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Anharmonic effects in carbon nanotubes: from thermal expansion to phonon lifetimes N. BONINI, N. MOUNET, N. MARZARI, Department of Materials Science and Engineering, MIT, Cambridge, MA, USA, M. LAZZERI, F. MAURI, Institut de Minéralogie et Physique des Milieux Condensés, Paris, France
— We study anharmonic effects in carbon nanotubes using a combination of density-functional theory and density-functional perturbation theory. In particular, we investigate thermal expansion and phonon lifetimes, which are key quantities that govern mechanical and transport properties in these systems. The thermal expansion coefficients are calculated from a minimization of the vibrational free energy in the quasi-harmonic approximation. Our results show that carbon nanotubes contract both in the axial and radial directions at low and room temperature and expand at higher temperatures. The role of different phonon modes in the thermal contraction is discussed together with their Grüneisen parameters. Anharmonic phonon lifetimes are evaluated from the cubic terms in the interatomic potential, using density-functional perturbation theory and the 2n+1 theorem. Finally, we discuss the possibility of estimating anharmonic effects using downfolding from graphene.

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