Molecular Modeling and Computer Simulation involving the Encapsulation of β-carotene in Boron Nitride Nanotubes

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INTRODUCTION

The possibility of applying functionalized nanotubes with β-carotene in the form of nanocrystalline dyes in photovoltaic-type cell (DSSC) is the motivating element of this work. It is now known that the addition of nanocrystalline organic dyes possibly increase the efficiency of these electronic devices in converting solar energy into electrical energy. Vale, in due course, referencing the recent work of Grätzel at al [7, 8, 9] on this subject.

On the one hand, we have the β-carotene (BC), orange pigment that has molecular formula C40H56. It is a natural dye that shows the photoluminescence phenomenon, property proven by spectroscopy. On the other hand, pointed out the boron nitride nanotubes (BNNTs). These nanostructures have been predicted theoretically shortly after the discovery of carbon nanotubes (CNTs), by Rubio et al in 1994, and were manufactured experimentally by Chopra et al, 1995[5]. All BNNTs are broadband semiconductor with gaps of approximately 5.5 ev [2, 3, 4]. Its high ionicity and high energy gap gives greater uniformity to the electronic properties and explain the use of these materials in the electronics field. In addition, BNNTs stand out for their chemical inertness and high thermal stability, potentially interesting properties for applications in biomedicine field and engineering of biomaterials [3]. Unfortunately, it is noted that the applications of this and other boron nitride materials of biological fields remain largely unexplored [6].

Our study uses the resources to perform computational molecular modeling molecular dynamics simulations and describe a process known as "encapsulation" of the β-carotene molecule into single-layer boron nitride nanotubes (SWBNNT). Our results have confirmed such encapsulation in conditions imposed. In addition, we rely on density functional approximations associated with the Tight-Binding method to investigate possible changes in the electronic structure of the materials involved.

Thus, an interesting line of research is that which proposes the replacement of mesoporous titanium oxide by a sensitizer higher efficiency. Nanotubes functionalized with BC are potentially promising in this regard.

METHODS

we propose a theoretical analysis of the BC molecule encapsulation within a SWBNNT, a form of chemical functionalization, in which use mathematical tools combined with molecular modeling and simulation Computational as Force Field Classical and Molecular Dynamics with results based on Functional Tight-Binding Density (TBFD +). To perform these simulations, the Materials Studio is used, a computer simulation package Cerius as desktop.

The Molecular Mechanics (MM) is a classic and simple method that uses newtonian mechanics equations to describe the potential energy surface (PES) and the physical properties of molecular systems through energy conformation calculation. In other words, you want to with the application of MM, get the optimized settings of the systems under study. The option of working with the so-called Universal Force Field (UFF) is conveniently categorical since the process that

want to play involves the interaction of an organic system with an inorganic system. The simulations describe the encapsulation of β-carotene into two specific nanotubes: a chiral SWBNNT (13,5) and a Armchair SWBNNT (9,9), with lengths and diameters are compatible with conditions already described in the literature for CNTs.

The encapsulation process occurs with the application of molecular dynamics (MD). This is the method used to describe the time evolution of systems, through numerical integration of Newton's laws. The results obtained by this means information provided for calculating its elastic energy, characterized possible deformations and enables estimated on the process spontaneity.

Finally, one obtains quantum properties of systems through application of TBFD + module, Cerius compound in the package. The TBFD + uses the Tight-binding method (TB) associated with the Density Functional Theory (DFT) to gain accuracy and efficiency. The TB is in turn an approximation method suitable to the first neighboring situation. From this, analyzes of energy and DOS our original systems and encapsulated allow us to make inferences about the gaps and other changes in the electronic structure of the same.

RESULTS AND DISCUSSIOS

In this study, we tried initially to get the optimized and isolated structures of β-carotene molecule and the nanotubes (13, 5) and (9, 9). This optimization procedure involves the application of force field (UFF). Nanotubes were selected with both ends open and lengths greater than the length of the molecule, so that avoid edge effects. The BNNTs also have diameters compatible with the diameters of CNTs described in the experimental work of Yanagi et al. [1].

Obtained the structures in their most stable conformations, urges the structures in place appropriate conditions for initial development dynamics. Other procedures, and the choice of NVT ensebly and the randomness of the initial velocities are intended to reproduce the experimental conditions under which the process occurs normally.The power stabilizing complexes SWBNNT + BC is obtained by comparing the energies of the complex before and after encapsulation. Stabilizing energy calculations confirmed the occurrence of encapsulation in its spontaneously in both cases studied. Figure 1 and Figure 2 show, in sequence, the frames that are evident in the BC SWBNNT tunnel (13,5) and SWBNNT (9,9). Similarly, the elastic energy of the encapsulated BC was obtained by comparing the free energy of the molecule with the energy of the encapsulated molecule. This energy results predict the emergence of geometric deformations in the molecule, resulting from weak interactions the same with the walls of the nanotubes.

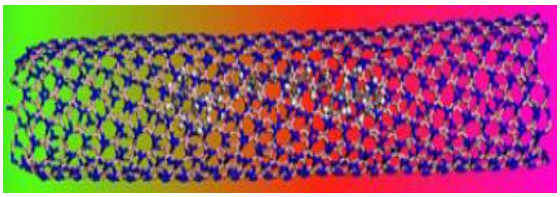

Figure 1. Frame in which notes the BC encapsulated in SWBNNT (13,5).

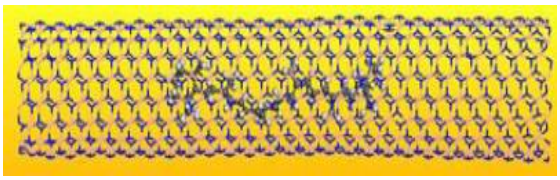

Figure 2. Frame in which notes the BC encapsulated in SWBNNT (9, 9).

Data on energy and the DOS of encapsulated SWBNNT complex (13, 5) + BC and SWBNNT (9.9) + BC have also been generated by application of DFTB + method. Figure 3 and Figure 4, relating the normalized DOS per unit state with the energy of corresponding nanotube.

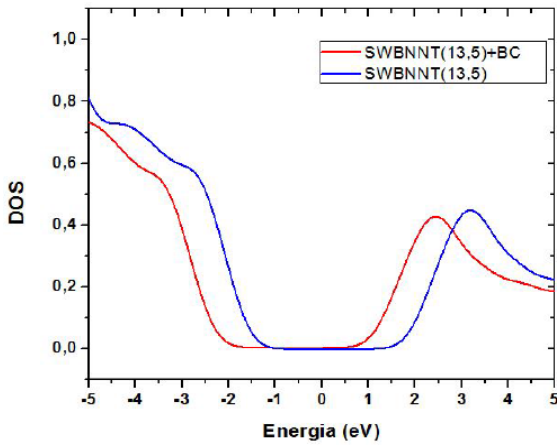

Figure 3. Of the curve giving the states by unit depending on the power to the SWBNNT (13,5). The blue line represents the pure nanotube and the red line represents the functionalized nanotube.

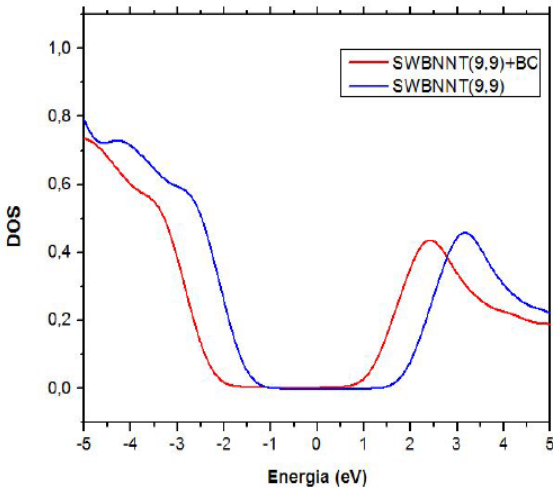

Figure 4. Of the curve giving the states by unit depending on the power to the SWBNNT (9,9). The blue line represents the pure nanotube and the red line represents the functionalized nanotube.

So we can compare the gaps of the nanotube with the gap of the encapsulated complex. Each figure highlights the region near the Fermi zone. The difference between the gap of the nanotube before and after encapsulation, is indicative of the BC electronic coupling involving in both cases.

CONCLUSIONS

Our simulations showed that BC is encapsulated in SWBNNT nanotubes (13,5) and (9,9). Calculations relating to stabilization energies suggest that this process is spontaneous. Estimates of the elastic deformation energy of the BC link systems.

Analysis of the investigated DOS systems, obtained by applying the TBFD + code, suggest the occurrence of electronic coupling due to the superposition of molecular orbitals.

There was, therefore, changes in the electronic structure of the two nanotubes. Despite this evidence, the difference is remarkably small, so that both keep their nanotubes semiconductor properties.

ACKNOWLEDGMENTS

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