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The Phonostat: Thermostating Phonons in Molecular Dynamics Simulations RAJAMANI RAGHUNATHAN, ALEX P. GREANEY, JEFFREY C. GROSSMAN[1], DMSE, MIT, Cambridge, MA02139 — We present a new phonostat algorithm to regulate temperature within molecular dynamics (MD) simulations. Our technique couples vibrational degrees of freedom of a group of atoms to a thermal reservoir allowing us to regulate an athermal population of various vibrational modes. In this phonostat algorithm, first the normal modes of vibrations are obtained using the frozen phonon calculation. Then we track modal energy in various vibrational modes by projecting the velocities and displacements of the group of atoms within each and every MD time step on to the corresponding normal mode. The modal energies are then coupled to a Nose-Hoover thermostat to regulate the temperature. We then emply this technique to understand the distribution and relaxation of vibrational modes in carbon nanotubes.

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