Density functional theory study on the adsorption of AsH$_3$ gas molecule with monolayer (AlN)$_{21}$ (including pristine, C, B doped and defective aluminium nitride sheet)

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Abstract
The interactions between graphene-like aluminium nitride (AlN)$_{21}$ nan ribbons doped and defect (AlN)$_{21}$Sheet, (AlN)$_{20}$-C, (AlN)$_{19}$-C$_2$, (AlN)$_{20}$--B, (AlN)$_{19}$--B$_2$, D-(AlN)$_{20}$, D-(AlN)$_{19}$--C, D-(AlN)$_{18}$--C$_2$, D-(AlN)$_{19}$--B, D-(AlN)$_{18}$--B$_2$), molecules and small toxic gas molecules (AsH$_3$), were built for two different adsorption sites on graphene-like aluminium nitride P(AlN)$_{21}$, have been done by employing BLYP density functional theory (DFT) with 6-31G(d,p) using Gaussian 09 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 AsH$_3$. In this research we got the adsorptions of AsH$_3$ on P(AlN)$_{21}$, (AlN)$_{20}$-C, (AlN)$_{19}$--C, D-(AlN)$_{20}$ and D-(C, B)atoms-doped P(AlN)$_{19}$ sheet are weak physisorption with an adsorption energy (E$_{ad}$) (-0.427197 eV), (-0.43536 eV), (-0.405364 eV) and (-0.456738 eV) respectively, while (E$_{ad}$) of AsH$_3$ on the center ring of the P(AL-N)$_{21}$, (C) atoms-doped P(AL-N)$_{20}$ sheet, D-P(AL-N)$_{20}$ and D-(C, B)atoms-doped P(AL-N)$_{19}$ sheet are (-0.479179 eV), (-0.43536 eV, -0.405364 eV), (-0.484338 eV, -0.476175 eV, -0.454407eV, -0.495222 eV) and (-0.481617 eV) respectively, otherwise doped aluminium nitride for this atom could be a good sensor for this gas AsH$_3$, except the adsorption of AsH$_3$ on B atoms-doped P(AlN)$_{20}$ sheet are a strong chemisorption, in this case, the B atoms-doped P(AL-N)$_{20}$ sheet could catalysis or activate, suggesting the possibility of P(AL-N)$_{20}$ as a metal-free catalyst, the total Mulliken charge on the molecules, and positive number means charge transfer from gas to P(AlN)$_{21}$. 

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 adsorbates. 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)21 sheet 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)21 sheet {8,9}. Theoretical studies indicate that the replacement of atom by doping or deforming can alter the band structure of (AlN)21 sheet 18,19, 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}.

**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 Per dew, 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 (B and N) -doped (Al-N) sheet and deformation was created.. The $E_{ad}$ of molecules on the P(Al-N) sheet ($E_{ad}$ (gas+ P(Al-N) sheet)) and (B or C)-doped (Al-N) sheet $E_{ad}$ (gas+ (B or C)-doped P(Al-N) sheet) is defined as:

$$E_{ad}$ (gas+ P(Al-N) sheet) = $E_{ad}$ (gas+ (B or C)-doped P(Al-N) sheet) = $E_{ad}$ (gas+ P(Al-N) sheet) + $E_{gas}$$

$$E_{ad}$ (gas+ (B or C)-doped P(Al-N) sheet) = $E_{ad}$ (gas+ (B or C)-doped P(Al-N) sheet) + $E_{gas}$$

where $E_{ad}$ (gas+ P(Al-N) sheet) and $E_{ad}$ (gas+ (B or C)-doped P(Al-N) sheet) are the total energies of the relaxed molecule on the P(Al-N) sheet and (B or C)-doped P(Al-N) sheet {8,9}, respectively, $E_{ad}$ (P(Al-N) sheet) and $E_{ad}$ (B or C)-doped P(Al-N) sheet are the energies of the isolated P(Al-N) sheet and (B or C)-doped P(Al-N) sheet and $E_{gas}$ 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 (B or C)-doped P(Al-N) sheet and adsorbed molecule on (B or C)-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

The (Al-N)$_{21}$ sheet has typical graphene-like structure. The optimized length of Al-N bond is 1.80 Å, which is consistent with the findings in recent studies. Our discussion begins with adsorption gas molecule, after relaxation, the optimized configurations obtained from the different initial states are compared to identify the most energetically stable one. The most stable configurations of the AsH$_3$ molecule on the pristine (P-), boron (B-), carbon (C-) and defective (D-) (Al-N)$_{21}$ sheet are summarized in figure 1. There are twelve different adsorption sites, which are the hollow center of the Al-N hexagon and defective (D-) (Al-N)$_{21}$, the top of the N atoms and defective (D-) (Al-N)$_{21}$. Moreover, one typical orientation of gas molecule with respect to the Al-N surface is considered. The gas molecule is initially placed with its center of mass exactly located at these sites. AsH$_3$ molecule is initially placed either vertically to the surface of Al-N sheet for all possible adsorption sites. For all gas molecule Al-N systems, the adsorption energy is defined as

$$E_a = E_{gas} + E_{Al-N} - E_{gas/AlN} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots 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of the doped atom (C-doped P(AlN)\textsubscript{20}) on the distance (1.78 Å) it noted that on the fig c, fig(d) gas molecular on the center ring C-doped P(AlN)\textsubscript{20}. on the distance (3.98 Å), the gas AsH\textsubscript{3} of the doped atom (B-doped P(AlN)\textsubscript{20}) on the distance (1.97 Å) is observed that on the fig e, fig(f) gas molecular on the center ring B-doped P(AlN)\textsubscript{20}, for the distance (1.94 Å\textdegree), the gas AsH\textsubscript{3} of the N atom in the D-P(AlN)\textsubscript{20} sheet for the distance (1.81Å\textdegree) we see that on the fig (g), fig(h) gas molecular on the center ring the D-P(AlN)\textsubscript{20} sheet, on the distance (2.52Å\textdegree), the gas AsH\textsubscript{3} of the C atom in D-(AlN)\textsubscript{19}–C sheet on the fig(i) on the distance (2.63Å\textdegree), gas molecular on the center ring the D-(AlN)\textsubscript{19}–C sheet, on the distance (2.58Å\textdegree), we see that on the fig (j), the gas AsH\textsubscript{3} of the B atom in D-(AlN)\textsubscript{19}–B sheet on the fig(k) on the distance (2.52Å\textdegree), gas molecular on the center ring the D-(AlN)\textsubscript{19}–B sheet, on the distance (2.57Å\textdegree), we see that on the fig (l),

We study the adsorption of AsH\textsubscript{3} gas on P(AlN)\textsubscript{21} sheet and (B or C)-doped P(AlN)\textsubscript{21} sheet near the dopant site. After adsorption of these gases, we try to examine its effect on structural, and electronic properties of (B or C)-doped P(AlN)\textsubscript{21} sheet. One of the most attractive topics in surface science research is the adsorption of Arsine (AsH\textsubscript{3}) on P(AlN)\textsubscript{21} sheet. It is known that AsH\textsubscript{3} is a non-irritating and colourless gas, a highly toxic flammable chemical gas used as a chemical weapon in wars when it enters the body of the human, AsH\textsubscript{3} combines with blood haemoglobin that prevents the union of oxygen and haemoglobin, leading to body tissue hypoxia and suffocation. Our discussion begins with Adsorption one gas molecule, AsH\textsubscript{3} on the Al-N sheet. As shown in Fig. 1.

![Diagram of adsorption](image-url)
(AlN)\textsubscript{20}–C–AsH\textsubscript{3} center

(AlN)\textsubscript{20}–B–AsH\textsubscript{3} center

D-P(AlN)\textsubscript{20}–AsH\textsubscript{3} center

\begin{align*}
\text{Bond lengths:} & \\
\text{(AlN)\textsubscript{20}–C–AsH\textsubscript{3}} & : 1.78 \text{ Å} \\
\text{(AlN)\textsubscript{20}–B–AsH\textsubscript{3}} & : 1.97 \text{ Å} \\
\text{D-P(AlN)\textsubscript{20}–AsH\textsubscript{3}} & : 1.81 \text{ Å} \\
\end{align*}
When we see Table (1), it can be noticed that \( E_{\text{Tot}} \) for adsorption of AsH\(_3\) on (C, B) atoms-doped P(AlN)\(_{20}\) sheet, D-P(AlN)\(_{20}\) and D-(C, B) atoms-doped P(AlN)\(_{19}\) and (adsorption center) are smaller than adsorbed P(AlN)\(_{21}\) sheet, this indicates that \( E_{\text{Tot}} \) increases (in magnitude) with increasing the number of atoms, decreases (in magnitude) with decreasing the number of atoms. And adsorption energy (\( E_{\text{ad}} \)) of AsH\(_3\) on the P(AlN)\(_{21}\), (C, B) atoms-doped P(AlN)\(_{20}\) sheet, D-P(AlN)\(_{20}\) and D-(C, B) atoms-doped P(AlN)\(_{19}\) sheet are (-0.427197 eV), (-0.43536 eV), (12.524763 eV), (-0.405364 eV), (-0.456738 eV) and (-0.495222 eV) respectively. While \( E_{\text{ad}} \) of AsH\(_3\) on the center ring of the P(Al-N)\(_{21}\), (C, B) atoms-doped P(AlN)\(_{20}\) sheet, D-P(AlN)\(_{20}\) and D-(C, B) atoms-doped P(AlN)\(_{19}\) sheet are (-0.484338 eV), (-0.476175 eV), (-0.684338 eV), (-0.454407 eV), (-0.495222 eV) and -0.481617 eV) respectively, \( E_{\text{ad}} \) of a gas atom are found using equation (1). However, the \( E_{\text{g}} \) of AsH\(_3\) on the P(AlN)\(_{21}\), (C, B) atoms-doped P(AlN)\(_{20}\) sheet, D-P(AlN)\(_{20}\) and D-(C, B) atoms-doped P(AlN)\(_{19}\) sheet are (1.5754 eV), (2.7974 eV), (2.7373 eV), (2.1441 eV), (1.0475 eV) and (1.9917 eV) respectively. While \( E_{\text{g}} \) of AsH\(_3\) on the center ring of the P(AlN)\(_{21}\), (C, B) atoms-doped P(Al-N)\(_{20}\) sheet, D-P(AlN)\(_{20}\) and D-(C, B) atoms-doped P(AlN)\(_{19}\) sheet are (2.9849 eV), (2.8352 eV), (2.8951 eV), (1.5033 eV), (0.9305 eV), and (1.8094 eV), respectively, \( E_{\text{g}} \) of a gas atom are found using equation:

\[
E_{\text{g}} = H_{\text{LUMO}} - E_{\text{HOMO}}
\]

………..(4)

while the \( E_{\text{g}} \) for adsorption of AsH\(_3\) on D-(C, B) atoms-doped P(AlN)\(_{19}\) sheet are smaller than those pristine and no defect molecules, which indicates that the \( E_{\text{g}} \) decreases with the adsorption of AsH\(_3\) on
D-(C, B) atoms-doped P(AlN)_{19}. One can see from the overall results that are displayed in Table (1), that $E_{\text{ad}}$ of (B) atoms-doped P(AL-N)_{20} sheet (on atom B and center ring) is larger than $E_{\text{ad}}$ for another systems because decreasing the number of atoms leads to decrease the area surface on sheets. The $E_{\text{ad}}$ of (B) atoms-doped P(AlN)_{20} sheet, (on atom B and center ring) is larger than -0.59 eV, corresponding to strong chemisorption \cite{16}. The $E_{\text{ad}}$ for another systems (on atom B and center ring) is smaller than 0.519 eV, corresponding to weak physisorption \cite{17}. The $E_{\text{ad}}$ for (B) atoms-doped P(AlN)_{20} sheet (on atom B and center ring) are in agreement with the previous results \cite{18,19}. In general, the $E_{\text{ad}}$ in the results indicates that (B) atoms-doped P(AlN)_{20} sheet is strongly reactive to molecule AsH_{3}, the $E_{\text{ad}}$ is (-12.524 eV) and (-0.684 eV) center ring, respectively corresponding 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 as a sensor of AsH_{3}. Nevertheless, B-doped P(Al-N)_{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 AsH_{3} with B-doped P(AlN)_{20} and B-doped P(AlN)_{20} center ring are $E_{\text{ad}}$ of (-12.524 eV) eV and (-0.684 eV) center ring, respectively, the results $E_{\text{ad}}$ for B-doped P(AlN)_{20} are consistent with those reported in other studies. so is the adsorption of AsH_{3} on P(AlN)_{21}, (C) atom-doped P(Al-N)_{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 $E_{\text{ad}}$ of this molecules are smaller than -0.518 eV. Thus, P(AlN)_{21}, (C) atom-doped P(AlN)_{20} sheet, D-P(Al-N)_{20} and D-(C,B) atom-doped P(AlN)_{19} sheet (on atom B and center ring) can be used to detect AsH_{3} since the adsorption-desorption equilibrium of AsH_{3} on this sheets are easily built.
Table (1): Structural and electronic properties of adsorption of AsH₃ 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.

| structural     | Eₜ     | E_ads  | HO     | LU     | E₉     | Eᵣ     | Q multikn |
|----------------|---------|--------|--------|--------|--------|--------|-----------|
| P(AlN)₂₁-AsH₃ | -1534146193 | -0.427197 | -4.900251 | 1.575  | -4.112  | 0.137  |
| P(AlN)₂₁-AsH₃ center | -1534146764 | -0.484338 | -5.616144 | -2.631207 | 2.9849 | -4.1236 | -0.04     |
| (AlN)₂₀-C-AsH₃ | -1529591348 | -0.43536  | -5.458326 | -2.478831 | 2.9794 | -3.9685 | 0.058     |
| (AlN)₂₀-C-AsH₃ center | -1529591756 | -0.476175  | -5.606133 | -2.80551 | 2.8352 | -4.2229 | 0.03      |
| (AlN)₂₀-B-AsH₃ | -1525841402 | 12.524763  | -5.420200 | -2.704674 | 2.7373 | -4.0733 | 0.208     |
| (AlN)₂₀-B-AsH₃ center | -1525891483 | -0.684338  | -5.493999 | -2.598555 | 2.8951 | -4.0461 | -0.08     |
| Compound                | E (eV)          | E' (eV)         | E'' (eV)        | E''' (eV)       | EIV (eV)      |
|-------------------------|-----------------|-----------------|-----------------|----------------|---------------|
| P(AlN)$_{20}$-AsH$_3$   | -146815.6583    | -0.405384       | -5.265135       | -3.120987      | 2.1441        |
| P(AlN)$_{20}$-AsH$_3$   | -146813.7073    | -0.454407       | -4.70603        | -3.967218      | 0.5033        |
| (AlN)$_{19}$-C-AsH$_3$  | -146345.4776    | -0.456728       | -5.172621       | -4.125036      | 1.0475        |
| (AlN)$_{19}$-C-AsH$_3$  | -146338.4269    | -0.485222       | -5.300508       | -4.389926      | 0.9305        |
| (AlN)$_{19}$-B-AsH$_3$  | -146000.3188    | -0.495222       | -4.225713       | -2.233941      | 1.9917        |
| (AlN)$_{19}$-B-AsH$_3$  | -146000.3052    | -0.481617       | -4.190340       | -2.380875      | 1.8094        |
The Table (1) indicates that $E_{\text{HOMO}}$ and $E_{\text{LUMO}}$ for adsorption AsH$_3$ on, (C, B) atoms-doped P(AlN)$_{20}$ sheet, D-P(AlN)$_{20}$ and D-(C, B) atoms-doped P(AlN)$_{19}$ sheet (on the atom and the center ring) are smaller than the P(Al-N)$_{21}$ sheet. We found that high value of $E_{\text{HOMO}}$ is $(-5.616144)$ eV, this value indicates a tendency of the molecule to donate electrons, while the lower the value of $E_{\text{LUMO}}$ is $(-2.631207)$ eV, this value indicates a tendency of the molecule to accept electrons.

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 ($E_g$) 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 a 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 $E_g$ value of the, (C, B) atoms-doped P(AlN)$_{20}$ sheet, and D-P(AlN)$_{20}$ sheet with gas is greater (2.979 eV) (2.737 eV), (2.144 eV) than the pristine (1.575 eV), D-(C,B) atom-doped P(AlN)$_{19}$ sheet (1.047 eV) and (1.991 eV). Though the adsorption of gas on vacancy defected sheets have a larger than energy gap defects pristine before adsorption gas, it is significantly smaller than gas adsorption. Moreover, the Fermi level of doped and defected sheets are found to be shifted to $-4.69$ and $-4.80$ eV, $-5.05$eV, $-4.50$ eV, $-3.49$ eV 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.
\[ E_g = 1.590 \text{eV} \]

\[ P(\text{AlN})_{21} - \text{A}_3\text{H}_3 \]

\[ E_g = 2.9849 \text{eV} \]

\[ P(\text{AlN})_{21} - \text{A}_3\text{H}_3 \text{ center} \]

\[ E_g = 2.9794 \text{eV} \]

\[ (\text{AlN})_{20} - \text{C}-\text{A}_3\text{H}_3 \]

\[ E_g = 2.8352 \text{eV} \]

\[ (\text{AlN})_{20} - \text{C}-\text{A}_3\text{H}_3 \text{ center} \]
$E_g = 2.7373 \text{ eV}$

(AlN)$_{20}$-B-A$_3$H$_3$

$E_g = 2.8951 \text{ eV}$

(AlN)$_{20}$-B-A$_3$H$_3$

center

$E_g = 2.1441 \text{ eV}$

D-P(Al-N)$_{20}$-A$_3$H$_3$

$E_g = 0.5033 \text{ eV}$

D-P(AlN)$_{20}$-A$_3$H$_3$

center
Figure (2): shows the DFT calculation of HOMO and LUMO shapes for studied \( \text{AsH}_3 \) adsorption molecules.
Conclusion

The conclusions of the present study adsorption of gases AsH₃, can be summarized as follows:

For adsorption of gas AsH₃

1. The bond lengths of optimized structure for adsorbed system decrease with increasing of number of electrons in the elements.

2. The calculated $E_{\text{Tot}}$ for all systems increases (in magnitude) with increasing the number of atoms.

3. There is no distortion in the planar structure of P(AlN) sheet in the case of doping (C,B)-doped P(AlN). The adsorption of gas molecules on P(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 $E_{\text{ad}}$ ranging can be used to detecting gas molecules AsH₃.

4. Pristine P(AlN)$_{21}$, (C- atoms-doped P(AlN)$_{20}$ sheet , D-P(AlN)$_{20}$ and D-(C, B)atoms-doped P(AlN)$_{19}$ sheet can be used as a good sensor for AsH₃ and not suitable for usage as a gas sensor for B-doped P(AlN)$_{20}$.

5. The adsorption B-doped P(AlN)$_{20}$ sheet, on atom and center ring of gas molecule with AsH₃ undergo in a strong chemisorption interaction with $E_{\text{ad}}$ ranging from -0.696 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 $E_g$ decrease for adsorbed gases on molecular study

7. Pristine P(AlN) sheet, doped and defect are more sensitive to the AsH₃ 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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