Electronic Transport Between Platinum Contacts Through Graphene/Nanotubes Structures

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Recent studies have shown that good metallic contacts could be form between a platinum (Pt) contacts and carbon nanotubes (CNT) thanks to the formation of a graphene layer between them[1].

We study electronic transport properties of CNTs with Pt contacts using first principles calculations. We have considered two situations: one where a layer of graphene had formed (and to where the CNT is covalently linked[2]) (Figure 1a) and the other where the CNT was in direct contact with the Pt surface (Figure 1c). The simulations are performed within the density functional theory (DFT) and the Non-Equilibrium Green Function (NEGF) formalism. The calculations are performed with the SIESTA[3] code and its extention, TranSIESTA[4], for the electronic transport calculations, using strictly localised orbitals as basis sets.

After performing the relaxation in both systems, we found that the equilibrium distance between graphene sheet and a Pt surface is of the order of 3.14 Å and the stable distance between the CNT and a Pt surface being of 2 Å. This fact brings us to the conclusion that the graphene sheet is decreasing the interaction of the CNT with the Pt contacts due to the larger distance between the Pt surface and the nanotube. As a consequence the overall transmission (when considering a wide range of energy) is higher in the second case (CNT directly on the Pt surface).

We also perform transport calculations applying different voltages to the Pt contacts and we study the transmission eigenstates, the potential drop and the charge density drop.

References

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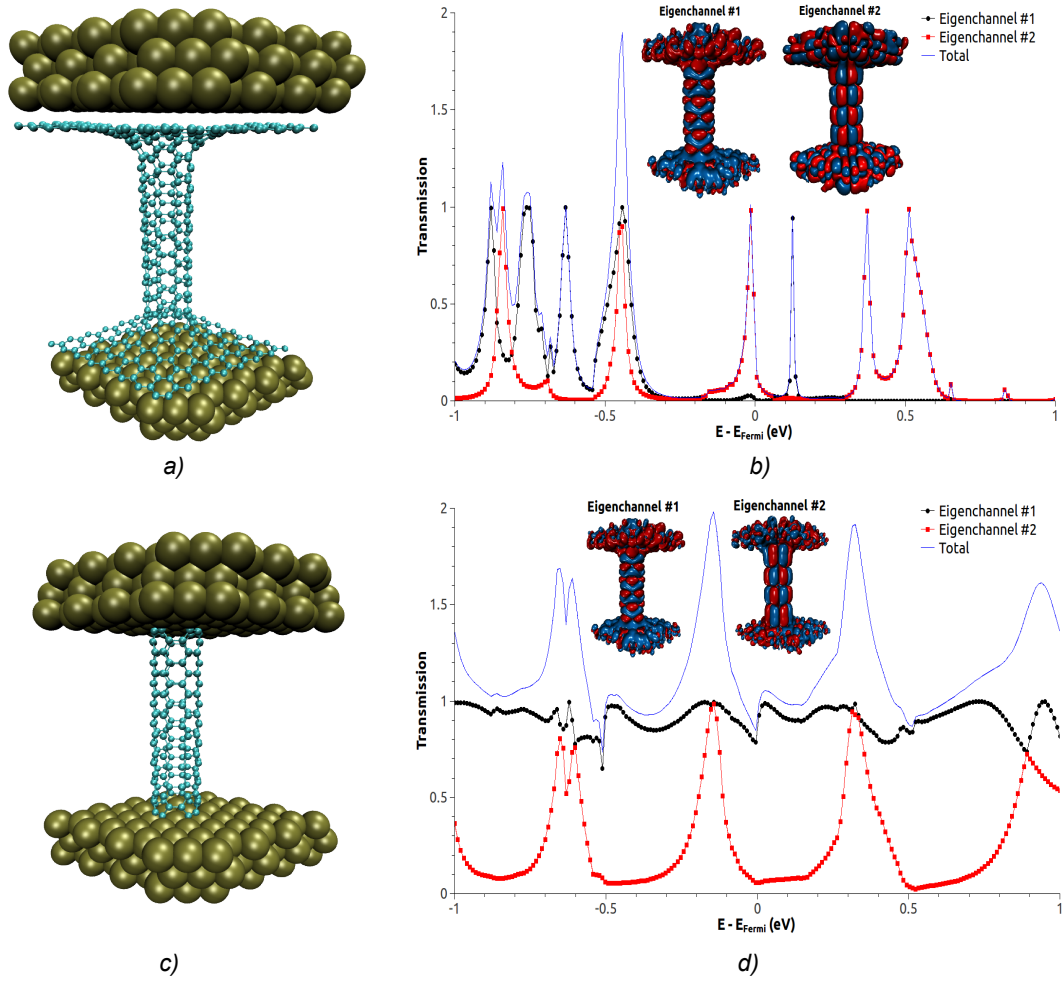**Figures**

a)

b)

c)

d)

Figure 1: a) Graphene/CNT/Pt structure, b) Graphene/CNT/Pt structure transmission at 0 V,
c) CNT/Pt structure, d) CNT/Pt structure transmission at 0 V.