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Anharmonic phonon lifetimes in graphene, graphite and carbon nanotubes NICOLA BONINI, NICOLA MARZARI, Department of Materials Science and Engineering, MIT, Cambridge, MA, USA, MICHELE LAZZERI, FRANCESCO MAURI, Institut de Mineralogie et Physique des Milieux Condenses, Paris, France — We present a density-functional study of anharmonic phonon lifetimes in low-dimensional graphitic structures. Phonon lifetimes are evaluated from the cubic terms in the interatomic potential, using density-functional perturbation theory and the 2n+1 theorem. We show that in graphene and graphite the phonon lifetimes of the E_{2g} LO mode at Γ and the A'_1 mode at **K** due to phonon-phonon scattering are larger than those due to the electron-phonon interaction. We discuss the relevance of this finding for the transport properties and the implications for carbon nanotubes. We also present the results for the temperature-dependent frequency shift of the Raman G mode, in which third- and fourth-order anharmonic terms contribute equally.

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