Electron-phonon interactions in low-dimensional carbon systems: superconductivity and charge-density waves

Abstract

In this thesis work I investigated the effects of the electron-phonon interactions in low-dimensional carbon allotropes from first principles. In particular I focused on the emergence of superconductive phase transitions when doping systems via field effect and the occurrence of charge-density waves (CDW) due to the reduced dimensionality. In order to do so, I exploited density functional theory (DFT) and its linear response extension (DFPT), taking also into account electronic correlations via hybrid exchange-correlation functionals and the GW approximation. Furthermore, when studying the CDW transition, I also took into account the anharmonic phonon-phonon interaction via the stochastic self-consistent harmonic approximation (SSCHA).

Chapter 1 gives a short review of the different carbon allotropes, since they represent the core of the present work. In particular I give a classification based on their dimensionalities, describing how they affect their electronic and vibrational properties, focusing more on the allotropes of interest for this thesis.

Chapter 2 reviews the electron-phonon interactions from a many-body point of view. I discuss the implication of the Migdal approximation to the electron-phonon vertex and the random phase approximation (RPA) to the phonon propagator. Finally I briefly derive the multi-band Migdal-Eliashberg theory of superconductivity and I discuss its main approximations.

Chapter 3 presents a general description of the field-effect (FET) doping technique from both the experimental and the theoretical point of view, discussing also the theoretical models for FET architectures implemented in plane-wave ab-initio codes. Finally, I investigate the field-effect induction of superconductive proximity effect in three phonon-mediated superconductors.

Chapter 4 studies if it is possibile to induce a superconductive phase transition in diamond thin films via field-effect doping using both a semi-empirical approach (McMillan/Allen-Dynes equation) and a many-body approach (solving the multi-band Migdal-Eliashberg equations). I first analyze how FET doping affects both the electronic and the vibrational properties of the system. Electron-phonon interactions are then computed ab-initio over all the Brillouin zone through a Wannier interpolation scheme. High temperature superconductivity ($T_c \sim 40$ K) is expected for relatively high doping ($n_{2D} \sim 6 \times 10^{14}$ cm^{-2}).

Chapter 5 deals with a possibile superconductive phase transition in few-layers graphene when stacked in a rhombohedral configuration induced via field-effect doping for sufficiently high values of the induced charge density. Due to flat bands at the Fermi level, electronic correlations are expected to play a key role also for electron-phonon interactions. Therefore, electron-phonon matrix elements are computed through finite differences by also taking into account different percentages of exact exchange interaction among electrons (i.e. with hybrid functionals). Standard DFPT severely underestimates the deformation potential in this case and the inclusion of electronic correlation boosts the electron-phonon coupling constant approximately by a factor 2. Nevertheless, no phonon-mediated superconductive phase transition is observed.

Chapter 6 focuses on the lattice instability of the linear acetylenic carbon chain. The Landau-Peierls distortion of carbyne from an ordered metallic to a distorted insulating phase is re-investigated, departing from the harmonic description of lattice dynamics and taking into account electronic correlations. Moreover, thanks to the stochastic self-consistent harmonic approximation (SSCHA), the temperature dependent free energy landscape is studied by including phonon-phonon anharmonic interactions in a non-perturbative way. Finally, I also perform ab-initio computation of the optical properties of polyyne both in the G_0W_0 approximation and solving the Bethe-Salpeter equation.