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Atomic simulations of nonlinear lattice dynamics in PbTe YUE CHEN, CHRIS MARIANETTI, Columbia Univ — PbTe is of great interest as a thermoelectric material and for displaying signs of strong phonon interactions. Inelastic neutron scattering experiments reveal a signature of strong anharmonicity as evidenced in anomalous temperature dependence of the phonon spectra. Here we perform molecular dynamic simulations using a 4th-order interatomic potential deduced from first-principles calculations. The temperature dependent phonon spectra are successfully reproduced from first-principles for the first time. The emergence of a new mode at the zone center is unambiguously shown, as observed in experiment. Furthermore, we confirm that there is not a local spontaneously broken symmetry, clarifying recent controversy among experimental results. Phonon self-energies at different temperatures are computed to show the origin of the phonon anomalies.

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