO3 perovskite (CaPv) is the third most abundant mineral in the Earth's lower mantle and is a major component of mid-ocean ridge basalt (MORB). This perovskite is stable only at high pressures, it is highly anharmonic, and undergoes a tetragonal to cubic transition at conditions that are still debated. We have used a recently developed hybrid method combining ab initio molecular dynamics with vibrational normal mode analysis to compute its free energy, thermal equation of state, and phase boundary at relevant geophysical conditions. These results are essential for understanding several aspects of mantle convection.

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