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The electrical and structural study of interaction HCN gas with SiCNTs: A DFT approach

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ABSTRACT

In this research, we investigate the interaction of HCN gas with SiCNTs to making new absorber and sensor for HCN gas. All stable adsorption structures are individually optimized by using density function theory at the cam-B3LYP level of theory using the Gaussian 09 set of programs. From optimized structures the DOS plots, MEP plot and quantum molecular descriptors: gap energy, chemical potential (μ), global hardness (η), electrophilicity index (ω), and electronegativity (χ) of the nanotubes are calculated. The results indicate that the adsorption of HCN from N and H head in the vertical direction of surface of SiCNTs is favorable than other those models in thermodynamically approach. The quantum parameters demonstrate that the SiCNTs is a good candidate for detecting HCN gas.

Keywords: SiCNTs, DFT, HCN interaction, quantum parameters

1. Introduction

Hydrogen cyanide (HCN) is highly lethal to man and animals, so the monitoring and control of its exposure in both industrial and residential environments are of special interest. Therefore, effective methods for monitoring and suppressing the HCN concentration have

been highly demanded for atmospheric environmental measurements and controls [1]. Since the discovery of carbon nanotubes (CNTs), extensive studies have focused on the application of CNTs in sensors. Prepared CNT sensors have advantages of low power consumption, fast response and easy recovery capability over the traditional bulk material sensors. [2-3] Silicon carbide nanotubes (SiCNTs) is one of the important nanotube that it is used to making sensor. The surface-to-volume ratio of the SiCNTs is higher than that f the bulk SiC materials. These results indicate that SiCNTs are good candidates for HCN detecting. The theoretical results show that the BNNTs and AlNNTs is a good candidate to detection HCN molecule [4-6].

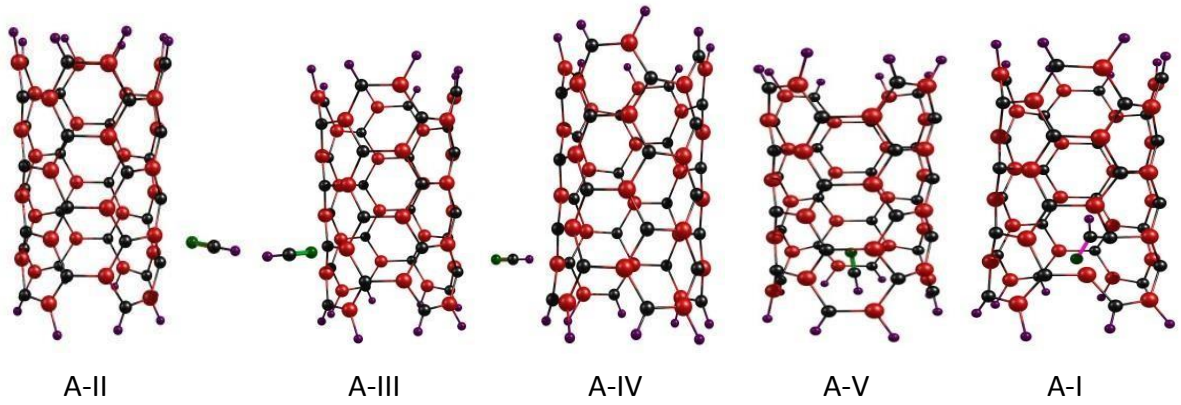

Fig 1. 2D geometrical structures for adsorption HCN molecule on SiCNTs

3. Results and discussion

The adsorption energy for HCN adsorption on surface of undoped and B-doped SiCNTs at representative (A-I to B-V) models are tabulated in table 1. Inspections of results show that the adsorption energy of all considered models is in range -3.7to 23.7 kcal/mol. It is notable that the adsorption energy of B-III models is more negative than other those models and so the adsorption of HCN molecule at this model is favorable than other models. Whereas the adsorption energy of B-II is more positive than other models and so this model is unspontaneously in view of thermodynamic approach.

Table 1. The adsorption energy for adsorption HCN gas on the surface of SiCNTs

Eads(Kcal/mol)	**A-I**	**A-II**	**A-III**	**A-IV**	**A-V**
Pristin	*-2/7*	*-2/7*	*-3/7*	*4/4*	*32/7*
B-Doped	**B-I**	**B-II**	**B-III**	**B-IV**	**B-V**
	-0/1	*31/1*	*-4/2*	*9/0*	*11/8*

The electrophilicity index (ω) determines maximum flow of electron from donor to acceptor species and supplies data connected to structural stability, reactivity and toxicity of chemisorbed on the surface of nanotube, a fairly large charge transfer occurs between two related species, thus their electronic transport properties could be significantly changed upon physisorption of HCN gas. The results show that the electrophilicity index of B- doped adsorption models increase significantly from original values.

Table 2. The NBO charge around HCN gas after adsorption

Pristine	**A-I**	**A-II**	**A-II**	**A-IV**	**A-V**
ΔρNBO	0.15	0.15	-0.015	0.022	-0.451
B DOPED	B-I	B-II	B-II	B-IV	B-V
ΔρNBO	-0.001	-0.208	-0.014	0.024	-.05
N DOPED	C-I	C-II	C-II	C-IV	C-V
ΔρNBO	0.15	-0.46	-0.023	0.035	-0.36
N B DOPED	D-I	D-II	D-II	D-IV	D-V
ΔρNBO	0.01	-0.018	-0.007	0.035	-0.34

The molecular electrostatic potential results reveal that the negative charge densities are localized on the surface of nanotube and positive charge are dispersed around HCN. Thereby in this adsorption process HCN gas has donor electron effects and so the gap energy, NBO, DOS plot (see Fig. 2) change significantly from original values and the electrical parameters of system is suitable for making sensor for HCN gas.

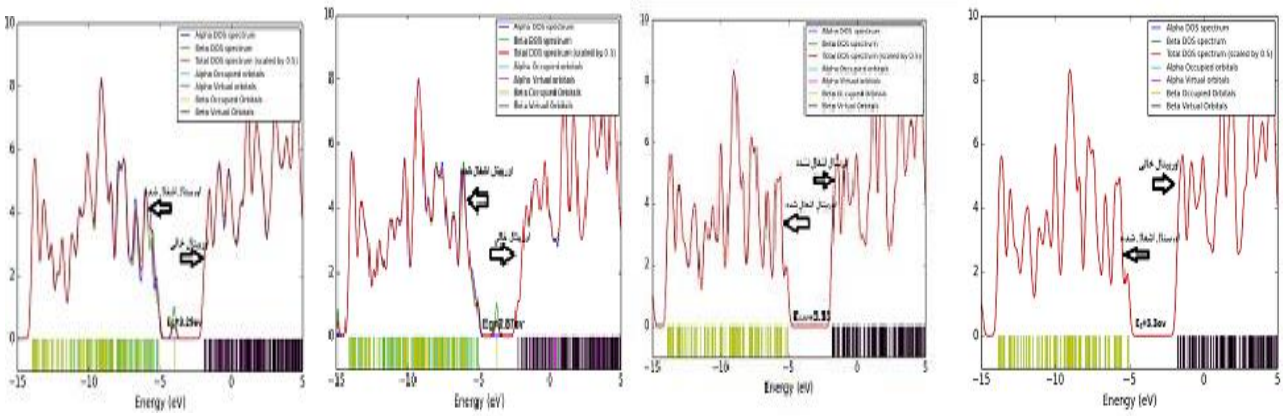

Fig 2. 2D DOS plots for adsorption HCN molecule on SiCNTs

4. Conclusions

The structural parameters reveal that the bond lengths (Si- C) of neighbourhood of doping and adsorbing sites undergo increase and bond angles (Si-Si) undergo decrease. The band gaps of HCN adsorption on the surface of undoped and B-doped SiCNTs reduced. The adsorption energy of the HCN gas shows that the adsorption process is weak physorption in thermodynamic approach. These results demonstrate that SiCNTs is not a good candidate to making HCN absorber. The quantum calculation is shown that the pristine SiCNTs is a good candidate to making HCN sensor.

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