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Theoretical study of the composites CNTs/ polyaniline

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Abstract – An important application of conducting polymers and carbon nanotubes (CNTs) is their usage in electrical devices, such as sensors, circuits and capacitors. The combination of these materials in the formation of the composites, such as for example, the combination of polianiline with carbon nanotubes (CNTs/polianiline) constitutes a material with important applications. In this work, a theoretical model was studied of the interaction between these structures, analyzing the stabilization energy, Gap (Homo-Lumo), charge distribution as well surfaces of HOMO and LUMO orbitals.

The conducting polymers, carbon nanotubes (CNTs) and fulerenes are among the principal components of this new class of advanced materials based on carbon. Among these compounds the combination of polymers and nanotubes have the potencial to be used in a variety of devices, such as low cost circuits, super-capacitors and sensors for solar cells. The formation of composites polymer/nanotubes is considered as a promising incorporation of nanotubes in devices with technological potential. Many polymers have been used as matrices in composites CNT/polymers for various applications, such as carbon nanotubes and polyanilines (PANI) with potential usage in photovoltaic devices. The PANI is one of the most important conducting polymers due to the relative facility in the processing, electrical conductivity and environmental stability [1, 2].

In this work we investigated the structure of polyaniline, of the CNTs and the composite CNT/polyaniline (Figure 1) using the HF and DFT methods with the 6-31G basis. The interaction energy was calculated using equation 1.

$$\text{Polianiline} + \text{CNT} \rightarrow \text{CNT/Polianiline} \quad \Delta E = E_{CNT/Polianiline} - E_{Polianiline} - E_{CNT} \qquad (1)$$

The polyanilines used in this interaction have 4 to 15 rings and the carbon nanotubes have zigzag and armchair configurations: (5,0); (5,5); (12,0) e (6,6). It was observed in the analysis the stabilization of the system with the lowering of the gap (HOMO-LUMO) in relation to the isolated structures, indicating in this form an improvement of the conductivity of the interacting system in relation to the two isolated structures. We also analyzed the charge distribution of the system such as the surfaces of the HOMO and LUMO orbitals.

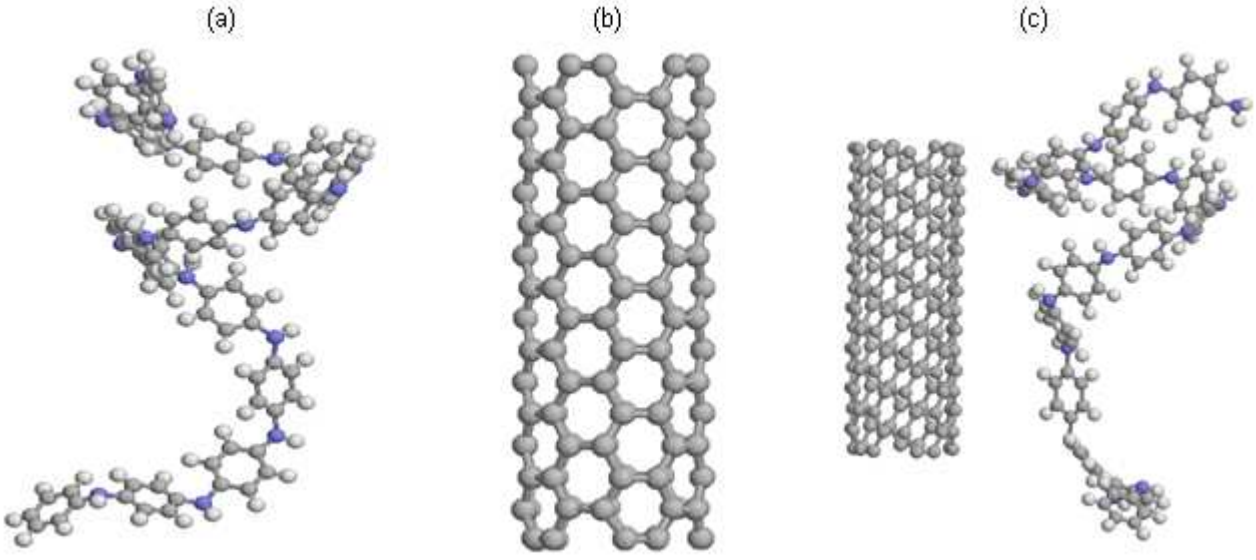

Figure 1. Models used in the study of the composites CNTs/polyaniline: (a) Polyaniline with 15 rings; (b) Carbon nanotube (5,5) with 8 levels (c) Interacting system CNT/polyaniline.

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