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Phonon lifetimes and thermal conductivity of graphene from first-principles NICOLA BONINI, DMSE-MIT, JIVTESH GARG, MechE-MIT, NICOLA MARZARI, DMSE-MIT — Carbon nanostructures, such as graphene and carbon nanotubes, are particularly promising materials for thermal management applications because of their very high thermal conductivity. A clear understanding of the transport properties of these materials is a key step in view of their possible integration into future devices. Here, we present a first-principles study of the thermal transport properties of graphene. We use density-functional theory and density-functional perturbation theory to determine both harmonic and cubic anharmonic terms in the crystalline potential—the key ingredients to calculate phonon frequencies and phonon lifetimes. Our results show that the long-wavelenght longitudinal and transverse in-plane acoustic phonon modes of graphene have an anomalously small lifetime, that leads to a significant underestimation of the thermal conductivity computed within the single mode relaxation time approximation. We will discuss the effect of strain and graphene-substrate interaction on the lifetime of the acoustic modes, and we will present results for the thermal conductivity determined by directly solving the linearized Boltzmann transport equation.

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