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Adsorption of Anticancer Drug Molecule on Single Wall Carbon Nanotube: An ab-initio Study

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Introduction

Curcumin is a natural compound known as a potent antioxidant, anti-tumor and anti-inflammatory agentwith nontoxic side effects compared to chemotherapeutic agents [1]. However, curcumin has low bioavailability and solubility due to its hydrophobic nature. Hence Single Walled Carbon NanoTubes (SWCNTs) have been utilizedexperimentally as nanocarriers to overcome these issues due to their nano-hollow-tubular structure and high surfacearea [2]. In this work, we are interested in the theoretical insights of(n,0) zigzag SWCNTs as delivery systems in attempt to getaround the curcumin biodisponibility problems. The binding energies, electronic properties, and nature of interaction were carried out using Density Functional Theory (DFT).

Theoretical Study

All simulations were done based on DFT as implemented in the OpenMX 3.8 package [3]. The exchange-correlation was described with the Perdew- Burke-Ernzerhof (PBE) within the generalized gradient approximation (GGA). The energy cutoff for the plane waves was set to 100 Ry. Along the □-Z direction in the Brillouin zone, 11 k-points were considered. The van der Waals interactions were included by the DFT-D2 approachproposed by Grimme. The periodic boundary conditions were applied to simulate infinitely long tubes.

Results and Discussion

Side view of curcumin @ (10,0) CNT is shown in figure 1. The binding energy value for the most stable complex is -18.93 eV. The energy band gap for isolated (10,0) CNT is 1.15 eV meanwhile the energy band gap of (10,0) CNT after functionalization with curcumin is 1.00 eV. We can notice that the energy band gap decreased with adsorption of the molecule but that doesn't affect the semiconducting behavior of the nanotube.

From the total density of state (DOS) spectra, (The Fermi level was set at 0 eV) in the presence of adsorbed molecule,an occupied state and DOS peak appears below the Fermi level.

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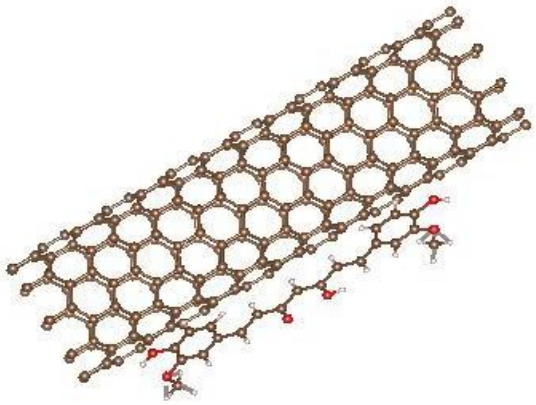

Fig1: Atomic structures of curcumin @ (10,0) CNT.

Conclusion

We can conclude that the curcumin weakly binds to theouter surface of the SWCNTs and the small interactionobtained quantitatively in terms of binding energies. However, our research is still ongoing to identify the moststable systems and to get more accuracy results when the diameter of CNTs increases.

References

1. Z. Hussain, H. E. Thu, M. W. Amjad, F. Hussain, T. A.Ahmed, S. Khan, *Mater. Sci. Eng. C*, **77** 1316 (2017)**.**
2. S. Mahajan, A. Patharkar, K. Kuche, R. Maheshwari, P. K. Deb, K. Kalia, R. K. Tekade, *Int. J. Pharm*, **548** 540(2018).
3. T. Ozaki, H. Kino, J. Yu, M. J. Han, M. Ohfuchi, F. Ishii,et al. User's manual of OpenMX version 3.8. http://www.openmx- square.org/openmx_man3.8/openmx.html.

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