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Theoretical study of interaction between Mexiletine drug and pristine, Si-, Ga- and Al-doped boron nitride nanosheet.

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ABSTRACT

In this study, the adsorption behavior of pristine, -Si, -Ga and -Al doped boron nitride nanosheet (BNN) is investigated toward the mexiletine drug 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* basis set. The adsorption energy (E_{ad}) between mexiletine and the pristine, Si-, Ga- and Al-doped BN nanosheet was changed in the following order: Ga-Complex-N(NH_2) > Al-Complex-N(NH_2) > Si-Complex-O. The E_{ad} of the mexiletine/BNN complex is −4.73kcal/mol, which is very low interaction so that the adsorption is not suitable. The E_{ad} of the mexiletine/Si-doped BNN complex is −22.14kcal/mol, which is a suitable interaction so that the desorption may be occurred readily. Besides, the E_g significantly increased from 4.47 eV to 5.68 eV and the rate of the change is % ΔE_g = −27.20% which shows the suitable sensitivity of the Si-doped BN nanosheet to the adsorption of drug. Therefore, it can be concluded that the Si-doped BN nanosheet can be a promising candidate to being a sensing ability over the mexiletine drug from both E_{ad} and E_g parameters.

1. Introduction

Mexiletine is a medication used to treat abnormal heart rhythms, chronic pain, and some causes of muscle stiffness. Common side effects include abdominal pain, chest discomfort, drowsiness, headache, and nausea. It works as a non-selective voltage-gated sodium channel blocker and belongs to the Class IB group of anti-arrhythmic medications [1].

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 of plants, soil, humans and animals and creates problems through manufacturing processes, agriculture and waste disposal. The drug is often released into the environment. These toxic compounds eventually enter the body of organisms through nutrition and drinking water. When a drug is released in large quantities into the environment and nature, it is dangerous and requires sensing to determine where the drug accumulates, for example in water and soil and in the environment in general, and therefore sensors are used. These sensors can be nanoparticles. As a result, nano-scale methods have been developed to identify drug compounds to address environmental pollution and concerns about human health [2-6]. With the advent of nanotechnology, due to their surface/volume ratio, which is much higher than conventional micro detectors [7, 8]. Nanostructures have received a great deal of attention as chemical sensors [9-16].

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 [17]. A sheet is not essentially completely flat but it is considered by a plate-like form or structure. There are various kinds of nanosheets including boron nitride nanosheets (BNN) which show suitable character in the stability and electronic properties comparing with carbon nanosheet [18-20].

Due to their excellent structural, electronic and optical properties, the BNN have attracted attention in recent years [21, 22]. The BNN indicate a size controllable energy band gap which enables them as promising materials for different technological applications. For instance, there are several evidences which indicate the suitable interaction of toxic gases with the BNN [23, 24]. Moreover, surface modifications, such as doping with suitable atoms could remarkably improve the surface reactivity of BNN [25, 26]. Modification of the surface of nanostructures by placing impure atoms is a promising way to improve their sensitivity to drugs or gas molecules [27].

-Khaleqian *et al.* studied the interaction of the single-walled BN nanotube with theophylline theoretically [28].

-In 2016, another study by Vessally *et al* [29] the interaction of an aspirin (AS) molecule with the external surface of a boron nitride fullerene-like nanocage (B12N12) is studied by means of density functional theory (DFT) calculations.

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, Ga and Al is a useful way to improve the electronic properties. Also, we examined the interaction between mexiletine from NH_2 and O head and the pristine BNN and the 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 study were performed using the DFT method at the theoretical level of B3LYP/6-31G* and also using the GaussView 05 and GAMESS program [30]. To ensure the lowest energy for the BNN/mexiletine complex rather than a local minimum, the potential energy surface (PES) scans were performed with respect to various dihedral angles (D). The Gauss sum was used for drawing the DOS plots [31].

The adsorption energy (E_{ad}) is calculated as follows:

$$E_{ad} = E(\text{drug/adsorbent}) - E(\text{adsorbent}) - E(\text{drug}) + E(\text{BSSE}) \quad (1)$$

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 [32]. In this study, 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 HOMO–LUMO energy gap (Eg) of the structures under study is computed as follows [33-46]:

$$Eg = ELUMO - EHOMO \quad (2)$$

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

$$\%\Delta Eg = [(Eg2 - Eg1)/Eg1] * 100 \quad (3)$$

3. Results and Discussion

3.1. The BN nanosheet characterization

The optimized structure of the BN nanosheet is shown in Fig. 1, in which different types of B-N bonds can be identified with corresponding equilibrium distances of 1.44 and 1.45 A. 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 Fig. 1, the HOMO energy of the BN nanosheet is −6.31 eV and that of the LUMO is −0.37 eV (Table 1, Fig. 2). Thus, the E_g is approximately 5.94 eV (Table 1). Fig. 2 indicates that the HOMO and LUMO levels are mainly located on the N and B atoms, respectively. The nitrogen atoms in BNN are electron donors and boron atoms are electron acceptors.

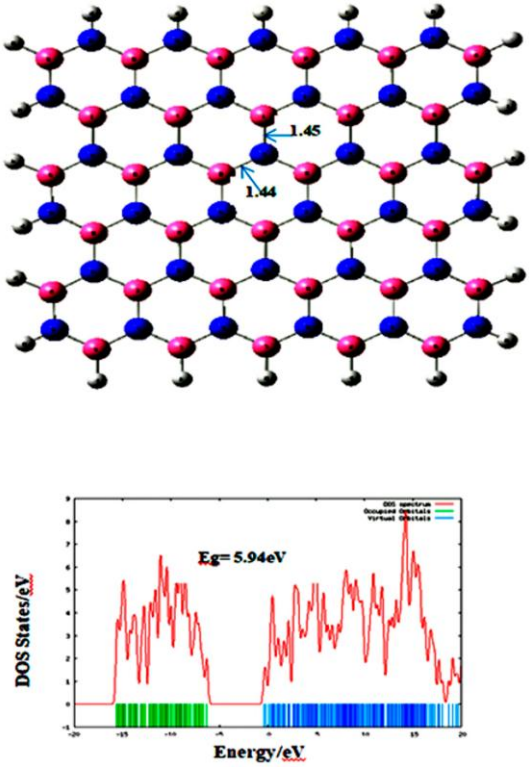

Figure 1. Optimized structure of BN nanosheet and density of state (DOS) plot.

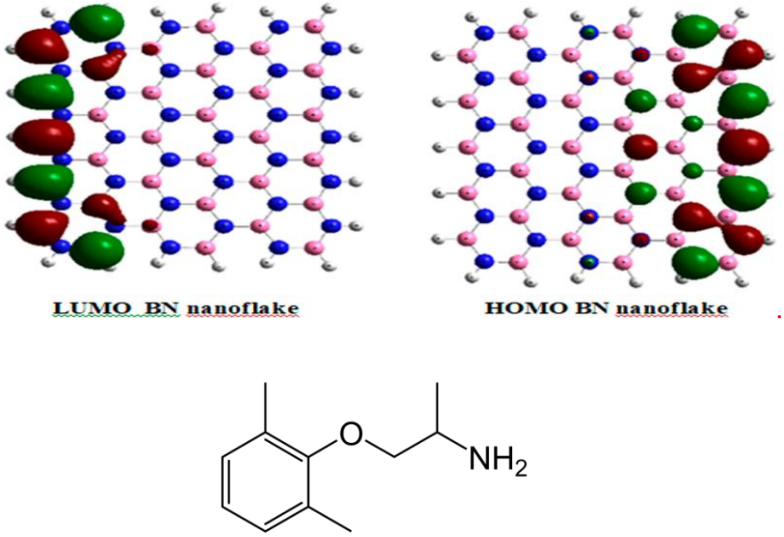

Figure 2. The HOMO and LUMO profiles of BN nanosheet

3.2. The adsorption of mexiletine on the BN nanosheet

3.2.1. BN nanosheet-mexiletine complex

The optimization process proceeds to reach the actual optimal mexiletine structure which has less energy (Figure 3). In order to find the stable configurations (global minima) of mexiletine adsorbed on the BN nanosheet, various studies have been carried out. Finally, two active sites for the drug are predicted, including the -NH_2 and-O heads which the drug can be adsorbed onto the B atom of the BNN nanosheet. As shown in Figure 4, we obtained two types of complexes that indicate the interactions between -NH_2 and -O in mexiletine and the B atom of BN nanoshet. The density of state plot (DOS), LUMO and HOMO have been presented in Figure 5 for the most stable complexes. It has been found that there are two important parameters including the E_{ad} and E_g parameters in the drug sensing potential by nanostructures. In the most stable complex-O, the drug adsorbed from the N atom onto the BN nanosheet with a distance of 3.66A^0. The adsorption energy is -4.73kcal/mol which shows a weak interaction.

In Figure 3, the HOMO of mexiletine is more focused on all three atoms and more on the ring focused whereas LUMO broadly surrounded the ring then the -O and slightly -NH2 functional groups. The DFT calculations showed that the electronic properties of the BN nanosheet have been changed during the adsorption of the drug molecule. According to Table 1 and Figure 5, the HOMO has been changed from-6.31in the BN nanosheet to -6.12 eV in the complex and the LUMO has been changed from - 0.37 to - 0.35 eV Slightly changed. This molecule of the drug donates a pair of electrons from its oxygen atoms to the boron atom, which is electron-deficient at the boron nitride nanosheet surface. These changes are to the extent that the LUMO and HOMO are located on the drug atoms. The drug molecule donates a pair of electrons from its nitrogen atoms to the boron atom which has electron-deficiency on the BN nano sheet surface.

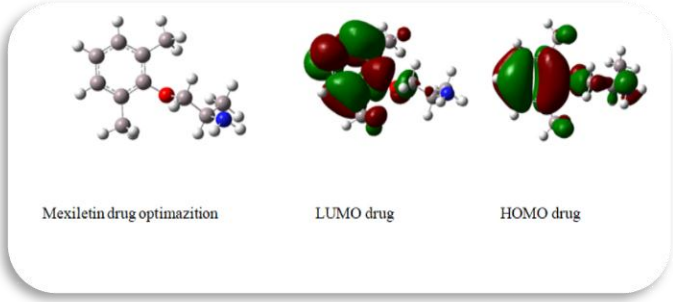

Figure 3. Optimized structure of mexiletine and its HOMO, and LUMO profiles.

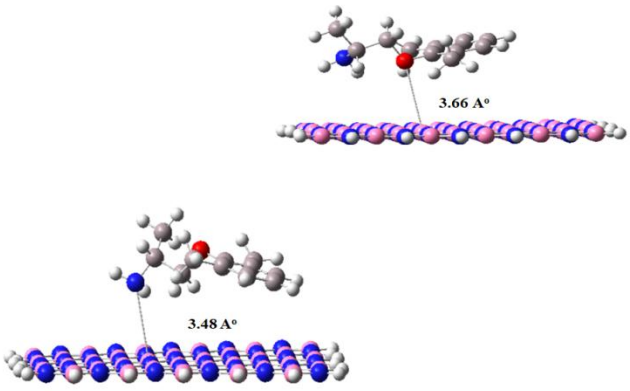

Figure 4. Optimized structures of BNN-mexiletine complexes. Distances are in Å.

As mentioned, there are two important parameters, *i.e.* E_{ad} and *E*g, in the drug sensing potential by nanostructures. The adsorption of mexiletine onto to BNnanosheet 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 [47, 48]:

$$\tau = \nu 0 – 1 \exp(–E_{ad}/kT) \quad (4)$$

Here τ is the recovery time and $\nu 0$ is the attempt frequency, T is the temperature, and *K* is the Boltzmann constant [49]. 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 [50]. Vacuum-UV is applied for the recovery of drugs from the surface of BN nanosheet.

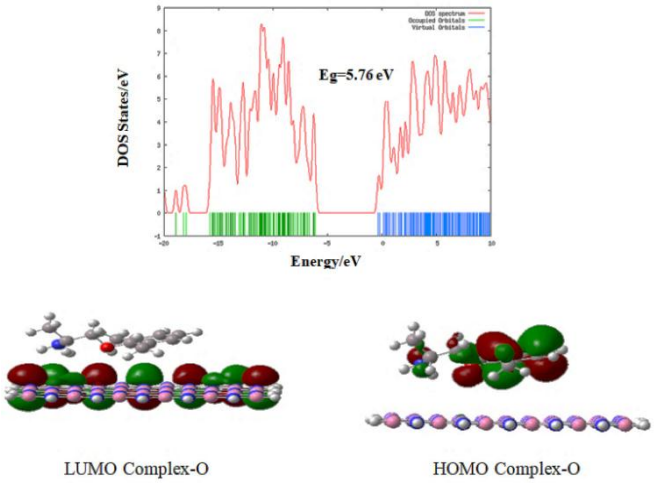

Figure 5. Density of states (DOS) plot of BNN-mexiletine complex-O, and the HOMO, and LUMO profiles of complex-O.

The second most important factor in sensing character is the HOMO–LUMO energy gap (*E*g) of the BN nanosheet in the presence of mexiletine. 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 mexiletine 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:

$$\sigma = AT3/2 \exp(–Eg/2kT) \quad (5)$$

where *k* is the Boltzmann constant, and A (electrons/m3K3⁄2) is a constant. There is an acceptable correlation between the obtained results of this procedure and experimental techniques reported in the literature [51].

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 [52, 53].
The *E*g of the BN nanosheet decreased when it adsorbed the drug, changing the *E*g significantly from 5.94 eV to 5.76 eV in the complex with %Δ*E*g of -2.89% which shows the low sensitivity of the BN nanosheet to the adsorption of mexiletine. The change in *E*g is not suitable for the sensing ability and the adsorption energy, E_{ad}, of −4.73kcal/mol is so weak that the BN nanosheet can not effectively adsorb the drug. So, the BN nanosheet does not a suitable sensing ability with respect to the adsorption energy and %Δ*E*g for mexiletine (Table 1).
-In the Complex-NH2, mexiletine is adsorbed from the N of NH2 onto the B atom of BNN nanosheet with a distance of 3.48A^0. The adsorption energy is −3.03 kcal/mol, indicating very week adsorption, But its effect on the ability of sensing (electrical sensitivity) is appropriate, with good Δ*E*g of -2.26% (Figure 7).

Table 1. Energy of HOMO, LUMO, HOMO–LUMO gap (*E*g) in eV, and the change of *Eg* up on the mexiletine drug adsorption on the BN nanosheet structures. The adsorption energy (E_{ad}) is in kcal/mol. % Δ*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 (eV)	%ΔE_g
BN sheet	----	-6.31	-0.37	5.94	-----
Complex-O	-4.73	-6.12	-0.35	5.76	-2.89%
Complex-N (NH2)	-3.03	-6.128	-0.32	5.80	-2.26%

3.3. Mexiletine adsorption onto the Si-, Al- and Ga-doped BN nanosheet
3.3.1. Si-doped BN nanosheet-mexiletine complex

Here, the interactions between mexiletine and Si-doped BNnanosheet are investigated. Two types of complexes were found that indicate the interactions between -O, -NH2 in mexiletine and the Si atom of Si-doped BN nanosheet (Figure 6 and Table 2). The corresponding density of state (DOS) is also shown in Figure 9. In the strongest interaction, the Si atom of Si-doped BN nanosheet interacts from the -O head of mexiletine with E_{ad} of -22.14kcal/mol with the Si . . . .O distance of 1.65A^0. The high adsorption energy in the Si-BNN/mexiletine complex may be due to the greater curvature of the nanosheet. The HOMO changes from -4.86 in Si-BNN to -6.08 eV in the Si-BNN/mexiletine complex and the LUMO slightly changes from -0.38 to −0.39 eV. The HOMO is localized on the mexiletine atoms while the LUMO remains unchanged on the surface of the BN nanosheet. The *E*g significantly increased from 4.47 eV to 5.68 eV and the rate of change is % Δ*E*g = −27.20% which shows the suitable sensitivity of the Si-doped BN nanosheet to the adsorption of drug. The insignificant change in *E*g which is suitable for the sensing ability, the E_{ad} of −22.14 kcal/mol is suitable that the Si-doped BN nanosheet suitable adsorbs mexiletine, which shows that the recovery time is suitable. Hence, the Si-doped BNN does show a suitable sensing ability with respect to suitable % ΔEg and suitable adsorption energy for mexiletine.
-In the Si-Complex-NH2, mexiletine is adsorbed from the N of NH2 onto the Si atom of Sidoped BN nanosheet with a distance of 1.72 A^0. The adsorption energy is −2.12kcal/mol, indicating very week adsorption, But its effect on the ability of sensing (electrical sensitivity) is appropriate, with good %Δ*E*g of -27.80 (Figure 7).

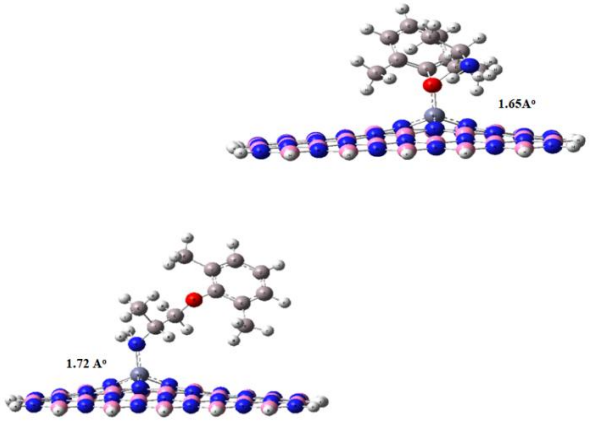

Figure 6. Optimized structures of Si-doped BNN-mexiletine complexes. Distances are in Å.

3.3.4. Ga-doped BN nanosheet-mexiletine complex

Here, the interactions between mexiletine and Ga-doped BNnanosheet are investigated.Two types of complexes were found that indicate the interactions between -O, -NH2 in mexiletine and the Ga atom of Ga-doped BN nanosheet (Figure 7 and Table 2). The corresponding density of state (DOS) is also shown in Figure 9. In the strongest interaction, the Ga atom of Ga-doped BN nanosheet interacts from the -NH2 head of mexiletine with E_{ad} of -43.47 kcal/mol with the Ga. . . .NH2 distance of 2.06A^0. The high adsorption energy in the Ga-BNN/mexiletine complex may be due to the greater curvature of the nanosheet. The HOMO changes from -6.32 in Ga-BNN to -5.96eV in the Ga-BNN/mexiletine complex and the LUMO slightly changes from -0.39 to −0.22 eV. the HOMO remains unchanged on the surface of the BN nanosheet , While LUMO was found on the surface of BN nanosheet and slightly on the surface of the drug. The *E*g decreased from

5.92eV to 5.73 eV and the rate of change is ΔEg = −3.29% which shows the weak sensitivity of the Ga-doped BN nanosheet to the adsorption of drug. The change in *E*g which is not suitable for the sensing ability, the E_{ad} of −43.47 kcal/mol is highly. As a result, the system may not be suitable for the sensor in terms of adsorption energy because the recovery time is prolonged and thus helps to decompose this compound and decompose and remove this compound.

-In the Ga-Complex-O, mexiletine is adsorbed from the -O onto the Ga atom of Ga-doped BN nanosheet with a distance of 2.03A^0. The adsorption energy is −35.92 kcal/mol, indicating a strong interaction. Partial sensing ability (electrical sensitivity) and ΔEg = -8.07% (Figure 6).

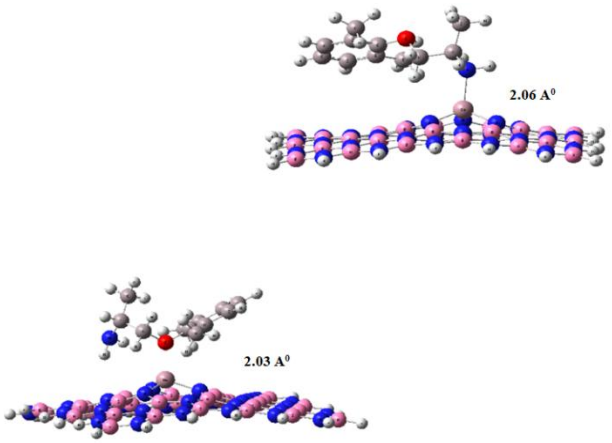

Figure 7. Optimized structures of Ga-doped BNN-mexiletine complexes. Distances are in Å.

3.3.5.Al -doped BN nano sheet-mexiletine complex

Here, the interactions between mexiletine and Al-doped BN nanosheet are investigated. Two types of complexes were found that indicate the interactions between -O, -NH2 in mexiletine and the Al atom of Al-doped BN nanosheet (Figure 8 and Table 2). The density of state (DOS) is also shown in Figure 9. In the strongest interaction, the Si atom of Si-doped BN nanosheet interacts from the -O head of mexiletine with E_{ad} of –36.05kcal/mol with the Al….NH2 distance of 2.04 A^0. The high adsorption energy in the Al-BNN/mexiletine complex may be due to the greater curvature of the nanosheet. The HOMO slightly changes from -6.29 in Si-BNN to -5.99 eV in the Al-BNN/mexiletine complex and the LUMO changes from -0.77 to −0.22 eV. The HOMO is on the surface of BN nanosheet and slightly localized on the mexiletine atoms while the LUMO remains unchanged on the surface of the BN nanosheet. The *E*g increased from 5.51 eV to 5.76 eV and the rate of change is % ΔEg = −4.56% which shows the weak sensitivity of the Al-doped BN nanosheet to the adsorption of drug. The weak change in *E*g which is not suitable for the sensing ability, the E_{ad} of −36.05 kcal/mol is highly. A very strong interaction is not suitable for a sensor. The recovery time is long and therefore can help to break down and remove this compound.

-In the Al-Complex-O, mexiletine is adsorbed from the -O onto the Al atom of Al-doped BN nanosheet with a distance of 1.98 A^0. The adsorption energy is −25.64 kcal/mol, indicating a suitable adsorption, But its effect on the ability of sensing (electrical sensitivity) is weak with %ΔEg of -0.68 (Figure 7).

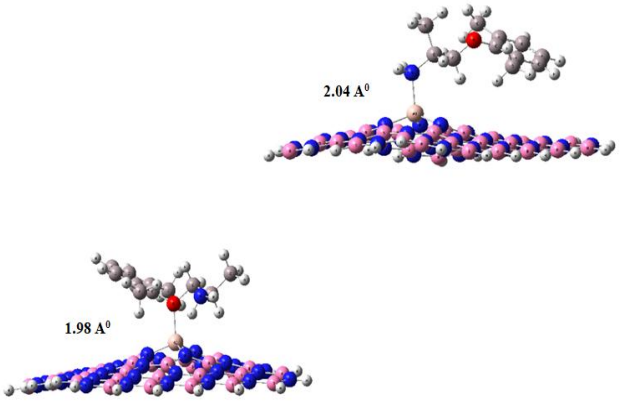

Figure 8. Optimized structures of Al-doped BNN-mexiletine complexes. Distances are in Å.

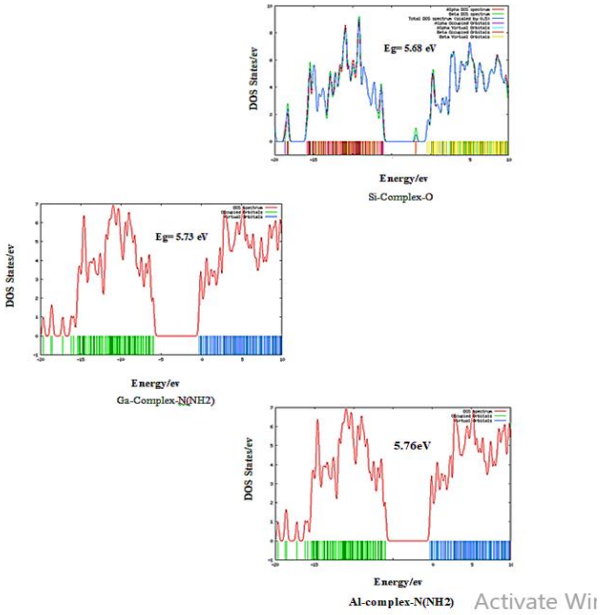

Figure 9. Density of states (DOS) plots of (a) Si-Complex-O, (b) Ga-Complex-NH2, (c) Al-Complex-NH2.

Table 2. Energy of HOMO, LUMO, HOMO–LUMO gap (E_g) in eV, and the change of E_g up on the mexiletine drug adsorption on the BN nanosheet structures. The

adsorption energy (E_{ad}) is inkcal/mol.% ΔE_g indicates the percentage of the change in E_g after the drug adsorption.

Structures	E_{ad} (kcal/mol)	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)	$\%\Delta E_g$
Si-BN Sheet	----	-4.86	-0.38	4.47	-----
Si-Complex-O	-22.14	-6.08	-0.39	5.68	- 27.20%
Si-Complex-N (NH_2)	-2.12	-6.07	-0.36	5.71	-27.80%
Ga-BN Sheet	-----	-6.32	-0.39	5.92	----
Ga-Complex-O	-35.92	-6.04	-0.59	5.44	-8.07%
Ga-Complex-N (NH_2)	-43.47	-5.96	-0.22	5.73	-3.29%
Al-BN Sheet	----	-6.29	-0.77	5.51	-----
Al-Complex-O	-25.64	-5.97	-0.50	5.47	-0.68%
Al-Complex-N (NH_2)	-36.05	-5.99	-0.22	5.76	-4.56%

4. Conclusions

In this resarch, the energy of interactions and the sensing ability between mexiletine and the pristine, Si-, Ga- and Al-doped BN nanosheets are investigated. Also, the adsorption behavior of Si-, Ga- and Al-doped BN nanosheets is investigated toward mexiletine. The adsorption energy (E_{ad}) between mexiletine and the pristine, Si-, Ga- and Al-doped BN nanosheet is changed in the following order:

Ga-Complex-N(NH2) > Al-Complex-N(NH2) > Si-Complex-O

The E_{ad} of the mexiletine/BNN complex is −4.73kcal/mol which has a low adsorption energy for the sensing ability. The interaction between mexiletine and the pristine BN nanosheet has a weak E_{ad} which can conclude that it isphysically absorbed and has no sensing ability.

The *E*g significantly increased from 4.47 eV to 5.68 eV and the rate of change is % ΔEg = −27.20% which shows the suitable sensitivity of the Si-doped BN nanosheet to the adsorption of drug. The insignificant change in *E*g which is suitable for the sensing ability, the E_{ad} of −22.14 kcal/mol is suitable that the Si-doped BN nanosheet suitable adsorbs mexiletine.

The *E*g decreased from 5.92 eV to 5.73 eV and the rate of change is % ΔEg = −3.29% which shows the weak sensitivity of the Ga-doped BN nanosheet to the adsorption of drug. The change in *E*g which is not suitable for the sensing ability, the E_{ad} of −43.47kcal/mol is highly. As a result, the system may not be suitable for the sensor in terms of absorption energy.

The *E*g increased from 5.51 eV to 5.76 eV and the rate of change is % ΔEg = −4.56% which shows the weak sensitivity of the Al-doped BN nanosheet to the adsorption of drug. The weak change in *E*g which is not suitable for the sensing ability, the E_{ad} of −36.05 kcal/mol is highly. A very strong interaction is not suitable for a sensor.

References

[1] M. J. Marmura, Intravenous lidocaine and mexiletine in the management of trigeminal autonomic cephalalgias. *Current. Pain. Headache. Reports.*, 14 (2010) 145-50.

[2] W. Baran, E. Adamek, J. Ziemia-nska, Effects of the presence of sulfonamides in the environment and their influence on human health. *J. Hazard. Mater*., 196 (2011) 1–15.

[3] X. Zhang, X. Sun, T. Lv, Preparation of PI porous fiber membrane for recovering oil-paper insulation structure. *J. Mater. Sci. Mater*., 31 (2021) 13344–13351.

[4] R. Chen, Y. Cheng, P. Wang, Enhanced removal of Co(II) and Ni(II) from highsalinity aqueous solution using reductive self-assembly of three-dimensional magnetic fungal hyphal/graphene oxide nanofibers. *Sci. Total. Environ*., 756(2021) 143871.

[5] R. Chen, Y.Cheng, P. Wang, Facile synthesis of a sandwiched Ti3C2TxMXene/nZVI/fungal hypha nanofiber hybrid membrane for enhanced removal of Be(II) from Be(NH2)2 complexing solutions. *Chem. Eng. J*., (2021)129682.

[6] A. Białk-Bieli-nska, S. Stolte, J. Arning, Ecotoxicity evaluation of selected sulfonamides. *Chemosphere*. 85 (2011) 928–933.

[7] S. F. Rastegar, A. A. Peyghan, H. Ghenaatian, NO2 detection by nanosized AlN sheet in the presence of NH3: DFT studies. *Appl. Surf. Sci*., 274 (2013) 217–220.

[8] J. He, X. Liu, L. Song, High annealing stability of in AlZnOnanofiberfield-effecttransistorswith improvedmorphology byAldoping. *J. Phys. Chem.Lett*., 59 (2021)1339–1345.

[9] Y. V. Berdinsky, A. V. Shevtsov, S. V. Okotrub, Sensor properties of fullerene films and fullerene compounds with iodine. *Chem. Sustain. Dev*., 8 (2008) 141–146.

[10] Z. Wang, T. Zhang, Large-scale one-pot synthesis of water-soluble and biocompatible upconversion nanoparticles for dual-modal imaging. *Colloids. Surf. B.*, 198 (2021) 111480.

[11] P. Dong, T. Zhang, H. Xiang, Controllable synthesis of exceptionally small-sized superparamagnetic magnetite nanoparticles for ultrasensitiveMR imaging and angiography. *J. Mater. Chem. B Mater. Biol Med*., 9 (2021) 958–968.

[12] S Zhang, S. Zhao, S. Huang, Photocatalytic degradation of oxytetracycline under visible light by nanohybrids of CoFe alloy nanoparticles and nitrogen-/sulfur-codoped mesoporous carbon. *Chem. Eng*., 420 (2021)130516.

[13] A. A. Peyghan, M. Moradi, First-principle study of methanol adsorption on Ni(Pd)-decorated grapheme. *J. Iran. Chem. Soc*., 12 (2015) 751–756.

[14] Z. Li, In situ chemical lithiation transforms diamond-like carbon into an ultrastrong ion conductor for dendrite-free lithium-metal anodes. *Adv. Mater*., (2021)

[15] H. Wang, T. Song, Z. Li, Exceptional high and reversible ammonia uptake by two dimension few-layer BiI3 nanosheets. *ACS. Appl. Mater. Interfaces*., 13 (2021) 25918–25925.

[16] T. Oku, M. Kuno, H. Kitahara, Atomic structures andproperties of boronnitride andcarbon nanocage fullerene materials. *Int. J. Inorg. Mater*., 3 (2001) 597–612.

[17] J. He, X. Liu, L.Song, HighAnnealing Stability of InAlZnONanofiber Field-EffectTransistors with Improved Morphology by Al Doping. *J Phys Chem Lett*., 12 (2021) 1335–1345.

[18] C. Zhi, Y. Bando, C. Tang, Boron nitride nanotubes/polystyrene composites. *J. Mater. Res*., 21 (2006) 2794–2800.

[19] R. Faramarzi, M. Falahati, M. Mirzaei, Interactions of fluorouracil by CNT and BNNT: DFT analyses. *Adv. J. Sci. Eng*. 1 (2020) 62–66.

[20] S. Prodhan, S. Mazumdar, S. Ramasesha, Correlated electronic properties of a graphene nanoflake. *coronene. Molecules*., 24 (2019) 730.

[21] D. Lee, S. Song, J. Hwang, (2013). Enhanced mechanical properties of epoxy nanocomposites by mixing noncovalently functionalized boron nitride nanoflakes. *Small*., 9 (2013) 2602–2610.

[22] A. Pakdel, Y. Bando, D. Golberg, Nano boron nitride flatland. *Chem Soc Rev*., 43 (2015) 934–959.

[23] M. Samadizadeh, A.A. Peyghan, S. F. Rastegar, ensing behavior of BN nanosheet toward nitrous oxide: A DFT study. *Chin Chem Lett*., 26 (2015) 1042–1045.

[24] A. C. Srivas, S. K. Bhat, P. K. Jain, (2015). Electronic transport properties of BN sheet on adsorption of ammonia (NH3) gas. *J Mol Model*., 21 (2015) 39.

[25] S. Noorizadeh, E. Shakerzadeh, (2012). Formaldehyde adsorption on pristine, Al-doped and monovacancy defected boron nitride nanosheets: a first principles study. *Comput Mater Sci*., 56 (2021) 122–130.

[26] F. Behmagham, E. Vessally, B. Massoumi, A computational study on the SO2 adsorption by the pristine, Al, and Si doped BN nanosheets. *Superlattice. Microst*., 100 (2016) 350–357.

[27] R. N. Goyal, V. K. Gupta, N. Bachheti, Fullerene-C60-modified electrode as a sensitive voltammetric sensor for detection of nandrolone – an anabolic steroid used in doping. *Anal. Chim. Acta*., 597 (2007) 82–89.

[28] H. Yin, C. Han, Q. Liu, Recent Advances and Perspectives on the Polymer Electrolytes for Sodium/Potassium-Ion Batteries. Small., 17 (2021) 2006627.

[29] E. Vessally, M. D. Esrafili, R. Nurazar, p. Nematollahi , A. Bekhradnia, A DFT study on electronic and optical properties of aspirin-functionalized B12N12 fullerene-like nanocluster. *Struct. chemist*., 28 (2017) 735-748.

[30] M. Schmidt, K. Baldridge, J. BoatzGeneral atomic and molecular electronic structure *system. J. Comp. Chem*., 14(1993) 1347–1363.

[31] N. OBoyle, A. Tenderholt, K. Langner, A library for package independent computational chemistry algorithms. *J. Comput. Chem*., 29 (2008) 839–845.

[32] S. F. Boys, F. Bernardi, (1970). Calculation of smallmolecular interactions by differences energies – some procedures with reduced errors. *Mol Phys*. 19 (1970) 553–566

[33] F. Gharibzadeh, E. Vessally, E. Edjlali L, A DFT study on Sumanene, Corannulene and nanosheet as the anodes in Li−ion batteries. *Iran J Chem Chem Eng*., 39 (2020) 51–62.

[34] E. Vessally, M. Babazadeh, F. Alipour, A computational study on the some small graphene-like nanostructures as the anodes in Na−ion batteries. *Iran J Chem Chem Eng.*, 40 (2021) 691–703.

[35] E. Vessally, P. Farajzadeh, E. Najafi, Possible sensing ability of boron nitride nanosheet and its Al– and Si–doped derivatives for methimazole drug by computational study. *Iran J Chem Chem Eng*., 40 (2021) 1001–1011.

[36] M. R. PoorHeravi, S. Habibzadeh, A. G. Ebadi, Substituent effects of fusedHammick silylenes via density functional theory survey. *J Phys Org Chem*., (2021) 4264.

[37] Z. Rostami, M. Asnaashariisfahani, S. Ahmadi, Adensity functional theory investigation on 1H-4-germapyridine-4-ylidene & the unsaturated heterocyclic substituted ones. *J Mol Struct.,* 1238 (2021) 130427.

[38] A. Hassanpour, S. Yasar, A. Ebadi, Thermodynamic stability, structural and electronic properties for the C 20-n Al n heterofullerenes (n=1–5): a DFT study. *J Mol Model*., 27 (2021) 1–12.

[39] A. Hassanpour, P. D. K. Nezhad, A. Hosseinian, Characterization of IR spectroscopy, APT charge, ESP maps, and AIM analysis of C20 and its C20−nAln heterofullerene analogous (*n*=1–5) using DFT. *J. Phys Org Chem*., (2021) 4198.

[40] A. Hassanpour, S. Ebrahimiasl, L. Youseftabar-Miri , A DFT study on the electronic detection of mercaptopurine drug by boron carbide nanosheets. *Comput Theoret Chem*., 1198 (2021) 113166.

[41] A. Hassanpour, S. Ahmadi, P. D. K. Nezhad, Sensing properties of Al-and Si-doped HBC nanostructures toward gamma-butyrolactone drug: a density functional theory study. *Comput . Chem*., 1197 (2021) 113163.

[42] A. Hassanpour, N. Farhami, M. Derakhshande, Magnesium and calcium ion batteries basedon the hexa-peri-hexabenzocoronene nanographene anode materials. *Inorg. Chem. Comm*., 129 (2021)108656.

[43] M. R. J. Sarvestani, S. Majedi, A DFT study on the interaction of alprazolam with fullerene (C20). *J. Chem. Lett*. , 1 (2020) 32–38.

[44] M. Kamel, A. Morsali, H. Raissi, Theoretical insights into the intermolecular and mechanisms of covalent interaction of flutamide drug with COOH and COCl functionalized carbon nanotubes: a DFT approach. *Chem. Rev. Lett*., 3 (2020) 23–37.

[45] M. R. J. Sarvestani, R. Ahmadi, B. F. Rik, Procarbazine adsorption on the surface of single walled carbon nanotube: DFT studies. *Chem. Rev. Lett.*, 3 (2020) 175–179.

[46] M. R. J. Sarvestani, Z. Doroudi, Fullerene (C20) as a potential sensor for thermal and electrochemical detection of amitriptyline: a DFT study. *J. Chem. Lett*., 1 (2020) 63–68.

[47] A. Redondo, Y. Zeiri, J. J. Low, Application of transition state theory to desorption fromsolid surfaces: ammonia on Ni(111*). J. Chem. Phys*., 79 (1993) 6410–6415.

[48] R. Kumar, N. Goel, M. Kumar, UV-activatedMoS2 based fast and reversibleNO2 sensor at room temperature. *ACS. Sens*. , 2(2017) 1744–1752.

[49] A. Bano, J. Krishna, D. K. Pandey, An ab initio study of sensing applications of MoB2 monolayer: a potential gas sensor. *Phys. Chem. Chem. Phys*., 21 (2019) 4633–4640.

[50] J. Li, Y. Lu, Q. Ye, Carbon nanotube sensors for gas and organic vapor detection. *Nano. Lett*., 3 (2003) 929–933.

[51] N. L. Hadipour, A. A. Peyghan, H. Soleymanabadi, Teoretical study on the Al-doped ZnO nanoclusters for CO chemical sensors. *J . Phys. Chem* C., 119 (2015) 6398–6404.

[52] A, Ahmadi, N. L. Hadipour, M. Kamfiroozi, Theoretical study of aluminum nitride nanotubes for chemical sensing of formaldehyde. *Sens. Actuators. B*., 161(2012) 1025–1029.

[53] J. Beheshtian, A. A. Peyghan, Z. Bagheri, Detection of phosgene by Sc-doped BN nanotubes: a DFT study. *Sens. Actuators. B*., (2012) 846–852.