Spin dependent electron transmission through single-walled carbon nanotubes of the zigzag type

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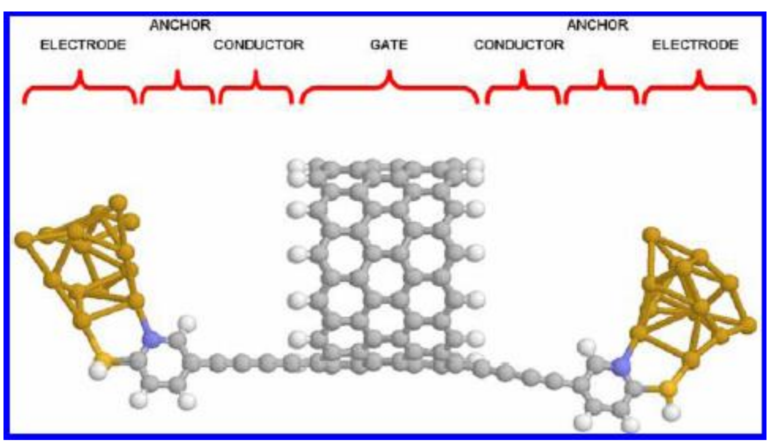
Magnetic carbon nanostructures hold great promise for potential applications in nanodevices based on spintronics [1], operating with spin currents rather than currents of electric charge, as employed in conventional electronics. Extended carbon structures may acquire magnetic ground states as a consequence of dimensional reduction. The focus of this contribution is on axially confined single-walled carbon nanotubes of the zigzag type (zSWCNTs) where magnetism is induced by unpaired electrons at the edges of the tube [2,3].

This contribution addresses the challenge of applying zSWCNTs in spintronics. Utilizing a zSWCNT as a transmission element in a nanoelectronic circuit requires designing conductive junctions that connect the tube to metal electrodes while leaving the spin polarization at the tube edges unquenched. Density-functional theory (DFT), with both plane-wave and atom-centered Gaussian bases, was used to model a circuit consisting of a zSWCNT as a gate with attached transacetylene chains anchoring 2-mercaptopyridine residues as conducting junctions, and gold clusters as electrodes [4], as shown in the figure. The emphasis of this presentation is on spin dependent electron transport through the zSWCNT gate. In particular, spin effects in transmission spectra and current-voltage (I-V) profiles, obtained by use of a non-equilibrium Green's Function (NEGF) procedure, will be discussed.



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