

Abstract Submitted
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Temperature dependent anharmonic lattice dynamics OLLE HELLMAN, SERGEI SIMAK, IGOR ABRİKOSOV, Linköping Univ - Linköping — We have developed a thorough and accurate method of determining anharmonic properties in solids, the temperature dependent effective potential technique (TDEP). It is based on ab initio molecular dynamics followed by a mapping onto a model Hamiltonian that describes the lattice dynamics. The effective Hamiltonian contains implicit temperature dependence, electron phonon coupling and renormalized anharmonicity to arbitrary order, making it suitable for strongly anharmonic systems. We show excellent results for a host of thermoelectric materials (PbTe, SnTe, Bi₂Te₃, FeSi, ScN), reproducing temperature dependent phonon spectra, thermal conductivity, and phonon self energies.

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