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Lattice dynamics of cubic $CaSiO_3$ perovskite at high temperatures and pressures[1] TAO SUN, DONG-BO ZHANG, RENATA M. WENTZCOVITCH, Department of Chemical Engineering and Materials Science, University of Minnesota — Cubic $CaSiO_3$-perovskite is a minor but important phase of the Earth's lower mantle. It is a mechanically unstable phase at low temperatures but it is stabilized at lower mantle temperatures. We have investigated its vibrational properties at high pressures and temperatures of the lower mantle. We have projected ionic velocities from ab initio molecular dynamics trajectories onto vibrational normal modes and computed the mode-mode correlation function from which we extract phonon frequencies and life times at finite temperatures. These correlations clearly indicate that normal modes with imaginary frequencies at 0 K are stabilized with increasing temperature. To overcome the finite size effect inherent in molecular dynamics simulations, a renormalized second-order force constant matrix in real space is constructed from the phonon frequencies at finite temperature and the phonon polarization vectors. Phonon dispersions and vibrational density of states are then determined by Fourier interpolation using the renormalized force matrix. These temperature dependent dispersions allow us to investigate thermodynamics and thermal elastic properties at lower mantle conditions.

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