A Density Functional Theory Study on Possible Sensing of Boron Nitride Nanosheet and Its Doped Derivatives over the Amantadine Drug

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ABSTRACT: *This study deals with the interaction between the Amantadine drug (Ad) and the Boron Nitride NanoSheet (BNNSh). The interactions between the Ad molecule and BNNSh, doped Si-BNNSh, Ge-BNNSh, and Ga-BNNSh were carried out at the RCAM-B3LYP method with 6-31G(d) basis set using the Gaussian 09 program. The DFT calculations clarified a weak interaction between the Ad drug and BNNSh. The doped Si, Ge, and Ga-BNNSh were examined to obtain a suitable interaction between the Ad drug and BNNSh to make a suitable sensing device. The adsorption energy (E_{ad}), as well as the gap energy between HOMO and LUMO (Eg), were calculated for the Ad drug and BNNSh and its doped Si-, Ge-, and Ga-BNNSh. The DFT calculations indicated that the E_{ad} of the Ge-BNNSh/Ad complex is -19.67 which was suitable adsorption energy for the sensing ability with low recovery time. Also, the change of % ΔE_g for the Ge-BNNSh/Ad is -21.50% which shows a high sensitivity of Ge-BNNSh to the Ad drug. This study showed that Ge-BNNSh is a promising candidate for being a possible sensor of the Ad drug.*

KEYWORDS: *Computational; Boron nitride; Amantadine; DFT calculations; Sensor.*

INTRODUCTION

One of the serious threats to human life is the presence of unused medicinal compounds in the environment. When unused drugs come into soil and water, these drugs accumulate in animals, humans, and plants' bodies. Also, the drugs are released into the environment through waste disposal, agriculture, and manufacturing processes. The release of large quantities of drugs into the environment is very dangerous. Therefore, it is very important to sensing and analyzing the unused drugs which accumulate in soil or water [1-2]. Thus, the design of a method or system to sense the drugs in the environment is very important. The amantadine drug (Ad) can be one of those drugs that need to sense in the environment. The Ad drug is the most known functionalized adamantane (1-aminoadamantane) which is an antiviral and anti-Parkinson drug. Ad is used to treat the symptoms

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of Parkinson's disease. Ad also is used to treat symptoms of the influenza A virus and for treatment of respiratory infections caused by the influenza A virus. Ad controls movement problems by increasing the amount of dopamine in certain parts of the body.

Nanoparticles are a class of important materials for various applications including sensing drugs and toxic gases and batteries [3-5]. Nanoparticles have attracted the attention of researchers due to their high surface-to-volume ratio which is considerably increased the efficiency and performance [6-15]. The BN nanoparticles have been used as electronic materials due to their unique characteristics such as oxidation resistance, high thermal conductance, low dielectric constant, high-temperature strength, and high stability [16]. Among BN nanoparticles, the boron nitride nanosheets (BNNSh) have high stability and good electronic properties which can be used to sense and detecting of drugs and gases [17–20]. The surface modification of nano-particles was modified and improved by replacing impurity atoms and doping elements [20].

Dust Mohammadi and co-workers have reported the possibility of detecting the amantadine molecule onto the outer surface of pristine boron nitride nanosheet, as well as its Al, Ga, P, and As-doped structures. In this work, the B3LYP-D3 (BJ)/6-31G (d) method has been used to consider the contribution of scattering interactions to energy analysis, natural bond orbital, and quantum theory of atoms in the molecules [24].

Suna and co-workers have tried to find a suitable sensor for amantadine and they have examined the interaction between amantadine and $Al_{12}N_{12}$ and $B_{12}N_{12}$ nanoclusters. The amantadine molecule was adsorbed on $Al_{12}N_{12}$ and $B_{12}N_{12}$ by two different mechanisms, including electrostatic and charge transfer, respectively [25].

The synthesis of the boron nitride nanosheet and its doping composite have been investigated [26-27] and are widely applied as a catalyst and electronic devices. *Yan* and *co-workers* have synthesized the doped boron nitride nanosheet and used it as an electrocatalyst for ambient nitrogen reduction.

Following up on the previous works, in this research, the sensing character of a BNNSh and its doped derivatives was investigated over the amantadine drug. The novelty of this work is to study two main parameters involved in the sensing process including the adsorption energy (E_{ad}) and gap energy between HOMO and LUMO (E_g) for BNNSh/Ad system. Also, the role of the doped atoms such as the Si, Ge, and Ga atoms instead of a B atom in BNNSh were investigated to enhance the sensing character of BNNSh to the Ad drug.

THEORETICAL SECTION

Computational methods

All calculations were performed through the DFT method at the RCAM- B3LYP /6-31G* level of theory through GAMESS software [11].

The potential energy surface (PES) scans were carried out through various dihedral angles (D) to obtain the minimum energy of BNNSh/Ad. We also employed the Gausssum to draw the DOS plots [12].

The energy of adsorption (E_{ad}) was obtained as follows:

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

E(adsorbent) relates to the total energy on an extrinsic or intrinsic molecule. *E*(drug/adsorbent) relates to the total energy of the drug molecule which was adsorbed on the surface of BNNSh.

E_{BSSE} relates to the Basis Set Superposition Error (BSSE) that should be corrected for all adsorption energies through the counterpoise method [13].

Theory

Sensors are devices that exhibit suitable interactions under certain conditions. The energy of the HOMO-LUMO gap (E_g) of the structures was calculated as below:

$$E_{ad} = ELUMO - EHOMO \quad (2)$$

When the electronic sensitivity of nanoparticles is evaluated, the differences between the HOMO and the LUMO energies are computed as follows:

$$\Delta E_g = \left[\left(E_{g2} - E_{g1}\right)/E_{g1}\right] \times 100 \quad (3)$$

EXPERIMENTAL SECTION

The boron nitride nanosheet. (BNNSh) and Amantadine drug (Ad)

The molecular structure of the boron nitride nanosheet (BNNSh) was optimized in which two types of B-N bonds were observed with bond lengths of 1.44 and 1.45Å. The BNNSh have 33 B and 33 N atoms which the end atoms were saturated with 22 hydrogen atoms for avoiding the boundary effects (Fig. 1). The HOMO and LUMO energies of BNNSh are -8.02eV and 1.42eV, respectively,

and thus the difference between HOMO and LUMO (E_g) is 9.44 eV (Table 1).

The DFT studies indicated that the HOMO and LUMO levels were mostly placed on the N and B atoms, respectively which indicates the electron-rich of the N atoms and electron-poor of the B atoms.

The amantadine drug (Ad) has a polar site such as $–NH_2$ that the N and H atoms can interact with the boron atoms of BNNSh.

Amantadine-boron nitride nanosheet complex (BNNSh/Ad)

The optimization process was done to obtain the global minima for amantadine (Ad), boron nitride nanosheet (BNNSh), and BNNSh/Ad complex (Fig. 2). Due to obtaining the most stable configurations (global minima) of BNNSh/Ad complex, the numerous computations were performed. Two active sites of Ad were predicted, such as -N and –H heads, which can be interacted with the B atom of BNNSh. For the most stable BNNSH/Ad, the density of state plot (DOS), LUMO, and HOMO were obtained. It was found that there were two significant parameters such as E_{ad} and E_g in the sensing process of BNNSh. The Ad drug in the BNNSH/Ad complex adsorbed from the N atom on the B head of BNNSh with a distance of 3.28Å. The E_{ad} of -3.61kcal/mol showed a weak interaction between the Ad drug and BNNSh. The HOMO of the Ad drug was more focused on the N atom which interacts with the B atom of BNNSh. The DFT computations showed that the electronic aspects of BNNSh were changed when the Ad molecule was absorbed. As shown in Table 1, the HOMO level was changed from -8.02 in the BNNSh to -7.82eV in the BNNSH/Ad, and the LUMO level was changed from 1.42 to -1.47eV which shifted to higher energy. A pair of electrons on the N atom of the Ad drug was donated to the B atom of BNNSh.

As mentioned above, E_{ad} and E_g are two important factors in the sensing potential of the drugs using the BNNSh nanoparticles. If the E_{ad} is in a suitable range, the adsorption of Ad on BNNSh can be reversible. Stronger interactions are not favorable in sensing of Ad since recovery time would be high and therefore the desorption of drugs on BNNSh becomes hard. As E_{ad} becomes more negative, there is an increase in recovery time (τ) that can be computed as follows [14, 15]:

$$\tau = \nu_0^{-1}\exp(-Ead/kT) \quad (4)$$

where τ, ν_0, T, K signify the recovery time, attempt frequency, temperature, and the Boltzmann constant respectively [16].

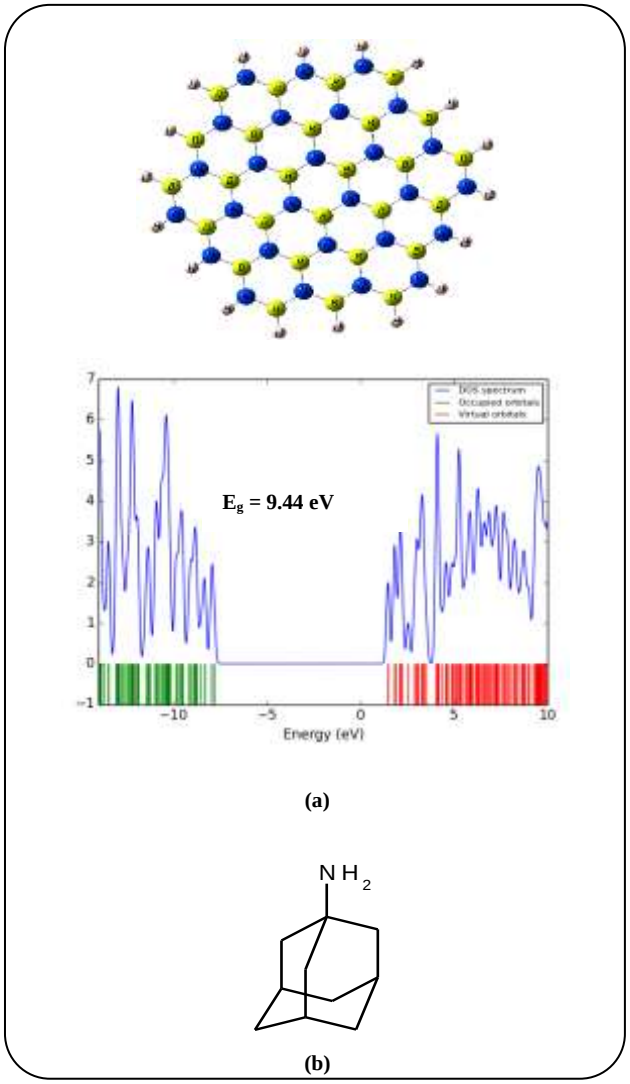

Fig. 1: (a) Optimized structures of BNNSh and density of state (DOS) plot; (b) Amantadine drug (Ad).

Based on equation (4), E_{ad} is exponentially related to τ. Sensor recovery is an important process that is possible to be used at higher temperatures than ambient temperature [17]. Vacuum-UV was employed for the recovery of the Ad molecule from the surface of BNNSh.

The energy of the HOMO–LUMO gap (E_g) of the BNNSh in the presence of Ad is the second significant parameter in the sensing capability. It has been demonstrated that E_g is proportional to the conduction electron population (σ) shown in Eq (5). When E_g decreases with the absorption of Ad on the BNNSh, the σ increases. The correlation between the Electrical Conductivity (EC) of nano-particles and E_g is as follows:

$$\sigma = A\,T^{3/2}\exp(-E_g/2kT) \quad (5)$$

Here k signifies the Boltzmann constant, and A (electrons/$m^3K^{3/2}$) signifies a constant. There is an acceptable correlation between the results obtained through this procedure and the experimental techniques reported in the literature [18].

The sensitivity of BNNSh to the Ad is determined using Equation (5). Hence, the decrease in the E_g can be led to make an electrical signal in the presence of the Ad molecule [22-24].

The E_g of BNNSh decreased after the adsorption of Ad over BNNSh which decreased from 9.44eV to 9.29eV with $\%\Delta E_g$ of -1.58%, indicating the low sensitivity of BNNSh to the Ad drug adsorption (Table 1 and Fig. 2). The HOMO of BNNSh/Ad was located on the drug surface and slightly on the surface of BNNSh, while LUMO was located on the surface of BNNSh (Fig. 2). Despite the change in E_g that is not suitable for the sensing capability, the E_{ad} of -3.61kcal/mol was so weak that BNNSh could not effectively adsorb Ad. Therefore, it can conclude that BNNSh is not a suitable sensing ability toward Ad since the E_g and E_{ad} parameters are not suitable.

Amantadine (Ad) adsorption over the Si-, Ge- and Ga-doped BNNSh

Amantadine-Ga-doped boron nitride nanosheet (Ga-BNNSh/Ad)

In Ga-BNNSh, the B atom of BNNSh was replaced with the Ga atom due to finding a nanoparticle with high sensitivity. The geometric structure and characteristics of Ga-doped BNNSh were investigated. Since the radius of Ga is larger than that of the B atom, the Ga atom was placed out of the Ga-BNNSh surface. The distance of Ga-N in Ga-BNNSh was 1.78 Å. DFT calculations clarified that there was no significant decrease in the HOMO from -8.00 in BNNSh to -7.58eV in Ga-BNNSh. However, there was a slight increase in the LUMO from 0.09 in the pure BNNSh to 1.66eV in the Ga-doped-BNNSh. The E_g changed from 9.44eV in the pristine BNNSh to 8.09eV in Ga- BNNSh which indicated that Ga—BNNSh nanoparticles became a slight semiconductor character (Table 1).

The interactions between Ad and Ga-doped BNNSh were also investigated. It found two active sites in the Ad drug, such as -N and –H heads, which could be adsorbed on the Ga atom of Ga-BNNSh (Fig. 3). The DOS plot was also calculated. The Ga atom of Ga-BNNSh strongly interacted with the N head of Ad by E_{ad} of -52.79 kcal/mol and Ga….N distance was 2.04Å.

The HOMO level was changed from -8.00 in Ga-

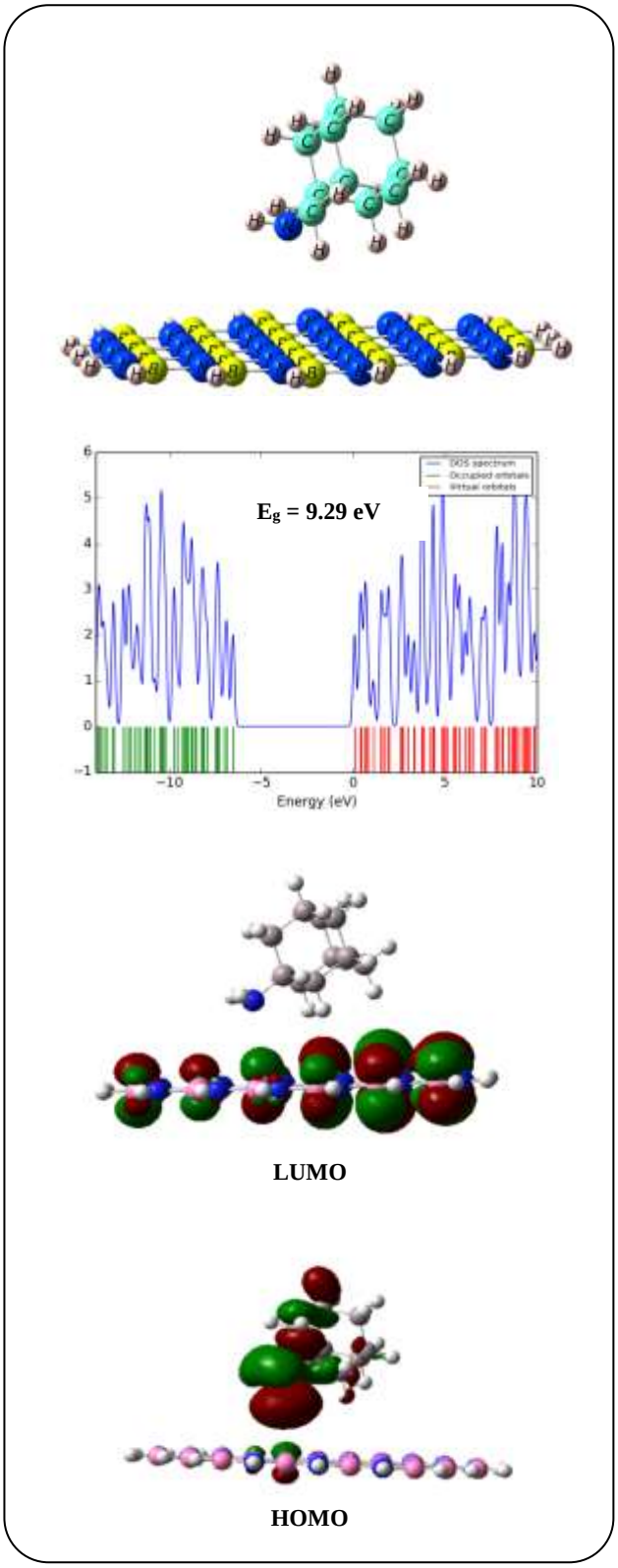

Fig. 2: Optimized structure of the Ad molecule on BNNSh and density of state (DOS) plot of BNNSh/Ad and the HOMO, and LUMO profiles of complex BNNSh/Ad (NH_2).

Table 1: Absorption energies (Eads), the energy of HOMO and LUMO orbitals, energy difference of HOMO and LUMO orbitals (E_g), Fermi level energy (EFL), electron transfer number (∆N) and dipole moment (DM) and working function for boron nitride nanosheet and its doped derivatives over the amantadine drug.

Systems	E_{ads} (kcal/mol)	E_{HOMO} (eV)	E_{FL} (eV)	E_{LUMO} (eV)	E_g (eV)	$^{*}\%\Delta E_g$	ΔN	DM (Debye)	Φ (eV)	$^{**}\Delta\Phi$ (eV)
B-BN	---	-8.02	-3.30	1.42	9.44	---	---	0.01	3.30	---
B-BN-Ad	-3.61	-7.82	-3.18	1.47	9.29	-1.58	-0.05	1.57	3.18	-3.91
Si-BN	---	-6.32	-2.47	1.39	7.72	---	---	0.84	2.47	---
Si-BN-Ad	-5.62	-5.71	-1.90	1.90	7.61	-1.41	-0.02	2.35	1.90	29.73
Ga-BN	---	-8.00	-3.95	0.09	8.09	---	---	0.14	3.95	33.63
Ga-BN-Ad	-52.79	-7.58	-2.96	1.66	9.24	12.39	-0.14	7.20	2.96	---
Ge-BN	---	-6.86	-2.72	1.42	8.28			0.41	2.72	----
Ge-BN-Ad	-19.67	-5.05	-1.80	1.45	6.50	-21.50	-0.04	4.36	2.07	31.36

BNNSh to -7.58eV in Ga—BNNSh/Ad, and the LUMO was significantly changed from 0.09 to 1.66eV. The HOMO did not change on the Ga-BNNSh surface while the LUMO was found on the surface of Ga-BNNSh. The E_g increased from 8.09 in Ga-BNNSh to 9.24 eV in Ga-BNNSh/Ad with the change rate of $\%\Delta E_g$ = +12.39%; indicating that Ga-BNNSh is not sensitive to the adsorption of Ad. The low change in E_g showed Ga-BNNSh was not suitable for the sensing ability. Besides, the E_{ad} of -52.79 kcal/mol was so high which indicated Ga- BNNSh strongly adsorbed Ad, which showed that the recovery time was high. Therefore, the Ga-BNNSh did not show a suitable sensing ability regarding lower $\%\Delta E_g$.

Amantadine-Ge-doped boron nitride nanosheet (Ge-BNNSh/Ad)

In Ge-BNNSh, the B atom of BNNSh is replaced with the Ge atom for finding a nanoparticle with high sensitivity. The geometric structures and characteristics of Ge-doped BNNSh were scrutinized. Since the radius of Ge was larger than that of the B atom, the Ge atom was placed out of the BNNSh surface. The distance of the Ge-N in Ge-BNNSh was 1.81 Å.

DFT calculations clarified that there was no significant decrease in the HOMO from -6.86 in BNNSh to -5.05eV in Ge-BNNSh while the LUMO increased from 1.42 in the pure BNNSh to 1.45eV in the Ge-BNNSh. The E_g changed from 8.28 eV in the pure BNNSh to 6.50eV in Ge-BNNSh which indicated that Ge-BNNSh became a semi-conductor in comparison with the pure BNNSh (Table 1).

The interactions between Ad and Ge-doped BNNSh were scrutinized. Two active sites including -N and –H heads of the Ad drug adsorbed to the Ge atom of Ge-BNNSh (Fig. 4 and Table 1). The DOS plot was also calculated. The Ge atom of Ge-BNNSh interacted suitably with the N head of Ad by E_{ad} of -19.67 kcal/mol and the Ge….N distance was 2.46Å.

The HOMO level was changed from -6.86 in Ge-BNNSh to -5.05eV in Ge-BNNSh/Ad complex and the LUMO was not significantly changed from 1.42 to 1.45eV. The HOMO on the N atom of Ad transferred to the Ge atom in Ge-BNNSh/Ad, while LUMO orbital was located on the Ge-BNNSh.

The E_g decreased significantly from 8.28 in Ge-BNNSh to 6.50eV in Ge-BNNSh/Ad and the rate of change was $\%\ \Delta E_g$= -21.50% which showed a good sensitivity of Ge-BNNSh to the adsorption of Ad. The high change in E_g and high sensitivity led to the design of a suitable sensing device. Besides, the E_{ad} of -19.67 kcal/mol was a suitable interaction amount that the Ge-BNNSh adsorbed Ad with a low recovery time which would be suitable for sensing ability. Therefore, the Ge-doped BNNSh was a promising candidate for a good sensing ability.

As above-mentioned, because of the suitable E_{ad} of -19.67kcal/mol which led to a lower recovery time and a high $\%\ \Delta E_g$ =-21.50%, it can be concluded that the Ge-doped BNNSh was a promising candidate for sensing the Ad drug.

Amantadine-Si-doped boron nitride nanosheet (Si-BNNSh/Ad)

In Si-BNNSh, the Si atom was replaced instead of the B atom in the BNNSh for finding a highly sensitive nanoparticle. The geometric structures and characteristics of Si–BNNSh were investigated. The DOS plot of Si–BNNSh was calculated. Since the radius of the Si atom was larger

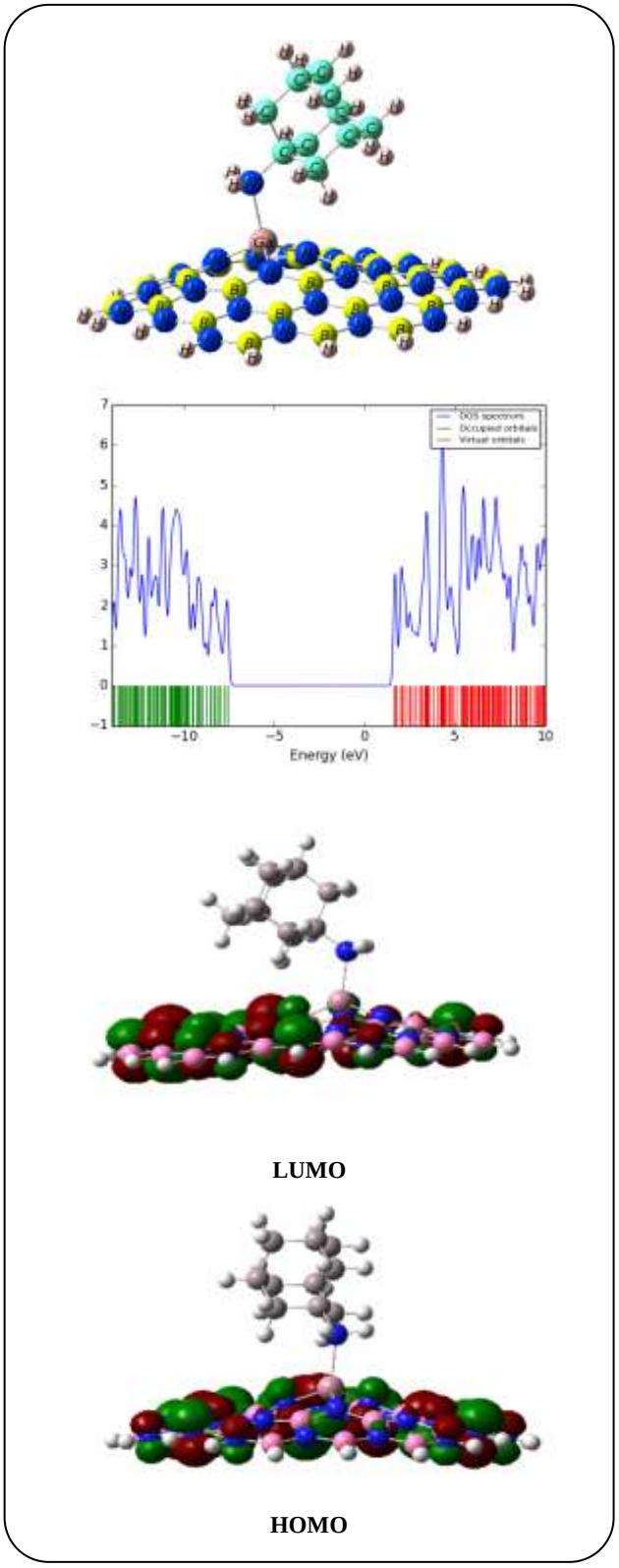

Fig. 3: Optimized structure of Ga-BNNSh/Ad and its density of state (DOS) diagram and the HOMO, and LUMO profiles of Ga-BNNSh/Ad.

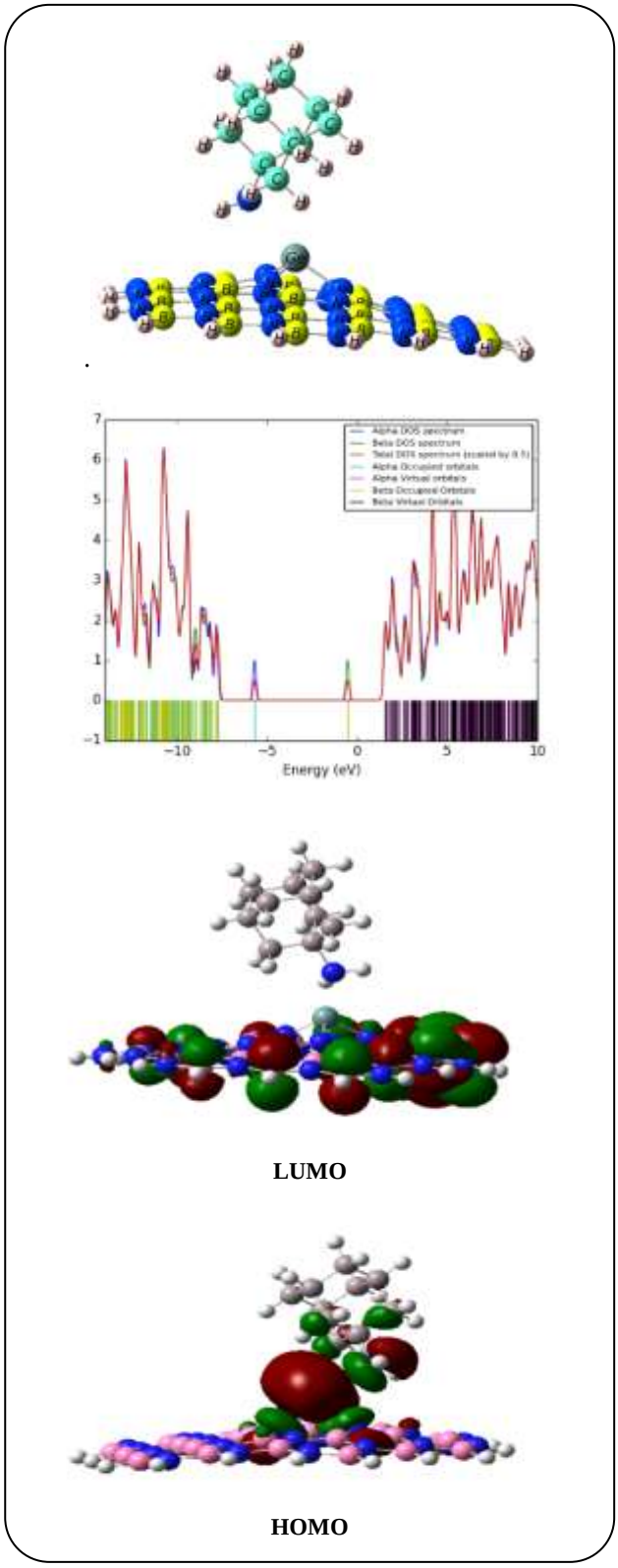

Fig. 4: Optimized structure of Ge-BNNSh/Ad and its density of state (DOS) diagram, and LUMO profiles of Ge-BNNSh/Ad.

than that of the B atom, the Si atom was placed out of the Si-BNNSh surface, and the distance of Si-N in Si-BNNSh was 1.72 Å. There was a considerable decrease in the HOMO from -6.32 in Si–BNNSh to -5.71eV in Si–BNNSh/Ad after adsorbing Ad (Fig. 5) while the LUMO increased from 1.39 in the Si–BNNSh to 1.90eV in the Si–BNNSh/Ad complex. There was not a significant increase in E_g from 7.72eV in Si–BNNSh to 7.61eV in Si–BNNSh/Ad. According to the DFT calculations, the E_g for Si–BNNSh slightly increased in the Si–BNNSh/Ad complex by $\%\Delta E_g$ of -1.41 (Table 1).

The Si atom of Si-BNNSh interacted with the N head of Ad (E_{ad} of -5.62 kcal/mol) and the Si….N distance was 2.86 Å. The E_{ad} for the Si–BNNSh/Ad was found to be low.

The HOMO changed from -6.32 in Si–BNNSh to -5.71eV in the Si–BNNSh/Ad complex while there was a slight change in the LUMO from 1.39 in Si–BNNSh to 1.90 eV in the Si–BNNSh/Ad. The HOMO was transferred to Si–BNNSh in the Si–BNNSh/Ad complex, but the LUMO did not change on the Si–BNNSh surface. There was a slight change in E_g from 7.72eV in Si–BNNSh to 7.61eV in the Si–BNNSh/Ad complex with the change rate of $\% \Delta E_g$= -1.41%, which demonstrated that the sensitivity of Si–BNNSh to the adsorption of Ad was very low. Very low of $\% \Delta E_g$ showed Si–BNNSh was not suitable for the sensing ability. The E_{ad} of -5.62 kcal/mol was also low so that the Si–BNNSh could not effectively adsorb Ad. Hence, the Si–BNNSh did not exhibit a suitable sensing ability regarding both lower $\% \Delta E_g$ and lower absorption energy, E_{ad}, for Ad.

CONCLUSIONS

In this wrk, the interaction energy and the sensing ability of the pure, Si-, Ga- and Ge-doped BNNSh over the Ad drug were investigated. The change in the adsorption energy (E_{ad}) between the pure, Si-, Ga- and Al-doped BNNSh and Ad were in the following order: Ga-BNNSh/Ad > Ge-BNNSh/Ad > Si-BNNSh/Ad > BNNSh/Ad. The E_{ad} of BNNSh/Ad and Si-BNNSh/Ad is -3.61 and -5.62 kcal/mol, respectively which indicated weak adsorption for the sensing ability. Besides, the $\% \Delta E_g$ of BNNSh/Ad and Si-BNNSh/Ad are -1.58 and -1.41, respectively which showed the low sensitivity of BNNSh and Si-BNNSh to the adsorption of Ad.

The E_{ad} of Ga-BNNSh/Ad is -52.79 which is very strong that showed a high recovery time which indicated this device is not suitable. Also, the $\% \Delta E_g$ for the Ga-BNNSh/Ad is +12.39 which shows a low sensitivity for sensing the Ad drug.

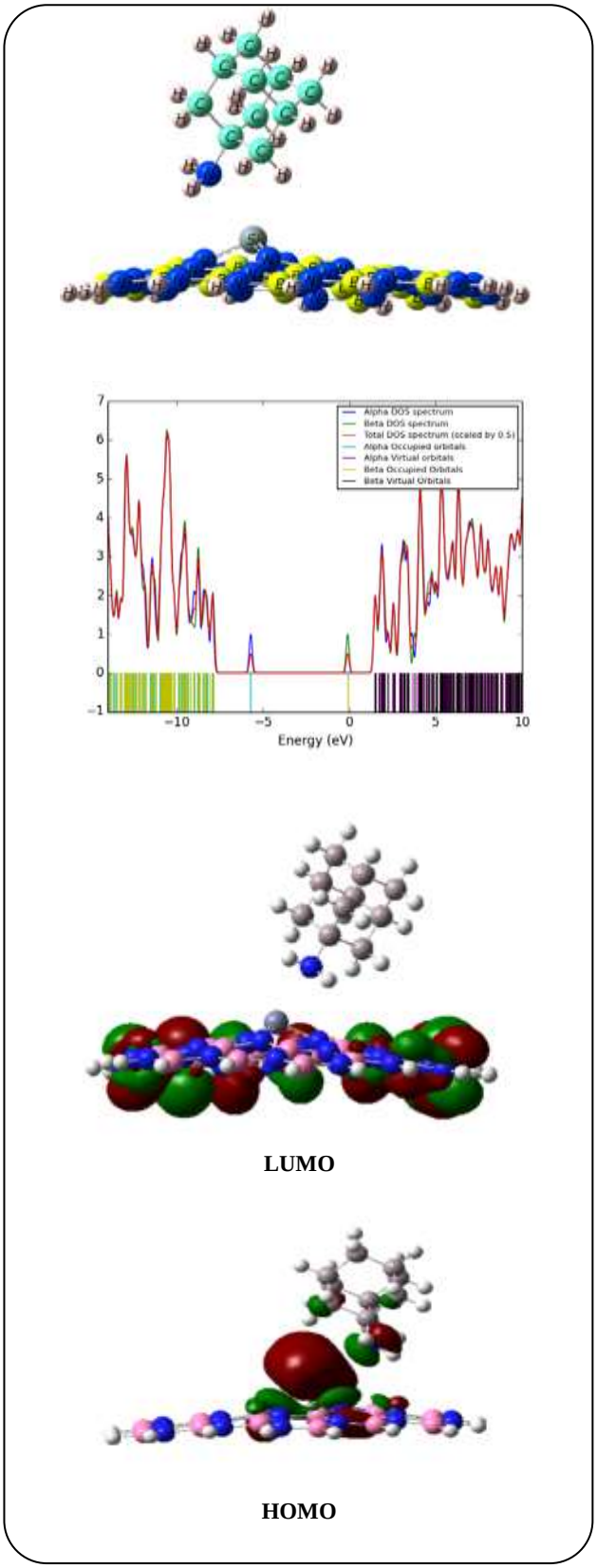

Fig. 5: Optimized structure of Si–BNNSh/Ad and its density of state (DOS) diagram. and LUMO profiles of Si-BNNSh/Ad.

Finally, the E_{ad} for Ge-BNNSh/Ad was -19.67, which indicated a suitable sensing ability. Also, the % ΔE_g for the Ge-BNNSh/Ad was -21.50 which showed a high sensitivity for sensing the Ad drug.

Therefore, this study implied that the Ge-BNNSh nanoparticle is an encouraging candidate for being a possible sensor of the Ad drug.

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