**Original Article**

**Density functional theory study on the adsorption of H2S gas molecule with monolayer (AlN)21 (including pristine, C and B doped and defective aluminium nitride sheet)**

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**Abstract**

The interactions between graphene - like aluminium nitride **P**(AlN)21 nano ribbons doped and defect (AlN)21Sheet, P(AlN)21, (AlN)20-C,(AlN)19–C2 , (AlN)20 –B,(AlN)19 –B2, D-P(AlN)20, D-(AlN)19 –C, D- (AlN)18 –C2, D-(AlN)19 –B, D-(AlN)18 –B2),molecules and small toxic gas molecules ( H2S), were built for two different adsorption sites on graphene like aluminium nitride **P**(AlN)21, have been done by employing B3LYP density functional theory (DFT) with 6-31G(d,p) using Gaussian viw5.08 package of programs and Nanotube Modeller program(2018), The most stable adsorption configurations, adsorption energies, charge transfers (total Mulliken charge), electronic and band structures are calculated to deeply understand to find the sensitivity of all studied sheets for toxic gas H2S.

In this research we got the adsorptions of H2S on P(AlN)21 , (C) atoms-doped P(AL-N)20 sheet , D-P(Al-N)20 , D-(C)atoms-doped (Al-N)19 and D-(B) atoms-doped(Al-N)19, (on atom) with a Ead (**-0.468**eV ),( **-0.473** eV),(**-0.457** eV), (**-0.478** eV) and (**-0.454** eV) respectively, (Ead)of H2S on the center ring of the P(AL-N)21 , (C) atoms-doped (Al-N)20 sheet , D-P(Al-N)20 and D-(C, B)atoms-doped (AL-N)19 sheet are (**-0.280** eV ),( **-0.465** eV ), (**-0.405** eV), (**-0.468** eV) and **-0.282** eV) respectively, are weak physisorption ,on the other hand **P**(AlN)21 could be a good sensor for H2S. However, the adsorptions of H2S, on the ((AlN)20 –B, (on atom N and center ring the sheet) are a strong chemisorption because the Ead larger than -0.5 eV, due to the strong interaction, the ((AlN)20 –B,   
could catalyst or activate, through the results that we obtained, which are the improvement of the sheet **P**(AlN)21 by doping and per forming a defect in ,it that can be used to design sensors .

**Introduction.**

Graphene like-material attracted tremendous scientific and technological attention as the new honeycomb. Its exceptional physical and chemical properties{1,3}, such as high surface area, superior electrical conductivity, and huge mechanical strength{2}, it has caused application in various fields of study, such as compound materials, solar-cell technology, liquid crystal devices, Catalyst, and gas adsorbent. Graphene-based nanostructures and Graphene like-material are well known to be great to improve the potential of various sensors. Normally pristine aluminium nitride (AlN)21 sheet, graphene like-material properties is a weak adsorbent/sensor device because it has two-dimensional (2D) structure{6,7} with the surface only and no volume, which exploits the interaction of surface dopants with adsorbents. Therefor to increase its sensitivity{4,5}, by deliberately doped pristine (AlN)21 sheet with B and C elements and deformation. It should be noticed that because of 2D structure of pristine (AlN)21 sheet{6}, there is a space limitation for nearing the large molecules on its surface. As a result, it may not be the best choice to use pristine (AlN)21 sheet for adsorption process of large molecules. To solving this problem, B and other elements-doped (AlN)21 sheet will be an ideal choice because of significant changing in the structure of(AlN)21 sheet. It has been recognized that C doping could attain the higher sensitivity of (AlN)21 sheet toward different chemicals, and the applications of (AlN)21 sheet could be mainly enhanced. Graphene and its relatives belong to the new active research area towards adsorption of gas molecules. It has been verified that the reinforcement in the charge concentration of (AlN)21 sheet after adsorption of gas molecule can be used to create highly sensitive sensors. The modifying in the resistivity due to gas adsorbed on (AlN)21(including pristine, B or C doped and defective aluminium nitride sheet) sheet corresponds to sensing properties that may be considered as acceptors or donors. In addition, special binding sites in (AlN)21sheet can help to understand of interactions near the surface. Several theoretical researches based on density functional theory (DFT) calculations has been done to demonstrate the energies of interaction between small molecules with a (AlN)21sheet {8,9}. Theoretical studies indicate that the replacement of atom by doping or deforming can alter the band structure of (AlN)21 sheet and thus, the applications of (AlN)21 sheet could be mainly enhanced and expanded. Based on the kind of dopant, they are many papers showing the enhanced properties of graphene{10,11} among them, B and C are one of the most used dopants toward doping process for different purpose {12}.

In the present work, DFT calculations are performed to simulate the adsorption of and (H2S) gas molecule on the surface of (AlN)21 sheet as well as (B and C)-doped(AlN)21sheet and investigate their effect on the electronic properties of these surfaces. It is doubted that the incorporation company alters the structure of graphene and raised its quality.

**Computational Details Of DFT**

In this work, All calculations are carried out using DFT{13}, the geometric structures were completely optimized using Gaussian 09 program package. We select the Perdew, Burke, and Ernzerhof (PBE) exchange-correlation functional{14},to describe the exchange and correlation energy in the structural optimizations and total energy calculations. The system is modeled including 21 (Al and N) atoms of Pristine as well as (C and B) -doped (Al-N) sheet and deformation was created.. The Ead of molecules on the P(Al-N) sheet (Ead (gas+ P(Al-N) sheet)) and (C or B)-doped (Al-N) sheet Ead (gas+( C or B)-doped P(Al-N) sheet) is defined as:

Ead (gas+ P (Al-N) sheet)= E(gas+ P(Al-N) sheet) - (E P(Al-N) sheet + Egas) (1)  
Ead (gas+ (C or B)-doped P(Al-N) sheet)= E(gas+ (C or B)-doped P(Al-N) sheet) - (E(C or B)-doped P(Al-N) sheet + Egas) (2)

where E(gas+P(Al-N) sheet) and E(gas+(C or B)-doped P(Al-N) sheet) are the total energies of the relaxed molecule on the P(AL-N) sheet and (C or B)-doped P(AL-N) sheet{8,9}, respectively, E P(Al-N) sheet and E(C or B)-doped P(Al-N) sheet are the energies of the isolated P(AL-N) sheet and (C or B)-doped P(AL-N) sheet and Egas is the energy of isolated gas molecule. The diversity of relative energy of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of free (C or B)-doped P(AL-N) sheet and adsorbed molecule on (C or B)-doped P(AL-N) sheet gives the mechanism of interaction. The HOMO can be defined as an electron donor because of having the excess of electrons whereas the LUMO is lacking electrons and therefore it has a power of accepting electrons{10,11}.

**Result and discussion**

**Electronic Properties of Adsorbed H2S Molecule on P(AlN)21, (C, B)-doped P(AlN)20 , D-P(AlN)20 and D-(C, B)-doped P(AlN)19**

The AlN sheet has typical graphene-like structure. The optimized length of Al-N, Al- C, Al-B, bond is 1.868 Å,1.936 Å,2.025 Å, which is consistent with the findings in recent studies {15}. Our discussion begins with adsorption H2S gas molecule, on the P(AlN)21 sheet. As shown in Fig.(1), there are two different adsorption sites,(on the atom and the hollow center ring) which are the hollow center of the Al-N hexagon (a), the hollow center ring of Al-N (b), the top of the C atoms (c) , the top of the hollow center ring of( Al-C) atoms (d), the top of the B atoms (e) the hollow center ring of Al-B (f), the top of the N atoms with defect P(AlN)20sheet (g) , the hollow center ring of defect P(AlN)20 sheet (h) , the top of the N atoms with defect P(AlN)19 –C sheet (i) , the hollow center ring of defect P(AlN)19 –C sheet (j) , the top of the N atoms with defect P(AlN)19 –B sheet (k) , the hollow center ring of defect P(AlN)19 –B sheet (l) . The gas molecule is initially placed with its the top of the atoms center of mass exactly located at these sites. For each site, configurations with gas are then examined. Gas molecule is initially placed vertically to the surface of AlN sheet for all the possible adsorption sites. For the gas molecule/AlN systems, the adsorption energy is defined as.

Ea = Egas +‏ EAlN - Egas/AlN (3)

which basically decrease and increase of electrons decrease and increase in the elements . from fig.(1) (a) the side view of gas molecules H2S adsorb on atom of P(AlN)21 on the distance (2.66 Å), the fig (b) shows that the gas H2S on the center ring of P(AlN)21 with (2.64 Å) the gas H2S of the doped atom (C- doped P(AlN)20) on the distance (2.85 Å) it note that on the fig c , fig(d) gas molecular on the center ring C- doped P(AlN)20. on the distance (2.57 Å), the gas H2S of the doped atom (B- doped P(AlN)20) on the distance (1.91 Å) is observed that on the fig e , fig(f) gas molecular on the center ring B- doped P(AlN)20, for the distance (2.63 Aº), the gas H2S of the N atom in the D-P(AlN)20 sheet for the distance (2.91Aº) we see that on the fig (g) , fig(h) gas molecular on the center ring the D-P(AlN)20 sheet, on the distance(2.55Aº), the gas H2S of the C atom in D-(AlN)19 –C sheet on the fig(i) on the distance(2.39Aº), gas molecular on the center ring the D-(AlN)19 –C sheet, on the distance(2.61Aº), we see that on the fig (j), the gas H2S of the B atom in D-(AlN)19 –B sheet on the fig(k) on the distance(2.21Aº), ), gas molecular on the center ring the D-(AlN)19 –B sheet, on the distance(2.65Aº), we see that on the fig (l),

|  |  |
| --- | --- |
| a  P(AlN)21-H2S  2.66Aº | b  P(AlN)21-H2Scenter  2.64 Aº  2.63 Aº  1.07Aº  1.0 6 Aº  2.63 Aº  1.07Aº  1.0 6 Aº  2.63 Aº  1.07Aº  1.0 6 Aº  2.63 Aº  1.07Aº  1.0 6 Aº  2.63 Aº  1.07Aº  1.0 6 Aº |
| c  (AlN)20 –C-H2S  2.85 Aº | d  2.57 Aº  2.63 Aº  1.07Aº  1.0 6 Aº  (AlN)20 –C-H2S center |
| (AlN)20 –B-H2S  e  1.91 Aº | f  (AlN)20 –B-H2S center  2.63 Aº |
| g  D-P(AlN)20 –H2S  2.91Aº | h  D-P(AlN)20-H2S center  2.55Aº |
| i  2.39Aº  D-(AlN)19 –C-H2S | j  2.61Aº  D-(AlN)19 –C-H2S center |
| k  2.21Aº  D-(AlN)19 –B-H2S | l  2.65Aº  D-(AlN)19 –B-H2S center |

**Figure (1): Initial structures of the studied complexes with H2S gas**.

When we see Table (1), it can be noticed that ETot for adsorption of H2S on (C, B) atoms-doped P(AlN)20 sheet , D-P(AlN)20 and D-(C, B)atoms-doped P(AlN)19and (adsorption center) are smaller than adsorbed P(AlN)21 sheet, this indicates that ETot increases (in magnitude) with increasing the number of atoms, decreases (in magnitude) with decreasing the number of atoms. And adsorption energy (Ead)of H2S on the P(AlN)21 , (C, B) atoms-doped (AlN)20 sheet , D-P(AlN)20 and D-(C, B)atoms-doped P(AlN)19 sheet are (**-0.468**eV ),( **-0.473** eV ),( **-0.696** eV), (**-0.457** eV), (**-0.478** eV) and (**-0.454** eV) respectively. While (Ead)of H2S on the center ring of the P(AlN)21 , (C, B) atoms-doped (AlN)20 sheet , D-P(AlN)20 and D-(C, B)atoms-doped (AlN)19 sheet are (**-0.280** eV ),( **-0.465** eV ),( **-0.646** eV), (**-0.405** eV), (**-0.468** eV) and **-0.282** eV) respectively, Ead of a gas atom are found using equation (3), However, the Eg of H2S on the P(AlN)21 , (C, B) atoms-doped (AlN)20 sheet , D-P(AlN)20 and D-(C, B) atoms-doped (AL-N)19 sheet are (**2.948** eV ),( **2.231** eV ),( **2.895** eV), (**1.420** eV), (**1.984** eV) and (**2.587** eV) respectively .While (Eg)of H2S on the center ring of the P(AlN)21 , (C, B) atoms-doped P(AlN)20 sheet , D-P(AL-N)20 and D-(C, B)atoms-doped P(AlN)19 sheet are (**2.930** eV), (**2.805** eV),( **2.084** eV), (**0.718** eV), (**1.297** eV), and (**1.929** eV), respectively, Eg of a gas atom are found using equation:

(4) while the Eg for adsorption of H2S on D-(C, B)atoms-doped P(AlN)19 sheet are smaller than those pristine and no defect molecules, which indicates that the Eg decreases with the adsorption of H2S on D-(C, B)atoms-doped P(AlN)19. One can see from the overall results that are displayed in Table (1), that Ead of (B) atoms-doped P(AlN)20 sheet (on atom B and center ring) is larger than Ead for another systems because decreasing the number of atoms leads to decrease the area surface on sheets. The Ead of (B) atoms-doped P(AlN)20 sheet , (on atom B and center ring) is larger than -0.59 eV, corresponding to strong chemisorption {16}. The Ead for another systems (on atom B and center ring) is smaller than - 0.519 eV, corresponding to weak physisorption {17}. The Ead for (B) atoms-doped P(AlN)20 sheet (on atom B and center ring) are in agreement with the previous results {18,19}. In general, the Ead in the results indicates that (B) atoms-doped P(AlN)20 sheet is strongly reactive to molecule H2S, the Ead is (-0.696 eV)and (-0.646 eV) center ring, respectivelycorresponding to a strong chemisorption. Therefore, due to gas slow desorption from (B) atoms-doped P(AlN)20, the B-doped P(AlN)20 is not suitable . Nevertheless, B-doped P(AlN)20 could catalyst or activate this adsorbate due to the strong interaction, suggesting the possibility of B-doped P(AlN)20 as a catalyst. For B-doped P(AlN)20 and B-doped P(AlN)20) center ring, the binding strength of H2S with B-doped P(AlN)20 and( B-doped P(AlN)20) center ring are Ead of (-0.696 eV)eV and (-0.646 eV) center ring, respectively, the results Ead for B-doped P(AlN)20 are consistent with those reported in other studies {20}. so is the adsorption of H2Son P(AlN)21 , (C) atom-doped P(AlN)20 sheet , D-P(AlN)20 and D-(C,B) atom-doped P(AlN)19 sheet(on atom B and center ring) are weak physisorption, because the Ead of this molecules are smaller than -0.518 eV. Thus, P(AlN)21 , (C) atom-doped P(AlN)20 sheet , D-P(AlN)20 and D-(C,B) atom-doped P(AlN)19 sheet(on atom B and center ring) can be used to detect H2S since the adsorption-desorption equilibrium of H2Son this sheets are easily built

**Table (1): Structural and electronic properties of adsorption of H2S molecules on P(AlN)21 , (C, B) atoms-doped P(AlN)20 , D-P(AlN)20 and D-(C, B)atoms-doped P(AlN)19 sheets.**

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| --- | --- | --- | --- | --- | --- | --- | --- |
| sutructural | ET  eV | Eads  eV | HO  eV | LU  eV | Eg  eV | Ef  eV | Q mulekn |
| P(AlN)21-H2S | **-103452.8173** | **-0.468012** | **-5.512746** | **-3.314178** | **2.9485** | **-4.4134** | **-0.062** |
| P(AlN)21-H2Scenter | **-103452.6295** | **-0.280263** | **-5.627028** | **-2.696511** | **2.9305** | **-4.1617** | **-0.07** |
| (AlN)20-C-H2S | **-102997.33** | **-0.473454** | **-5.186226** | **-2.955006** | **2.2312** | **-4.0706** | **-0.164** |
| (AlN)20-C-H2S center | **-102997.3219** | **-0.465291** | **-5.463768** | **-2.658417** | **2.8053** | **-4.0610** | **-0.097** |
| (AlN)20-B-H2S | **-102635.5187** | **-0.696576** | **-5.455605** | **-2.560461** | **2.8951** | **-4.0080** | **-0.075** |
| (AlN)20-B-H2S center | **-102635.2683** | **-0.646244** | **-5.444721** | **-3.360435** | **2.0842** | **-4.4025** | **-0.087** |
| D-P(AlN)20-H2S | **-96851.86718** | **-0.457128** | **-5.591655** | **-4.171293** | **1.4203** | **-4.8814** | **-0.164** |
| D-P(AlN)20-H2Scenter | **-96851.81548** | **-0.405429** | **-4.149525** | **-3.431181** | **0.7183** | **-3.7903** | **-0.093** |
| D-(AlN)19-C-H2S | **-96396.57041** | **-0.478896** | **-5.744031** | **-3.795795** | **1.9482** | **-4.7699** | **0.142** |
| D-(AlN)19-C-H2S center | **-96396.55953** | **-0.468012** | **-5.403906** | **-4.105989** | **1.2979** | **-4.7549** | **-0.1** |
| D-(AlN)19-B-H2S | **-96038.43511** | **-0.454407** | **-5.186226** | **-2.598555** | **2.5876** | **-3.8923** | **0.152** |
| D-(AlN)19-B-H2S center | **-96038.26369** | **-0.282984** | **-4.228434** | **-2.299245** | **1.9291** | **-3.2638** | **-0.089** |

Figure (2) DFT calculation of HOMO and LUMO shapes for studied adsorption molecule on the sheet. In the P(AlN)21  sheet lobe. The calculated HOMO, LUMO, energy gap (Eg) values and the corresponding Fermi energies for the pristine, P(AlN)21  sheet ,doped pristine, P(AlN)21 sheet and defective pristine, P(AlN)21 sheets along with gas are summarized in Table (1). The orbital energy shape (Figure 2) shows a considerable change in HOMO and LUMO regions upon adsorption of gas in the pristine, doped and defective P(AlN)21 sheets, which illustrates the influence of gas .Both HOMO and LUMO energies of pristine ,doped and defective P(AlN)21  sheets are increased upon the adsorption of gas.This indicates the enhancement of electron donating and accepting ability of the P(AlN)21  sheet and gas. Furthermore, the gas adsorbed P(AlN)21 sheet has large shift in HOMO and LUMO values Table(1) due to the high charge transfer than the other gas.Since the increase in energy gap values suggests that the gas are freely entering into the P(AlN)21  sheets resulting in the accumulation of charges. Besides from Table (1). The Eg value of the P(AlN)21  sheets with gas is greater, (C, B) atoms-doped P(AlN)20 sheet , and D-P(AlN)20 sheet). Though the adsorption of gas on vacancy defected sheets have a larger than energy gap defects pristine before adsorption gas,. The influence of defects on the shape of pristine and defective sheets before the adsorption of gas are shown in Figure (2).From shape, D-( B) atom-doped P(AlN)19 sheet have minor variations while the other doped and defective have significant variations in the valence band region. Initially, the Fermi level of the pristine sheet is located at(−4.413 eV), (−4.161 eV) center and the inclusion of defect. leads to the minimize of the valence band, which subsequently shifts the Fermi level to( −3.263 eV). Moreover, the Fermi level of doped and defected sheets, are found to be shifted to −4.70 eV , −4.008 eV −4.881 eV, (−4.769 eV), (−4.892 eV) and (−4.061 eV) center (−4.402 eV) center (-3.790eV) center, (-4.754 eV) center,(-3.263 eV) center ,respectively. Thus, the inclusion of vacancy defected sheet is responsible for the height reduction of shape lobs in the valence band region. Moreover, the Fermi energy upshifts during the interaction of gas with pristine and defective sheets, indicating the electron gain from gas. The charge transfer between gas and P-sheets was obtained from Mulliken population analysis (Table 1).The total Mulliken charge on the molecules, and negative number means charge transfer from sheet to molecule gas.

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| --- | --- | --- |
| HOMO | Eg=2.948 eV  P(AlN)21-H2S | LUMO |
| HOMO | Eg=2.9305 eV  P(AlN)21-H2S  center | LUMO |
| Eg=2.2312 eV  HOMO | (AlN)20-C-H2S | LUMO |
| HOMO | (AlN)20-C-H2S center  Eg=2.8053 eV | LUMO |
| HOMO | (AlN)20-B-H2S  Eg=2.8951 eV | LUMO |
| HOMO | (AlN)20-B-H2S  Eg=2.0842 eV  center | LUMO |
| HOMO | Eg=1.4203 eV  D-P(AlN)20-H2S | LUMO |
| HOMO | Eg=0.7183eV  D-P(AlN)20-H2S  center | LUMO |
| HOMO | Eg=1.9482 eV  D-(AlN)19-C-H2S | LUMO |
| HOMO | Eg=1.2979 eV  D-(AlN)19-C-H2S  center | LUMO |
| HOMO | Eg=2.5876 eV  D-(AlN)19-B-H2S | LUMO |
| HOMO | Eg=1.9291 eV  D-(AlN)19-B-H2S  center | LUMO |

**Figure (2): shows the DFT calculation of HOMO and LUMO shapes for studied H2S adsorption molecules.**

**Conclusion**

The conclusions of the present study adsorption of gases H2S, can be summarized as follows:

1. The bond lengths of optimised structure for adsorbed system decrease with increasing of number of electrons in the elements.
2. The calculated ETot for all systems increases (in magnitude) with increasing the number of atoms.
3. There is no distortion in the planar structure of **P**(AlN) sheetin the case of doping (C,B)-doped **P**(AlN) . The adsorption of gas molecules onP(AlN)21 , (C- atoms-doped P(AlN)20 sheet , D-P(AlN)20 and D-(C, B)atoms-doped P(AlN)19 sheet undergoes a weak physisorption interaction, this Ead ranging can be used to detecting gas molecules H2S .
4. Pristine P(AlN)21 , (C- atoms-doped P(AlN)20 sheet , D-P(AlN)20 and D-(C, B)atoms-doped P(AL-N)19 sheet can be used as a good sensor for H2S and not suitable for usage as a gas sensor for B-doped **P**(AlN)20 .
5. The adsorption B-doped **P**(AlN)20sheet, on atom and center ring of gas molecule with H2S undergo in a strong chemisorption interaction with Ead ranging from -0.69 eV to 12.5 eV , so it presumably unsuitable for usage as a gas sensor for these gases, and could catalyse or activate.
6. The values of Eg decrease for adsorbed gases on molecular study
7. Pristine **P**(AlN) sheet, doped and defect are more sensitive to the H2S based toxic gases.
8. The electronic properties of **P**(AlN) can be modified by doped **P**(AlN) and defective **P**(AlN) sheets.

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