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An efficient method for calculating high PT elastic constants ZHONGQING WU, University of Minnesota — First-principles quasi-harmonic calculations play a very important role in mineral physics because they can accurately predict the structure and thermodynamic properties of materials at pressure and temperature conditions that are still challenging for experiments. It also enables calculations of thermoelastic properties by obtaining the second-order derivatives of the free energies with respect to strain. However, these are exceedingly demanding computations requiring thousands of large jobs running on 10^1 processors each. Here we introduce a simpler approach that requires only calculations of static elastic constants and phonon density of states for unstrained configurations. This approach decreases the computational time by more than one order of magnitude. We show results on MgO and forsterite that are in very good agreement with previous first-principles results and experimental data.

Zhongqing Wu
University of Minnesota

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