Development of nanofilters and nanosensor for environmental control

Mirele Bastos (PG)*, Ihosvany Camps (PQ)

Laboratório de Modelagem Computacional – LaModel. Unifal-MG.

Palavras Chave: *nanoestructure, metallic ions and electronic properties.*

Introdução

In recent decades, the importance of environmental control is growing mainly because industries dump their waste inappropriately in aquatic ecosystems. Concerns about the presence of heavy metals in wastewater are mainly due to the possibility of the death of biota and the gradual accumulation in the human body through the food chain[1]. Thinking in this problem, the aim of this work is to develop efficient heavy metal filters and sensors made of organic nanostructures. Therefore, the toxic metals used in this study were Cd (cadmium), Ni (nickel) and the organic nanostructures consist in carbon nanotubes (CNTs) with various chiralities and hydrogen-passivated in they pure phase and randomically functionalized with different organic groups. In this work we have performed a theoretical investigation using ab initio calculations based on the density-functional theory (DFT) and the generalized gradient approximation developed by Perdew, Burke and Ernzerhof (GGA-PBE)[2] for the exchange-correlation functional as implemented in the SIESTA[3] code. Using the DFT approach we studied free CNTs and combined systems i.e. CNTs plus metallic ions. The electronic properties such as the energy band structure and the density of states where calculated for all the systems together with the interaction energy for the combined ones. From the comparison of the electronic properties between the pure CNTs and the combined systems, our results shown the viability of CNTs as strong candidates to be used as the core of heavy metal filters an sensor devices.

Resultados e Discussão

Initially, we constructed a pure zigzag (10,0) carbon nanotube (pCNT) of five unit cells which results in a CNT with a diameter of 7.83Å and a length of 21.30Å. Energy convergence studies were carried out varying the MeshCutOff parameter resulting in 480 and 600 Ry for the complex CNT-Ni and CNT-Cd, respectively. The single point energy was calculated for the pCNT and for the complex systems. For the combine systems, the single point energy was calculated varying the metallic ions distance from the CNT surface and aligned with the ring center.The interaction energy (E_{int}) between the metallic ion and the carbon nanotube was calculated using the expression $E_{int}=E_{combine}-E_{pCNT}-E_{ion}$, were $E_{combine}$ is the complex energy, E_{pCNT} is the energy for the pure CNT and E_{ion} is the ion energy. Our results shown that for the Ni ion, we get the minimum interaction energy of -1.69eV around 9.20Å (see figure 1, graph (a)). For the Cd ion, the interaction energy was lower with a value equal to -1.44eV at a distance of 10.6Å (see figure 1, graph (b)).

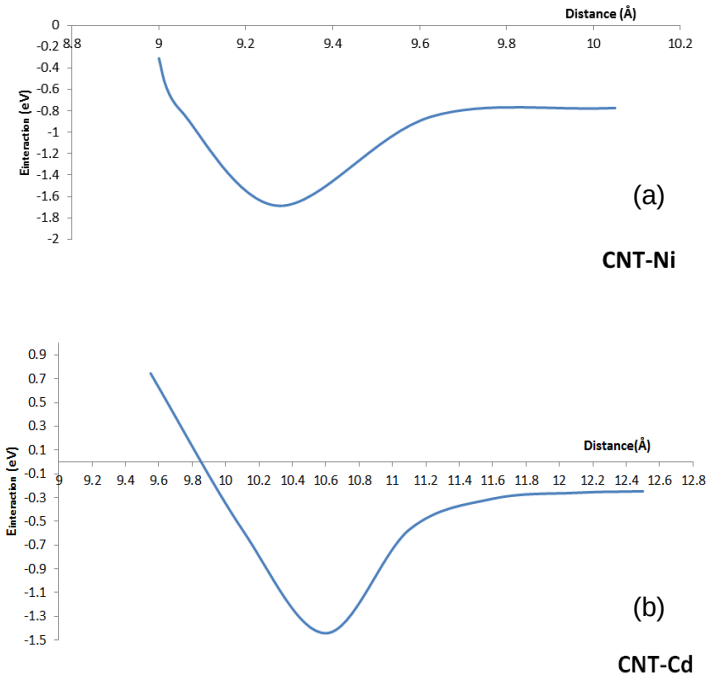

Figure 1. Potencial energy curve calculated for the complex CNT-Ni (a) and CNT-Cd (b).

Conclusões

The results of calculations of the binding energy on the distance to the CNT indicated that CNT (10,0) interacting with the metals Cd and Ni do not provide a good option as sensors for these metals, since the lowest binding energy was measured at a distance of approximately 10Å to Ni end 10.6Å for Cd. Other studies were conducted including analysis of the band structure and density of states for other CNT chiralities and for functionalized CNT with carboxyl and hydroxyl groups. The results obtained in this work indicate that the nanostructures used here are able to successfully work as the core of nanofilters to remove metallic ions.

Agradecimentos

We thank Unifal-MG, FAPEMIG, CNPq and CAPES for their support.

[1] GOEL, L.; *et al.* J. Hazard Mater, v. 125B, p. 211-220, **2005**.
[2] FUCHS, M.; *et al.* Matter Phys. Review, v. 57, p. 2134-2145, **1998**.
[3] SOLER, J. M.; *et al.* J. Phys.: Condensed Matter, v. 14, p. 2745-2779, **2002.**