Designing a spin filter circuit based on a finite single-walled carbon nanotube of the zigzag type

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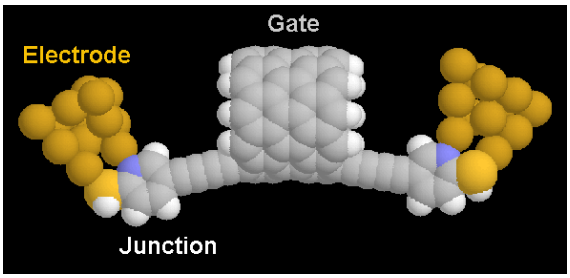
Zigzag-edge single-walled carbon nanotubes (zSWCNTs) of finite size are well-known candidates for conductors in nanoelectronic circuits,[1] since they are chemically inert and mechanically stable, and thus can be easily handled and exposed to relatively high operating temperatures. Recently, it has been predicted that H-terminated zSWCNTs can also be used as gates in a spin valve or spin filter circuit due to the antiferromagnetic nature of their electronic ground state, characterized by unpaired electrons with opposite spin orientation at either end of the tube.[2] However, problems may arise when making a junction between the zSWCNT and electrodes, as this junction could quench the spin polarization of the system. This is a non-trivial issue, as formation of a covalent bond with any of the carbon atoms of the zSWCNT might quench the spin density at the respective end of the tube.[3] The challenge addressed in this work is defining a junction, which, while being electrically conductive, can be attached both to the ends of the zSWCNT and to the surface of an electrode without substantially compromising the zSWCNT magnetic properties.

Specifically, we discuss a complete circuit, consisting of a zigzag-edge single-walled carbon nanotube (zSWCNT) as a gate with attached transacetylene chains anchoring 2-mercaptopyridine residues as conducting junctions, and gold clusters as electrodes. This system is modeled by density-functional theory (DFT), with both plane-wave and atom-centered Gaussian bases. Spin polarization is found to be preserved in zSWCNT upon covalent grafting of the conducting substituents, and spin conductivity is observed through the entire circuit. These findings are relatively insensitive to the zSWCNT diameter and the gold cluster size. This suggests that the present design may be an interesting candidate for a nanotube-based spin filter prototype.



(1) Liu, L.; Ma, W.; Zhang, Z. Macroscopic Carbon Nanotube Assemblies: Preparation, Properties, and Potential Applications. *Small*, 2011, *7*, 1504–1520.

(2) Wu, J.; Hagelberg, F. Magnetism in Finite-Sized Single Walled Carbon Nanotubes of the Zigzag Type. *Phys. Rev. B*, **2009**, *79*, 115436.