Electron-phonon interaction in carbon-based materials: from superconducting diamond to single-layer graphene[†]

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Recent years have witnessed a surge of interest in the electron-phonon problem, mainly in connection with the discovery of strong electron-lattice effects in high-temperature superconductors, new phonon-mediated superconductors, and the observation of phonon-limited mobilities in carbon-nanotube field-effect devices. The first-principles investigation of phenomena induced by electron-phonon interaction requires an accurate sampling of electron and phonon scattering processes in proximity of the Fermi surface. This computationally demanding task can only be performed nowadays on simple systems with a few atoms per unit cell. In this talk I will first introduce a recently developed methodology based on electronic and lattice Wannier functions which reduces by several orders of magnitude the computational cost of such first-principles calculations. Then I will discuss the application of this method to two classes of carbon-based materials, superconducting boron-doped diamond and single-layer graphene, which are currently being considered as potential candidates for novel electronic and spintronic device concepts. In the case of superconducting boron-doped diamond, theoretical investigations have come to a consensus about a conventional phonon-mediated paring, however the nature of the phonon mechanism involved is still a controversial issue. I this talk will show that the localized vibrational modes associated with the boron atoms are crucial to the superconducting pairing insofar they enable scattering processes with large momentum transfer. In the case of single-layer graphene, photoemission experiments revealed an unexpected dependence of the hole linewidths on binding energy. Here I will show that the electron-phonon interaction accounts for a major fraction of the measured linewidths, as well as for a significant renormalization of the Dirac velocity.

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