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Anomalous Anharmonic Phonons in PbTe Reproduced from First-Principles Calculations YUE CHEN, CHRIS MARIANETTI, Columbia University in the City of New York — PbTe is of great interest due to its thermoelectric properties. Inelastic neutron scattering experiments reveal a signature of strong anharmonicity as evidenced in an anomalous temperature dependence of the phonon spectra. Novel approaches based on first-principles calculations have been developed for computing anharmonic phonons at elevated temperatures in recent years, though these techniques do not include lifetime effects and hence cannot address the anomalies observed in experiment. Here we perform first-principles molecular dynamics which includes the anharmonic terms at lowest order. The temperature dependent phonon spectra is computed and compared to experimental measurements, yielding insight on the origin of the observed anomalies.

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