Abstract Submitted
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Real-time *ab initio* simulations of excited carrier dynamics in carbon nanotubes.[1] YOSHIYUKI MIYAMOTO, Fundamental and Environmental Res. Labs. NEC, ANGEL RUBIO SECADES, Universita Pais Vasco, DAVID TOMANEK, Michigan State University — Combining time-dependent density functional calculations for electrons with molecular dynamics simulations for ions, we investigate the dynamics of excited carriers in a $(3,3)$ carbon nanotube at different temperatures. Following an $h\nu = 6.8$ eV photo-excitation, the carrier decay is initially dominated by efficient energy transfer to the electronic degrees of freedom. About 200 fs after the photoexcitation in a nanotube initially at room temperature, the electron-hole gap is reduced to nearly half its initial value and the decay mechanism becomes dominated by coupling to phonons. We show that the onset point and damping rate within the phonon regime change with the initial ion velocities, which is a manifestation of a temperature dependent electron-phonon coupling.

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