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Adsorption of gas molecules on (BN) Monolayer as potential SO, SO2 NO, and NO2 gases sensor: A DFT study

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Abstract

In this work, a solar concentrator was constructed using liquid crystalline material of the isotropic type to increase the To explore the sensitive characteristics of gas molecules (SO, SO2, NO, NO2) on a Boron Nitride(BN) monolayer and Aluminum(Al) -doped Boron Nitride(BN) monolayer, the B3PLYP functional and 6-311G (d, p) basis set computations were utilized, Gaussian 09 and Nanotube Modeller (2018) programs utilized. Significantly, these gases contribute to the degradation of the environment. From three options of monolayer : the center of the ring, nitrogen atom, and bridge(B-N) , adsorption energy, distance, and charge transfer factors allowed us to choose the best location for adsorption. Various gas molecules (SO, SO2, NO, and NO2) have had chemical adsorptions on a Boron Nitride (BN) monolayer and Aluminum(Al)-doped Boron Nitride (BN) monolayer. There is no physical adsorption of NO gas in bridge(B-N) , NO2 in nitrogen atom for BN monolayer, and NO2 gas in Bridge for Aluminum(Al) -doped Boron Nitride(BN) monolayer. The findings of this work further show that following adsorption, there is a large amount of charge transfer between gas molecules and a Boron Nitride(BN) monolayer and an Aluminum(Al) -doped Boron Nitride(BN) monolayer, with the exception of one location where the adsorption energy is weak and the charge transfer is weak (NO gas /pristine Boron Nitride(BN). This means that a Boron Nitride(BN) monolayer and an Aluminum(Al)/doped Boron Nitride(BN) monolayer are more vulnerable to SO, SO_2, NO, and NO_2 adsorption than pristine and doped graphene, and that gas adsorption on the Aluminum(Al)/doped Boron Nitride(BN) monolayers is stronger to other gases. Furthermore, small gas molecule adsorption clearly modifies the band -gap and work function of a Boron Nitride(BN) and Aluminum(Al) -doped Boron Nitride(BN) monolayer to variable degrees. Our study will give theoretical guidance for practical implementations.

Keyword: Boron Nitride (BN), Aluminum(Al)/doped BN monolayer gas adsorption, DFT, HOMO, LUMO..

1. Introduction

In the past few years, Scientists expanded their study and interest Graphene-like material, and managing and doing research about it, Because on the necessary and large applications it has, Graphene-like nanomaterial's such as Boron Nitride(BN) a structure of two dimensions is gained large attention from (people who work to find information), because of its electronic properties ,low cost, its fast response time and high sensitivity at room temperature[1-3]. Previous researches on graphene-like nanomaterial's suggests that these materials are necessary or candidate, for sensing poisonous gases and harmful gases (CO, CO_2, NO, NO_2) that factories release in vast amounts into the atmosphere, causing issues such as smog and acid rain, as well as other pollutants that are hazardous to humans and the environment, which shows high electron ability to move around Experimentally[4,5]. However, this work exhibit that Boron Nitride(BN) is an exciting candidacy for utilization as a gas sensor due to its tremendous sensitivity, permanency durability. Similar according to the good sensor properties of CNTs, BN, a single atomic layer , is considered to be an worthy sensor material due to its special properties , Boron Nitride(BN) sample has been mentioned to be used as a very sensitive gas sensor[6,7]. Donor or acceptor molecules on Boron Nitride(BN) have been shown to be able to substantially alter electronic properties by using DF-T[8-13]. And as the gas molecules are adsorbed on the BN layer, there are variations in resistance that make it possible for Boron Nitride(BN) to be a solid-state sensor to detect the actual gas from others. The transfer of charge between the gas molecules and the BN layer applies to the direction of the gas molecules with

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respect to the BN layer and has little to do with the adsorption site[14,15]. In view of the above, we studied the various positions of the CO molecules in order to find the most optimal arrangement of the adsorption. Most of the previous analysis centered on pristine graphene and projected comparatively low adsorption energy compared to the critical requirements of gas sensing applications[16,17]. The measurable range and sensitivity of the single wall Boron Nitride(BN) layer have been reported to be expanded and improved by doping technologies.

2. Modeling and Computational Details

In this work, DFT calculations were completed using Gaussian 09 package [13]. This software package is using the standard and modern quantum mechanics basics and there are different types from these. The B3LYP/6-311G (d, p) base set is used for geometry optimization in SO, SO_2, NO and NO_2 gas absorption effect of single-layer Boron Nitride(BN) [14]. One theoretical level commonly used for the structure of the nanotube is the B3LYP / 6-311G Functional level (d, p)[15]. As shown below, the chemical potential of complexes or Fermi energy (E_F) was obtained:

$$E_F = (E_{HOMO} + E_{LUMO})/2 \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

Where:

-E_{HOMO}: is the energy of the higher occupied molecular orbital.

-E_{LUMO}: is the energy of the lower unoccupied molecular orbital.

In addition, the energy gap in the energy levels (for example) of the system is recognized as follows:

$$E_g = E_{LUMO} - E_{HOMO} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (2)$$

The adsorption energy (E_{ads}) was calculated using the following pretty close expression:

$$E_{ads} = E_{(COMPLEX)} - (E_{(MOLECULE)} + E_{(GAS)}) \quad \ldots\ldots\ldots\ldots \quad (3)$$

[17]

Where:

- $E_{(COMPLEX)}$: The actual molecule energy with gas adsorption.
- $E_{(MOLECULE)}$: The total energy without absorption of the studied molecule.
- $E_{(GAS)}$: Gas molecule's total energy [18].

3. Results and Discussion

Adsorption configurations

The Boron Nitride(BN) monolayer has a single layer, as seen in Fig. 1. There are three types of adsorption sites in the BN monolayer and Al-doped Boron Nitride(BN) monolayer. The distance between the Boron Nitride(BN) - substrate and the gas molecules is initially fixed at 2.5 Å before optimization. Furthermore, the gas molecule's starting location is perpendicular to the substrate .Multiple insertion geometries must be considered since gas molecules adsorb in a variety of configurations. To do this, one (SO, SO_2,NO, and NO_2,) gas molecule is employed at a distance of 2.5 Å over the nitrogen atom, center, and bridge. However, one initial orientation of the triatomic (NO_2), SO_2, is taken into account. The S atom of gas points to the nitrogen atom in the first direction, the B-N bridge is in the second, and the center ring in the third, whereas the S atoms of SO_2 and nitrogen atom of NO gas point to the BN layer in the same ways. Then, all of systems will be totally relaxed. The molecules' absorption energies can be used to determine how they interact with the BN monolayer and Al-doped BN monolayer. According to the formula. The higher the E_{ads} value, the more gas molecules adsorb onto the BN. The most energy-appropriate adsorption configurations are chosen for future inquiry.

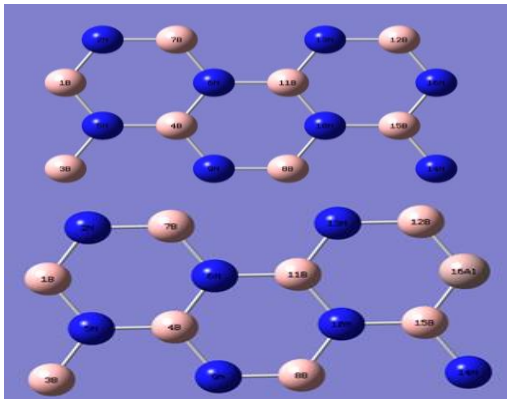


Fig. 1. Geometric structures of pristine and Al-doped BN monolayer.

The adsorption energy (E_{ads}), electronic characteristics of the investigated molecules such as HOMO, LUMO, total energy (E_{tot}), energy gap (E_g), and Fermi energy (E_F) were discovered after optimizing the geometry, as shown in Table 1.

Table 1: Structural and electronic properties of pristine and Al-doped BN monolayer.

model	site	HOMO	LUMO	E_g eV	E_F eV
	bridge(B-N)	-6.693	-4.163	2.53	-5.428
SO/pristine BN	nitrogen atom	-6.149	-4.367	2.101	-5.258
	center of the ring(B-N)	-6.312	-4.271	2.041	-5.2915
	bridge(B-N)	-6.176	-4.163	2.013	-4.339
SO/Al-doped BN	nitrogen atom	-6.149	-4.163	1.986	-4.285
	center of the ring Al-doped (B-N)	-6.084	4.135	1.449	-4.285
	bridge(B-N)	-6.312	-2.448	3.864	-4.38
SO_2/pristine BN	nitrogen atom	-6.312	-2.864	3.918	-4.353
	center of the ring(B-N)	-6.339	-2.204	3.435	-4.271
	bridge(B-N)	-4.435	-4.135	0.3	-4.666
SO_2/Al-doped BN	nitrogen atom	-6.231	-3.047	3.184	-4.639
	center of the ring Al-doped (B-N)	-6.095	-2.775	3.32	-4.435
	bridge(B-N)	-6.584	-4.190	1.394	-5.387
NO/pristine BN	nitrogen atom	-6.748	-4.952	1.36	-5.898
	center of the ring(B-N)	-6.748	-4.952	1.396	-5.85
	bridge(B-N)	-4.788	-3.319	1.469	-4.053
NO/Al-doped BN	nitrogen atom	-4.788	-3.319	1.469	-4.053
	center of the ring Al-doped (B-N)	-4.788	-3.319	1.469	-4.053
	bridge(B-N)	-6.938	-4.326	2.204	-5.428
NO_2/pristine BN	nitrogen atom	-6.938	-4.108	2.83	-5.523
	center of the ring(B-N)	-6.285	-4.329	2.212	-5.432
	bridge(B-N)	-6.639	-3.401	3.238	-5.02
NO_2/Al-doped BN	nitrogen atom	-6.639	-3.401	3.238	-5.019
	center of the ring Al-doped (B-N)	-6.639	-3.401	3.238	-5.001

The adsorption energies of several gas molecules considered in this work on BN monolayer and Al-doped BN monolayer are summarized in Table 2. We ignore the varied orientations of adsorbed gas molecules since we are only interested in the effect of gas adsorption on the electronic structure of the BN monolayer. The research of electronic structure, on the other hand, is almost entirely independent from the research of direction and adsorption sites.The adsorption energies of SO, SO_2, NO, and NO_2 are substantially greater, showing a strong bond between these two molecules and Al-doped BN monolayer.

Table 2: Adsorption energies $\mathbf{E_{ads}}$ **eV**, adsorption height **D(A°)**, sum of covalent atomic radii **r (A°)** and transfer charges **Q |e|** for adsorption configurations.

model	site	D°A	r ° A	E_{ads} eV	Q |e|
	bridge(B-N)	1.53465	3.35	-3.0134	-0. 26
SO/pristine BN	nitrogen atom	1.84521	3.35	-2.8366	1.275
	center of the ring(B-N)	1.83009	3.35	-2.7169	-0. 5
	bridge(B-N)	3.04591	3.35	-2.7984	0.23
SO/ Al-pristine BN	nitrogen atom	2.19495	3.35	-3.0230	0.12
	center of the ring Al-doped (B-N)	2.19495	3.35	-3.0230	-0.001
	bridge(B-N)	1.78817	3.35	-3.6053	0.26
SO_2/pristine BN	nitrogen atom	1.79425	3.35	-3.6706	-0.56
	center of the ring(B-N)	1.70728	3.35	-3.7121	0. 56
	bridge(B-N)	1.92118	3.35	-3.7821	0.211
SO_2/ Al-pristine BN	nitrogen atom	2.85293	3.35	-3.3849	-0.001
	center of the ring Al-doped (B-N)	2.89885	3.35	-3.8855	-0.231
	bridge(B-N)	3.77550	3.1 N-N	-0.1231	-0.003
NO/pristine BN	nitrogen atom	1.42344	3.1 N-N	-3.6367	-0.011
	center of the ring(B-N)	1.42368	3.47 B-N	-3.5890	-0.011
	bridge(B-N)	1.80967	3.1	-2.5631	0.875
NO/ Al-pristine BN	nitrogen atom	1.80988	3.1	-2.5631	0.697
	center of the ring Al-doped (B-N)	1.80986	3.1	-2.5631	0.001
	bridge(B-N)	1.408	3.44 B-O	-3.7698	0.2
NO_2/pristine BN	nitrogen atom	3.189	3.44 B-O	-0.2623	-0.001
	center of the ring(B-N)	1.425	3.44 B-O	-3.6760	-0.2
	bridge(B-N)	3.37660	3.1	-0.1493	0.001
NO_2/ Al-pristine	nitrogen atom	2.50391	3.1	-3.1373	-0.416
NO_2/ Al-pristine	center of the ring Al-doped (B-N)	2.06050	3.1	-3.1131	0.1

Adsorption of SO gas on pristine and Al-doped BN monolayer.

The adsorption of SO molecules on pristine and Al-doped Boron Nitride(BN) monolayers was examined. Figure (2) shows the most stable adsorption

configuration for the SO/BN complex. The SO molecule is positioned perpendicular to the Boron Nitride(BN) plane at different positions, namely the N atom, the middle ring, and the B-N bridge. Adsorption energies are -0.754, -1.749, and -1.945 eV, respectively for pristine and (-3.7223,-3.6345,-3.652)for Al-doped Boron Nitride(BN) monolayer. The distance between SO gas and Boron Nitride is 1.885, which is less than the sum of covalent atomic radii of S-N (3.35), the atom-atom distance (S-N bond length) between SO gas and Al-doped Boron Nitride monolayer is (2.19495), and the atom-atom distance between SO and the middle ring Boron Nitride (BN) monolayers is 1.83, which is less than the sum of covalent atomic (3.35 Å)for pristine. SO gas and Al/doped Boron Nitride (BN) have an atom-atom distance of (S-N bond length) of (2.19495Å), which is less than the sum of covalent atomic radii of S-N (3.35 Å). and distance of atom-atom from SO to the bridge B-N is 1.534, which is less than the length of the S-N dimer bond (3.35)for pristine and the atom-atom distance (S-N bond length) between SO to the bridge Al-doped BN is(3.04591Å), which is less than the sum of covalent atomic radii of S-N (3.35 Å) . These findings indicate that the SO gas on pristine Boron Nitride(BN) is chemically Adsorption , Adsorption energies is strong . Furthermore, the relationship of SO gas and BN results in a charge shift of (-0. 26-1.275) eV from the BN layer to SO gas and layer to SO gas molecule . A charge shift SO and Al/doped BN monolayer is(0.23 to -0.01) e from the Al/doped BN layer to SO gas and layer to SO gas . These findings indicate that the SO gas is strong chemically Adsorption for Al-doped BN monolayer.

SO_2 Adsorption on pristine and Al/doped BN monolayer.

The adsorption of SO_2 on pristine BN and Al/doped BN monolayers is more complicated than the other chemicals investigated. The pure BN and Al/doped BN monolayers, as well as the SO_2 gas, display substantial structural changes after adsorption on the pristine and Al/doped BN monolayers.

The most stable adsorption structure of the SO_2/BN complex is depicted in Figure (2).Three sites on the SO_2 molecule are vertical to the BN plane: the N atom, the center ring BN, and the B-N bridge. The associated adsorption energies for pristine are -3.6053, -3.6706, and -3.7121 eV and adsorption energies for Al/doped BN monolayers are (-3.3849, -3.8855 and -3.7821). The average atom-atom distance (S-N bond length) between SO_2 and pristine BN is 1.78817 Å , which is less than the S-N dimer bond length (3.35 Å), and the minimum atom-atom distance between SO_2 and the bridge B-N is 1.79425 Å, which is less than the S-N dimer bond length (3.35 Å) ,the atom-atom distance between SO_2 and the center ring BN is 1.707 Å, which is less than the length of the S-N dimer bond (3.35 Å). The average atom-atom distance (S-N bond length) between SO_2 and Al/doped BN monolayers are 1.79425 Å, which is less than the S-N dimer bond length (3.35 Å), and the minimum atom-atom distance between SO_2 and the bridge B-N in Al/doped BN is 1.78817 Å, which is less than the S-N dimer bond length (3. 35 Å) ,the atom-atom distance between SO_2 and the middle ring B-N in Al/doped BN is 1.70728 Å is less than the S-N dimer bond length (3.35 Å). These findings indicate that SO_2 is chemically adsorbing on the pristine BN and Al/doped BN monolayers. Furthermore, the SO_2/BN reaction transfers charges of 0.26, -0.56, and 0.56 e from the BN layer to the SO_2 or from the SO_2 to the BN layer. The SO_2-Al/doped BN reaction transfers charges of 0.1, -0.1, and 0.2e from the Al/doped BN layer to SO_2 or from SO_2 to t BN layer.

NO gas adsorption on BN monolayers pristine and doped with Al

When NO is exposed to the BN layer, it takes an oblique path with regard to the BN level, as shown in Figure (2). The N atom in the NO gas indicates the N atom in the BN. It must be remembered that the distance of N-N (1.42 Å) in NO/BN complex is smaller than length of the (3.1Å) N-N bond, and the monolayer is completely different from that of graphene. For NO, the E_{ads} values on pristine BN were Specific to be -3.6367 and -3.5890 eV for atom-atom and center and are greater than those on graphene with 1.1-2.9 eV[16].Demonstration of the covalent bonding amid pristine BN and NO Adsorption leads to a strong artificial pull between the molecule and its adsorbents. Table 1 summarizes the adsorption energies of the different structures. The adsorption energy obtained for NO gas on pristine BN is much higher than that recorded for native graphene (0.30eV) and N-doped graphene (0.40eV) [16]. It's also comparable with the NO gas absorption energy recorded on B-doped graphene (1.07 eV)[17] for atom-atom and center position but the adsorption energies of bridge is weak -0.1231eV. When NO gas is absorbed onto the pristine BN sheet, a clear charge of -0.003,-0.011and -0.011e of the pristine BN sheet is transferred to NO gas. It's also comparable with the NO gas absorption energy recorded on Al/doped BN . When NO gas is absorbed on to the Al/doped BN sheet, a clear charge of 0.001, 0.697 and 0. 875 e of NO is transferred to the Al/doped BN sheet and inverse with strong adsorption energy(-2.5631,-2.5631 and -2.5631) eV .These findings indicate that NO is chemically adsorbing on the Al/doped BN

monolayers .Gas adsorption on the Al/doped BN monolayers is better than other gases.

NO_2 Adsorption on pristine and Al/doped BN monolayer.

The process of NO_2 gas adsorption on virgin and Al/doped BN monolayers is more complicated than that of the other molecules discussed above. Absorption on the pristine BN and Al/doped BN monolayers induces significant structural changes in both the pure and Al/doped BN monolayers, as well as the NO_2 molecule. This indicates that the molecule is entirely segregated during absorption in the NO_2 and O species.

In both the pure and Al/doped BN monolayers, as in Figure (2) the chemical absorption NO2 isolated is quite close to the NO2 molecule. The NO2 absorption energies on the pristine and Al /doped BN monolayers and the adsorption energy measured for NO2-in both the pristine and Al /doped BN monolayers is lower than that calculated for NO2/ graphene. Most interestingly, the Eads scale of NO2 on both the pristine and Al/doped BN monolayers is greater than that recorded for NO2 absorption on graphene (0.48 eV), N-doped graphene (0.98 V)and B-doped graphene (1.37 eV)[17].Furthermore, a large charge of 0.1 and -0.416 e of NO2 molecule is transferred to the pristine but charge of 0.001e is transferred for atom-atom with adsorption energy -3.1373eV . This wide charge transfer corresponds to the high NO2 adsorption energies over the pristine and Al/doped BN monolayers.

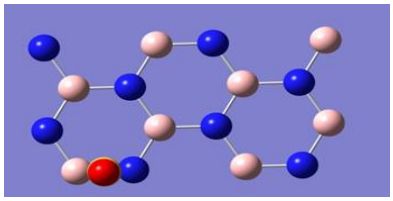
The electronic structure of the BN **monolayer**

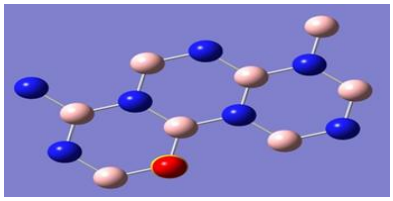
The HOMO and LUMO orbits lie close to the Fermi plane, which allowed us to learn about the acquaintance of electron states at the Fermi surface as well as the acquaintance of transported electrons. The distribution of the HOMO and LUMO orbitals can be seen in Figure 3. We discovered that the electron cloud distribution meaning in these two orbits is concentrated toward the edge of pure graphene, where the electrons are concentrated.

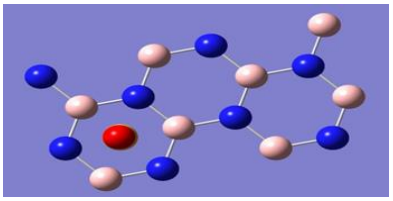
Figure 3 shows the HOMO and LUMO energies of the virgin and Al-doped BN monolayers following gas absorption. SO_2, SO, NO, and NO_2 had no influence on the E_f of the pristine BN and Al/doped BN monolayers systems because to the short absorption distance, high charge transfer, and low absorption energy.

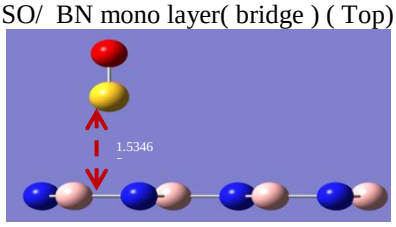
4. Conclusion

In summary, the DFT theoretical results reveal that during the exposure to natural gas and pollutant particles, the original and Al- doped Boron Nitride(BN monolayers exhibit a variety of behaviors. The original and pristine Al-doped Boron Nitride(BN monolayer has a higher affinity for SO_2, SO, NO, and NO_2 molecules. The chemical adsorption characteristic of the adsorption of SO2, SO, NO and NO_2 can be clearly seen with its wide E_{ads} but in NO , at bridge positions ,NO_2 at atom-atom positions both of them in pristine on together with NO at bridge positions in Al-doped Boron Nitride(BN) monolayer it is physical-_adsorption because of the adsorption energies value is low then (-0.5), charge transfer and short adsorption distance. This indicates that the original, Al-doped BN monolayer is ideal for use as SO, SO_2, NO and NO_2 gas sensors and that the best sensor is the (NO andSO_2 /Al-doped Boron Nitride(BN) and pristine Boron Nitride(BN) layer for other monolayers.

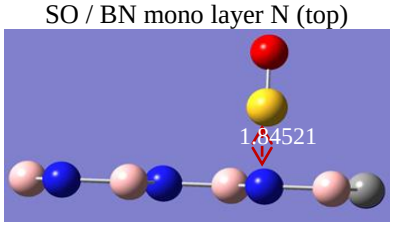

SO/ BN mono layer(bridge) (Top)


SO / BN mono layer N (top)

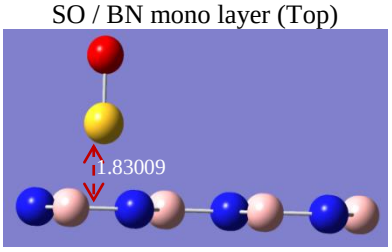

SO / BN mono layer (Top)



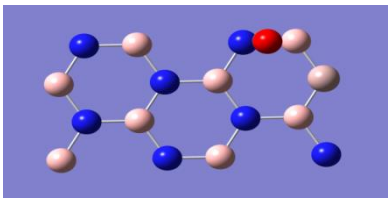
SO/ BN mono layer (bridge) (side)

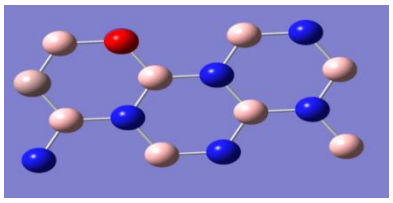


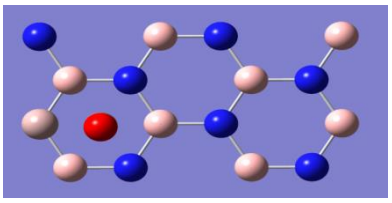
SO/ BN mono layer N(side)

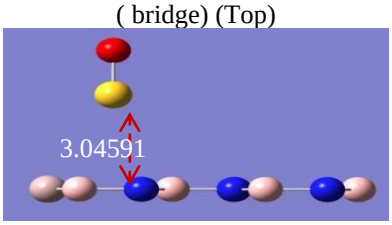


SO/ BN mono layer center (side)

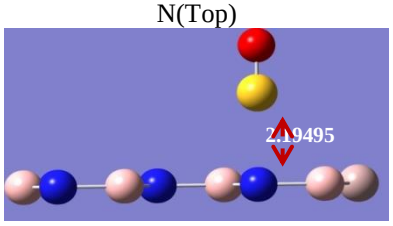

SO / Al-doped BN monolayer (bridge) (Top)


SO/ Al-doped BN monolayer N(Top)

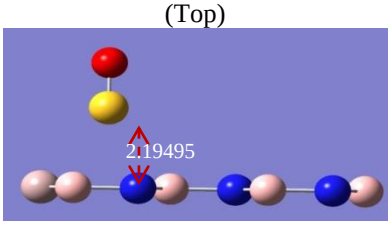

SO/ Al-doped BN monolayer center (Top)



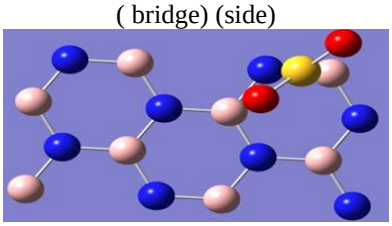
SO / Al-doped BN monolayer (bridge) (side)

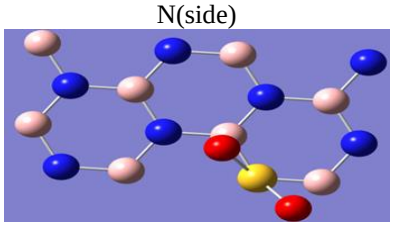


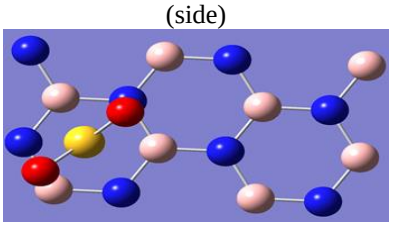
SO/ Al-doped BN monolayer N(side)

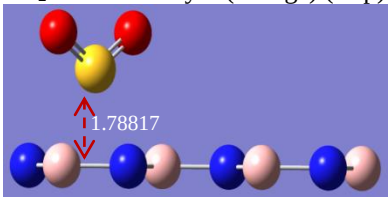


SO/ Al-doped BN monolayer center (side)

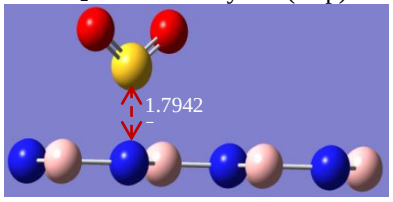

SO_2/ BN monolayer (bridge) (Top)


SO_2/ BN monolayer N(Top)

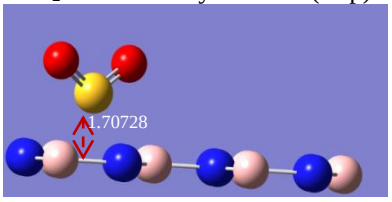

SO_2/ BN monolayer center (Top)



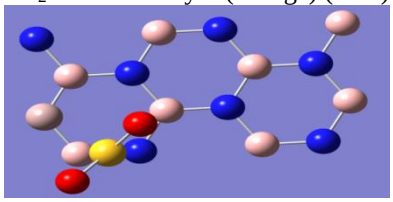
SO_2/ BN monolayer (bridge) (Side)

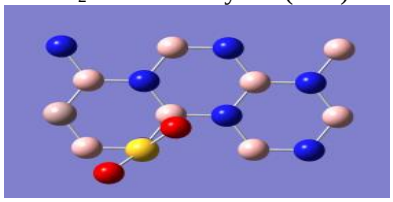


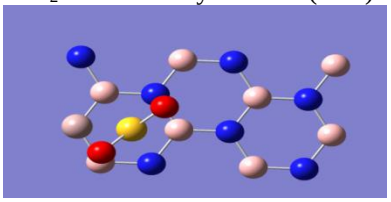
SO_2/ BN monolayer N(Side)

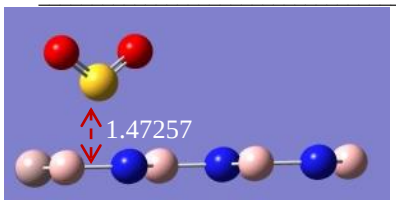


SO_2/ BN monolayer center (Side)

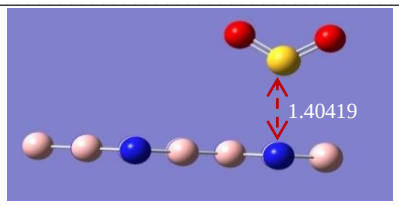

SO_2/ Al-doped BN monolayer (bridge) (Top)


SO_2/ Al-doped BN monolayer N(Top)

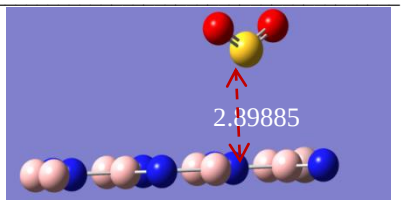

SO_2/ Al-doped BN monolayer center (Top)



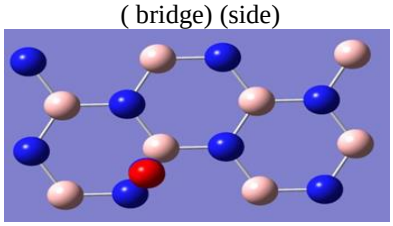
SO_2/ Al-doped BN monolayer (bridge) (side)



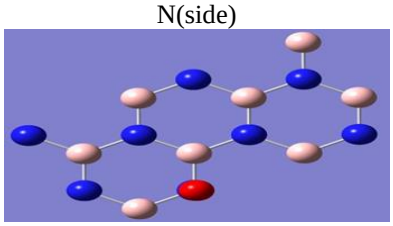
SO_2/ Al-doped BN mono layer N(side)



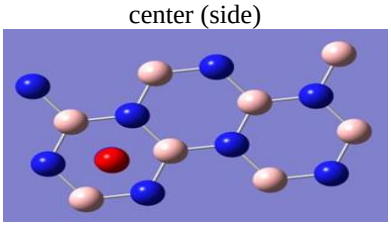
SO_2/ Al-doped BN monolayer center (side)



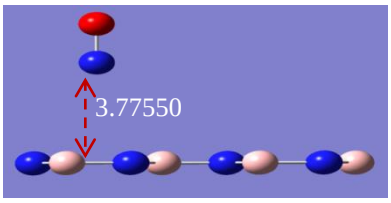
NO/ BN monolayer (bridge) (Top)



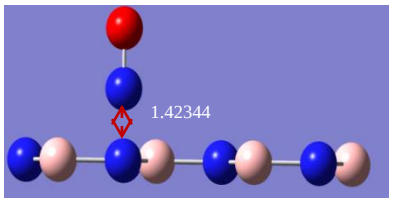
NO/ BN monolayer N(Top)



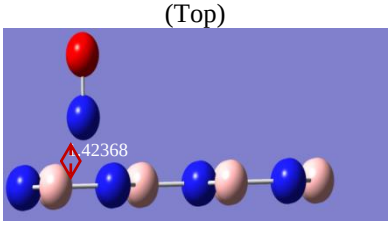
NO/ BN monolayer center (Top)



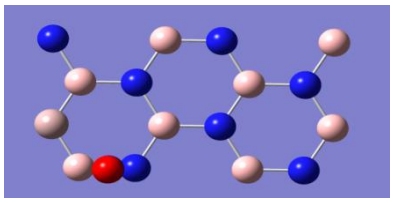
NO/ BN monolayer (bridge) (side)



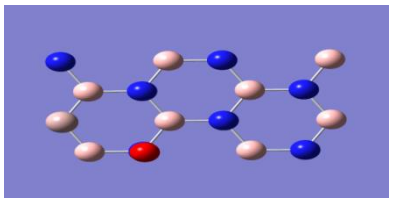
NO/ BN monolayer N(side)



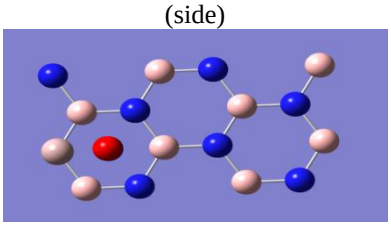
NO/ BN monolayer center (side)



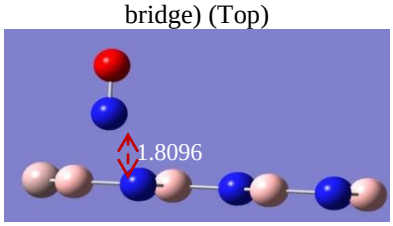
NO/ Al-doped BN monolayer(bridge) (Top)



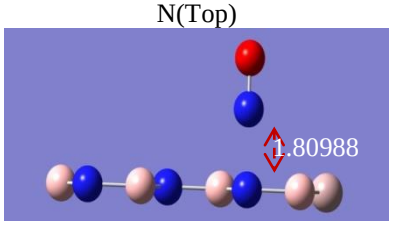
NO/ Al-doped BN monolayer N(Top)



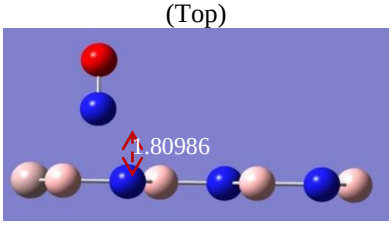
NO/ Al-doped BN monolayer center (Top)



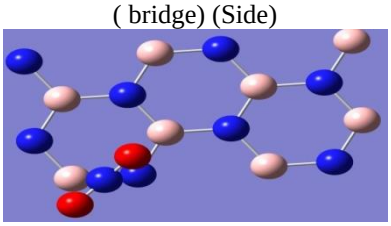
NO/ Al-doped BN monolayer (bridge) (Side)



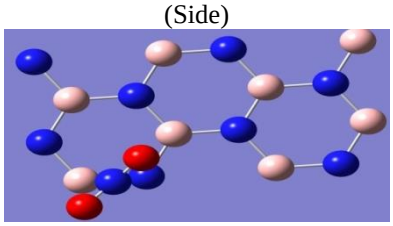
NO/ Al-doped BN monolayer N (Side)



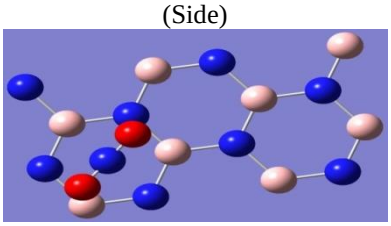
NO/ Al-doped BN monolayer center (Side)



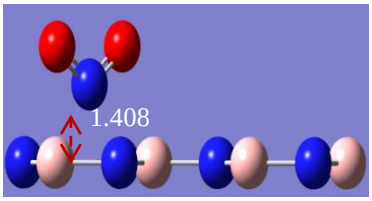
NO_2/ BN monolayer (bridge) (Top)

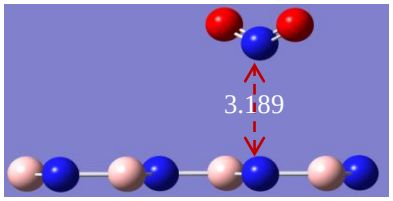


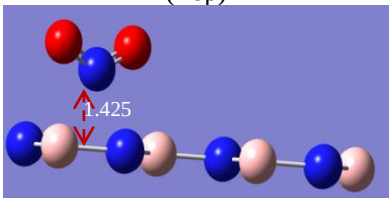
NO_2/ BN monolayer N(Top)



NO_2/ BN monolayer center (Top)







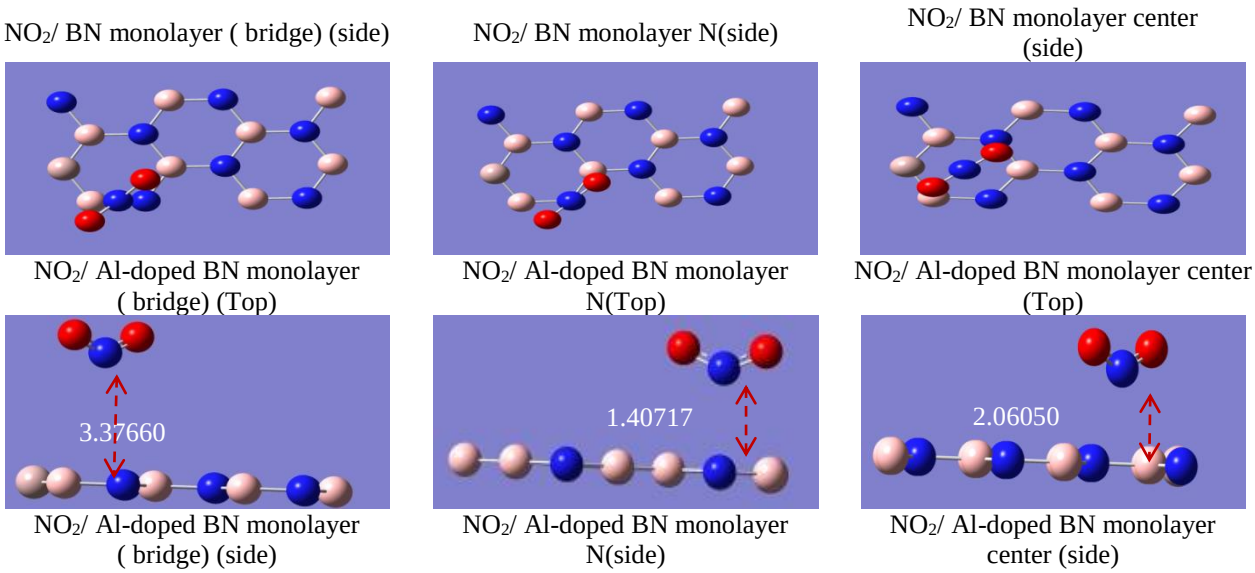
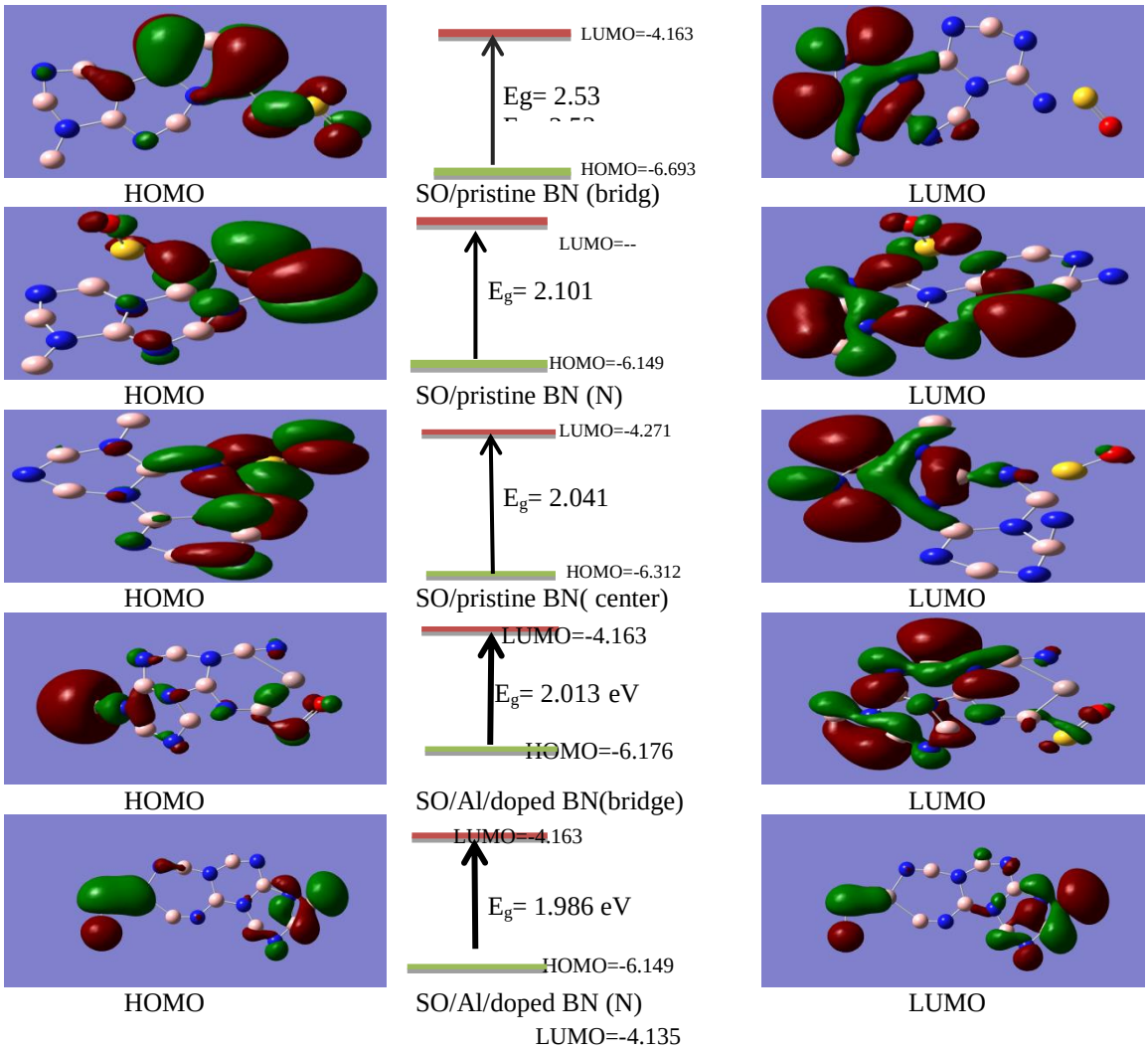
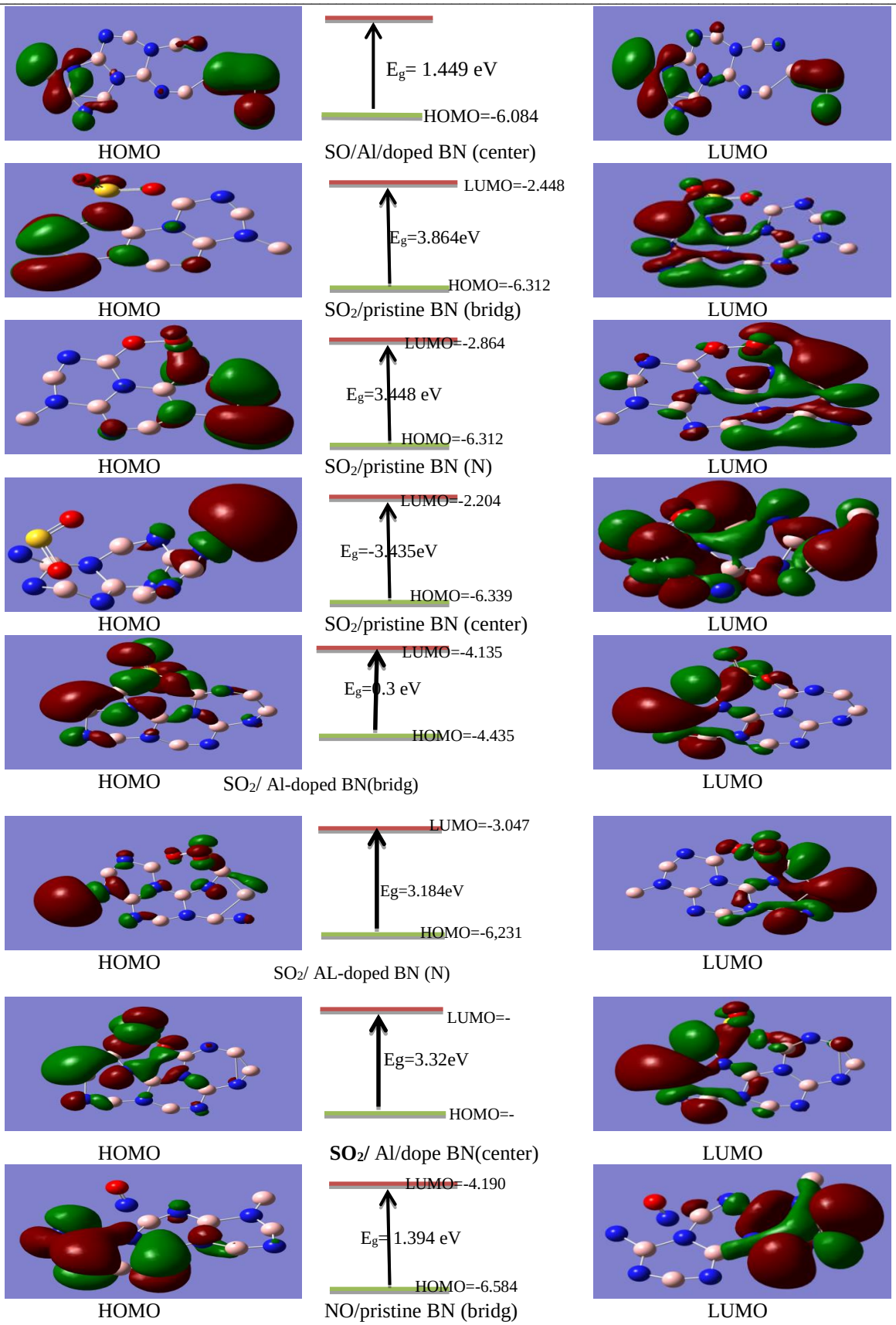
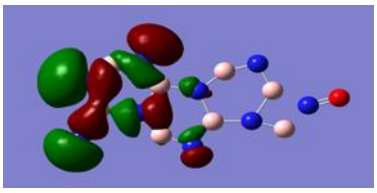
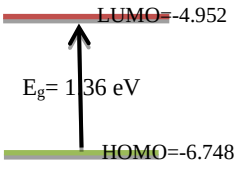


Fig.2: A top view and side view of most stable configurations of (a) bridge(B-N), (b) N atoms, (c) center of the ring(B-N), pristine and Al-doped BN monolayers adsorbed gases on the top site of monolayers.

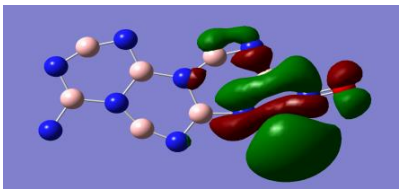


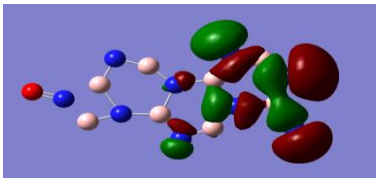

HOMO
Eg= 1.449 eV
HOMO=-6.084
LUMO
SO/Al/doped BN (center)
HOMO
LUMO=-2.448
Eg=3.864eV
HOMO=-6.312
LUMO
SO2/pristine BN (bridg)
HOMO
LUMO=-2.864
Eg=3.448 eV
HOMO=-6.312
LUMO
SO2/pristine BN (N)
HOMO
LUMO=-2.204
Eg=-3.435eV
HOMO=-6.339
LUMO
SO2/pristine BN (center)
HOMO
LUMO=-4.135
Eg=0.3 eV
HOMO=-4.435
LUMO
SO2/ Al-doped BN(bridg)
HOMO
LUMO=-3.047
Eg=3.184eV
HOMO=-6,231
LUMO
SO2/ AL-doped BN (N)
HOMO
LUMO=-
Eg=3.32eV
HOMO=-
LUMO
SO2/ Al/dope BN(center)
HOMO
LUMO=-4.190
Eg=1.394 eV
HOMO=-6.584
LUMO
NO/pristine BN (bridg)


HOMO



NO/pristine BN (N)


LUMO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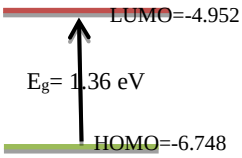
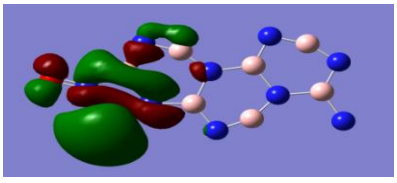


NO/pristine BN (center)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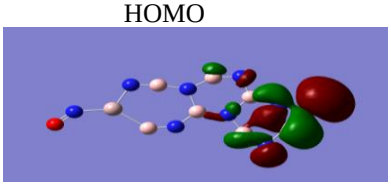
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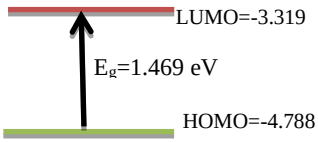
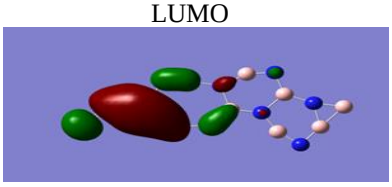


NO/ Al/doped BN(bridg)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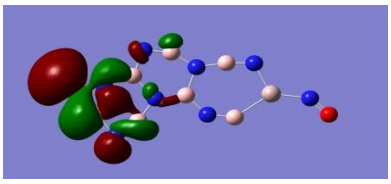
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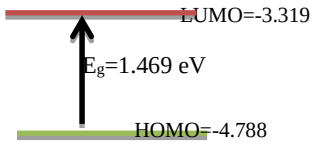
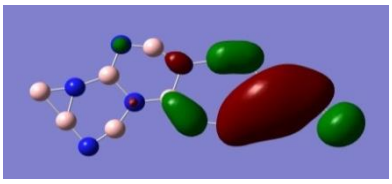
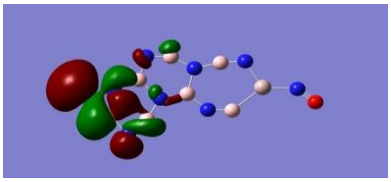


NO/ AL-doped BN(N)


LUMO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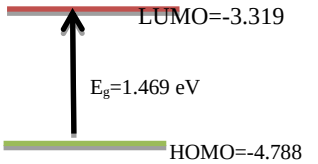
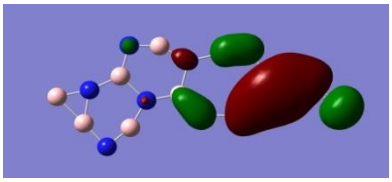
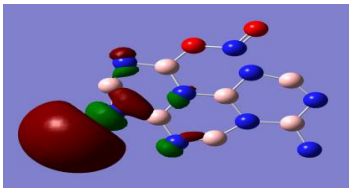


NO/ Al/dope BN(center)


LUMO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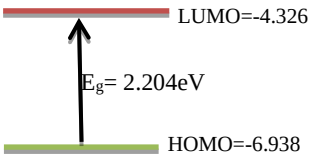
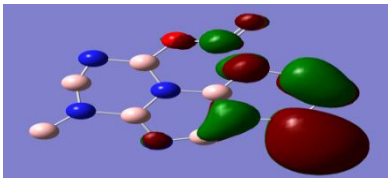


NO_2/pristine BN (bridg)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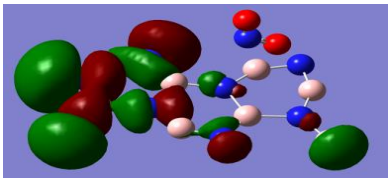
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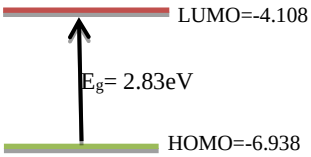
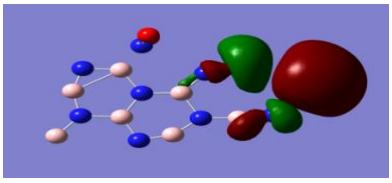
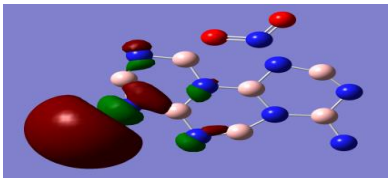
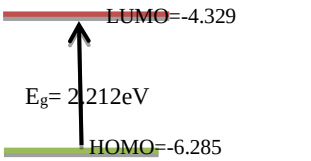


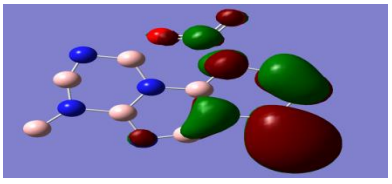
NO_2/pristine BN (N)


LUMO


HOMO



NO_2/pristine BN (center)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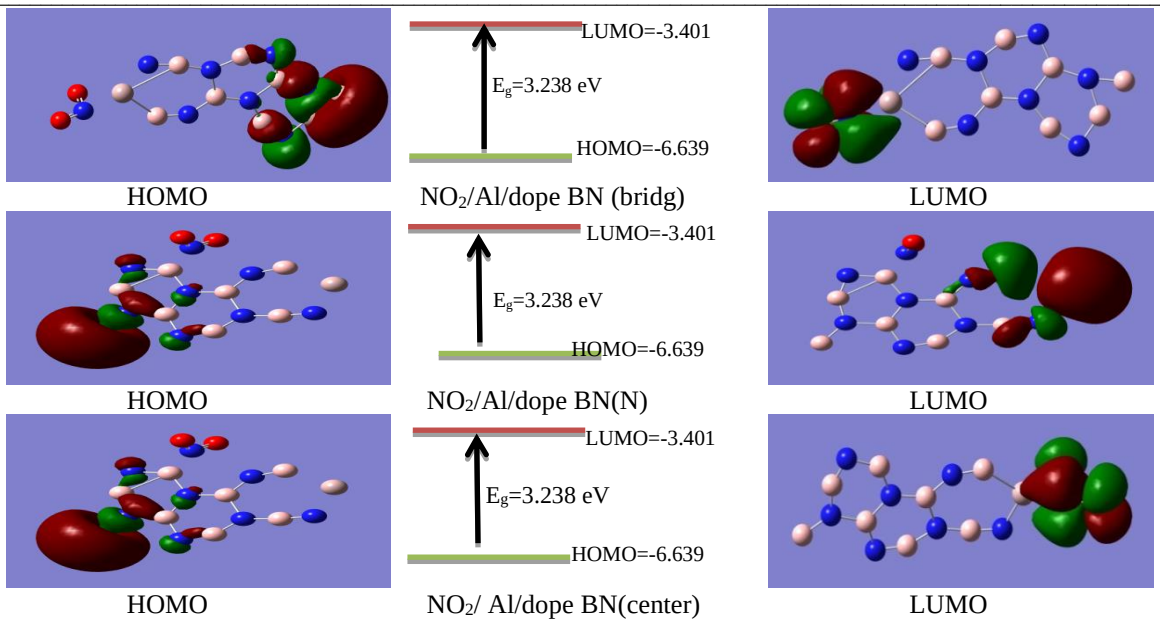

Fig.3: Shows the DFT calculation of HOMO and LUMO shapes for studied the pristine and Al-doped BN monolayers adsorption molecules

Conflicts of interest

There are no conflicts to declare.

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The funding sources by authors.

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