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Energy Transfer and Resonance Enhancement at the Nanoscale.[1]

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Classical molecular dynamics (MD) simulations of carbon nanotubes are used to elucidate important phenomena in the transfer of (lattice) vibrational energy between nanoscale objects. We study in particular the transfer of energy between specific vibrational modes. The calculations show efficient transfer of energy between modes that are in resonance and the time scale over which energy is transfered is set by the weak van der Waal's coupling between nanotubes. These observations provide the mechanistic basis for a new theoretical framework for describing energy transfer at the nanoscale. The insight gained from this theoretical picture is used to propose several novel nanomechanical devices with applications in chemical sensing and wireless communications that function by the exchange of vibrational energy. The operation and feasibility of these devices is demonstrated by further MD simulations.

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