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Research Article

REMOVAL OF CYANOGEN TOXIC GAS FROM ENVIRONMENTAL SYSTEMS BY USING BN NANOSHEET

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ABSTRACT
Electrical sensitivity of a boron nitride nanosheet (BNNS) was examined toward cyanogen (C_2N_2) molecule by using density functional theory (DFT) calculations at the B3LYP/6-31G (d) level, and it was found that the adsorption energy (E_{ad}) of cyanogen on the pristine nanotubes is a bout -0.76kcal/mol. However when nanotube has been doped with Si and Al atoms, the adsorption energy of cyanogen molecule was increased. Calculation showed that when the nanosheet is doped by Si, the adsorption energy is about -85.62 to -87.43kcal/mol and also the amount of HOMO/LUMO energy gap (E_g) will reduce significantly. Boron nitride nanosheet is a suitable adsorbent for cyanogen and can be used in separation processes cyanogen. It is seem that nanosheet (BNNS) is a suitable semiconductor after doping. The doped BNNS in the presence of cyanogen an electrical signal is generating directly and therefore can potentially be used for cyanogen sensors.

Keywords: *Sensor, Nanosheet, DFT, Cyanogen*

INTRODUCTION
Cyanogen is a toxic gas that is smell like bitter almonds. Molecules with cyanogen groups are common species in several D-class asteroids (Cruikshank *et al.*, 1991), and in chemical models for circumstellar envelopes involving CN reactions (Mebel *et al.*, 2002).
Since the discovery of carbon nanotube (CNT) by Iijima (1991) the properties and applications of this novel material have been investigated extensively (Hummer, 2007; Zhu *et al.*, 2011; Hung *et al.*, 2004). CNTs have recently emerged as a promising substitute for materials of different properties and various applications in hydrogen storage, gas sensors, textiles and many more (Fam *et al.*, 2011; Cabria *et al.*, 2006).
BN nanomaterials, including BN nanosheets (BNNSs), BN nanotubes (BNNTs) and BN nanoparticls (BNNPs) are of potential use in nano-dimensional electronic devise and nanofillers for composites in termsof their unique physical and mechanical properties (Zhic *et al.*, 2010; Cho *et al.*, 2013; Kusunose *et al.*, 2002).
BN sheet has aroused extensive research interest due to its many in triguing properties such as high chemical stabilities, excellent mechanical properties and high conductivity (Wu *et al.*, 2005; Gard *et al.*, 2008).
Previously adsorption different molecules toward nanostructures have been studied (Moghimi and Baei, 2012; Peyghan *et al.*, 2013; Beheshtian *et al.*, 2013; Noei *et al.*, 2013). In this study, the adsorption of cyanogen on the pristine case BNNS while Si and Al atoms are in its structure has been investigated.

MATERIALS AND METHODS
Computational Methods
Computation procedures are including the following**:**
We have optimized the cyanogen molecule and BNNS at the B3LYP/6-31G (d) level of theory. BNNS is made up of 39N, 39B atoms were saturated by 24 hydrogen atoms which are in initial and end part of nanosheet. The reason for this act had been done to decrease the boundary effects (Figure 1).

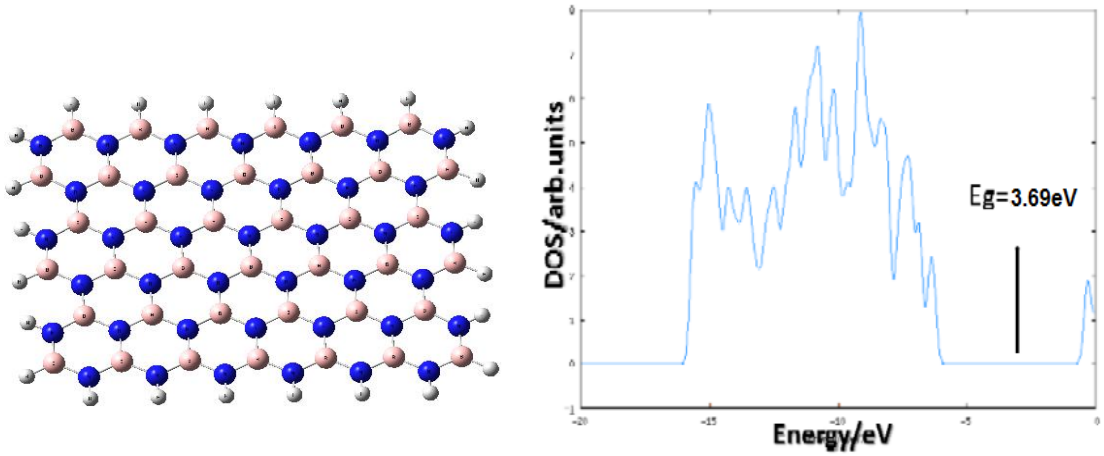


Figure 1: BNNS and DOS diagram for E_g of nanosheet

The GAMESS software (Schmidt, 1993) is used to perform these calculations. The B3LYP is demonstrated to be a reliable and commonly used functional in the study of different nanostructures (Beheshtian *et al.*, 2012; Owens, 2011; Fokin and Schreiner, 2009). We made cyanogen molecule from different positions of the site to be close to the nanosheet (Figure 2).

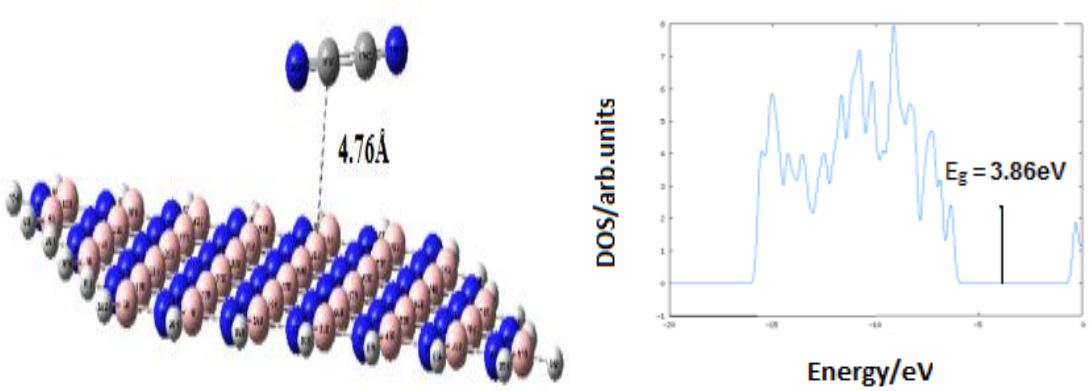


Figure 2: Cyanogen adsorption on the BNNS and DOS diagram for observing E_g of nanosheet .Distance is in Å

And it's adsorption has been calculated by using the Eq.(1).

$$E_{ad}=E_{Nanosheet\ +\ Cyanogen} - [E_{Cyanogen} + E_{Nanosheet}] + \delta_{BSSE} \quad (1)$$

According to the mentioned equation $E_{Cyanogen}$ is cyanogen molecule's energy, $E_{Nanosheet}$ is the nanosheet energy and $E_{Nanosheet\ +\ Cyanogen}$ is the nanosheet's energy with cyanogen. In addition, δ_{BSSE} is representing the basis set super position error. In the following steps Si and Al atoms in the nanotube structure have been doped to examine the cyanogen adsorption on the nanosheet and conductivity that which is doping with Si and Al atoms.

RESULTS AND DISCUSSION

Figure 1, shows the structure of boron nitride nanosheet (BNNS), in order to obtain the most stable adsorption mode of cyanogen molecule on different positions of BNNS, the most stable configuration is shown in Figure 2 , that carbon atom of cyanogen is 4.76Å far from nitrogen atom of the nanosheet .
Detailed information of the structure and electronic properties of the BNNS including the HOMO/LUMO energy gap (E_g) are shown in Table 1 in which adsorption energy (E_{ad}) for mentioned configuration of

cyanogen and nanotube is about -0.76kcal/mol and then we calculated the HOMO/LUMO energy gap (E_g) for pristine nanotube since the cyanogen molecule is adsorbed on the nanosheet (Table 1). Diagram which shows HOMO/LUMO energy gap (E_g) has been calculated, and the diagram which shows E_g has been obtained by using density of state (DOS) software.

Table 1: E_{ad}(kcal/mol), eV for the others

System	E_{ad}	E_{HOMO}	E_{LUMO}	E_g
BNNS	-	-6.28	-0.35	3.69
C_2N_2/BNNS	-0.76	-6.29	-2.45	3.86
Si_N	-	-4.47	-0.46	4.01
Si_N-C_2N_2	-87.43	-5.83	-2.44	3.39
Si_B	-	-1.86	-0.45	1.41
Si_B-C_2N_2	-85.62	-5.29	-2.35	2.94
Al_N	-	-5.11	-2.47	2.64
Al_N-C_2N_2	-15.61	-5.07	-2.42	2.65
Al_B	-	-6.29	-0.25	4.01
Al_B-C_2N_2	-7.52	-6.27	-2.56	3.71

Adsorption OF C_2N_2 ON Al Doped BNNS

The sensitivity of the adsorption of C_2N_2 on surface of BNNS has been examind two times, once with B atom doped by Al and in the other N atom by Al atom has been doped. Doped calculation of Al on BNNS shows that the value of HOMO/LUMO energy gap (E_g=2.64eV) is less than the pristine nanotube with E_g=3.69eV (Fig.3) and the best adsorption energy (E_{ad}=-15.61kcal/mol) is obtained when Al sitting instead of N and cyanogen has been adsorbed.

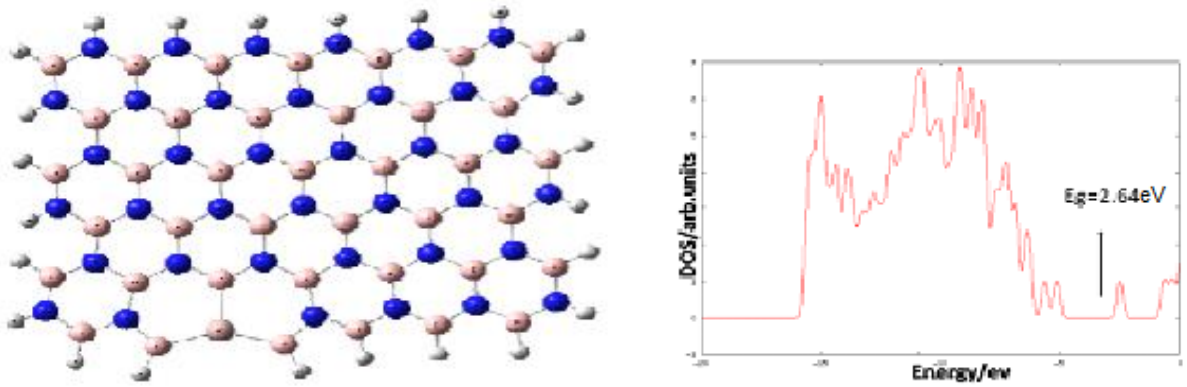
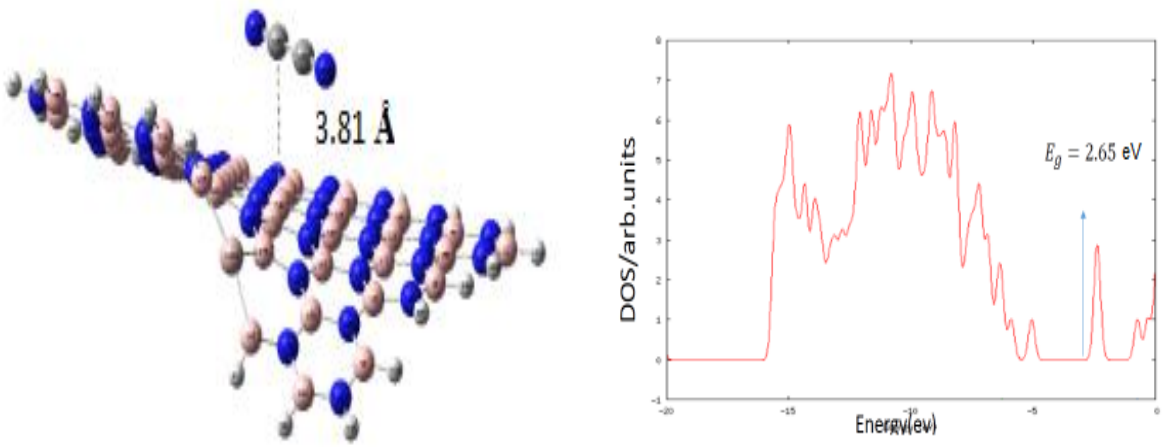


Figure 3: Doped nanosheet by Al_N and DOS diagram for E_g of nanosheet

When Al doping on BNNS in the presence of cyanogen electrical signal is generation directly and therefore can potentially be used for cyanogen sensors. DOS diagram clearly shows that when Al is doped on the BNNS (Figure 3) it will become a semiconductor (E_g=2.64eV). Optimizations of these types of interactions are desirable for gas detection because such strong interactions mean the BNNS is a suitable absorbent for cyanogen molecule (Figure 4).

a)



b)

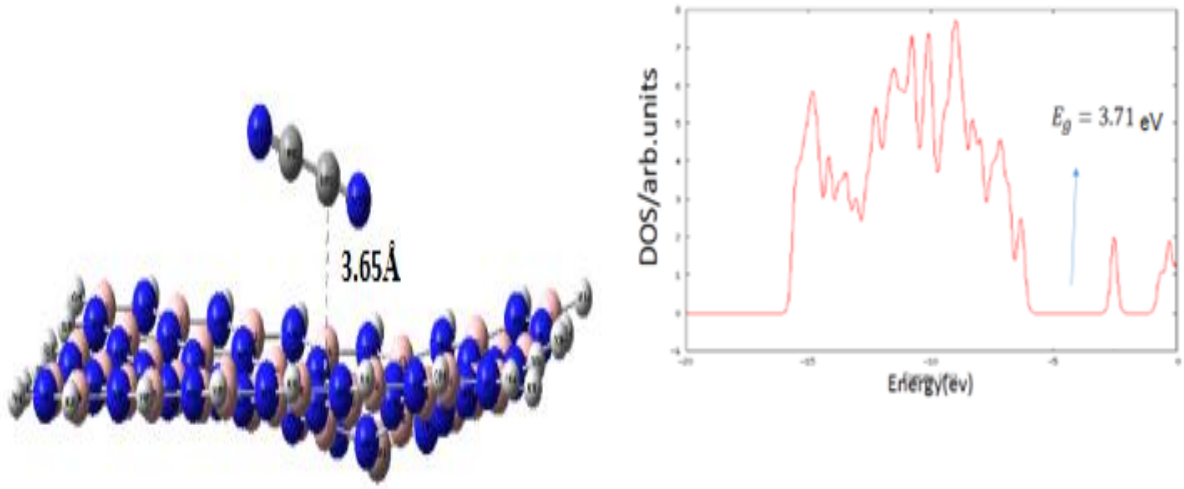


Figure 4: a) Cyanogen adsorption on doped nanosheet by Al_N and DOS diagram for observing E_g of nanosheet. b) Cyanogen adsorption on doped nanosheet by Al_B and DOS diagram for observing E_g of nanosheet. Distance is in Å

If E_{ad} is significantly increased then it is expected that recovery will be so long, meanwhile according to transition state theory and recovery time can be explain as Eq.(2)

$$\tau = \upsilon_0^{-1} \exp(-E_{ad}/kT) \quad (2)$$

Where T is the temperature, k is the Boltzmann's constant, and υ_0 is the attempt frequency.

According to this equation as long as adsorption energy (E_{ad}) is increasing the recovery time becomes longer and calculation in Table1.

Adsorption OF C_2N_2 ON Si Doped BNNS

At this stage doping has been studied with another element.

First, instead of B atom in the boron nitride nanosheet a Si atom and then instead of N atom a Si atom replaced in a nanosheet (Figure 5), and then geometrical structures and electronic properties of BNNS are doped and their adsorption behavior are studied (Figure 6).

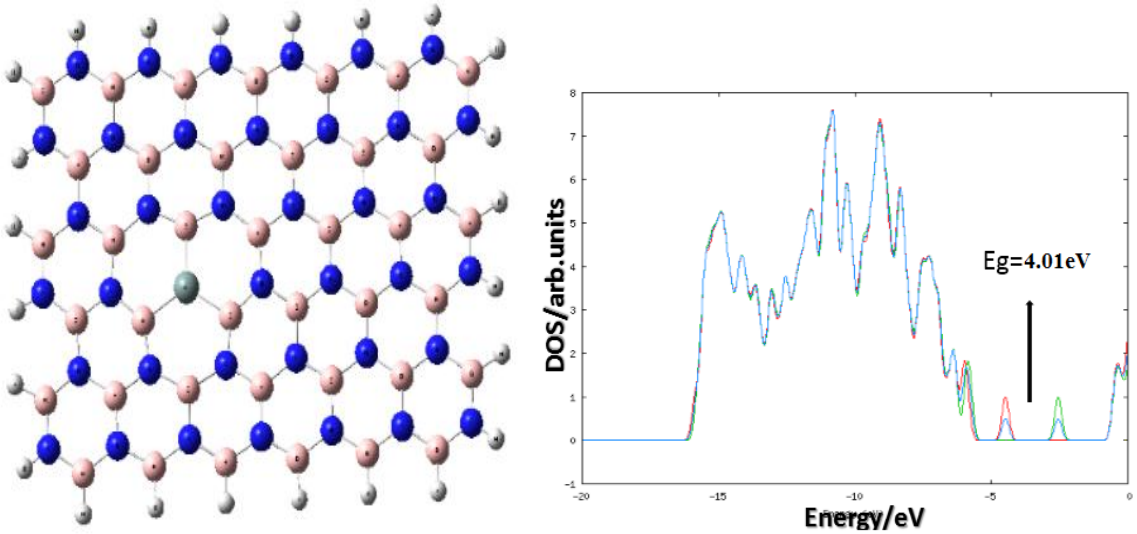
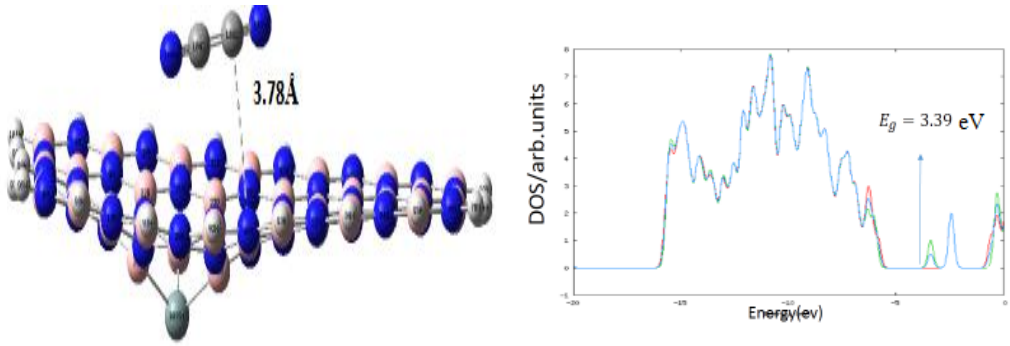


Figure 5: Doped nanosheet by Si_N and DOS diagram for E_g of nanosheet

Computations shows that when B atom replaced by Si in BNNS the HOMO/LUMO energy gap will become less of pristine BNNS (E_g=3.96eV), (Figure 6).

a)



b)

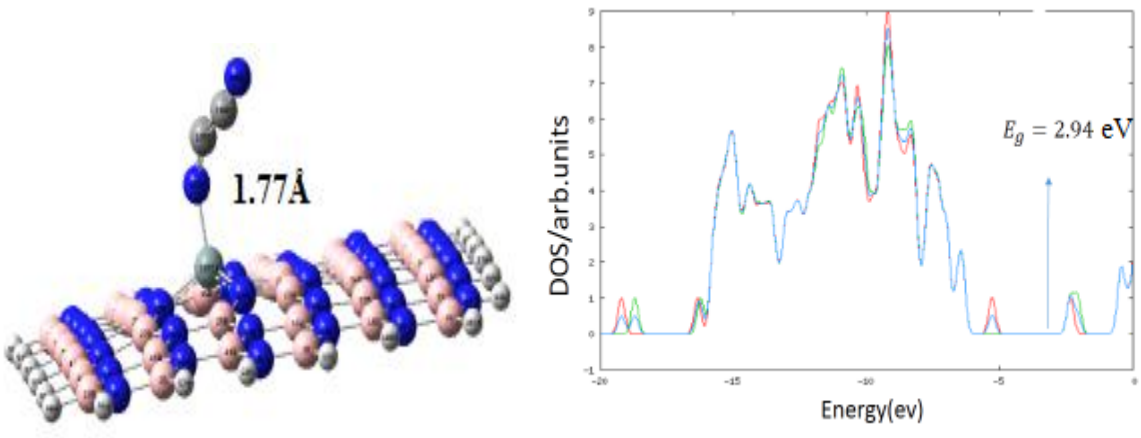


Figure 6: a) Cyanogen adsorption on doped nanosheet by Si_N and DOS diagram for observing of E_g nanosheet. b) Cyanogen adsorption on doped by Si_B and DOS diagram for observing of E_g nanosheet. Distance is in Å

When Si is sitting of N and B, the adsorption energy of cyanogen on nanotube is more (E_{ad}=-87.43kcal/mol) than when we just use the pristine nanotube (E_{ad}= -0.76kcal/mol). After adsorption of C_2N_2 on the mentioned nanosheet that has doped by Si the HOMO/LUMO energy gap (E_g=3.39eV) will decrease the pristine of nanosheet and therefore a substantial increase will occur in conductivity and this phenomenon can be explain as Eq. (3), (Beheshtian *et al.*, 2012)

$$\sigma \propto \exp(-E_g/2kT) \quad (3)$$

Where σ is conductance, T is temperature, k is Boltzmann constant. According to this equation as long as E_g is smaller, the conductivity to be more it can be concluded that, so the Si atom is a suitable for doping in BNNS.

Conclusion

The adsorption of an cyanogen (C_2N_2 molecules on the surface of BNNS (boron nitride nanosheet) has been studied by using density functional theory (DFT) and then we doped the Al atom in the structure of the nanosheet, the results show it is clearly possible to modify the nanosheet as an effective adsorbent of cyanogen molecule in gas sensors which are sensitive about cyanogen. These results may open new doors to chemically modify the nanosheets thereby expanding their applications in industry and technology.

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