Study the Adsorption of Letrozole Drug on the Silicon Doped Graphdiyne Monolayer: a DFT Investigation

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Abstract

In the current study, by employing first-principles computations, the adsorption behavior of letrozole (LET) was investigated on the pristine graphdiyne nanosheet (GDY) as well as Si-doped graphdiyne (SiGDY). According to the adsorption energy, charge transfer value, and the change in the band gap energy, the tendency of the pristine GDY towards LET is insignificant. However, the interaction of LET with SiGDY was strong and the adsorption energy was approximately -19.20 kcal/mol. In addition, the associated electrical conductivity with SiGDY increased by approximately 23.53 % following the adsorption of LET. The results show that SiGDY can be employed as an electronic sensor to detect LET. Furthermore, LET is detected by SiGDY in the water phase based on the magnitude of solvation energy. Finally, a considerable charge-transfer between LET and SiGDY is a precondition for the adsorption of the LET molecule with proper binding energies, which delivers the Si atoms with a significant positive charge.

Keywords Graphdiyne nanosheet · Electrical conductivity · Solvation energy · Electronic sensor

1 Introduction

Recently, deaths from various cancers are more significant than other diseases. Prescribing anticancer drugs to the target cell improves patient survival and limits further tumor proliferation [1–7]. One of the side effects on the natural cell is increasing anti-cancer drugs in the patient body [8–14]. For this reason, we need to control and diagnose the concentration

of anti-cancer drugs [15–19]. Improvement of clinical efficacy and helping to prescribe drugs for malignant cells are the results of the development of the drug sensing system. The importance of the drug sensing system for the incomplete diagnosis of drug concentrations to normal cells is too great [20–23]. Also, different methods were developed for the detection of different drug and biomaterials [4, 24–28].

For many applications such as biosensors, chemical sensors, and catalysts, the recent developments in the carbonaceous material such as graphane, graphyne, and graphdiyne are the pioneers in the research field [29–36]. In addition, in recent years the detection of many different viruses was important for controlling disease spread [37–41]. According to molecular dynamics, Barraza-Lopez and Kaloni have been considered the water dissociation on the monolayer monochalcogenides of group IV, like phosphorene, GeS, GeTe, and GeSe [42–47]. Graphdiyne (GDY) is the new carbon allotrope of the graphyne family. Graphyne is the assembled low dimensional layer of sp and sp² hybridized C-atoms, which is prone to energy materials use. Moreover, GDY is synthesized using hexaethynylbenzene by way of cross-coupling on the copper foil surface [48–51]. GDY sheet consists of carbon-carbon triple bond with benzene rings in its structure while the connection of this benzene ring to the six adjacent benzene rings is through carbon-carbon triple bonds.

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It has an exceptional electronic structure and chemical stability, due to sp and sp² hybridized carbon atoms [52–57].

For improvement the properties of carbon based material were used different methods such as defect, doping and etc. [58–60]. Among of all doped material metallic compounds are very interesting based on the specific properties [61]. We choice silicon atom because silicon is the most abundant electropositive element in the Earth's crust. Due to the interesting features of SiGDY, such as thermal stability, mechanical reaction, optical enhancement, and thermal conductivity, the presence of silicon centers uniformly in a distributed carbon network constructs additional connection points for metal centers [62].

We have employed density functional theory (DFT) computations to study its potential application of GDY and SiGDY as a high effectual sensor material for sensing of letrozole (LET) anti-cancer drug. We have also studied and reported the quantum molecular descriptors, including Fermi level, charge analysis, and electrical conductivity in the recent research. To investigate drug solubility in an aquatic solution, we studied solvation energy for the SiGDY nanosheet and LET drug.

2 Computational Details

The optimization of structures and all quantum molecular descriptors such as electrical conductivity, charge transfer, and density of states (DOS) analyses were executed by the B3LYP-D functional 6-31G (d) basis set. By addition grimme dispersion term “D” to B3LYP functional the weak interactions was considered [63]. Researches reviews indicate that B3LYP is a reliable and proper density functional for the anticipation of the optic, structural, energetic, and electronic characteristics of various nanostructures [64, 65]. All of the computations were executed by the GAMESS suit of program [66]. The adsorption energy (E_{ad}) for the mustard drug interaction with the graphyne is calculated by the following equation:

$$E_{\text{ad}} = E_{(\text{complex})} - E_{(\text{GDY or SiGDY})} - E_{(\text{LET})} + E_{\text{BSSE}} \quad (1)$$

where E (GDY or SiGDY) is the energy of GDY (SiGDY) sheet. E (complex) is the energy of each GDY (SiGDY) with a mustard gas adsorbed on its surface. The counterpoise approach had predicted the base set superposition error energy (EBSSE) [67]. The HOMO-LUMO energy gap (E_g) of all structures was computed as follows:

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

The GaussSum program was applied to draw the DOS plots [68].

3 Results and Discussion

3.1 GDY Nanosheet Geometric Optimization and Electronic Properties

The suggested project includes GDY nanosheet as a base material, which was used to adsorb the TPA drug. Figure 1 demonstrates the bond distance between different carbons namely (d_1 , d_2 , d_3 , and d_4) on GDY compounds. The calculated bond distances were diagnosed 1.419 Å, between different carbons in the hexagonal ring [69]. Further, the sp–sp hybridization bond length was observed 1.213 Å in acetylenic links [69]. The binding length among sp²–sp² differs between each C–element pairs which are depicted in Fig. 1.

We really would desire to demonstrate the basic things for the GDY sheets, which mostly contain two different pores: (i) quasi-triangular pore found in the acetylene linkers; (ii) On six-member carbon ring the hexagonal pore was observed. Because the GDY sheets of carbon materials was used to absorb drugs, the structural stability of the base materials must first be well established. The structural stability of the pure GDY sheet was investigated by the term below with the cohesive energy (E_{coh}) provided [70]:

$$E_{\text{coh}} = (1/m) (E_{(\text{GDY-NS})} - m E_C) \quad (3)$$

Where E (GDY sheet) expresses the overall energy of GDY, while $E(C)$ depicts the energy of the lone C-atom, ‘ m ’ represents the total C-elements assembled in the substance GDY. It is estimated that the E_{coh} of the GDY sheet is – 7.391 eV / atom, which possibly agrees with the published research (– 7.20 eV / atom) [70]. GDY nanosheets are stable in its structure by the obvious anticipation of the negative E_{coh} . GDY sheet also possesses the energy band gap E_g of 2.61 eV.

Fig. 1 Optimized structure of GDY nanosheet

3.2 LET Adsorption on Pristine GDY Nanosheet

We discuss the interaction of LET drug in GDY with three important parameters, which are adsorption energy, energy gap change (E_g), and charge transfer (Q). As demonstrated in Fig. 2, the complex of LET drug on GDY surface. Before starting the study of drug adsorption on GDY sheets, we conducted adsorption studies at various sites that exceeded carbon atoms, triangular pores, and hexagonal pores. Based on the adsorption energy and distance between drug and GDY versus energy, only one set is minimal in terms of global position. All the other sites of drug adsorption on GDY sheets are excluded from the discussion. The adsorption energy, charge transfer (Q), and average energy gap variation (E_g^a) of GDY-LET complex are summarized in Table 1. The adsorption energy of the LET-GDY complex is computed -7.64 kcal/mol at the current research. The binding of the drug on the GDY sheet is obviously inferred by negative adsorption energy. In addition, the absorption energy causes the physical absorption of drug molecules on GDY sheets and is a weak value. By the way, the lower value of adsorption energy classifies the process as physisorption mainly due to slightly weak van der Waal forces.

Charge transfer is of critical importance in adsorption process of LET over GDY sheet [71–73]. An important point to note is the charge carrier. In this research, the magnitude of the charge carrier for the adsorption site of the drug is positive. This means that the charge is carried from the LET drug to the GDY sheet. Can be note, when charges are carried from drugs to GDYs, there may be a slight distortion of the lattice, which

Table 1 Adsorption energy (E_{ad} , kcal/mol for LET drug adsorption on the GDY and SiGDY)

Structure	E_{ad}	E_{HOMO}	E_F	E_{LUMO}	E_g	$\Delta E_g(\%)$	Q
GDY	-	-5.22	-3.89	-2.58	2.60	-	-
LET/GDY	-7.64	-4.11	-2.96	-1.82	2.29	12.31	0.089
SiGDY	-	-4.55	-3.25	-1.96	2.59	-	-
LET/SiGDY	-19.20	-2.97	-1.97	-0.99	1.98	23.83	0.903

Energy of Fermi level (E_F), HOMO, and LUMO, and HOMO-LUMO energy gap (E_g) in eV. The ΔE_g indicates the change of E_g after the adsorption process. Charge transfer value (Q)

is reflected in the change in the band gap. In addition, the charge transfer depends on the structure of the drug that absorbs it into the GDY sheet. The Q value could be insignificant for the LET-GDY complex. The trivial amount of Q was created due to the place where the charge is not effectively absorbed and transferred.

We are changing our focus on the GDY band gap on LET drug interaction [74, 75]. The energy gap of GDY gets decreased from 2.61 eV for the pristine form to 2.29 eV in the LET-GDY complex upon the adsorption of the aforesaid drugs. The average energy band gap also changes $E_g^a \%$, which is negligible for the LET-GDY complex. Therefore, adsorption energy, Q and $E_g^a \%$ results show that the GDY sheet cannot be used as a competent efficient device for LET drug sensing. We used another strategy to increase the sensitivity of the GDY sheet to the LET drug in the next section.

Fig. 2 The optimized structure of LET/GDY complexes

3.3 SiGDY Nanosheet Geometric Optimization and Electronic Properties

Figure 3 shows the SiGDY optimized structure. In this analysis, the BGDY monolayer consisted of the following two C-C bond types with a length of 1.419 Å and 1.417 Å and the Si-C bond of 1.861 and 1.834 Å. SiGDY maintains a semiconducting characteristic with an energy gap of 2.59 eV in pristine form. Mostly on the Si-doped site is the HOMO electron density is shown in Fig. 3.

3.4 LET Adsorption on Pristine SiGDY Nanosheet

The optimized structures of LET with the S side on the SiGDY sheet as illustrated in Fig. 4. All of the electronic characteristics of SiGDY about the interaction of LET drug similar to pristine GDY as indicated in Table 1. The adsorption energy of LET on the SiGDY sheet is computed −19.20 kcal/mol. Besides, the charge carrier possesses a positive magnitude comparable to the pure GDY for the drug adsorption site. The charge transfer magnitude for LET on the SiGDY sheet is higher than for GDY. The outstanding magnitude of Q creates a more positive charge due to the presence of the Si-doped site, in which charge transfer and adsorption occur efficiently. Also, the energy gap of SiGDY is decreased on the adsorption of the aforesaid LET drug from 2.59 eV for the pristine form to 1.98 eV and that is corresponding to the $E_g^a\%$, which has been changed significantly. It can be used as a sensitive sensor in the diagnosis of LET drugs, unlike pristine GDY, based on what we have calculated. In the Table 2, the physical parameters obtained in the current study were contrasted with the results of reports from articles on the measurement of the different drug by employing theoretical methods. Based on Table 2, the adsorption energy of

Fig. 3 Optimized structures of SiGDY nanosheet

Fig. 4 The optimized structure of LET/SiGDY complex

the different drug on different two-dimensional, with regard to the differences in the calculation method, is generally in the physical adsorption range. And this result was also obtained for the adsorption of SiGDY in the current study. In addition to acceptable absorption energy, the decrease in the E_g band gap is also another important quantity of the sensor capability. The decrease in E_g in the current study is comparable with the reduction in E_g reported by two-dimensional materials in Table 2. Also, the amount of charge transfer from the drug to the adsorbent surface is another important quantity in confirming the interaction between the adsorbed surface and the adsorbent. The charge transfer in the SiGDY@LET system is also higher than the charge transfer reported for similar systems. Ganjali and et al. [76] by preparation of PVC membrane electrode successfully were determined LET in some pharmaceutical formulations. The PVC membrane electrode sensor response was about 1943 in the low range concentration of LET drug. In this work, the value of Si-GDY sensor response for LET drug by DFT is about 1462 and comparable to the above experimental method.

3.5 DOS Spectrum Studies of SiGDY Upon the Interaction of LET Drug

As illustrated in Fig. 5, the density of states profile show the main role in the adsorption properties of LET drugs on SiGDY sheets [80, 82, 83]. The pristine SiGDY sheet also shows the energy gap of 2.59 eV. Contrary, by the adsorption of LET drug in the SiGDY surface, band gap of SiGDY was reduces. The reason for the change in the structure of the band after drug absorption is as follows: The molecules such as the LET drug, due to their unique structure, clearly reduce the

Table 2 Summary of different drug detection with different materials based on the theoretical methods

Compound	Method	Parameters			Ref
		E_{ad} (Kcal/mol)	ΔE_g (%)	Charge transfers (e)	
Al-BNNT	DFT/ B3LYP/6–31G*	-42.89	-38.01	-0.13	[77]
BNNCS	DFT/ B3LYP-D/6–311G**	-41.02	-38.68	-0.11	[78]
GO	DFT/ M05-2X/6–31G**	-79.58	-49.61	-0.14	[79]
BNNCS	DFT/ B3LYP-D/6–31G*	-11.90	-30.70	-0.21	[80]
ZnO sheet	DFT/ B3LYP-D/6–31G*	-19.20	-23.83	-0.909	[81]
Si-GDY	DFT/ B3LYP-D/6–31G*	-21.74	-35.89	-0.549	This work

band gap compared to the isolated SiGDY sheet. In addition, LET has an N atom, after absorption for complex SiGDY-LET, the band gap is reduced to 1.98 eV. A comparison between DOS of SiGDY and SiGDY-LET indicates a charge transfer during LET adsorption. Additionally, a significant shift of valence and conductance bands can be observed for SiGDY-LET complex. According to DOS analysis band structure of adsorption complex, an electron transfer is dedicated between LET and SiGDY while these changes are negligible when GDY is examined as LET adsorbent substrate. As a result, the DOS spectrum show that the absorption of

LET leads to the transfer of electrons between drug molecules and SiGDY sheet materials (unlike virgin GDY), which is observed from the peak change and change in the DOS spectrum at different energy levels. In Fig. 6 can be seen the correlation between the parameters energy of adsorption, the charges transfer, and the variation of the electrical conductivity for GDY and Si-GDY after drug adsorption. According to Fig. 6, the value of the energy of adsorption and the variation of the electrical conductivity was increased about twice in the Si-GDY than to GDY after LET drug adsorption. While the charges transfer in Si-GDY was increase about tenfold as compared to pristine GDY.

Fig. 5 The partial density of states for SiGDY and LET/SiGDY complex

3.6 Solvation Energy Investigation

Solvation energy is used to validate the solubility of LET drug in the water medium, which plays a critical role in the

Fig. 6 Correlation between of physical parameters after LET drug adsorption in the GDY and Si-GDY surface

presence of the drug and SiGDY nanosheets in water. We placed the whole system in the aqueous phase to investigate the solubility factors of the drug and SiGDY sheet on water. The dielectric constant of water was simulated by keeping at 78.8. According to the following equations, the solvation energy is computed [84]:

$$E_{ad}^{Gas} = (E_{complex} - E_{SiGDY} - E_{drug}) \quad (4)$$

$$E_{ad}^{Solv} = (E_{complex-hyd} - E_{SiGDY-hyd} - E_{drug-hyd}) \quad (5)$$

$$E_{ad}^{Solv} = (E_{complex} + E_{complex}^{solv}) - (E_{SiGDY} + E_{SiGDY}^{solv}) - (E_{drug} + E_{drug}^{solv}) \quad (6)$$

$$E_{ad}^{Solv} = E_{ads}^{Gas} + E_{complex}^{solv} - E_{SiGDY}^{solv} - E_{drug}^{solv} \quad (7)$$

where, E_{SiGDY} , E_{comp} , and E_{drug} attributes the energy of isolated SiGDY nanosheet, SiGDY-LET complex and the energy of drugs, respectively. Similarly, $E_{SiGDY-hyd}$, $E_{comp-hyd}$, and $E_{drug-hyd}$ indicate the corresponding energy of hydrated SiGDY, hydrated drugs, and hydrated complex, respectively. The solvation energy was computed about -60.74 kcal/mol for SiGDY-LET complex. In addition, the solvation energy of the LET drug on the SiGDY sheet reveals the solubility of the aforesaid drugs in the aqueous phase. This result proved that SiGDY can be used as a sensitive sensor for LET drugs in the aqueous phase. The response of SiGDY sensor to different molecules which are present in the environment, such as methanol (CH_3OH), water (H_2O), and acetone (CH_3COCH_3) was investigated. All of these molecules were absorbed on the SiGDY. Compared to the LET drug, the interaction of the aforementioned molecules with SiGDY was weaker and the variation of electrical conductivity is low.

4 Conclusions

The interaction of LET drugs with GDY and SiGDY surface were investigated by considering of different parameters such as energy of adsorption, the charges transfer, and the variation of the electrical conductivity based on the DFT calculations. The low-value energy of adsorption of LET drugs on the GDY sheets is observed and the low amounts weaken the binding of the drug to the GDY sheets. Furthermore, the amount of charge transfer and variation electrical conductivity was slight, in the process of absorbing LET on the GDY sheet. While, the value of LET absorption energy has increased to -19.20 kcal/mol by doping Si atom in the GDY sheet. Also, the electrical conductivity of SiGDY was increased about 23.53 % during the adsorption process of LET drug compare to pristine GDY.

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Data Availability Confirm.

Declarations

Conflicts of Interest None.

Ethical Approval Not required.

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