11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

Analysis of nanotube p-n doping of $[(CC)_n]_m$, $[(GeGe)_n]_m$, and $[(SiSi)_n]_m$ using semiempirical, HF, and DFT methods

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Abstract – The p-n junction in carbon nanotubes have been analyzed theoretically, indicating that the distance of 2.50 Å between doped nanotubos yields an increase of the Gap (HOMO-LUMO), suggesting that these structures can be used as diodes.

The p-n junctions are of fundamental importance for modern semiconductor devices. They are the basis for most of the optical transition devices. The carbon single walled nanotubes (SWNTs) are a class of materials with potential importance for electronic devices, such as transistors, memory devices, sensors, and diodes, through the formations of p-n type junctions. It has been shown experimentally that the doping of individual nanotubes to form a p-n junction could be done, yielding near ideal diode characteristics [1].

The models were constructed considering Ge and P as a n type dopant and B as a p type dopant (Figure 1). The distances were optimized for the nanotubes, yielding in this manner the lowest energy among them (Figure 2), analyzing also the Gap (HOMO-LUMO) in relation to the interaction distance (Figure 3).

Figures 2 and 3 shows that the distance of smallest energy between the nanotubes is 2.50 Å, with an increase of the Gap (HOMO-LUMO) to 12.91 eV. This trend is not shown by the carbon non-doped nanotubes. Thus the doped structures can be used as diodes with observed experimentally.

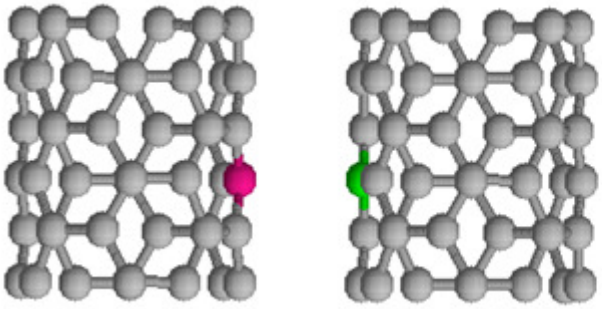

Figure 1. Interaction between carbon nanotubes with p type doping (B) and n type (Ge)

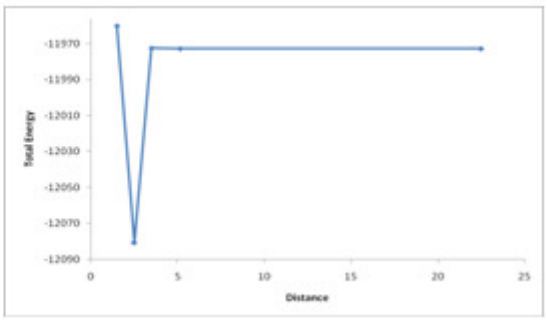

Figure 2. Relation between the nanotubes and total energy

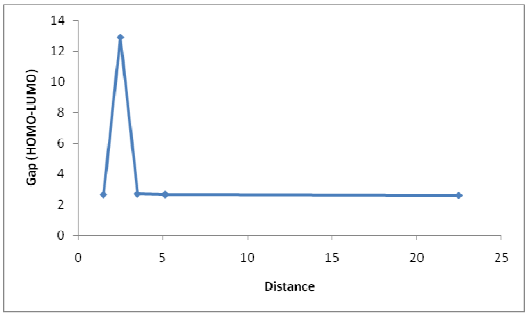

Figure 3. Relation between the Gap, (HOMO-LUMO) and the interaction distance

[1] J. U. Lee, P. P. Gipp and C. M. Heller, Appl. Phys. Lett. 85 (2004).