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Investigation Effect Adsorption Glycine (Gly) Amino Acid on Carbon NanoCone (240) by Computational Methods

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Abstract: Carbon Nanocone (CNC), in compared with other carbon nanotubes, show investigation novel properties and can be used as a significant complement in Nano-technology. The structure of Nanocone and Glycine and complex between CNC and Gly were Geometry optimizations were carried out at the B3LYP/6-31G* level of theory using the Gaussian 09 suite of programs. We present the nature of the Gly interaction in selected sites of the CNCs(240).Binding energies corresponding to adsorption of the Gly are calculated to be in the range 4–21 kJ mol-1. More efficient binding energies cannot be achieved by increasing the CNCs diameter. We also provide the effects of Gly adsorption on the electronic properties (DOS) of the CNCs.

Keywords: adsorption, Gly, CNCs, DFT, DOS

INTRODUCTION

Since the discovery of carbon nanotubes (CNTs) [1], single walled carbon nanotubes (SWCNTs) have attracted great interest owing to their physical and chemical properties [1–3] and applications as a fascinating novel material [4, 5]. Glycine is the smallest of the amino acids. It is ambivalent, meaning that it can be inside or outside of the protein molecule. In aqueous solution at or near neutral pH, glycine will exist predominantly as the zwitterions. The isoelectric point or isoelectric pH of glycine will be centered between the pKas of the two ionizable groups, the amino group and the carboxylic acid group. In estimating the pKa of a functional group, it is important to consider the molecule as a whole. For example, glycine is a derivative of acetic acid, and the pKa of acetic acid is well known. Alternatively, glycine could be considered a derivative of amino ethane.

COMPUTATIONAL METHODS

In the present work, adsorption behaviors of the Gly on the SWCNCs were studied by using the representative models of (240) zigzag SWCNCs in which the ends of the NanoCone are saturated by hydrogen atoms. The hydrogenated (240) zigzag SWCNCs have 56 (C46H7NO2), atoms. In the first step, the structures were allowed to relax by all atomic geometrical optimization at the DFT level of B3LYP exchange-functional and 6-31G* standard basis set. The Optimized structures have diameters of 4.80, 5.63, and 6.33 A. The BE of an Gly on the CNCs wall was calculated as follows: where E CNCs_Gly was obtained from the scan of the potential energy of the CNCs–molecular glycine structure, E CNCs is the energy of the optimized CNCs structure, and EGly is the energy of an optimized Gly. All the calculations were carried out by using the Gaussian 03suite of programs [6-10].

RESULTS AND DISCUSSION

In order to investigate the interaction between glycine (Gly) amino acid as a nano cone (240) as nanometer-scaled structures, we have examined the adsorption capability of Gly with Nanocone(240) by means of ab

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initio calculations based on the generalized gradient approximation (GGA) with the Becke's three parameter (B3) exchange functional together with the Lee–Yang– Parr (LYP) non-local correlation functional [2] in density functional theory and 6-31g,6-31g* basis set. For this purpose, we have considered the binding of the glycine on the exterior surface of the Nanocone (240). After full structural optimization of the considered systems, the obtained results reveal that the binding of glycine to the cage generates more stable complex with binding energy of -0.25 eV (-5.76 Kcal/mol) via its hydroxyl oxygen active site, suggesting the involvement of no covalent interactions in the adsorption, see Fig. 1(a).

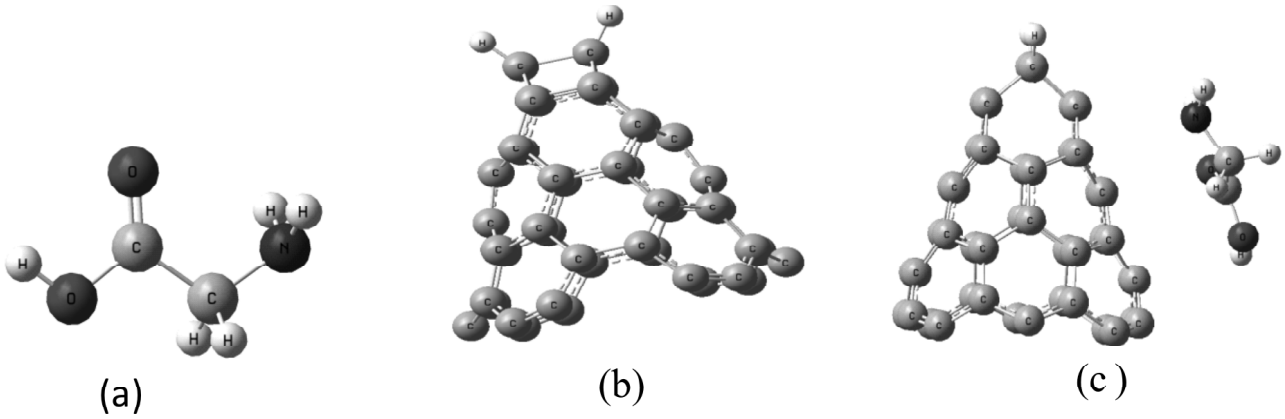

Figure 1: Atomistic configurations of interaction Gly on surface CNCs.

Table 1
The HOMO and LUMO energies and their energy gaps for the most favorable states for interaction of the configurations

Model	*Basis set*	*HOMO*	*LUMO*	*Energy gap(ev)*
CNC	3-21g	-0.23843	-0.10046	-0.13797
	6-31g	-0.23211	-0.09703	-0.13508
	6-311g	-0.24446	-0.10857	-0.13589
Gly	3-21g	-0.37830	0.00914	-0.38744
	6-31g	-0.39242	-0.01076	-0.38166
	6-311g	-0.40081	-0.01888	-0.38193
CNC-Gly	3-21g	-0.22677	-0.09538	-0.13139
	6-31g	-0.22763	-0.09339	-0.038
	6-311g	-0.23902	-0.10395	-0.13507

ELECTRONIC PROPERTIES

Finally, we studied the influence of Gly adsorptions on the electronic properties of the CNCs. The calculated band gaps of the clean perfect (240) zigzag SWCNCs are about 0.83 eV, respectively. The effects of the Gly on adsorption energies in the CNCs relate to their electronic structure.

When the Gly is adsorbed on the CNCs, the interaction between them being very weak, the electronic properties of these tubes are not changed obviously and the band gaps are calculated to be about 0.84 eV, respectively. But for the method 6-31g(6,0) zigzag SWCNTs,the interaction between them being further from the CNCs, the band gap is calculated to be about 0.96 eV.However, the adsorption of Gly on the Al-doped SWCNCs slightly increases the energy gap of the pristine CNCs, and reduces their electrical conductance.

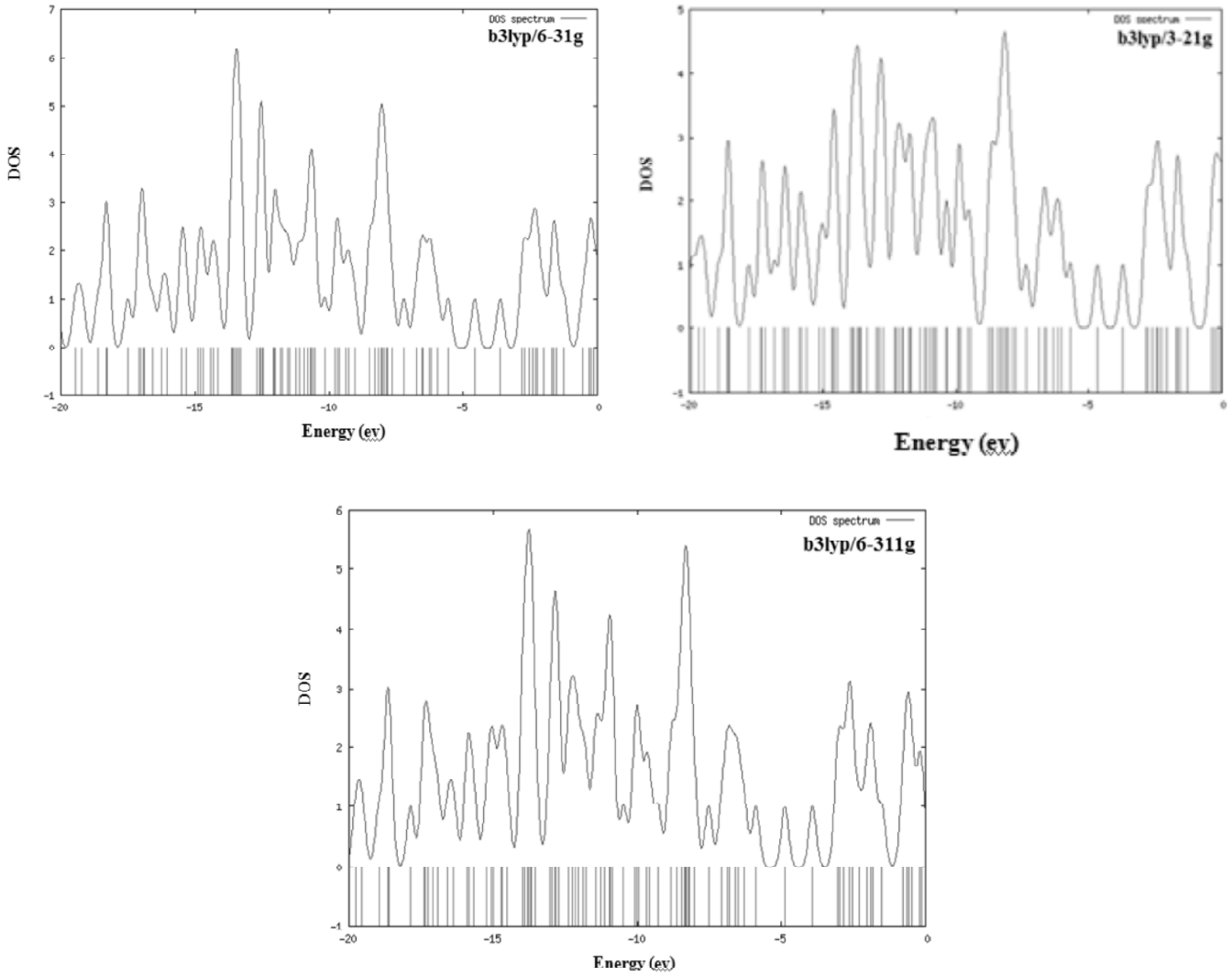

Fig 2.(a) The most stable configuration of CNCs/Gly complex via OH active site. (b) Calculated density of states (DOS) foran isolated Gly, an isolated CNCs and the combination of the two at equilibrium geometry for Gly-CNCs system. Furthermore, charge analysis based on Mulliken population reveals that there is about 0.05 e transfer from glycine to the CNCs cage for respective complex indicating the physically adsorption of the glycine on the CNCs cage due to week interaction of corresponding species. Compared with pristine C60 fullerene, the CNCs system has slightly higher binding energy value. Results from binding energies indicate, however, that adsorption property is typical for the physisorption. In addition, the calculated density of states (DOS), as shown in Fig. 1. (b), and HOMO/LUMO isosurfaces show that there is no significant orbital hybridization between glycine and CNCs molecules.

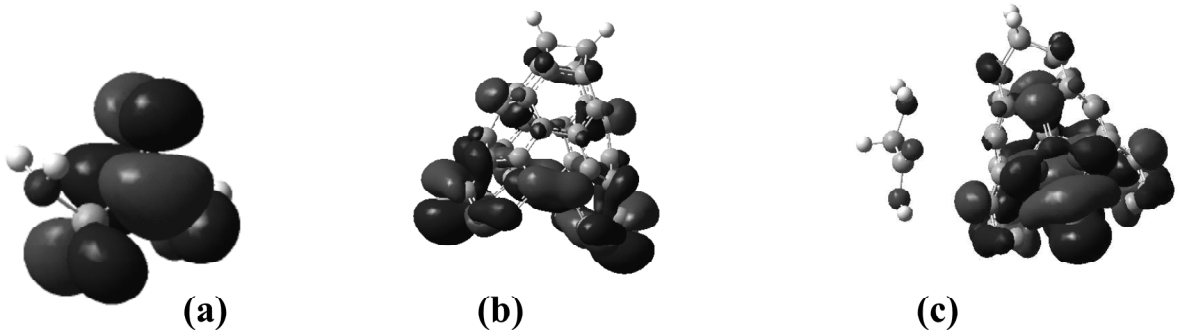

Figure 2: DFT calculated HOMO-LUMO orbitals for(a)Gly and (b) CNCs(240) and (c)Gly-CNCs

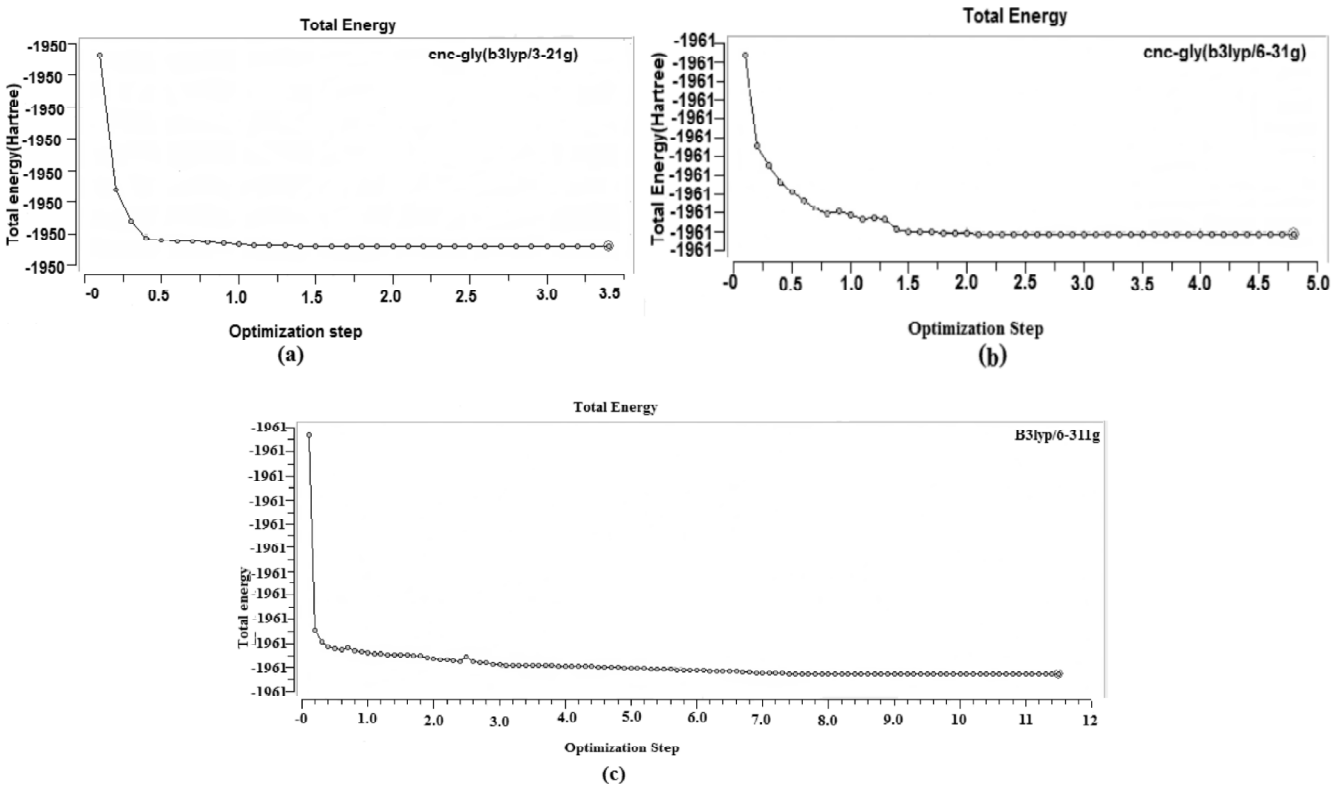

Figure 3: Interaction energy curves of a Gly molecule on surface the CNCs 240 Nano cluster obtained by the optimization calculation B3lyp/3-21g, 6-31g (a), 6-311g (b)

CONCLUSION

We have studied the interaction Gly on CNCs configurations of (240) means of DFT calculations. On the basis of our calculations, comparing all the BE curves of Gly interacting with all possible sites of adsorption on carbon NanoCone and in several structural configurations, it seems that the pristine SWCNTs cannot be used as an Gly storage medium. For the CNCs, the calculated BE for Gly in N-down is a little more than that in O-down, but for the SWCNCs, the BE in O-down is a little more than that in N-down. We showed that more efficient binding could not be achieved by increasing the nanotube diameter. Furthermore, in this study the presence of the Gly on the CNCs slightly increases the energy gap of pristine CNCs and reduces their electrical conductance.

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