574e A Toolbox for Spintronics: Ab-Initio Evidence of a Carbon Nanotube-Based Material for Spin-Polarized Electron Transport

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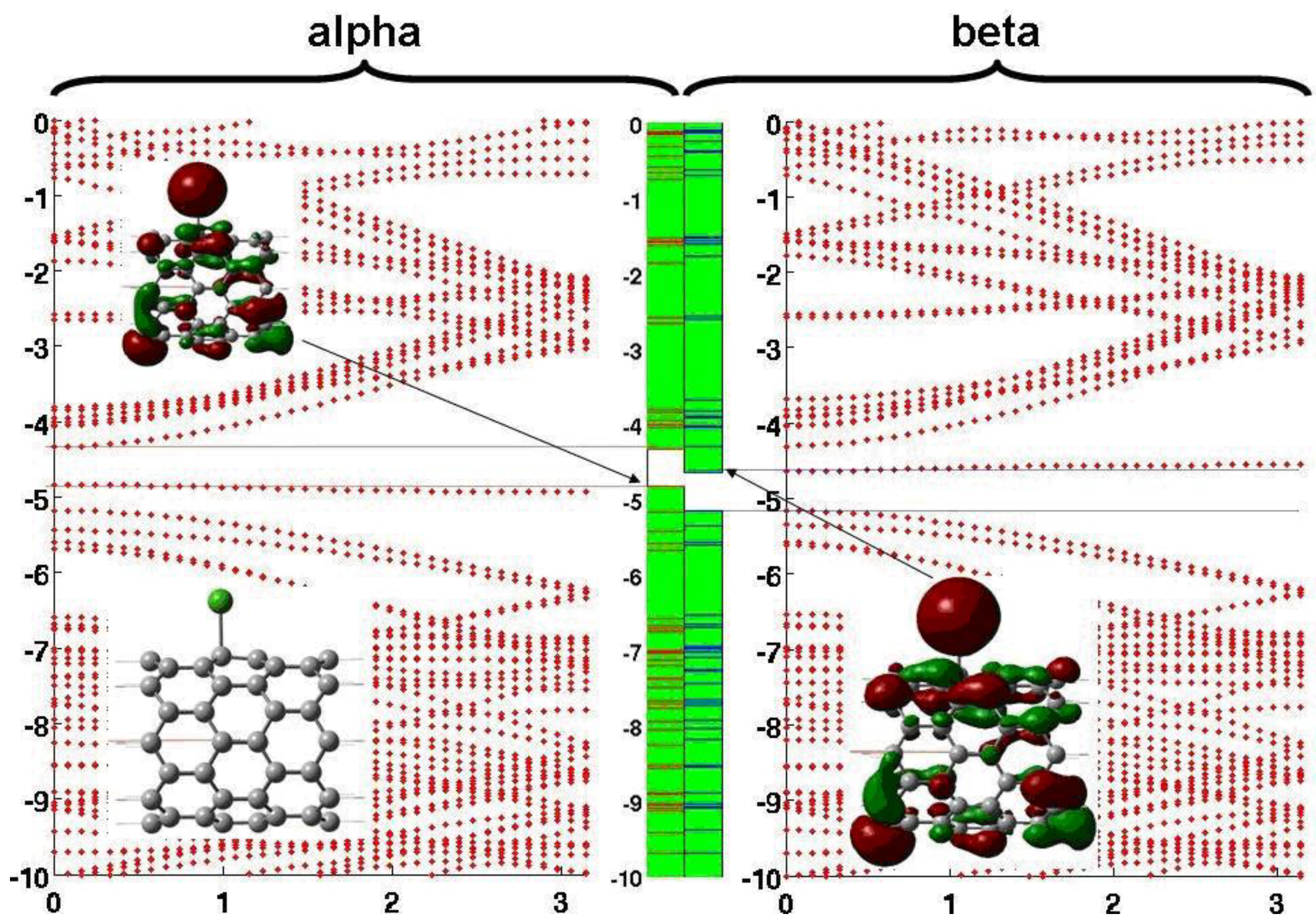
In a conceptual open-loop design of a spintronic device three stages would be needed: a source of spin-polarized electrons, a controller able to do some processing according to the spin of the current, and a plant sensitive to the spin of the electrons. We present a carbon nanotube- (CNT) based molecular system that allows a separation of spin current; with α-electrons moving exclusively through the valence band and β-holes through the conduction band. The calculation of infinitely long semiconducting (8,0) CNT with Au atoms adsorbed is carried out using periodic boundary conditions as implemented in Gaussian 03 with the PW91/LANL2DZ level of theory. The primitive cell for the system under study is shown in the lower left part of Figure 1. A flat band translates into an infinite effective mass and zero mobility, thus, carriers dwelling on those bands will be immobile for transport purposes. The valence and conduction bands show a finite curvature (finite effective mass), allowing the movement of carriers whenever electric field is applied. Since these bands have similar curvature, the hole and electron mobility will be also of similar value, and lower than for the case of pure (8,0) CNT. The band structures are calculated at 0 K. At some applied temperature, the thermal energy will cause β-electrons to jump from the β-HOCO band to the β-LUCO band, where they will remain immobilized, leaving behind β-hole type carriers in the valence band, as in p-type material. On the other hand, immobile α-electrons jump from the α-HOCO band to the valence band, forming α-electron type carriers, as in n-type material.

Figure 1 Band structured for a periodic system of Au atoms adsorbed on a (8,0) CNT. The unit cell is shown in the lower left part. The geometry was optimized using the PW91 functional for exchange and correlation and LANL2DZ basis set for all atoms. Crystal orbital energy levels (for k=0) are zoomed and displayed in green, with the band gaps readily visible, for both alpha and beta spins. Vertical units in eV and horizontal quantities are in (1/a) units. Where a is the lattice constant of the system (8.6 Å).



alpha
beta