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Adsorption behavior of mephentermine on the pristine and Si, Al, Ga- doped boron nitride nanosheets: DFT studies

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ABSTRACT

In this research, the adsorption behavior of pristine, Si- and Al- and Ga-doped boron nitride nano sheet are investigated toward mephentermine using density functional theory (DFT) calculations. Total energies, geometry optimizations were obtained and density of state (DOS) analysis was performed at B3LYP level of theory with the 6-31g (d) basis set. The adsorption energy (E_{ad}) between mephentermine and the pristine, Si- and Al- and Ga doped BNN is changed in the following order: Ga-Complex-N> Al-Complex-N>Si-Complex-N> complex -N. The E_{ad} of the BNN-mephentermine complex is -2.09 kcal/mol, which shows that the adsorption is weak physicaly. The E_{ad} of the Al-doped BNN-mephentermine complex is -34.06 kcal/mol, ΔE_g = -1.37%, indicating a low sensitivity of the Al-doped boron nitride nanosheet to the adsorption of mephentermine and is not suitable for sensing. As mentioned, due to the adsorption energy of −34.06 kcal/mol and the rather long recovery time, a strong interaction is not suitable for a sensor. The E_{ad} of the Ga-doped BNN-mephentermine complex is -46.46 kcal/mol, ΔE_g = -6.39%. the adsorption energy of -46.46 kcal/mol is not suitable for a sensor and indicates a long recovery time, As a result, it helps to decompose this compound and remove this compound.

1. Introduction

Mephentermine is a drug cardiovascular that It strengthens the heart and stimulates respiration. mephentermine helps release a chemical messenger that compresses blood vessels and also increases the heart's contractile power in pumping. The presence of medicinal compounds in the environment is considered a serious threat to humans and the entry of these substances into water and soil resources causes the pollution. Therefore A sensor is needed to detect the accumulation of drug waste. With the advent of nanotechnology, it was found that their surface /volume ratio is much higher than conventional micro-detectors [1, 2]. Nanostructures have received a great deal of attention as chemical sensors [3-10]. BN nanosheet is a two-dimensional structure of hexagonal boron nitride (h-BN) with a thickness of one to several atomic layers. It is geometrically similar to graphene, but has very different chemical and electronic properties [11]. BN nanosheets consist of sp^2-conjugated boron and nitrogen atoms that form a hexagonal structure [12, 13]. The BN nanostructures have a wide range of attractive properties such as stability high temperature strength, low dielectric constant, high thermal conductivity and oxidation resistance, which leads to a number of potential applications as electronic materials [14]. The BN nanosheet indicate a size controllable energy band Gap wich enable them a promising Materials for different thchnological application.

-In a study conducted in 2017 by Khaleghian and Azarbakhshi [15], the nonbonding interaction of single walled boron nitride nanotube with theophylline was studied theoretically, the effects of electron instability and bipolar interaction and spatial repulsion on structural and electronic properties and the amount Reactivity was investigated using quantum mechanics of density functional theory at the B3lyp theoretical level. Orbital analysis of natural bonding was performed and

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the results showed that the energy gap in the complex compared to theophylline only decreased and the amount of hardness parameter decreased while The softness parameter and semiconductor properties increased.

-In 2017, another study by Vessally et al [16], examined the interaction of an aspirin molecule with the outer surface of fullerene boron nitride, such as a nano-cage, using density functional theory calculations. Equilibrium geometry, electron properties, adsorption energy and thermodynamic stability are known for all forms of adsorption. At the M06-2X / 6-31 + G** level, the results showed that the doped aluminum on the nanostructure tends to increase the adsorption energy and the thermodynamic stability of the aspirin molecule on this nanocage.

-In a research in 2018 by siadati, rezazadeh [17], examined the Switching behavior of an actuator containing germanium, silicon-decorated and normal C20 fullerene, the results showed that in the case of the silicon-decorated C_{20} fullerene, changingthe system from state A to state B*via* changing the temperature(24.7 kcal mol^{-1}) is much easier than that of germanium-decorated (27.5 kcal mol^{-1}) or normal C_{20} fullerene (37.8 kcal mol^{-1}). It seems that further studies on this phenomenon, might be beneficial for designing the thermal sensor systems, and energy storage devices.

-In a research in 2017 byVessally et al [18], examined the selective sensing of ozone and the chemically active gaseous species of the troposphere by using the C_{20} fullerene and graphene segment , the results showed that the ozone could significantly change the electrical conductivity of C_{20} fullerene, for each adsorption step. Thus, this fullerene could clearly sense ozone in different adsorption steps; while, the graphene segment could do this only at the second step adsorption ($/\Delta E_{g\text{-}B}/$=0.016eV) (at the first adsorption step the $/\Delta E_{g\text{-}A}/$ is 0.00eV).

-Another study in 2016 by siadati et al [19], examined the a theoretical study on the possibility of functionalization of C20 fullerene via its Diels-Alder reaction with 1,3-Butadiene, the results showed that at least in this case, pericyclic reaction could carry out the functionalization of this small carbon cage with no need to a solvent engagement or any other accelerating agents such as catalysts, light or heat.

-In a study conducted in 2016 by Siadati [20], examined a Theoretical Study on the Possibility of Functionalization of C20 Fullerene Via its Diels-Alder Reaction with 1,3-Butadiene, the results showed
The present way seems to be faster than other methods which have been already reported on the functionalization of C20 fullerene. The results showed that at least in this case,
pericyclic reaction could carry out the functionalization of this small carbon cage with no need to a solvent engagement or any other accelerating agents such as catalysts, light or heat.

-In a study conducted in 2015 by Siadati and Ali Mirabi [21], examined the Diels–Alder versus 1,3-dipolar cycloaddition pathways in the reaction of C20 fullerene and 2-furan nitrile oxide, the results showed that 1,3-dipolar cycloaddition is faster than the Diels–Alder reaction for the functionalisation of C20 fullerene by 2-furan nitrile oxide.

-In a study conducted in 2017 by pakravan and siadati [22], the possibility of using C 20 fullerene and graphene as semiconductor segments for detection, and destruction of cyanogen-chloride chemical agent, the results showed that the electronic density of states DOS showed that C20 fullerene senses the existence of cyanogen chloride agent with a clearer signal (ΔEg=0.0110eV) compared to the graphene segment (ΔEg=0.0001eV).

Also the adsorption energy calculations showed that cyanogen chloride could be adsorbed by the fullerene in a multi-step process (Eads1=-0.852kcalmol-1; Eads2=-0.446kcalmol-1; Eads3=-2.330kcalmol-1).

In recent years, the use of computational chemistry and molecular modeling with the help of computers has attracted the attention of chemists. In this study, we showed that replacing a boron atom in BNN with Si and Al and Ga is a useful way to improve the electronic properties. Also, we examined the interaction between mephentermine from (NH) head and the pristine BNN and the BNN doped with Al, Ga (from Group IIIA) and Si (from group IVA) using DFT calculations.

2. Computational details

2.1. Methods

All calculations in this research, were performed using the DFT method at the theoretical level of B3LYP/6-31G∗ and also using the GaussView 05 and GAMESS program [23]. To ensure the lowest energy for the complexes rather than a local minimum, the potential energy surface (PES) scans were performed with respect to various dihedral angles (D). The Gausssum was used for drawing the DOS plots [24]. The adsorption energy (E_{ad}) is calculated as follows:

E_{ad}= E(drug/adsorbent) − E(adsorbent) − E(drug) (1)

where E(adsorbent) is the total energy on an intrinsic or extrinsic molecule. E(drug/adsorbent) is the total energy of the adsorbed drug molecule on the adsorbent surface.

E(BSSE) is the basis set superposition error (BSSE) corrected for all adsorption energies using the counterpoise method [25]. In this research, some reaction indicators that are useful for Analysis were evaluated.

2.2. Theory

Sensors are tools that show the expected and desired interactions under certain conditions. The LUMO – HOMO energy gap (E_g) of the structures under study is computed as follows [26-39]:

$E_g = ELUMO - EHOMO$ (2)

When we evaluate the electronic sensitivity of a nanostructure to a drug, the HOMO and LUMO energy differences are calculated as follows:

$\%\_\Delta E_g = [(E_{g2} - E_{g1})/Eg_1] * 100$ (3)

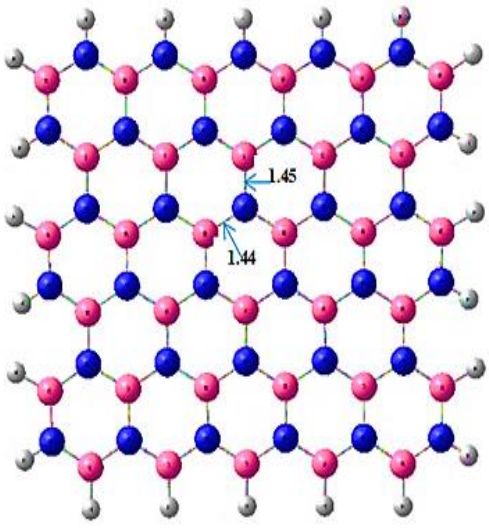
3. Results and Discussion

3.1. The Mephentermine drug adsorption on the BNnanosheet

The optimized structure of the BN sheet is depicted in Figure 1, in which different types of B-N bonds can be identified, with corresponding equilibrium distances of 1.44 and 1.45 A^0. It consists of 33 B, and 33 N atoms, and the end atoms were saturated with 22 hydrogen atoms to avoid the boundary effects. As shown by the DOS plot in (Figure 1). the HOMO energy of the BN nano sheet is approximately −6.31 eV and that of the LUMO −0.37 eV (Table 1). Thus, the E_g is approximately 5.94 eV (Table 1).

The DFT calculations showed that the der to adsorbed on the BN nanosheet, various possible initial adsorption geometries including different atoms of the drug which are close to B atom of BN sheet are considered. Finally, only one (global minimum) was predicted after the relaxation process as shown in (Fig 3).

In the complex, mephentermine was adsorbed from the N atom onto the boron atom of BN sheet at a distance of 4.03 Å and the adsorption energy is -2.09 kcal/mol, which indicates weak interaction (Fig 3). The density of state (DOS), LUMO and HOMO in the stable complex are presented in (Figure 4).



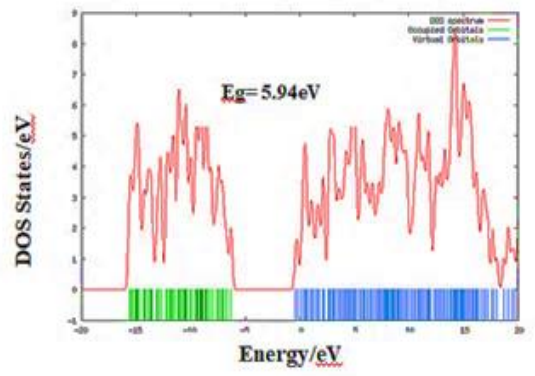


Figure 1. Optimized structure of BN nanosheet and density of state (DOS) plot.

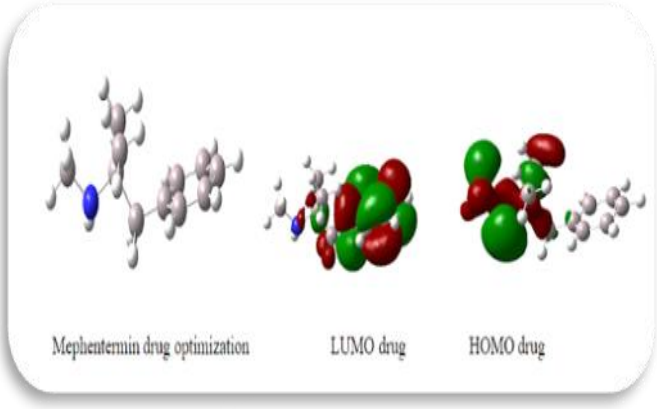


Figure 2. Optimized structure of mephentermine and its HOMO, LUMO profiles.

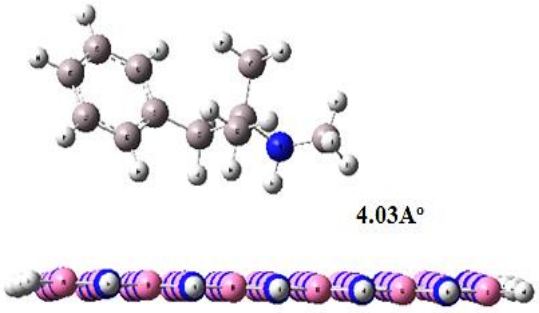


Figure 3. Optimized structures of BNN-Mephentermine complexes. Distances are in Å.

According to Table 1 and Figure 4, the HOMO has been changed from −6.31 in the BN sheet to -5.57 eV in the complex and the LUMO has been changed from −0.371 in the BN sheet to -0.370 in the complex. These changes are to the extent that the LUMO is located on the nano sheet and HOMO is located on the drug atoms. The drug molecule donates a pair of electrons from its nitrogen atoms to theBoron atomwhich has been electron deficiency on the BN nanosheet surface.

As mentioned, there are two important parameters, i.e. E_{ad} and E_g, in the drug sensing potential by nanostructures. The adsorption of mephentermine onto to BN nanosheet may be reversible if the E_{ad} is in a reasonable range. Strong interactions are not favorable

in drug sensing because of a long recovery time and thus hard desorption of a drug over a nanoparticle. With more negative E_{ad}, the recovery time (τ) is increased and this may be determined using the following equation[40, 41].

$$\tau = \nu 0^{-1} \exp(-Ead/kT) \quad (4)$$

Here τ is the recovery time and $\nu 0$ is the attempt frequency, T is the temperature, and K is the Boltzman constant [42]. According to this equation, there is an exponential relationship between E_{ad} and the recovery time. Sensor recovery is a major issue that can be addressed by heating the sensor at higher temperatures than room temperature [43]. Vacuum-UV is applied for the recovery of drugs from the surface of nano structure system.

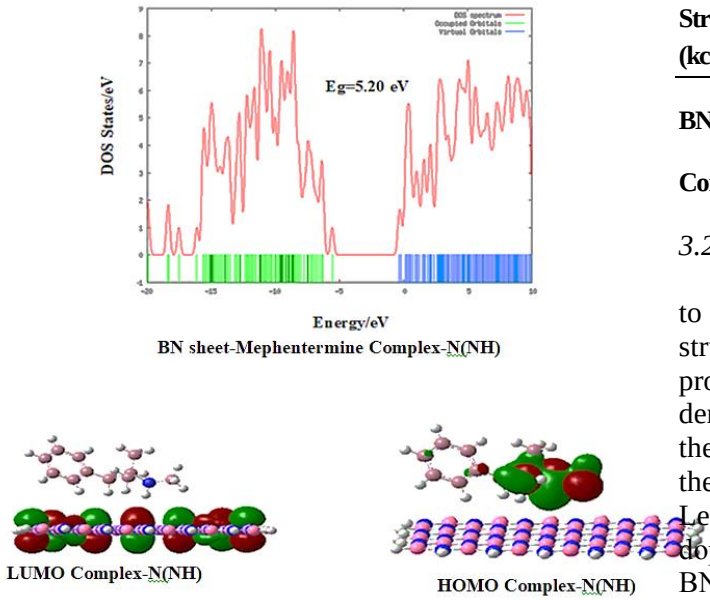


Figure 4. Density of states (DOS) plot of BNN-Mephentermine complex- N(NH), and the HOMO, and LUMO profiles of complex-N(NH).

The second most important factor in sensing character is the LUMO– HOMO energy gap (E_g) of the BN nanosheet in the presence of mephentermine. It has been indicated that the E_g is proportional to the conduction electron population (σ) presented in Equation (5). σ increases when the HOMO–LUMO energy gap (E_g) decreases with the absorption of mephentermine onto the BN nanosheet. On the other hand, when the $-\%\Delta E_g$ increases, the sensing potential also increases. The correlation between E_g and the electrical conductance of nanostructures is as follows:

$$\sigma = A\, T3/2 \exp(-Eg/2kT) \quad (5)$$

Where k is the Boltzmann constant, and A (electrons/m3K3/2) is a constant. There is a acceptable correlation between the obtained results of this procedure and experimental techniques reported in the literature [44]. Equation (5) is used to investigate the sensitivity of a nanostructure toward a drug. As a result, electrical conductivity can be converted into an electrical signal related to the presence of drug molecules [45, 46]. The E_g of the BN nanosheet decreased when it absorbed the drug, changing the E_g significantly from 5.94 eV to 5.20 eV in the complex with $\%\Delta E_g$ of -12.46 % which shows the sensitivity Almost weak of the BN nanosheet to the adsorption of Mephentermine. the adsorption energy is −2.09 kcal/mol that is so weak that the BN nanosheet cannot effectively adsorb the drug and absorption is a type of poor physical adsorption.

Table 1. Energy of HOMO, LUMO, (E_g) in eV, and the change of Eg up on the mephentermine drug adsorption on the BN nanosheet structures. The adsorption energy (E_{ad}) is in kcal/mol. $\%\Delta E_g$ indicates the percentage of the change in E_g after the drug adsorption.

Structure	E_{ad} (kcal/mol)	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g	$\%\Delta E_g$
BN Sheet	----	-6.31	-0.371	5.94	----
Complex –N(NH)	-2.09	-5.57	-0.370	5.20	-12.46%

3.2. Si- doped BN nanosheet

B atom of the BNsheet was replaced with the Si atom to find a highly sensitive nanostructure and the new structure was optimized. The structure and geometric properties of BN nanosheet was investigated and the density diagram (DOS) was shown in Figure 5. Due to the larger radius of the Si atom compared to the B atom, the Si atom is placed out of the nanosheet surface. Bond Length of the Si–N of nanostructure is 1.72 A^0. After doping with Si, the HOMO decreases from −6.31 in BNN to −4.86 eV in Si-doped BNN while the LUMO slightly increases from −0.37 in the BNN to −0.38 eV in the Si-doped BNN. The E_g changes significantly from 5.94 eV in the pristine BNN to 4.47 eV in Si-doped BNN. The DFT calculations clarify that the electrical conductivity in Si-doped BN nanosheet (Table 2).

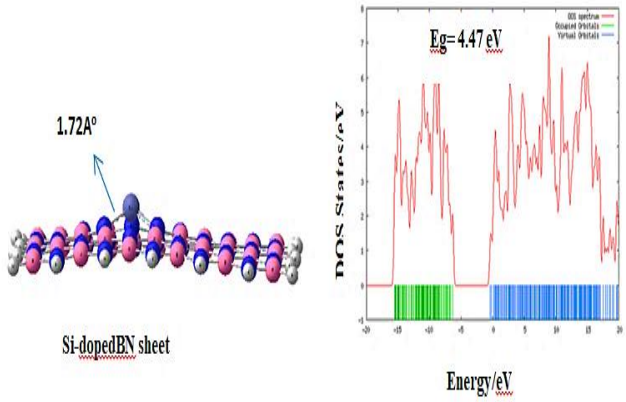


Figure 5. Optimized structure of Si- doped BN nanosheet. Distances are in Å and density of state (DOS) Plot.

3.3. The Mephentermine drug adsorption on the Si-doped BN nanosheet

In this case, the interactions between Mephentermine and Si-doped BNnanosheet are investigated. One type of complex was found that indicate the interaction between NH in Mephentermine and the Si atom of Si-doped BN nanosheet (Figure 6 and Table 2). In the strongest interaction, the Si atom of Si-doped BN nanosheet interacts from the NH head of mephentermine with E_{ad} of –2.67 kcal/mol with the Si …N distance of 3.69 A^0. HOMO was slightly from -4.86 in boron nitride doped with Si to -4.76eV in the complex of boron nitride doped with Si and the drug and in LUMO it was slightly shifted from -0.38 to -0.35 eV. HOMO was found on the surface of nanoparticles doped with Si and there is some on the drug, While LUMO remained unchanged at the nano surface of boron nitride. E_g decreases slightly from 4.47 eV to 4.41 eV and the change rate is ΔE_g = -1.31%, indicating a very low sensitivity of the Si-doped boron nitride nanosheet to the adsorption of mephentermine. A very small change in E_g is not suitable for sensing, the adsorption energy is -2.67 kcal/mol, which is a weak amount and does not have good adsorption. Therefore, this complex does not show good sensing ability due to lower $\%\Delta E_g$ and lower adsorption energy for mephentermine.

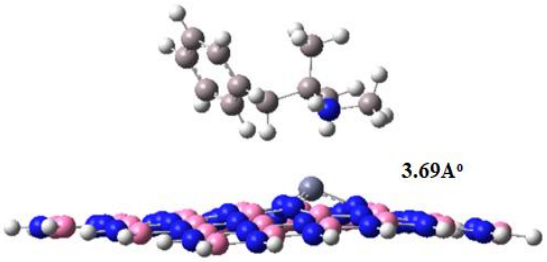


Figure 6. Optimized structure of The Mephentermine drug adsorption on the Si-doped BN nanosheet. Distance is inÅ.

3.4. Al -doped BN nanosheet

B atom of the BNsheet was replaced with the Al atom to find a highly sensitive nanostructure and the new structure was optimized. The structure and geometric properties of BN nanosheet was investigated and the density of state (DOS) was shown in Figure 7. Due to the larger radius of the Al atom compared to the B atom, the Al atom is placed out of the nanosheet surface. Bond length of the Al–N of nanostructure is 1.74 A^0. After doping with Al, the HOMO slightly decreases from -6.31in BNN to -6.29 eV in Al-doped BNN while the LUMO increases from −0.37 in the BNN to −0.77 eV in the Al-doped BNN. The E_g changes significantly from 5.94 eV in the pristine BNN to 5.51 eV in Al-doped BNN. The DFT calculations clarify that the electrical conductivity in Al-doped BN nanosheet (Table 2). According to DFT calculations, Al -dopd BN nanosheet increases electrical conductivity and becomes a semiconducto Compared to pristine boron nitride nanosheet.

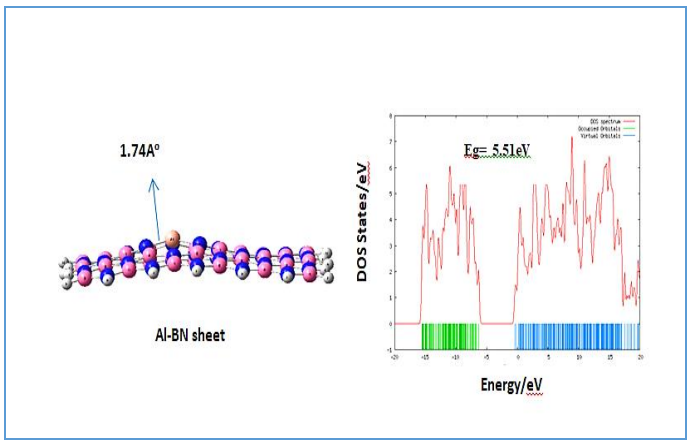


Figure 7. Optimized structure of Al -doped BN nanosheet. Distances are in Å and density of state (DOS) plot.

3.5. The Mephentermine drug adsorption on the Al-doped BN nanosheet

In this case, the interactions between mephentermine and Al-doped BNN are investigated. one type of complex was found that indicate the interaction between NH in mephentermine and the Al atom of Al-doped BNN (Figure 8 and Table 2). density of state (DOS) is shown in Figure 9. In the strongest interaction, the Si atom of Si-doped BN nanosheet interacts from the NH head of mephentermine with E_{ad} of –34.06 kcal/mol with the Al....N distance of 2.074 A^0. the HOMO chenges from -6.29 in the Al-doped BNN to -5.96 eV in the comlex, while the LUMO slightly changes from −0.77 in the Al-doped BNN to −0.37 eV in the complex. HOMO was found on the surface of nanoparticles doped with Al, While in LUMO drug transfer was seen. E_g decreases slightly from 5.51 eV to 5.58 eV and the change rate is ΔE_g = -1.37%, indicating a very low sensitivity of the Al-doped boron nitride nanosheet to the adsorption of mephentermine. A very small change in E_g is not suitable for sensing. As mentioned, due to the adsorption energy of −34.06 kcal/mol and the rather long recovery time, a strong interaction is not suitable for a sensor. A system with high adsorption energy can be a sensor at high temperatures and The recovery time is 48s. At high temperatures the recovery time is reduced and the sensing is improved.

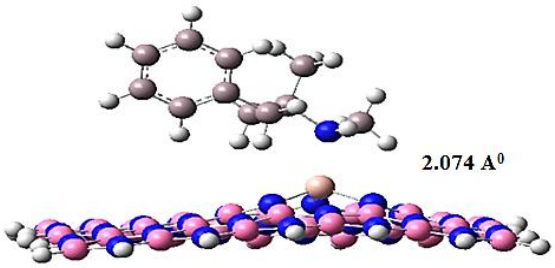
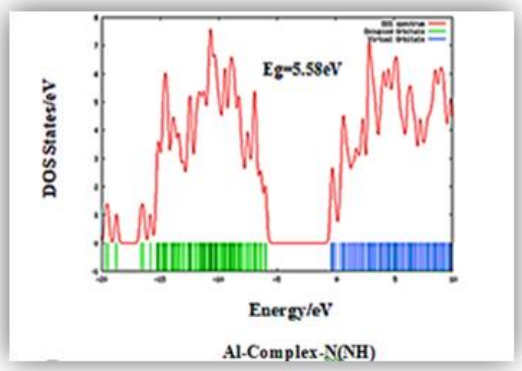
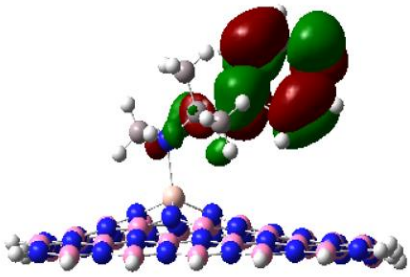
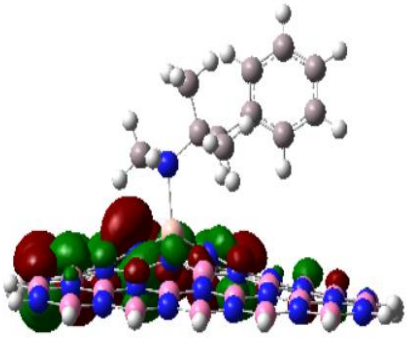


Figure 8. Optimized structure of The Mephentermine drug adsorption on the Al-doped BN nanosheet. Distance is in Å.





Al-Complex-N(NH)LUMO



Al-Complex-N(NH)HOMO

Figure 9. Density of states (DOS) plots of Al-Complex-N(NH) and the HOMO, LUMO profiles of Al-doped BN nanosheet.

3.6. Ga- doped BN nanosheet

B atom of the BNsheet was replaced with the Ga atom to find a highly sensitive nanostructure and the new structure was optimized. The structure and geometric properties of BN nanosheet was investigated and the density of state (DOS) was shown in Figure 10. Due to the larger radius of the Ga atom compared to the B atom, the Ga atom is placed out of the nanosheet surface. Bond length of the Ga–N of nanostructure is 1.74 A^0. After doping with Ga, the HOMO shifted slightly from -6.31 in BNN to -6.32 eV in Ga-doped BNN while the LUMO increase slightly from -0.37 in the BNN to -0.39 eV in the Ga-doped BNN. The E_g changes slightly from 5.94 eV in the pristine BNN to 5.92 eV in Ga-doped BNN. The DFT calculations clarify that the electrical conductivity of boron nitride nanosheet with Ga doping does not increase significantly and it can be concluded that boron nitride nanosheet doped with Ga does not have the ability to measure properly. the electrical conductivity in Ga-doped BN nanosheet (Table 2).

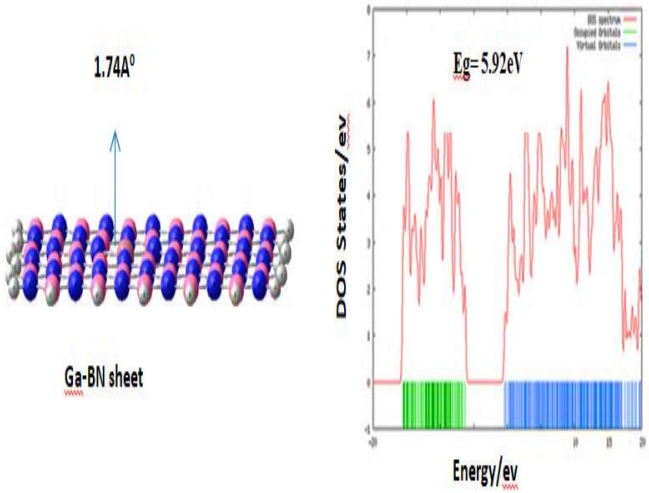


Figure 10. Optimized structure of Ga-doped BN nanosheet. Distances are in Å and density of state (DOS) plot.

3.5. The Mephentermine drug adsorption on the Ga-doped BN nanosheet

In this case, the interactions between Mephentermine and Ga-doped BNN are investigated. one type of complex was found that indicate the interaction between NH in Mephentermine and the Ga atom of Ga-doped BNN (Figure 11 and Table 2). density of state (DOS) is shown in Figure 12. In the strongest interaction, the Ga atom of Ga-doped BN nanosheet interacts from the NH head of mephentermine with Ead of -46.46 kcal/mol with the Ga…N distance of 2.078 A^0 the HOMO chenges from -6.32 in the Ga-doped BNN to -5.93 eV in the comlex, while the LUMO Slightly changes from -0.39 in the Ga-doped BNN to -0.38 eV in the complex. HOMO was found on the surface of nanoparticles doped with Ga, While in LUMO drug transfer was seen. E_g decreases from 5.92 eV to 5.55 eV and the change rate is ΔE_g= -6.36%, indicating a low sensitivity of the Ga-doped boron nitride nanosheet to the adsorption of mefentermin. A small change in E_g is not suitable for sensing. As mentioned, due to the adsorption energy of -46.46 kcal/mol and the rather long recovery time, a strong interaction is not suitable for a sensor.

A very strong interaction is not suitable for a sensor. Calculation of high temperature recovery time is 1.35×10^8 seconds. Helps prolong recovery and thus decompose the compound and decompose and remove the compound.

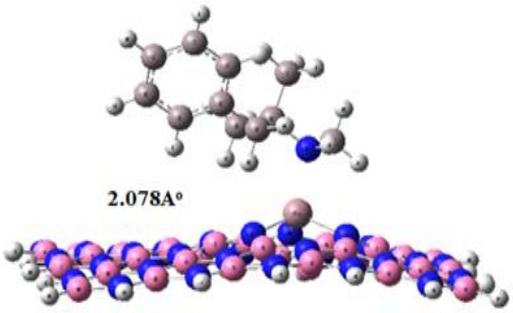


Figure 11. Optimized structure of The Mephentermine drug adsorption on the Ga-doped BN nanosheet. Distance is in Å.

Table 2. Energy of HOMO, LUMO, (E_g) in eV, and the change of *E*g upon the mephentermine drug adsorption on the Si and Al and Ga-doped BN nanosheet structures. The adsorption energy (E_{ad}) is in kcal/mol.% ΔEg indicates The percentage of the change of Eg after the EA adsorption.

Structures	E_{ad} (kcal/mol)	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)	$\%\Delta E_g$
Si-BNsheet	-----	-4.86	-0.38	4.47	-----
Si-Complex-N(NH)	-2.67	-4.76	-0.35	4.41	-1.31%
Al-BN sheet	-----	-6.29	-0.77	5.51	------
Al-Complex-N(NH)	-34.06	-5.96	-0.37	5.58	-1.37%
Ga-BN sheet	----	-5.93	-0.39	5.92	------
Ga -Complex-N(NH)	-46.46	-5.93	-0.38	5.55	-6.39%

4. Conclusions

Medicinal pollutions are adsorbed from the environment through food, drink and respiration, as well as the skin, and the indirect use of drugs in this way causes the body to become resistant and the subsequent dangerous effects. Due to the problems caused by the presence of pollutants that are not biologically eliminated, humans are looking for different solutions to identify and detect them. One of these solutions is to use sensors.

In this study, using DFT calculations, the adsorption behavior and sensing ability mefentermine with pristine and doped with Si and Al and Ga were investigated to find a suitable sensor. Pristine and doped boron nitride nanosheet with Si and Al and Ga with mefentermin: Ga-Complex-N(NH) > Al-Complex-N(NH) > Si-Complex- N(NH) > Complex-N(NH)

The best complex is Al-Complex-N(NH) in the mephentermine drug adsorption on the Al-doped BNN with adsorption energy -34.06 kcal/mol, which is related to the interaction of Al-doped BNN-mefantermite. This system with this adsorption energy can be a sensor suitable at higher temperatures. But the electrical sensivity is low and changing the E_g is not suitable for the sensor.

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