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Understanding and Controlling Intrinsic Dissipation in Driven Single Walled Carbon Nanotube Resonators[1] RAJAMANI RAGHUNATHAN, P. ALEX GREANEY, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology, Cambridge, MA 02139 — A "Phonostat" algorithm that can regulate total energy in a given internal degree of freedom within a molecular dynamics (MD) simulation is presented. The algorithm computes modal energies at every MD timestep, controls energy in a chosen vibrational mode with an external driving force and an internal damping. Using a test case of driven damped anharmonic oscillator, two different approaches of force correction are presented and various parameters that control the phonostat algorithm are analyzed. This algorithm is then employed to drive a chosen vibrational mode in carbon nanotube resonator to understand intrinsic dissipation under continuous driving, simultaneously computing its quality factor to mimic experimental conditions. The *gateway* modes that couple the driven mode to the thermal background are identified. Regulating these gateway modes hold the key to control intrinsic dissipation and improve quality factor for mass sensing application.

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Rajamani Raghunathan
Massachusetts Institute of Technology, Cambridge, MA 02139

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