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Adsorption Study of Cyanate Ion on the Single-wall BC_2N Nanotubes: a Computational Study

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Cyanate adsorption on the external surface of H-capped (6,0) zigzag single-walled BC_2N nanotube was studied by using density functional theory calculations. We present the nature of the cyanate interaction in different sites of the nanotube. This nanotube can absorb the cyanate ion in its pristine form without manipulating its structure through doping, chemical functionalization, making defect, etc, and the nanotube can be used as cyanate storage.

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1. INTRODUCTION

Adsorption of chemical species on nanotubes has attracted great interest for chemical sensing of molecules because of their high surface to volume ratio, high sensitivity, and quick response time toward several molecules. Many investigations have been studies about adsorption of cyanate on metal surfaces [1-2], whereas there are few studies about cyanate adsorption on nanotubes and semiconducting surfaces [3] and further study of the cyanate adsorption on nanotubes remains interesting. Improving the sensing performance of the pristine nanotubes and nano sheets by functional groups is formidable task and too expensive; and thus, finding high sensitive pristine nanotubes is of scientific interest. Among $B_xC_yN_z$ nanotubes, the single-wall BC_2N nanotube stoichiometry is the most stable stoichiometry [4]. The electronic structure properties of BC2NNTs have been theoretically studied by different groups [4-6]. Recently, theoretical calculations on the pristine $B_xC_yN_z$ compound nanotubes have shown that these nanostructures are very promising for energy-storage applications [7] and also for nanotube-based molecular sensors [8]. However, to our knowledge, no experiments and theoretical investigation have been reported for cyanate adsorption on the BC2N nanotube. Herein, the potential possibility of single-walled pristine BC2N nanotube as an absorbent or vehicle for adsorption and to transport cyanate across membranes into living cells is investigated. To this end, we have studied the interaction between the cyanate and BC2N nanotube using density functional theory calculations.

2. COMPUTATIONAL METHODS

In the first step, all the different OCN^-/ BC2NNT complex configurations were allowed to relax in the optimization at the DFT level of B3LYP exchange-functional and 6-31G* standard basis set. Then, adsorption of the cyanate on the optimized nanotube model was studied. The adsorption energy (E_{ad}) of cyanate on the optimized nanotube model was as follows:

$$E_{ad} = E_{OCN^-/BC2NNT-} [E_{BC2NNT} + E_{OCN^-}] + \delta_{BSSE}, \quad (1)$$

where $E_{OCN^-/BC2NNT}$ was obtained from full optimization of the OCN^-/ BC2NNT complex configurations, E_{BC2NNT} is the energy of the optimized BC2N structure, E_{OCN^-} is the energy of an optimized OCN^-, and δ_{BSSE} is the BSSE correction. A negative or positive value for *BE* is referred to exothermic or endothermic processes, respectively. All the calculations were carried out by using the Gaussian 03 suite of programs [9].

3. RESULT AND DISCUSION

For the adsorption of cyanate on the *zigzag* (6,0) BC2N nanotube (OCN^-/BC2NNT complex), various possible adsorption geometries was investigated by placing the O and N atoms of cyanate on the B, or N, and or C atom of BC2N nanotube, with the cyanate axis being perpendicular to the surface of the nanotube, and parallel to the B-C, C-C, C-N, and B-N bonds. Having done structural optimizations, we obtained four most stable adsorption configurations that are plotted in Fig.1

In the most stable configuration (Fig. 1A), i.e., the almost perpendicular approach of cyanate (N-down) to the *(6,0)* BC2N nanotube wall on the upper boron atom, the interaction distance between the N atom of the cyanate and B atom of the nanotube is 1.52 Å and the adsorption energy for this complex is -2.54 eV which characterize a exothermic process and almost strong interaction between the cyanate and the BC2N nanotube. Moreover, the adsorption of cyanate shows a local structural deformation on both the cyanate and the BC2N nanotube. The bond lengths of B–N and B-C in the pristine BC2N nanotube significantly increased from 1.44 and 1.54Å in the pristine model to 1.59 and 1.62 Å in the complex, indicating a bond weakening due to the interaction and also, the NBO hybridization of B atom shows a change from sp^2 to nearly sp^3. For the cyanate, the bond lengths of N-C and C-O decreased from 1.20 and 1.23Å in free cyanate to 1.19 and 1.20 Å in the adsorbed state.

For the configuration B, oxygen atom of the cyanate approach to the (6,0) BC_2N nanotube wall on the upper boron atom. It can be seen that the O atom in the configuration and the N atom in the most stable configuration (Fig. 1a) of the cyanate are bonded to the boron at-

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om of the BC2N nanotube. The major difference between the two configurations is dependent on orientations of cyanate (N-down or O-down). The adsorption energy for this configuration is – 1.89 eV with equilibrium distance 1.55 Å, indicate that the calculated adsorption energy for cyanate in N-down or configuration A (– 2.54eV) is more than that in O-down or configuration B (– 1.85eV). In addition, the bond lengths of B–N and B-C of nanotube for the configuration B are 1.56 and 1.61Å which is 0.03 and 0.01 smaller than that of configuration A.

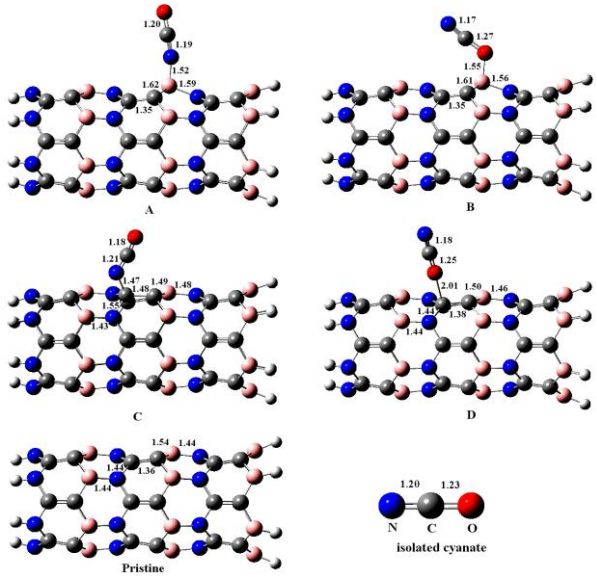

Fig. 2 – Two-dimensional (2D) views and adsorption configurations of CO

For the configurations B and C, nitrogen and oxygen atoms of the cyanate approach to the *(*6,0*)* BC2N nanotube wall on the upper carbon atom. The adsorption energies for the configurations are -1.79 and -0.22 eV with equilibrium distances 1.47 and 2.01Å, indicate that the calculated adsorption energies for cyanate in the configurations are smaller than that in the configurations A and B. In addition, in the configurations B and C, the calculated adsorption energy for cyanate in N-down is more than that in O-down.

4. CONCLUSION

We studied the adsorptions of cyanate on *zigzag* (6,0) BC2N nanotube by means of density functional theory (DFT) calculations to find the potential possibility of BC2N nanotube as an storage for cyanate adsorption. On the basis of our calculations, the cyanate can be strongly adsorbed on the surface of the BC2N nanotube. Also, pristine BC2N nanotube can be used as a cyanate storage medium as long as cyanate is adsorbed on the exterior walls of the BC2N nanotube because of the high adsorption energy.

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