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Anharmonic phonon lifetimes in carbon nanotubes, graphene and graphite NICOLA BONINI, Department of Materials Science and Engineering, MIT, Cambridge, MA, USA, MICHELE LAZZERI, FRANCESCO MAURI, Institut de Mineralogie et Physique des Milieux Condenses, Paris, France, NICOLA MARZARI, Department of Materials Science and Engineering, MIT, Cambridge, MA, USA — In this work we present a first-principles study of the anharmonic phonon lifetimes of the key vibrational modes that most strongly interact with electrons in carbon nanotubes, graphene and graphite. The calculations of both harmonic and anharmonic properties are performed using density-functional theory and density-functional perturbation theory. Our results—in excellent agreement with the available experimental data—provide a microscopic characterization of the energy relaxation mechanisms and of the relative importance of the individual decay channels. We will discuss the relevance of these results to elucidate the role of non-equilibrium phonon populations in high-field electronic transport.

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