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Phonons at finite temperature

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We present recent developments using the temperature dependent effective potential technique (TDEP) to model strongly non-harmonic materials. The method employs model Hamiltonians that explicitly depend on temperature. I will present applications pertaining to thermal conductivity, inelastic neutron spectra and phase stabilities. In addition, we investigate non-linear electron-phonon coupling and its influence on phonon spectra, and recent additions to that deal with nuclear quantum effects and efficient stochastic sampling.

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