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Reduced Backscattering in Potassium Doped Nanotubes

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INTRODUCTION

The integration of carbon nanotubes (CNTs) in electronic devices such as field-effect transistors (CNFETs) [1] has generated much experimental and theoretical work to understand the basic phenomena controlling the device performances. As a crucial ingredient, the doping of the semiconducting canal has been achieved following different strategies.

While substitutional doping certainly increases the carrier density in the CNTs, it also induces significant backscattering that can reduce the charge transmission capability of a given conduction channel [2], [3]. We study the conductance of metallic and semiconducting tubes doped either by K in adsorption or N in substitution.

TEORETICAL FRAMZWORK

A O(N) *ab initio* method is used to precisely compute the effect of isolated defects on the Landauer transmission. Our *ab initio* results are further used to construct an accurate $\pi - \pi^*$ effective model which allows to access, within the Kubo formalism, the conductance and elastic mean free path of tubes randomly doped over micron scales.

DISCUSSION

The case of a metallic C(6,6) and semiconducting C(7,0) nanotubes are considered (Fig. 1). In the case of K-doping, an important outcome of the present study is *the complete disappearance of the broad structure associated with the low energy (more bound) resonance state*. This is a clear indication that K-doped tubes, as compared to the N-doped systems, will display a ballistic-like behavior on a much larger gate-voltage range and for longer propagation length of charge carriers.

We also investigate more realistic cases of micrometers long nanotubes doped by a random distribution of scatterers. Such calculations have been carried on doped (10,10) CNTS ((Fig. 2). The MFP of the K-doped nanotube ($\ell_e \sim 24\mu$m) is found to be four times larger than the N-doped tube at $E_F \sim 0.5eV$ (energy of the deeper N quasibound state), and at the same impurity density.

CONCLUSION

On the basis of *ab initio* conductance calculations, K-impurities have been shown to induce much less backscattering as compared to nitrogen substitutions. By mapping the *ab initio* Hamiltonian onto a reduced $\pi - \pi^*$ model, the conductance and mean-free path of randomly doped micrometers long tubes was investigated within the Kubo formalism, confirming that K-doping leads to much longer mean free paths.

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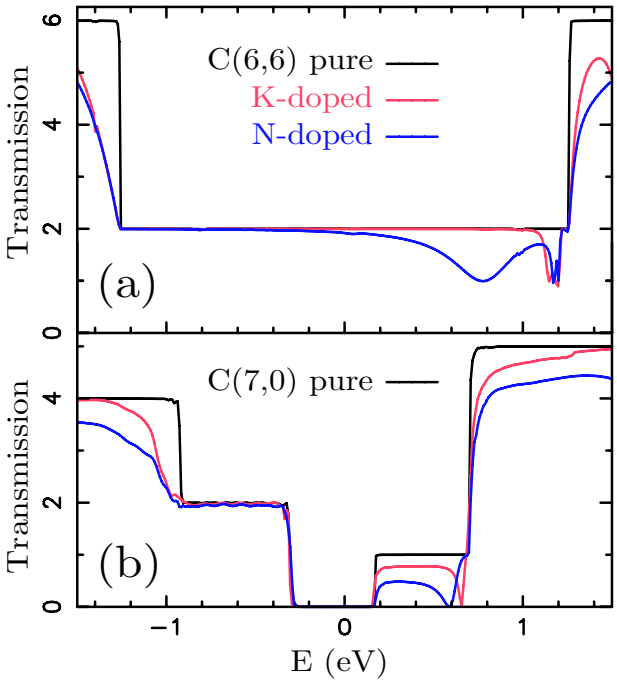

Fig. 1. Transmission for (a) a C(6,6) and (b) a C(7,0) nanotube. Undoped (black), nitrogen-doped (blue) and potassium-doped (red) tubes are considered.

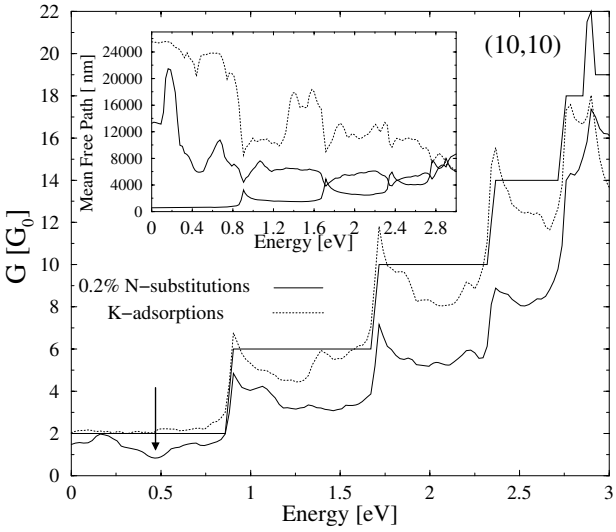

Fig. 2. Main frame: Conductance for the (10,10) nanotube with 0.2% of randomly substituted N-impurities (bold) or physisorbed K-impurities (dotted line). The number of quantum channels is also reported (solid line). Inset: Corresponding mean free paths together with the rescaled density of states (solid line).