Inelastic Disordered Transport Applied to Graphene Nanoribbons with Hydroxyl Impurities

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With the trend toward decreasing the dimensions of electronic devices, the interaction between electrons and ionic vibrations plays an important role in electronic transport. The electron-phonon coupling can cause the loss of the electron's phase coherence, the opening of new conductance channels and the suppression of purely elastic ones. From the technological viewpoint phonons might restrict the efficiency of electronic devices by energy dissipation, causing heating, power loss and instability.

Computer simulations can be an important tool for predicting and helping the design of new devices. However, another important feature of realistic electronic devices that should be taken into account is the fact that these devices most often can reach the 100 nm length scale with a large number of randomly distributed defects. This "disorder" can lead to a fundamentally new transport regime, namely the Anderson localization regime. Therefore, in order to perform quantitatively meaningful simulations of realistic devices, the method used should be able to consider tens of thousands of atoms with randomly positioned defects which, by means of *ab initio* methods, is not an easy task. Also, the combination of disordered systems with electron-phonon interaction might explain open questions such as the nature of conductivity in polymers.

In this work we present a method that allows one to compute the transport properties of realistic electronic devices with the two named features: large number of randomly distributed defects together with realistic electron-phonon interaction. Our method combines the accuracy and functionality of *ab initio* Density Functional Theory to determine the electronic structure with a recursive Green's functions formalism. We considered the case with weak and localized electron-phonon coupling strength. Approximating the contact broadening and the non-interacting retarded Green's functions as energy independent matrices, the current and power expressions can be expanded to second order in the electron-phonon couplings and the integration over energy performed analytically, the so-called Lowest Order Approximation [1,2]. We present results showing the effects produced by considering the electron-phonon interactions in toy models and in graphene nanoribbons with joint attachment of hydroxyl group.

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