Cyanogen, Methylacetylene, Hydroquinone, Ethylacetylene, Aniline, Pyrrole, and Ethanol Detection by Using BNNT: DFT Studies

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ABSTRACT: *Electrical sensitivity of a Boron Nitride Nano Tube (BNNT) was examined toward hydroquinone ($C_6H_4(OH)_2$), cyanogens (C_2N_2), methylacetylene (C_3H_4), ethylacetylene (C_4H_6), aniline ($C_6H_5NH_2$), ethanol (C_2H_5OH), pyrrole (C_4H_5N), molecules by using Density Functional Theory (DFT) calculations at the B3LYP/6-31G(d) level of theory. In considering the adsorption energy (E_{ad}) of those molecules on the BNNT are sequenced: $C_6H_5NH_2$(E_{ad}= -47.55kcal/mol)> C_4H_5N (E_{ad}=-26.66kcal/mol) >C_2H_5OH(E_{ad}= -25.91kcal/mol)> (CN)2(Ead=-20.70kcal/mol)> $C_6H_4(OH)_2$(E_{ad}= -20.21kcal/mol) >C_3H_4(E_{ad}=-12.73kcal/mol)> C_4H_6(E_{ad}=-11.19kcal/mol). According to this comparison aniline molecule with E_{ad}=-47.55 kcal/mol has the most adsorption energy among all molecules. Calculations showed that when the nanotube was doped by Si and Al atoms, the amount of HOMO/LUMO energy gap (E_g) reduced significantly. This reduced showed that BNNT is a suitable semiconductor after doping and the doped BNNT in the presence of those gases generates an electrical signal and therefore can be used potentially for gas sensors. Recent researches demonstrate that Boron nitride nanotube is a suitable adsorbent for detection and separation of those compounds.*

KEYWORDS: *Sensor; Nanotube; DFT; BNNT.*

INTRODUCTION

As a matter of fact, nowadays, nanotechnology has a significant impact on various industries and communities. The nanoparticles, as one the most applicable nanostructures, are used as the catalyst in many reactions [1]

The hydroquinone (HQ) as toxic phenolic compounds widely in nature, which have brought serious threats to biological systems and ecological environment [2].

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Methylacetylene is a toxic gas that is a lateral product industry and has been detected in the atmosphere.

Ethyl acetylene is very dangerous for nature and human thus ethyl acetylene detection and separation is very important [3]. This compound can be used in the synthesis of more complex organic molecules.

Cyanogen is a toxic gas that is smell like bitter almonds. Molecules with cyanogen groups are common species in several D-class asteroids and in chemical models for circumstellar envelopes involving CN reactions [4].

It is well known that substituted Pyrroles are an important class of heterocyclic compounds due to their remarkable biological and physical properties [5].

Aniline is a kind of common organic contaminant in industrial and it is noxious and harmful to human being and environment [6].

Ethanol from lignocellulosic feedstocks has received much recent attention for its potential role as a light-duty vehicle fuel due to volatile crude oil prices, ethanol's potential to reduce North America's dependence on imported petroleum and recent policies to reduce the carbon intensity of transportation fuels and to increase the production of biofuels [7], the properties and applications of this novel material have been investigated extensively [8].

Carbon Nano Tubes (CNTs) have many unique properties such as superior electronic conductivity and high capacity of hydrogen uptake and are attracting increasing attention as novel support media for heterogeneous catalysis [9]. The unique properties of these compounds including tensile strength, stiffness, drug delivery[10] and deformation are the feature of this nanotube [11].

During the past decade, Boron Nitride NanoTubes (BNNTs) have attracted considerable interests owing to their unique properties [12]. BNNT has composed by a single layer rotation of SP2 and they have particular and unique properties and also have a semiconductor behavior. This behavior reason is the total atomic number of B and N, that an interesting case for studding about these BNNTs is investigating their composite types [13]. Previously adsorption of different molecules toward nanostructures has been studied [14-17].Thus it's monitoring and control of exposure in both industrial and residential environments, are of special interest. People have been looking for good materials gas sensors with high sensitivity for a long time. As this study adsorption of several molecules on the surface of BNNT in order to find a suitable absorbent has been studied. Recently several studies in this field have been investigated which theory and empirical methods have been comparing [18-20].

THEORETICAL SECTION

We have optimized the molecules and BNNT at the B3LYP/6-31G (d) level of theory. BNNT is made up of 30N, 30B atoms were saturated with 10 hydrogen atoms which are in initial and end part of the nanotube. The reason for this act had been done to decrease the boundary effects and totally nanotube is involving 70 (Fig. 1).

All Computations are performed by means of GAMESS computational software [21]**.** The B3LYP is demonstrated to be a reliable and commonly used functionally in the study of different nanostructures[22]. We made molecules from different positions of the site to be close to the nanotube, and it's adsorption has been calculated by using the Equation(1)

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

According to the mentioned equation, $E_{Molecule}$ is molecule's energy, $E_{Nanotube}$ is the nanotube energy and $E_{Nanotube+Molecule}$ is the nanotube's energy with the molecule. In addition, δ_{BSSE} is representing the basis set superposition error. In the following steps, Si and Al atoms in the nanotube structure have been doped to examine the molecules adsorption on the nanotube and conductivity that which is doping with Si and Al atoms [23-26].

RESULTS AND DISCUSSION

Adsorption of Cyanogen on BNNT

The most stable configuration is shown in Fig. 2, that carbon atom of cyanogen is 3.98Å far from nitrogen atom of the nanotube. Detailed information of the structure and electronic properties of the BNNT 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 -1.62kcal/mol and then we calculated the HOMO/LUMO energy gap (E_g) for pristine nanotube since the cyanogen molecule is adsorbed on the nanotubes (Table 1). The 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: Calculated adsorption energy (E_{ad}, kcal/mol), HOMO and LUMO energies, HOMO-LUMO energy gap (E_g) of systems in eV.

System	E_{ad}	E_{HOMO}	E_{LUMO}	E_g
BNNT	-	-6.45	-2.76	3.69
BNNT/ C_2N_2	-1.62	-6.62	-2.11	4.51
Si_N	-	-6.06	-3.51	2.55
Si_N- C_2N_2	-9.03	-6.1	-2.17	3.93
Si_B	-	-5.73	-2.95	2.78
Si_B- C_2N_2	-9.10	-6.04	-2.06	3.98
Al_N	-	-5.54	-3.00	2.54
Al_N- C_2N_2	-11.23	-5.37	-2.59	2.78
Al_B	-	-6.41	-2.67	3.74
Al_B- C_2N_2	-20.70	-6.44	-2.37	4.07

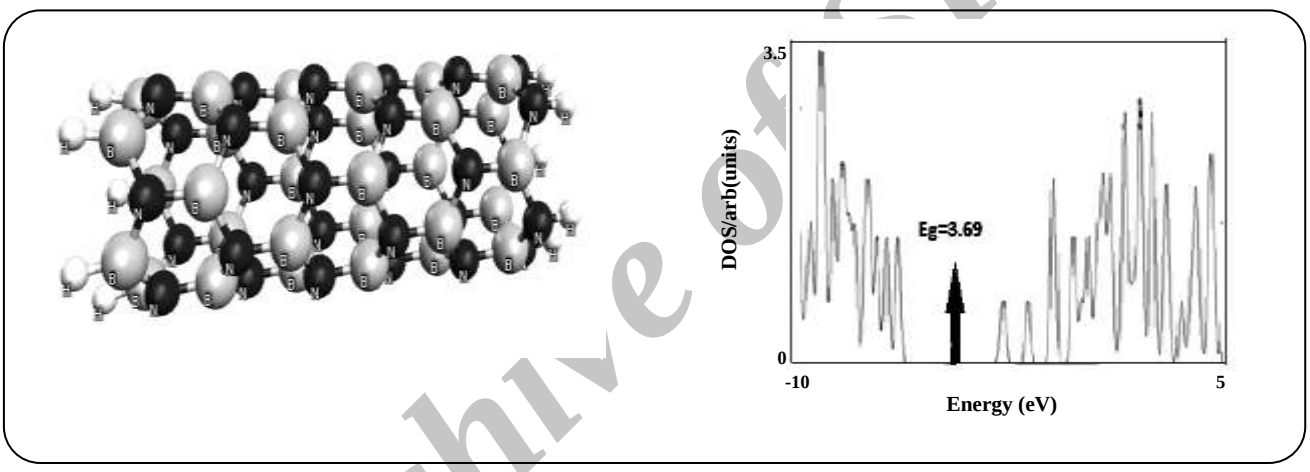

Fig. 1: Optimized structure and density of state (DOS) diagram of BNNT.

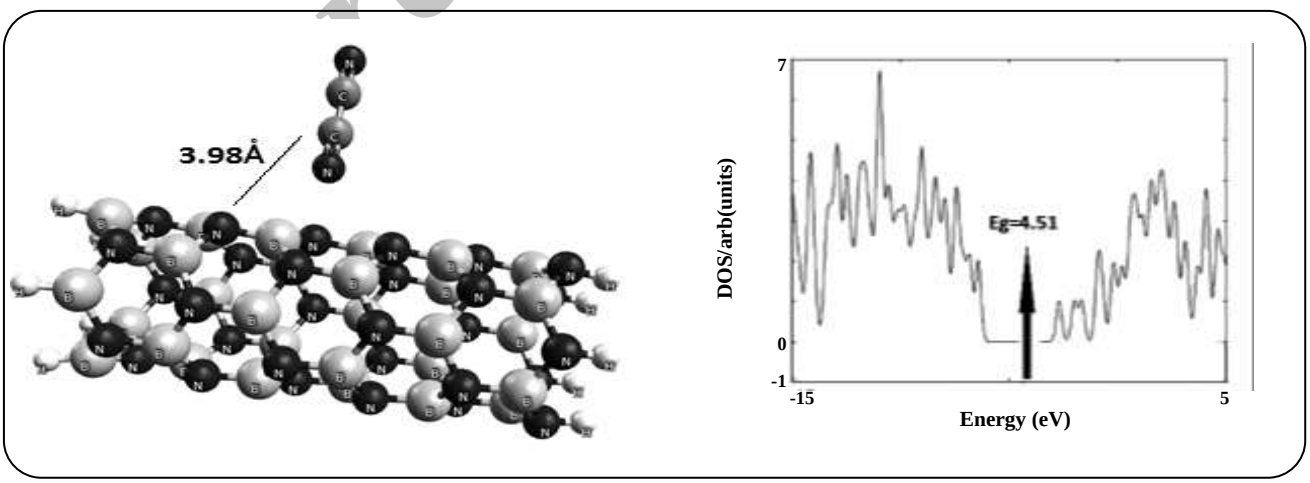

Fig. 2: Optimized structure of the C_2N_2 adsorbed BNNT and density of state diagram (DOS) of the complex. The distance is Å.

In order to evaluate the sensitivity of BNNT to adsorption of C_2N_2, this review was conducted twice, once B atom doped by Al atom and next time N atom by Al atom has been doped. In the optimized Al-doped nanotube, the Al atom has a larger size than the B and N atoms, accordingly to reduce stress due to its larger size, the Al atom impurity is projected out of the surface nanotube. The calculated bond lengths are 1.44 Å for B-N and 1.77 Å for Al-N and 2.09 Å for Al-B. Doped calculation of Al on BNNT shows that the value of HOMO/LUMO energy gap (E_g=4.07eV) is more than the pristine nanotube with E_g=3.69eV.The structural deformation results in a significant change in properties such as E_{ad}, E_g. The best adsorption energy (E_{ad}=-20.70 kcal/mol) is obtained when Al sitting instead of B and cyanogen has been adsorbed. When Al doping on BNNT 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 BNNT it will become a semiconductor (E_g=3.74). Optimization of these types of interactions is desirable for gas detection because such strong interactions mean that the BNNT is a suitable absorbent for cyanogen molecule. 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 explained by Equation(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 often as adsorption energy (E_{ad}) is increasing the recovery time becomes longer and calculation in Table 1. At this stage, doping has been studied with another element. First, instead of B atom in the boron nitride nanotube a Si atom and then instead of N atom a Si atom replaced in a nanotube, and then geometrical structures and electronic properties of BNNT are doped and their adsorption behavior are studied. The Si atom impurity is projected out of the surface nanotube in order to reduce stress due to its larger size compared to the B and N atoms. The calculated bond lengths are 1.44 Å for B-N and 1.73 Å for Si-N and 1.48Å for Si-B. Computations showed that when N replaced by Si in BNNT the HOMO/LUMO energy gap will become less (E_g=2.55eV).When Si is sitting of N, and the adsorption energy of cyanogen on nanotube is more (E_{ad}=-9.03kcal/mol) than when we just use the pristine nanotube (E_{ad}= -1.62kcal/mol). After adsorption of C_2N_2 on the mentioned nanotube that has doped by Si the HOMO/LUMO energy gap (E_g=3.93eV) will decrease the pristine of nanotube and therefore a substantial increase will occur in conductivity and this phenomenon can be explained as Equation (3), [27]

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

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

Adsorption of methylacetylene on BNNT

The most stable configuration is shown in Fig. 3, that carbon atom of methylacetylene is 3.96Å far from boron atom of the nanotube. Adsorption energy (E_{ad}) for mentioned configuration of methylacetylene and nanotube is about -1.78kcal/mol and then we calculated the HOMO/LUMO energy gap (E_g) for pristine nanotube since the methylacetylene molecule is adsorbed on the nanotubes (Table 2).

After adsorption of C_3H_4 on the mentioned nanotube that has doped by Al the HOMO/LUMO energy gap (E_g=3.67eV) will decrease and therefore a substantial increase will occur in conductivity and this phenomenon can be explained as Equation (2). when Al doping on BNNT in the presence of methylacetylene electrical signal is generated directly and therefore can potentially be used for methylacetylene sensors and the best adsorption energy (E_{ad}= -12.73kcal/mol) is when Al sitting instead of B and methylacetylene has been adsorbed. When Si is sitting on N and B, and the adsorption energy of methylacetylene on the nanotube is more (E_{ad}=-11.02kcal/mol) than when we just use the pristine nanotube (E_{ad}= -1.78kcal/mol).

Adsorption of hydroquinone on BNNT

The most stable configuration is shown in Fig. 4, that oxygen atom of hydroquinone is 4.26Å far from boron atom of the nanotube. Adsorption energy (E_{ad}) for mentioned configuration of hydroquinone and nanotube is about -7.77kcal/mol and then we calculated the

Table 2: Calculated adsorption energy (Ead, kcal/mol), HOMO and LUMO energies, HOMO-LUMO energy gap (Eg) of systems in eV.

System	E_{ad}	E_{HOMO}	E_{LUMO}	E_g
BNNT/C_3H_4	-1.78	-6.45	-2.75	3.71
Si_N-C_3H_4	-9.42	-6.37	-1.52	4.85
Si_B-C_3H_4	-11.02	-5.57	-1.43	4.14
Al_N-C_3H_4	-2.37	-5.56	-3.02	2.60
Al_B-C_3H_4	-12.73	-6.17	-2.41	3.67

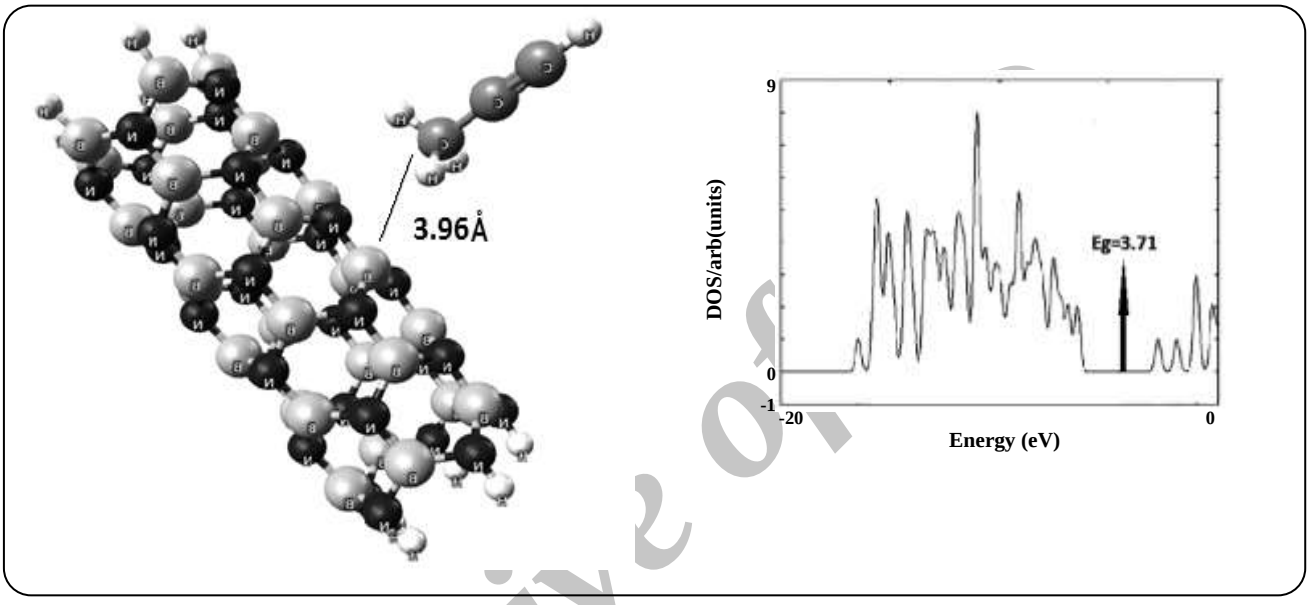

Fig. 3: Optimized structure of the C_3H_4 adsorbed BNNT and density of state diagram (DOS) of the complex. The distance is Å.

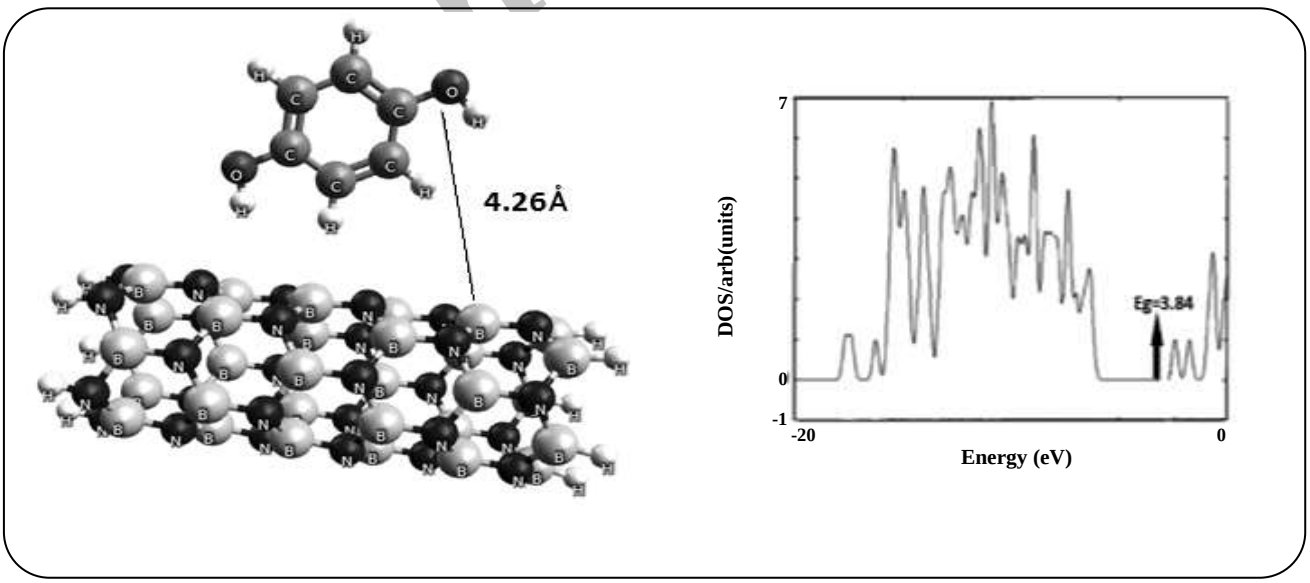

Fig. 4: Optimized structure of the $C_6H_4(OH)_2$ adsorbed BNNT and density of state diagram (DOS) of the complex. The distance is Å

Table 3: Calculated adsorption energy (Ead, kcal/mol), HOMO and LUMO energies, HOMO-LUMO energy gap (Eg) of systems in eV.

System	E_{ad}	E_{HOMO}	E_{LUMO}	E_g
BNNT/C_6H_4OH	-7.77	-6.24	-2.47	3.84
Si_N- C_6H_4OH	-8.05	-5.26	-2.75	2.51
Si_B- C_6H_4OH	-3.55	-5.5	-2.64	2.86
Al_N- C_6H_4OH	-19.70	-5.01	-2.42	2.59
Al_B- C_6H_4OH	-20.21	-6.12	-2.36	3.76

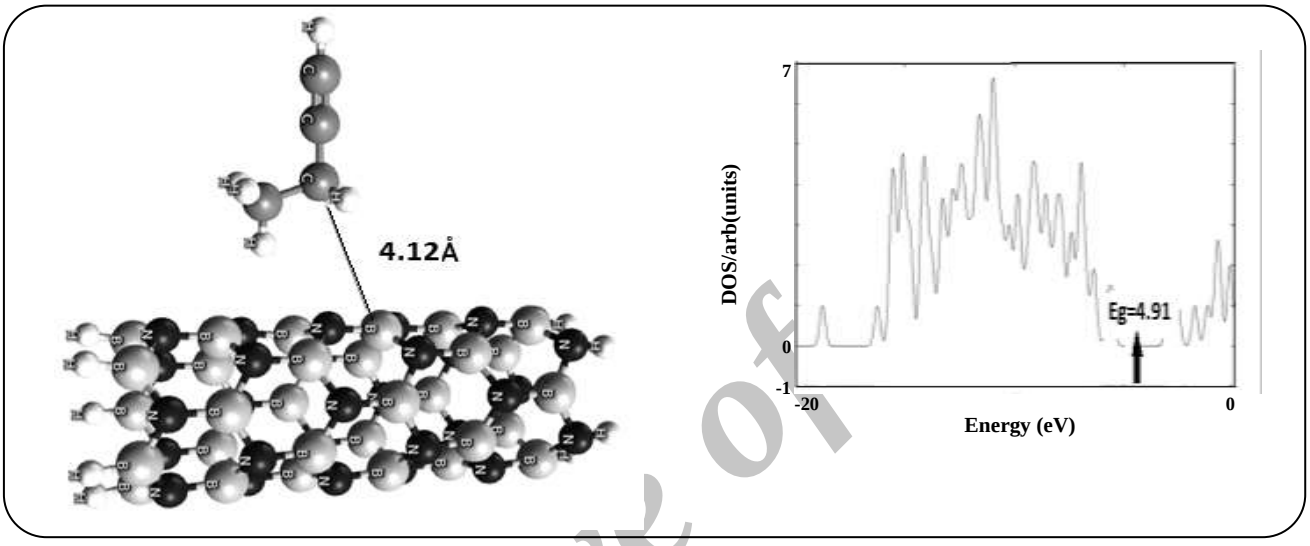

Fig. 5: Optimized structure of the C_4H_6 adsorbed BNNT and density of state diagram (DOS) of the complex. The distance is Å.

HOMO/LUMO energy gap (E_g) for pristine nanotube since the hydroquinone molecule is adsorbed on the nanotubes (Table 3).

After adsorption of hydroquinone on the mentioned nanotube that has doped by Al the HOMO/LUMO energy gap (E_g=2.59eV) will decrease and therefore a substantial increase will occur in conductivity and this phenomenon can be explained as Equation (2). when Al doping on BNNT in the presence of hydroquinone electrical signal is generated directly and therefore can potentially be used for hydroquinone sensors and the best adsorption energy (E_{ad}= -20.21kcal/mol) is when Al sitting instead of B and hydroquinone has been adsorbed.

Adsorption of ethylacetylene on BNNT

The most stable configuration is shown in Fig. 5, that carbon atom of ethylacetylene is 4.12 Å far from boron atom of the nanotube. Adsorption energy (E_{ad}) for mentioned configuration of ethylacetylene and nanotube is about -1.60kcal/mol and then we calculated the HOMO/LUMO energy gap (E_g) for pristine nanotube since the ethylacetylene molecule is adsorbed on the nanotubes (Table 4).

After adsorption of ethylacetylene on the mentioned nanotube that has doped by Al the HOMO/LUMO energy gap (E_g=3.76eV) will decrease and therefore a substantial increase will occur in conductivity and this phenomenon can be explained as Equation (2). when Al doping on BNNT in the presence of ethylacetylene electrical signal is generated directly and therefore can potentially be used for ethylacetylene sensors and the best adsorption energy (E_{ad}= -11.19 kcal/mol) is when Al sitting instead of N and ethylacetylene has been adsorbed.

Adsorption of aniline on BNNT

The most stable configuration is shown in Fig. 6, that nitrogen atom of aniline is 3.13 Å far from boron atom of the nanotube. Adsorption energy (E_{ad}) for mentioned

Table 4: Calculated adsorption energy (Ead, kcal/mol), HOMO and LUMO energies, HOMO-LUMO energy gap (Eg) of systems in eV.

System	E_{ad}	E_{HOMO}	E_{LUMO}	E_g
BNNT/C_4H_6	-1.60	-6.42	-2.75	4.91
Si_N-C_4H_6	-2.74	-5.96	-2.66	3.30
Si_B-C_4H_6	-1.96	-8.95	-1.28	7.67
Al_N-C_4H_6	-11.19	-6.17	-2.41	3.76
Al_B-C_4H_6	-1.64	-5.80	-1.85	3.95

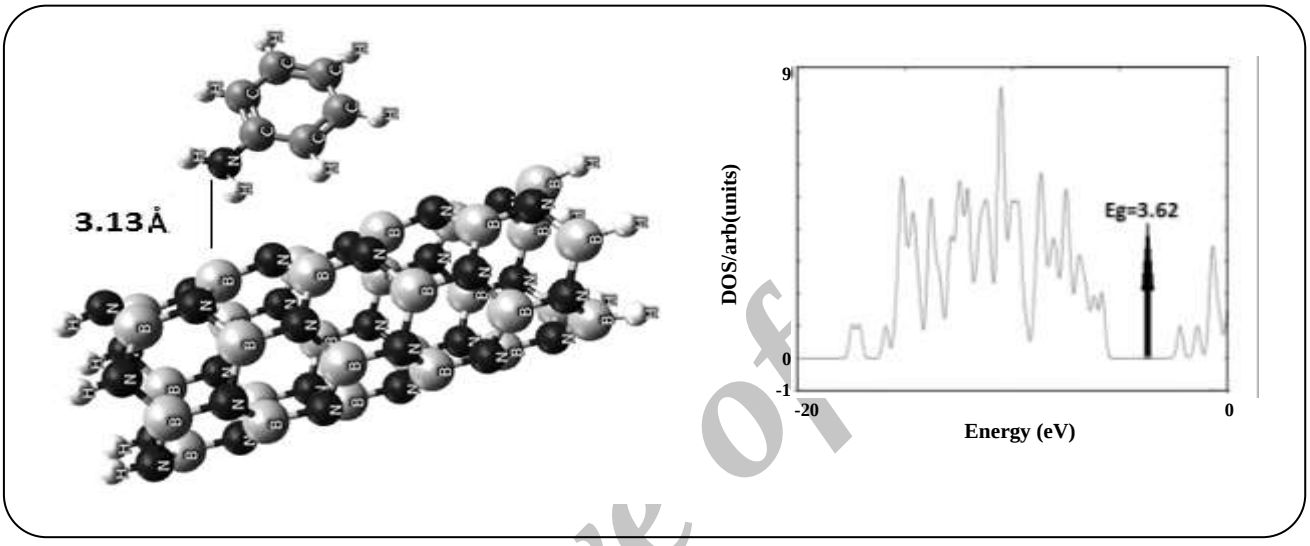

Fig. 6: Optimized structure of the $C_6H_5NH_2$ adsorbed BNNT and density of state diagram (DOS) of the complex. The distance is Å.

configuration of aniline and nanotube is about -19.03kcal/mol and then we calculated the HOMO/LUMO energy gap (E_g) for pristine nanotube since the aniline molecule is adsorbed on the nanotubes (Table 5).

After adsorption of aniline on the mentioned nanotube that has doped by Al the HOMO/LUMO energy gap (E_g=2.67eV) will decrease and therefore a substantial increase will occur in conductivity and this phenomenon can be explained as Equation (2). when Al doping on BNNT in the presence of aniline electrical signal is generated directly and therefore can potentially be used for aniline sensors and the best adsorption energy (E_{ad}= -47.75 kcal/mol) is when Al sitting instead of N and aniline has been adsorbed.

Adsorption of pyrrole on BNNT

The most stable configuration is shown in Fig. 7, that nitrogen atom of pyrrole is 3.16Å far from boron atom of the nanotube. Adsorption energy (E_{ad}) for mentioned configuration of pyrrole and nanotube is about -16.37kcal/mol and then we calculated the HOMO/LUMO energy gap (E_g) for pristine nanotube since the pyrrole molecule is adsorbed on the nanotubes (Table 6).

After adsorption of pyrrole on the mentioned nanotube that has doped by Al the HOMO/LUMO energy gap (E_g=2.80eV) will decrease and therefore a substantial increase will occur in conductivity and this phenomenon can be explained as Equation (2). when Al doping on BNNT in the presence of pyrrole electrical signal is generated directly and therefore can potentially be used for pyrrole sensors and the best adsorption energy (E_{ad}= -26.66kcal/mol) is when Al sitting instead of B and pyrrole has been adsorbed.

Adsorption of ethanol on BNNT

The most stable configuration is shown in Fig. 8, that hydrogen atom of ethanol is 2.07 Å far from nitrogen atom of the nanotube. Adsorption energy (E_{ad}) for

Table 5: Calculated adsorption energy (Ead, kcal/mol), HOMO and LUMO energies, HOMO-LUMO energy gap (Eg) of systems in eV.

System	E_{ad}	E_{HOMO}	E_{LUMO}	E_g
BNNT/ $C_6H_5NH_2$	-19.03	-5.81	-2.19	3.62
Si_N- $C_6H_5NH_2$	-24.91	-5.19	-2.36	2.89
Si_B- $C_6H_5NH_2$	-10.85	-5.06	-2.55	2.51
Al_N- $C_6H_5NH_2$	-27.73	-4.94	-2.27	2.67
Al_B- $C_6H_5NH_2$	-47.75	-6.12	-2.28	3.48

Table 6: Calculated adsorption energy (Ead, kcal/mol), HOMO and LUMO energies, HOMO-LUMO energy gap (Eg) of systems in eV.

System	E_{ad}	E_{HOMO}	E_{LUMO}	E_g
$BNNT_B$/ C_4H_5N	-16.37	-5.81	-2.59	3.22
Si_N- C_4H_5N	-24.29	-4.67	-2.41	2.26
Al_B- C_4H_5N	-26.66	-6.06	-2.26	2.80

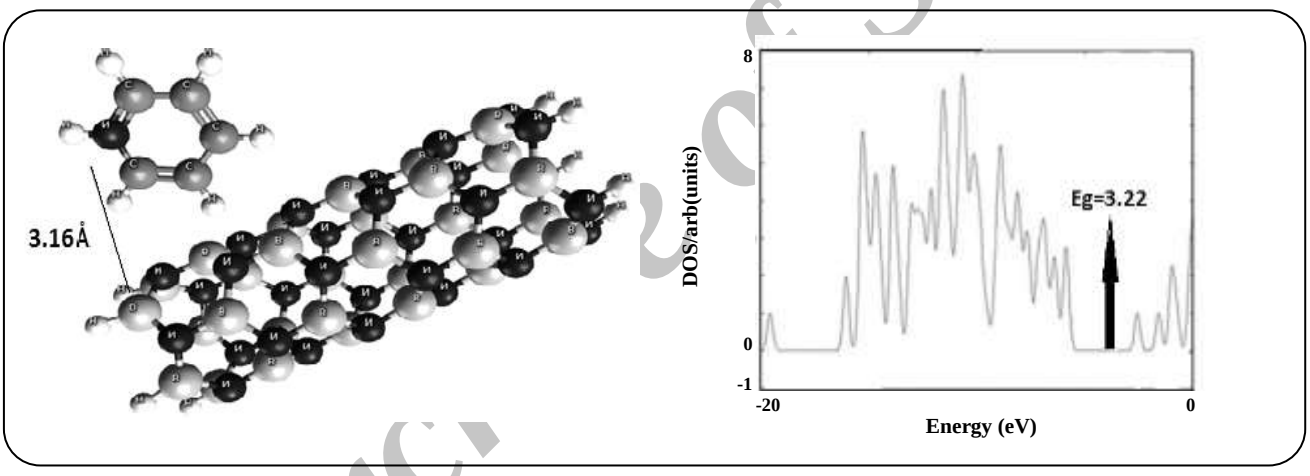

Fig. 7: Optimized structure of the C_4H_5N adsorbed BNNT and density of state diagram (DOS) of the complex. The distance is Å

mentioned configuration of ethanol and nanotube is about -12.26kcal/mol and then we calculated the HOMO/LUMO energy gap (E_g) for pristine nanotube since the ethanol molecule is adsorbed on the nanotubes (Table 7).

After adsorption of ethanol on the mentioned nanotube that has doped by Al the HOMO/LUMO energy gap (E_g=2.71eV) will decrease and therefore a substantial increase will occur in conductivity and this phenomenon can be explained as Equation (2). when Al doping on BNNT in the presence of ethanol electrical signal is generated directly and therefore can potentially be used for ethanol sensors and the best adsorption energy (E_{ad}= -25.09kcal/mol) is when Al sitting instead of B and ethanol has been adsorbed.

CONCLUSIONS

The adsorption of hydroquinone ($C_6H_4(OH)_2$), cyanogens(C_2N_2), methylacetylene (C_3H_4), ethylacetylene (C_4H_6), aniline ($C_6H_5NH_2$), ethanol (C_2H_5OH), pyrrole (C_4H_5N), molecules on the surface of BNNT (boron nitride nanotube) has been studied by using density functional theory (DFT) , and it was found that the adsorption energy (E_{ad}) of those molecules on the nanotube are according to this order: $C_6H_5NH_2$ > C_4H_5N >C_2H_5OH> C_2N_2>$C_6H_4(OH)_2$> C_3H_4 > C_4H_6. The results show clearly that modifying the nanotube could be as an effective adsorbent of those molecules in gas sensors which are sensitive to those molecules, when the BNNT

Table 7: Calculated adsorption energy (Ead, kcal/mol), HOMO and LUMO energies, HOMO-LUMO energy gap (Eg) of systems in eV.

System	E_{ad}	E_{HOMO}	E_{LUMO}	E_g
Si_N- C_2H_5OH	-19.70	-5.47	-2.96	2.51
Si_B- C_2H_5OH	-4.81	-3.02	-2.13	0.89
Al_N- C_2H_5OH	-24.52	-5.03	-2.32	2.71
Al_B- C_2H_5OH	-25.91	-6.18	-2.33	3.58
BNNT/ C_2H_5OH	-12.26	-6.2	-2.47	3.74

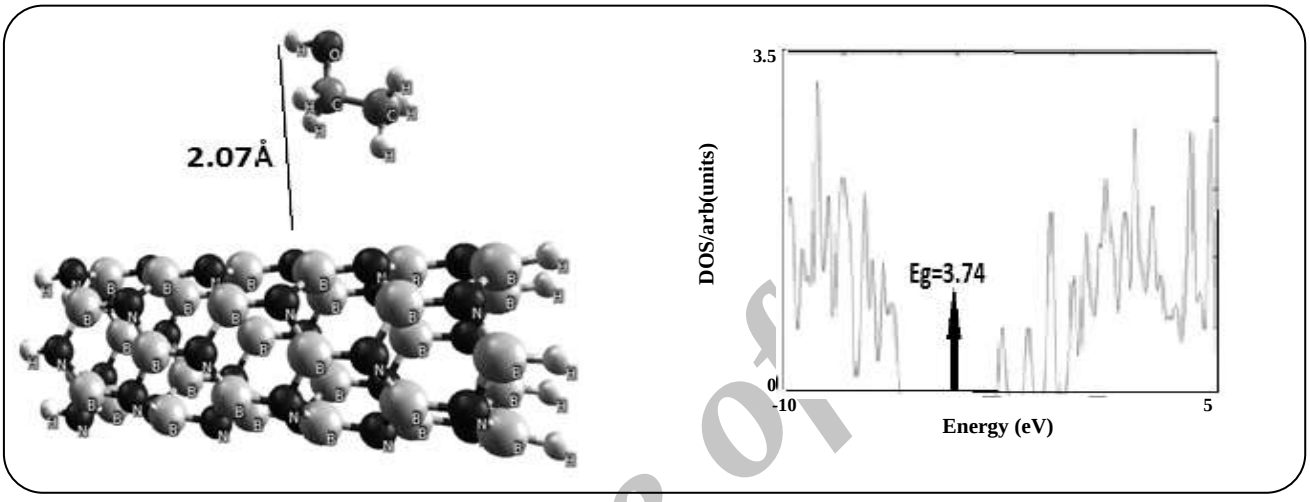

Fig. 8: Optimized structure of the C_2H_5OH adsorbed BNNT and density of state diagram (DOS) of the complex. The distance is Å

was doped by Al and Si atoms the HOMO/LUMO energy gap (E_g) values and the adsorption energy values improved. These results may be open a new gate to chemically modifying nanotubes in a way to expanding their applications in industry and technology.

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