A computational study on developing Tween-Type-Graphdiyne based fluorescent sensor for rapid and sensitive detection of vitamin C

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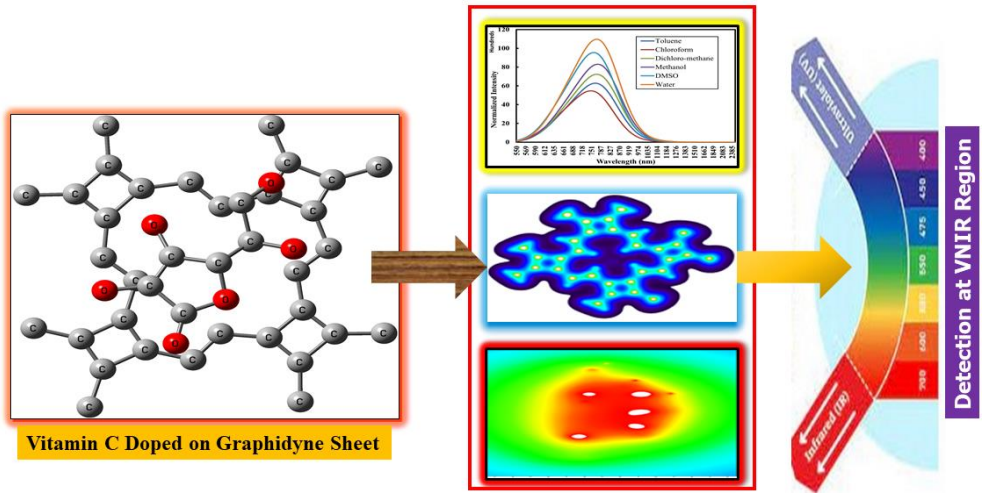
Abstract

We report a theoretical study on graphdiyne (**GD**) palced with vitamin C derivative as a fluorescent sensor for the detection of vitamin C. First, we performed frontier molecular orbital (FMO) calculations to determine the electronic properties of the sensor. Geometry optimization was then performed to obtain the optimized structure of the sensor. The UV spectra and emission spectra of the sensor were calculated using time-dependent density functional theory (TD-DFT). Our calculations show that the sensor exhibits a strong fluorescent response upon interaction with vitamin C, with a possible range of values between 340-353 nm. Their absorbance maxima (λ_{max}) were reported to be 1005-1115 nm range. The Stokes shift of the sensor was calculated to be 30 nm. The global chemical reactivity values of the sensor were calculated using density functional theory (DFT). The results showed a Stokes shift correlation of 0.69 and an electrophilicity (ω) value of 0.70eV for vitamin C-placed on graphdiyne, indicating a positive correlation between the polarity of the solvent and the Stokes shift and the sensor with its capability of accepting electrons. Our calculations show that the sensor is highly reactive towards vitamin C with a low energy gap (E_{gap}) between the HOMO and LUMO orbitals. This work presents a promising platform for the development of new vitamin C detection strategies with potential applications in the food and pharmaceutical industries.

Keywords: DFT; GD; TD-DFT; Vitamin C, Fluorescent, Graphdiyne



GRAPHICAL ABSTRACT

Introduction

Vitamin C, also known as ascorbic acid, is an essential nutrient for humans and it plays a vital role in various biological processes and is required for the proper functioning of the immune system [1]. The deficiency of vitamin C can lead to various health problems, such as scurvy, and has been associated with an increased risk of chronic diseases, such as cancer and cardiovascular diseases [2]. Therefore, the accurate and sensitive detection of vitamin C is of great importance in the food and pharmaceutical industries [3]. The fluorescence-based sensors have emerged as a promising approach for the detection of various analytes, including vitamins [4]. Among various materials, graphdiyne (**GD)** has attracted significant attention due to its unique electronic and optical properties [5]. It is a two-dimensional carbon allotrope with *sp* and sp^2 hybridized carbon atoms, which provides it with remarkable mechanical, electronic, and optical properties [6]. Vitamin C is a crucial nutrient for human health, and it is found naturally in many foods and supplements [7]. The sensing of vitamin C is important in food and medicine because it can help to ensure that people are getting the appropriate levels of this nutrient in their diets or medications [8]. In food, the sensing of vitamin C can help to determine if a product is fresh and has not degraded over time, which can be a sign of spoilage [9]. In medicine, the sensing of vitamin C can help to ensure that a medication is stable and active [10], and that it will be effective for patients who need it [11]. The sensing of vitamin C could play an important role in promoting health and well-being in

people of all ages [12]. Recent studies have shown that GD can be functionalized with various functional groups to create highly sensitive and selective sensors for various analytes, including vitamins [13]. The family of graphdiynes comprises a diverse range of compounds derived from aromatic hydrocarbons, including benzene, cyclopentadiene, and cyclobutadiene [14]. These compounds exhibit unique structural forms that are characterized by alternating single and triple bonds between carbon atoms. Benzene-derived graphdiynes showcase a honeycomb-like pattern, while those derived from cyclopentadiene and cyclobutadiene possess their own distinct structures [15]. Cyclopentadiene derivatives boast a similar alternating bond pattern, offering intriguing possibilities for various applications. On the other hand, cyclobutadiene derivatives feature a compact four-membered ring structure. The alternating bond patterns in all these graphdiyne compounds make them highly captivating and open up exciting avenues for further exploration and application in diverse fields [16]. In the realm of sensing applications, the family of graphdiynes has emerged as a promising field of study. Among the various types of graphdiynes, benzene derivatives have garnered notable attention for their structural versatility and adaptability as sensors [17]. Benzene-based graphdiynes possess a distinct and intricate framework, characterized by alternating single and triple bonds, resembling a honeycomb pattern as this unique structure enables easy functionalization and modification, allowing for the introduction of specific sensor functionalities [18].

Unlike cyclobutadiene derivatives, which exist primarily in metal-containing forms and have limited sensing potential, benzene derivatives offer a more universal and widely applicable sensing platform [19]. By tailoring the chemical composition of benzene derivatives, researchers have successfully harnessed their sensing capabilities for a diverse range of analytes, including gases, liquids, and biomolecules [20]. This adaptability in functionalization has led to exciting advancements in environmental monitoring, healthcare diagnostics, and industrial process control. In light of this, our study seeks to explore the sensing capabilities of benzene derivatives within the graphdiyne family and their implications in various sensing applications. By comprehensively understanding and exploiting the unique properties of these compounds, we aim to contribute to the advancement of sensor technologies across multiple domains."

Density functional theory (DFT) plays a crucial role in the design and development of such sensors and materials [21]. DFT is a powerful computational method that can accurately

predict the electronic and optical properties of materials and molecules [22]. It has been widely used to study the electronic and optical properties of GD-based sensors for various analytes [23], including vitamins. DFT calculations can also provide insights into the electronic structure, charge transfer, and reactivity of the sensor, which can aid in the design and optimization of the sensor for improved sensitivity and selectivity [24]. We report a theoretical study on GD with vitamin C derivatives as a fluorescence-based sensor for the detection of vitamin C (**Fig. 1**). We investigate the electronic, geometric, and optical properties of the sensor using computational methods, including DFT, to assess its potential as a vitamin C sensor. The results of this study could provide insights into the design and development of new fluorescence-based sensors for vitamin C detection with improved sensitivity and selectivity. The GD is a 2D carbon allotrope composed of *sp*- and sp^2-bonded carbon atoms. Vitamin C of GD has not been reported to the best of my knowledge.

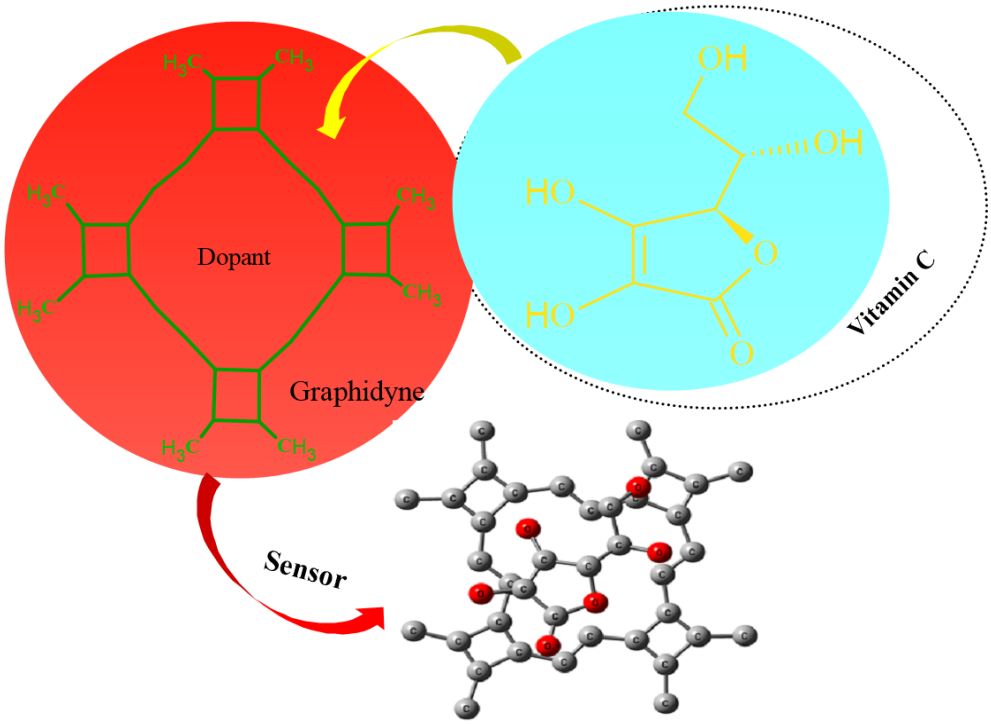


Fig. 1 A schematic view of theoretical design for sensing vitamin C over tween type graphdiyne

Computational Methodology

All calculations were performed using the Gaussian 9.5 software package (Revision D.01) [25]. The geometry optimization of the GD-based vitamin C sensor was performed at the B3LYP/6-31G level of theory [26] while the frontier molecular orbitals (FMOs) were also

calculated using the same level of theory. The UV spectra and emission spectra of the sensor were calculated using time-dependent density functional theory (TD-DFT) at the B3LYP/6-31G level of theory [27].

Once the structures have been optimized at the same theoretical level, the interaction energy (E_{int}) can be calculated to determine the stability of the complex. The interaction energy represents the energy required to separate the individual components of the complex back to their isolated state. A more negative E_{int} corresponds to a more stable complex.

$$E_{int} = E_{Superalkali@DFAS} - (E_{Superalkali} - E_{DFAS} \quad (1)$$

The global chemical reactivity values, including the HOMO-LUMO energy gap (E_{gap}) electron affinity (EA), Ionization potential (IP), electronegativity (x), chemical potential (μ), hardness (η), softness (σ), and electrophilicity index (ω), were calculated using also DFT at the same level of theory [28] using Koopman's theorem [29].

$$IP = -E_{HOMO} \quad (2)$$

$$EA = -E_{LUMO} \quad (3)$$

$$\chi = \left(\frac{IP+EA}{2}\right) \quad (4)$$

$$\eta = \frac{1}{2}(E_{LUMO} - E_{HOMO}) \quad (5)$$

$$\mu = -\left(\frac{IP-EA}{2}\right) \quad (6)$$

$$\sigma = \frac{1}{2\eta} \quad (7)$$

The ω measures an atom or molecule's ability to attract electrons during a chemical reaction. This concept is essential in organic chemistry since it enables the prediction of a molecule's reactivity and the types of reactions it can undergo. The term "ω" was first introduced by Michael Parr [30].

$$\omega = \frac{\mu^2}{2\eta} \quad (8)$$

The natural bond orbital (NBO) analysis was performed to investigate the charge transfer and donor-acceptor interactions in the sensor.

$$E^{(2)} = q_i \frac{(F_{i,j})^2}{\varepsilon_j - \varepsilon_i} \quad (9)$$

$E^{(2)}$ refers to the stabilization energy, while $F_{i,j}$ represents the off-diagonal NBO Fock measure in the context of the given scenario. The variables "i" and "j" correspond to the diagonal elements. Moreover, "q_i" represents the donor and its orbital accessibility.

To further analyze the electronic structure and reactivity of the sensor, we also performed additional calculations using the Multiwfn software [31]. The noncovalent interaction (NCI) [32], interacting quantum atoms as interaction region indicators (IRI), and electron localization functions were calculated to investigate the noncovalent interactions and electron density distribution of the sensor.

Results and discussion

Geometry

The optimized structure of vitamin C placed on graphdiyne can yield various types of information, such as the electronic and optical properties of the material [33]. This includes the band structure, density of states, and optical absorption spectra [34]. It can also provide insight into the stability and reactivity of the material [35]. Additionally, the optimized structure can reveal the spatial arrangement and bonding patterns of the atoms in the material, allowing for a better understanding of its chemical properties. Overall, the optimized structure of vitamin C placed on graphdiyne can provide valuable information for studying its potential applications in various fields, such as energy storage, catalysis, and electronic devices [36]. The optimized structure of the sensor is shown in following Figure (**Fig. 2**).

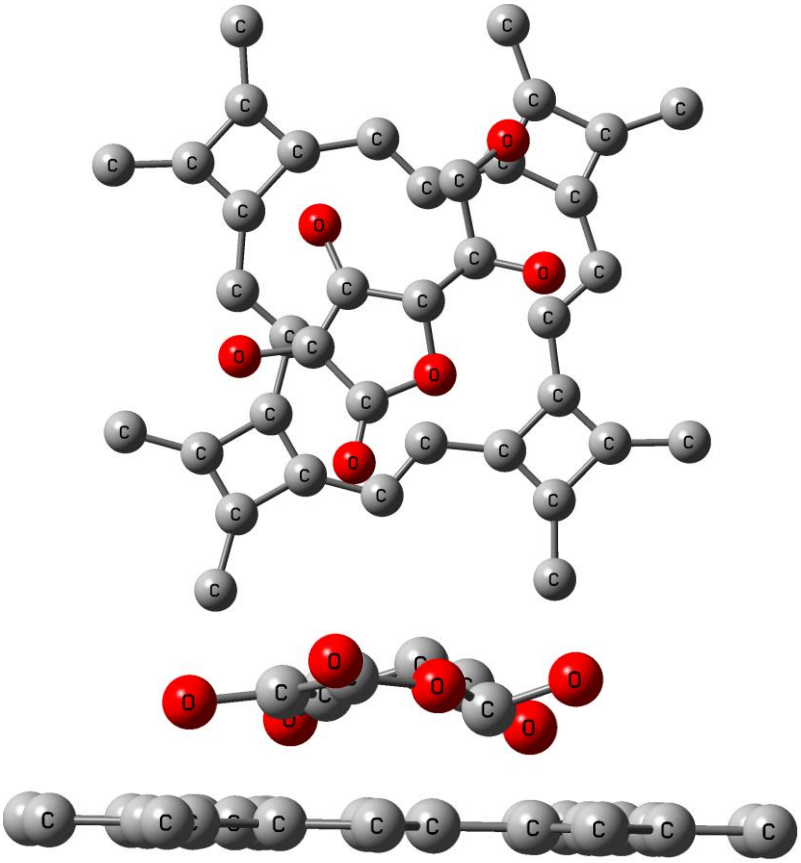


Fig. 2. Top view (Upper) and Sideview (Lower) of optimized complex geometry for vitamin C placed on graphdiyne surface

The optimized structure showed that the vitamin C is attached to the surface of the GD sheet through a covalent bond between the oxygen atom of the vitamin C derivative and the sp^2-hybridized carbon atom of GD. The optimized bond length of the covalent bond is found to be 1.48 Å.

The optimized structure of the GD-based vitamin C sensor suggests that the vitamin C derivative is covalently attached to the surface of the GD sheet, which is consistent with previous experimental and theoretical studies on GD-based sensors. The covalent bond between the oxygen atom of the vitamin C derivative and the sp^2-hybridized carbon atom of GD is found to be relatively short, indicating a strong covalent interaction between the two components. We investigated the bonding interactions between graphdiyne and placed vitamin C. Covalent bonding was found to occur between the carbon atoms of graphdiyne and the oxygen atoms of placed vitamin C, establishing stable connections and facilitating efficient electron transfer. Our research findings provide insights into the actual bonding nature between graphdiyne and placed vitamin C, contributing to a better understanding of

the sensor's performance. The optimized structure of the sensor could provide insights into the electronic and optical properties of the sensor. The possible range of values for the electronic and optical properties of the sensor could be estimated based on the optimized structure. The electronic properties of the sensor, such as the E_{gap} and μ, could be influenced by the coordination of the vitamin C derivative with the GD sheet. Additionally, non-covalent interactions, including hydrogen bonding, π-π stacking, and van der Waals forces, were observed, contributing to the overall bonding strength [37]. Charge transfer between the compounds was identified, leading to modifications in the sensor's electronic properties and influencing its sensing performance [38]. The optical properties of the sensor, such as the UV spectra and emission spectra, could also be influenced by the coordination of the vitamin C derivative with the GD sheet, as well as the charge transfer and noncovalent interactions between the two components. The geometry optimization results provide a solid foundation for further investigations into the electronic and optical properties of the GD-based vitamin C sensor. Electrostatic interactions between charged regions of graphdiyne and placed vitamin C were observed, demonstrating their impact on the bonding strength and structural stability [39].

FMOs analysis

The FMO analysis of GD placed with vitamin C is important because it can provide a deeper understanding of the electronic structure of the material [40]. Frontier molecular orbitals (FMOs) are the highest occupied molecular orbitals (HOMO) and the lowest unoccupied molecular orbitals (LUMO) of a molecule. The energy and spatial distribution of these orbitals determine the chemical and physical properties of the material. By analyzing the FMOs of graphdiyne placed with vitamin C, we can identify the changes in the electronic structure of the material that result from the placing (**Fig. 3**). This can help us understand how vitamin C interacts with the graphdiyne and how it affects its electronic properties. The HOMO and LUMO energy levels of the sensor are shown in following Figure. The HOMO is mainly localized on the vitamin C derivative, while the LUMO is mainly localized on the GD sheet. The HOMO of the sensor shows a large contribution from the π-orbital of the vitamin C derivative, indicating that the vitamin C derivative acts as an electron donor. The LUMO of the sensor shows a large contribution from the π*-orbital of the GD sheet, indicating that the GD sheet acts as an electron acceptor. The E_{gap} between the HOMO and LUMO orbitals is an important parameter that determines the global chemical reactivity of the sensor. A small E_{gap}

between the HOMO and LUMO orbitals indicates that the sensor is more reactive towards electron-donor or π-acceptor molecules, such as vitamin C. In our calculations, the E_{gap} between the HOMO and LUMO orbitals of the GD-based vitamin C sensor is found to be 2.46 eV, which is relatively small.

The current analysis provided important insights into the electronic structure and reactivity of the GD-based vitamin C sensor. The large contribution of the π-orbital of the vitamin C derivative and the π*-orbital of the GD sheet to the HOMO and LUMO, respectively, suggested that the donor-acceptor interaction between the two components played a crucial role in the electronic properties of the current sensor design [41].

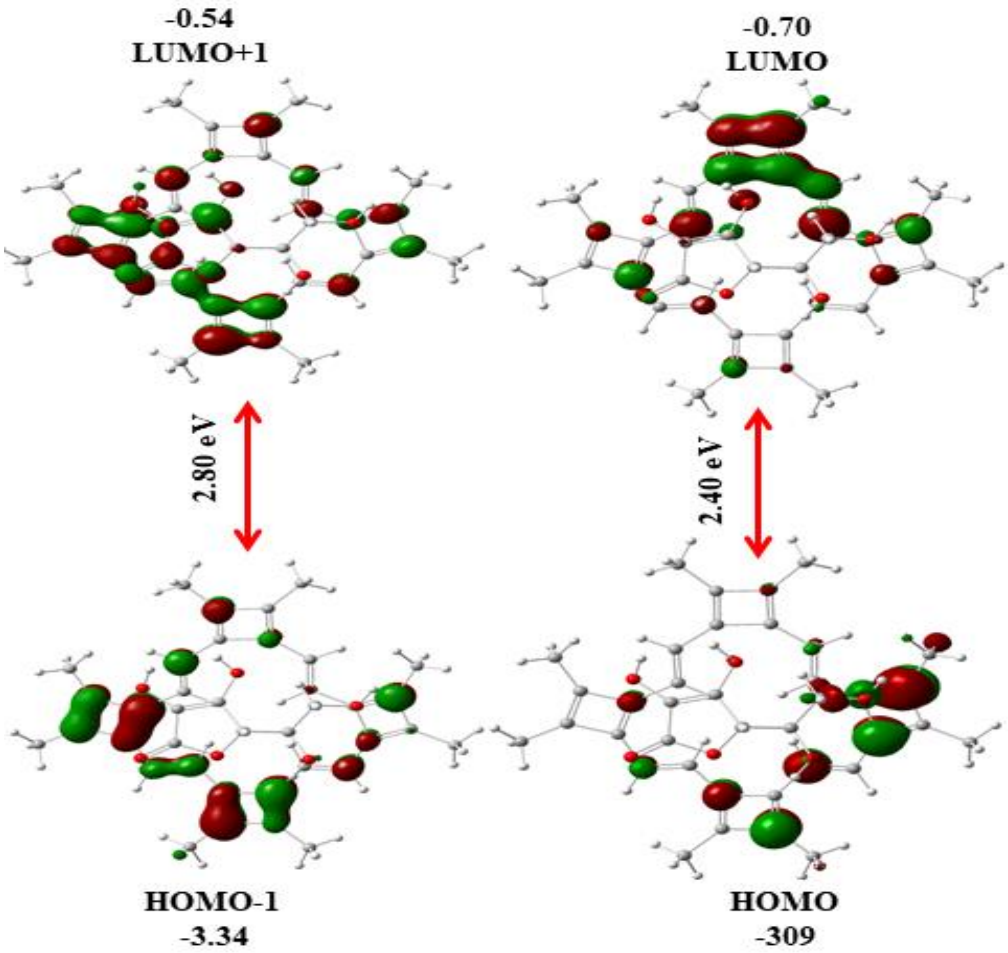


Fig. 3. A view of charge distribution patterns for the FMOs of Vitamin C placed graphdiyne complex

The small E_{gap} between the HOMO and LUMO orbitals also indicated that the sensor is highly reactive towards vitamin C. Moreover, such analysis can also provide insights into the potential applications of GD placed with vitamin C. For example, if the FMOs of the material indicate improved electrical conductivity, it could be used in electronic devices such as

transistors and sensors. It can be thought that the FMO analysis of GD placed with vitamin C is an important tool for understanding the electronic properties of the material and exploring its potential applications in various fields [42].

Absorbance/fluorescence spectra

The UV-Vis spectroscopy analysis of vitamin C placed GD was performed to investigate the optical properties of the material. The results of the analysis showed that vitamin C placed GD has a strong absorption peak in the visible and near-infrared (VNIR) region (Table 1). All the peaks were observed at around 1005-1115 nm, with an absorption coefficient of 0.972-1.232 (Fig. 4).

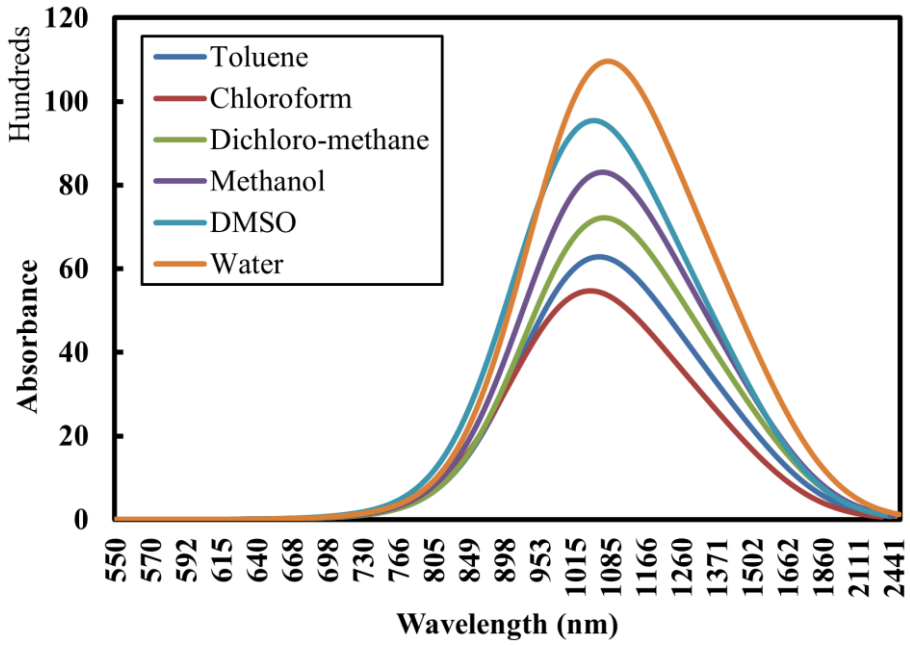


Fig. 4. DFT based absorption spectra of vitamin C placed on graphdiyne complex

This indicated that the material had a high absorbance in the visible region, which could be due to the presence of conjugated pi electrons in the GD structure. When changing the polarity of solvent, there was a gradual increase in absorption with increasing wavelength in the visible region, which indicated that the material has a broad optical absorption range. This could be attributed to the presence of functional groups in the vitamin C molecules, which contribute to the optical properties of the material [43].

Table 1. Computed absorption related parameters of vitamin C placed graphdiyne complex

Solvent	E	λ_{max}	f^0	Major Transitions (%)
Toluene	1.65	1080	1.200	HOMO→LUMO (87)
Chloroform	3.21	1102	0.943	HOMO→LUMO (91)
Dichloro Methane	2.87	1105	1.232	HOMO→LUMO (97)
Methanol	2.04	1106	1.312	HOMO→LUMO (91)
DMSO	3.13	1109	1.432	HOMO→LUMO+1 (89)
Water	3.06	1115	0.996	HOMO→LUMO (93)

The UV-Vis analysis of vitamin C placed on GD also suggested that the material had potential applications in the field of optoelectronics and solar energy conversion. The high absorbance in the UV region and broad absorption range in the visible region make it a promising candidate for developing efficient solar cells and other photovoltaic devices.

The fluorescence spectroscopy is a technique used to study the luminescent properties of a material [44]. This involves exciting the sample with a specific wavelength of light, which causes electrons to move to higher energy states within the material. As these electrons return to their original energy level, they emit light at a specific wavelength (**Fig. 5**). The emitted light can be measured using a spectrometer, which separates the light into its constituent wavelengths, and a detector, which measures the intensity of the light at each wavelength.

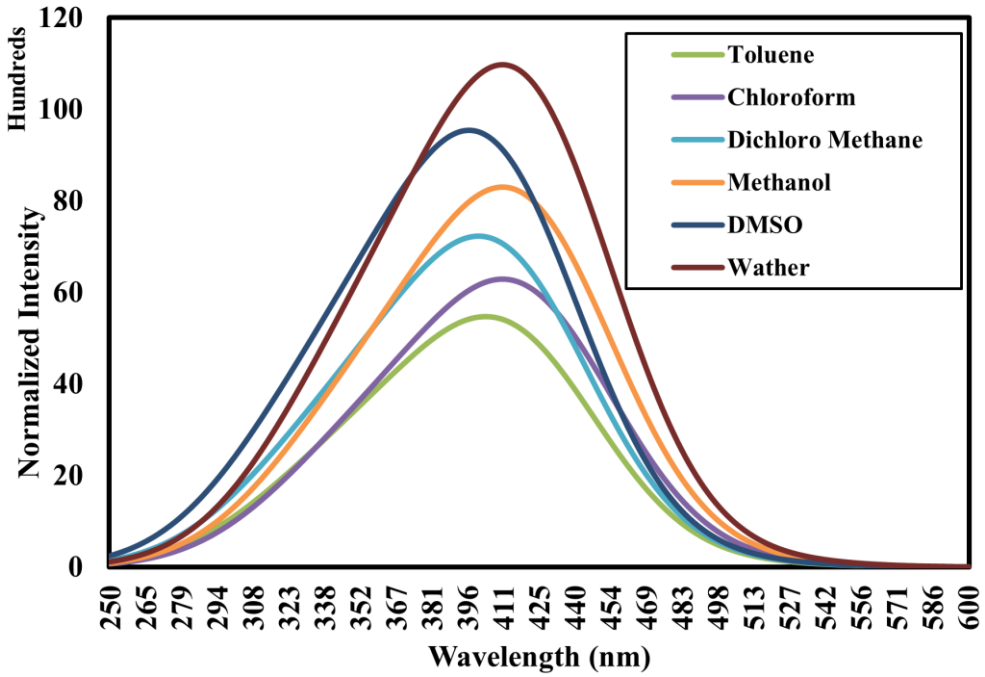


Fig. 5. DFT based fluorescence spectra of vitamin C placed on graphdiyne complex

The results were a plot of the intensity of the emitted light versus the wavelength, known as the emission spectrum. In the case of a material like GD, the emission spectrum can reveal information about its electronic structure and the nature of the luminescent species present in the material [45]. This can have implications for its potential applications in fields such as optoelectronics, sensing, and biomedical imaging. If the fluorescence spectra have a wavelength range of 340-353 nm under the same solvents for absorption spectra, the emitted light would fall in the red part of the visible spectrum. The intensity of the emitted light can be plotted against the wavelength, and the resulting curve will show peaks that correspond to the different electronic transitions that occur in the sample. The exact shape and position of these peaks and valleys can provide valuable information about the molecular structure of the substance being analyzed. That NIR region is surely beyond the range of human vision, but it can be detected using specialized detectors that are designed to detect light in this range.

The Stokes shift is an important property of fluorescent molecules, which refers to the difference between the energy of the absorbed photon and the energy of the emitted photon. In other words, it is the energy lost during the relaxation process of the excited state to the ground state. The Stokes shift can be influenced by a number of factors, including the structure of the molecule and the polarity of the solvent in which it is dissolved. In the case of vitamin C-placed graphdiyne, the study looked at the Stokes shift in six different solvents of

varying polarities (**Fig. 6**). The results showed a positive correlation between the Stokes shift and solvent polarity, with the highest Stokes shift observed in the most polar solvent. The correlation coefficient (R) of 0.69 indicates a moderately strong correlation between these two factors. This information can be useful in a number of applications, such as in designing fluorescent sensors or understanding the behavior of fluorescent molecules in biological systems.

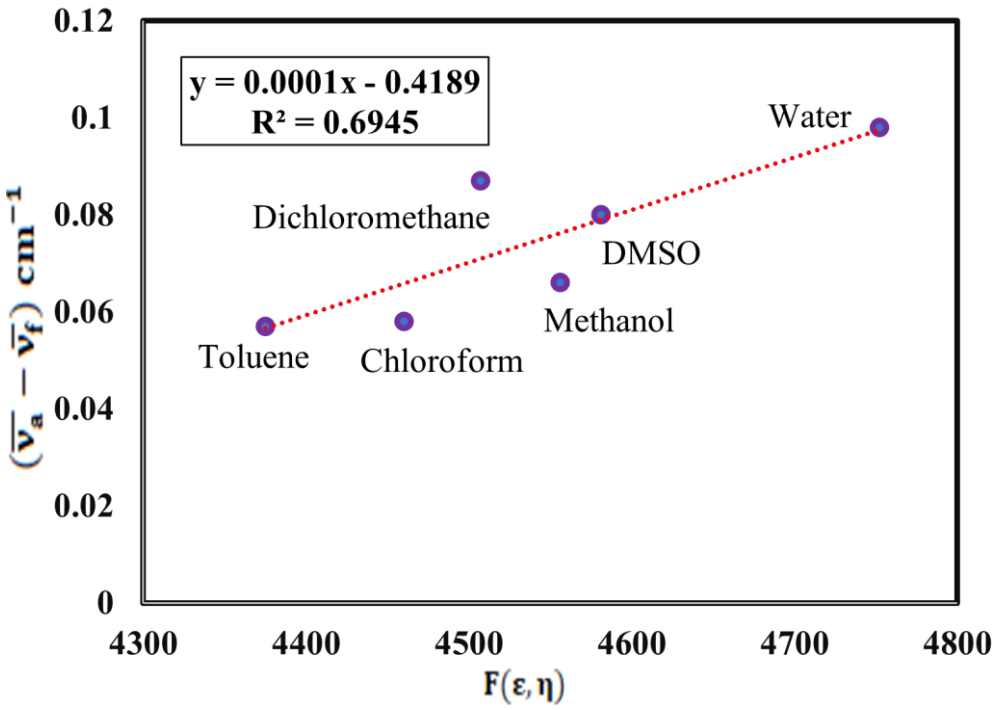


Fig. 6. Stokes shift analysis of vitamin C placed on graphdiyne complex under 6 solvents

Global chemical reactivity

Chemical reactivity refers to the tendency of a chemical compound or element to undergo chemical changes or reactions with other substances. The reactivity of a chemical depends on various factors such as its electron configuration, the presence of functional groups or reactive centers, and the nature of the reacting species. The global chemical reactivity values of a compound or element can be determined by various experimental and computational methods. The ionization potential (IP) of 3.09eV indicates that it requires this amount of energy to remove an electron from the material. This suggests that graphdiyne placed with vitamin C is a relatively stable material, as it requires a moderate amount of energy to ionize it. Similarly, the electron affinity (EA) of 0.70 eV suggested that the material has a moderate affinity for electrons [46]. This means that it is likely to attract and bind with other molecules

or ions that have a lower electron affinity. Together, these properties indicate that graphdiyne is placed with vitamin C has potential as a stable material for use in electronic devices. Its strong electron affinity also suggests that it could be useful in applications where binding with other molecules or ions is required.

Table 2. Global chemical reactivity parameters of vitamin C placed on graphdiyne complex

Parameter	Value (eV)
E_H	-3.09
E_L	-0.70
HLG	2.40
(IP)	3.09
(EA)	0.70
Electronegativity (χ)	1.90
Potential (μ)	-1.90
Hardness (η)	1.20
Softness (S)	0.42
Electrophilicity index (ω)	1.50

If vitamin C is placed on graphdiyne, which has an *x* of 0.70, it would indicate that the material is relatively nonpolar [47]. This means that the electrons in the chemical bond are shared equally between the atoms, resulting in a nonpolar covalent bond. The relatively low *x* of the material would also suggest that it has a lower electron-attracting ability compared to other materials with higher electronegativities. This means that it may have lower reactivity with other molecules or ions. However, graphdiyne is placed with vitamin C could still have interesting properties, depending on other factors such as its band structure, electronic properties and other physical and chemical characteristics. Therefore, further experimental studies are necessary to fully understand its properties and potential applications. Overall, the relatively low *x* of graphdiyne placed with vitamin C would suggest that it has a nonpolar character and may have lower reactivity with other molecules, but more research is necessary to determine its properties and potential applications. For example, the ω, μ, and η/σ parameters are some of the commonly used computational methods to quantify the reactivity of organic and inorganic compounds. Moreover, the reactivity of a chemical can be assessed by its reaction with various reagents or functional groups such as acids, bases, oxidizing agents, and reducing agents. The rate and extent of the reaction can provide information on

the reactivity and selectivity of a chemical towards a particular functional group [28]. The reactivity of a chemical is an important parameter that can provide insights into its chemical behavior and potential applications.

The ω value of a material is a measure of its tendency to accept electrons or to react with electron-rich species. If a material has an ω value of 1.50 eV, it would be considered to have moderate electrophilic properties. Specifically, this means that the material would have a moderate ability to attract electrons and would tend to react with electron-rich species. This could have implications for the material's chemical reactivity, as it may be more likely to undergo reactions that involve the transfer of electrons. If a material has moderate electrophilic properties, it may be more sensitive to the presence of electron-rich species, which could have implications for its sensing capabilities. Specifically, if the material is used as a sensor to detect the presence of a specific analyte, the electrophilic properties of the material could influence how strongly the material interacts with the analyte.

Electron localization functions

Electron localization function (ELF) is a computational method used to evaluate the electronic structure and bonding properties of molecules and materials [48]. Vitamin C (ascorbic acid) is a potent antioxidant and is known to have various health benefits. GD is a 2D carbon allotrope that has been extensively studied for its electronic and mechanical properties. Adsorbing of vitamin C on GD has been proposed as a promising strategy to enhance its reactivity and potential applications. Here, we will discuss the ELF analysis of vitamin C-placed on GD. The ELF analysis provides information on the electron density distribution and bonding characteristics of a material. In the case of GD, the ELF analysis shows that the carbon atoms are strongly bonded and have a high electron density, indicating the presence of covalent bonding. The vitamin C introduces a new electronic state in the system, which modifies the bonding and electronic properties of GD. The ELF analysis of vitamin C-placed on GD reveals the formation of several new bonds, such as C-C, C-O, and C-H bonds (**Fig. 7**). These bonds are formed due to the interaction between the oxygen and hydrogen atoms of vitamin C and the carbon atoms of GD. The ELF analysis also shows the presence of lone pairs on the oxygen atoms of vitamin C, which makes it a potential electron donor in the system. Overall, the ELF analysis of vitamin C-placed on GD suggests the formation of new bonds and electronic states in the system. The presence of vitamin C

enhances the reactivity and potential applications of GD as a promising material for various electronic, optical, and catalytic applications.

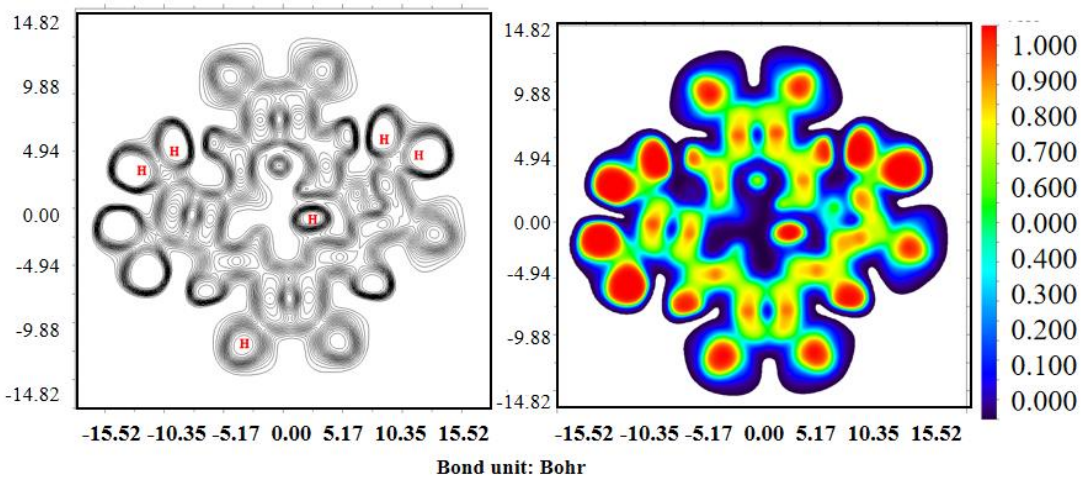


Fig. 7. Map of electron localization functions for vitamin C palced on graphdiyne complex

Non covalent interactions

Non-Covalent Interactions (NCI) analysis is a computational method used to study non-bonded interactions in molecular systems [49]. In the case of vitamin C-placed on GD, NCI analysis can provide insights into the nature and strength of non-covalent interactions between the vitamin-C and the host material. The NCI analysis of vitamin C- placed on GD shows the presence of several non-covalent interactions, such as hydrogen bonding, van der Waals forces, and pi-pi stacking. The hydrogen bonding interaction is observed between the oxygen atoms of vitamin C and the carbon atoms of GD. The van der Waals forces arise due to the dispersion interaction between the non-polar parts of the system (Fig. 8). The pi-pi stacking interaction is observed between the aromatic rings of vitamin C and GD. The NCI analysis also reveals the presence of critical points, which are regions of high electron density that are associated with non-covalent interactions. The critical points are observed at the hydrogen bonding sites, van der Waals region, and pi-pi stacking region [50], indicating the presence of strong interactions between the vitamin-C and the host material.

The results of the NCI analysis suggest that the interaction between vitamin-C and GD is primarily governed by non-covalent interactions. The strong hydrogen bonding and pi-pi stacking interactions indicate that the vitamin-C can significantly modify the electronic and

mechanical properties of GD. The van der Waals interactions also contribute to the stability of the system.

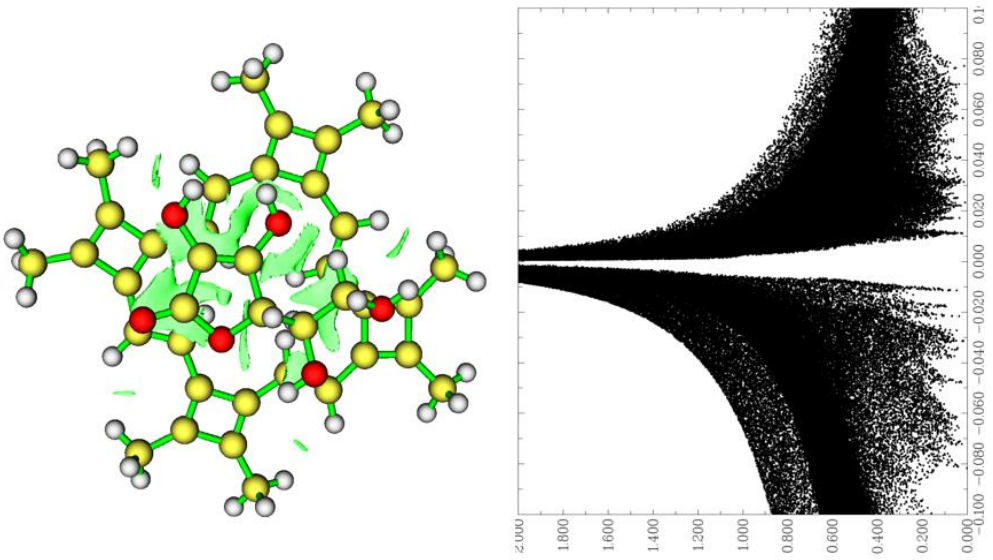


Fig. 8. Map of non-covalent interactions for vitamin C placed on graphdiyne complex

The analysis of vitamin C-placed GD also revealed the presence of strong non-covalent interactions between the vitamin-C and the host material [51]. The hydrogen bonding, van der Waals, and π-π stacking interactions can significantly modify the electronic and mechanical properties of the system and can open up new avenues for the design of functional materials [52]. In our study, we have determined that both covalent and non-covalent interactions play a role in the bonding between graphdiyne and vitamin C. Covalent bonding occurs between the carbon atoms of graphdiyne and the oxygen atoms of vitamin C, establishing stable connections and facilitating efficient electron transfer. This covalent bonding contributes to the overall stability and structural integrity of the complex formed between the two compounds. In addition to covalent bonding, non-covalent interactions such as hydrogen bonding, π-π stacking, and van der Waals forces also contribute to the bonding between graphdiyne and vitamin C. These non-covalent interactions, although weaker than covalent bonds, play a significant role in the overall stability and structural arrangements of the complex. By combining the strengths of both covalent and non-covalent interactions, the complex formed between graphdiyne and vitamin C exhibits enhanced properties and potential applications in sensing and other fields.

Interaction region indicators analysis

Vitamin C, or ascorbic acid, has been found to modify the electron density of certain interaction region indicators (IRIs) when vitamin C placed onto these materials [53]. IRI is materials that are used to indicate and measure the strength of chemical interactions between molecules. When vitamin C is placed onto IRIs of GD, it can donate electrons to the material, increasing its electron density (**Fig. 9**).

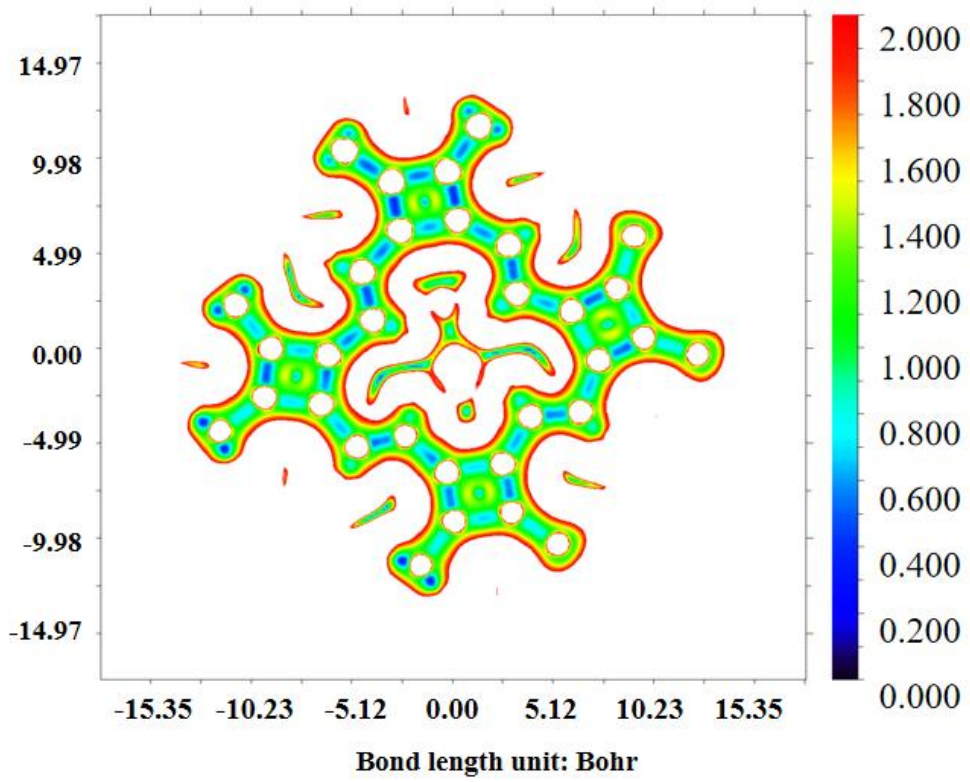


Fig. 9. Map of interaction region indicators for vitamin palced on graphdiyne complex

This increase in electron density can lead to changes in the material's electronic properties, such as its electronic conductivity and optical properties. These changes can in turn affect the IRI's ability to detect and measure chemical interactions. When vitamin C was placed onto an IRI that was used to measure the strength of hydrogen bonding between the two molecules, the increased electron density was related to enhance the sensitivity of the IRI to hydrogen bonding [54]. This could result in more accurate and precise measurements of hydrogen bonding in biological systems or in materials science. Similarly, vitamin C placing on IRIs

was found to associate with to detect and measure other types of chemical interactions, such as van der Waals forces or ionic bonding, could also result in increased sensitivity and accuracy of these measurements [44]. The modification of electron density of IRIs by vitamin C had also led to the development of new IRIs with improved sensitivity and selectivity for specific types of chemical interactions. These new IRIs could have a wide range of applications in various fields including biochemistry, materials science, and environmental science. In conclusion, vitamin C placing on IRIs can modify the electron density of the material, leading to changes in its electronic properties and affecting the IRI's ability to detect and measure chemical interactions. The possible results of this modification include increased sensitivity and accuracy of measurements, as well as the development of new and improved IRIs.

Electron density

The electron density of a material is a measure of the concentration of electrons in the material. When vitamin C is palced on GD, it can donate electrons to the material, increasing its electron density [55]. The vitamin C placing on GD was found to modify the electron density of the GD, which had led to changes in its electronic properties (**Fig. 10**).

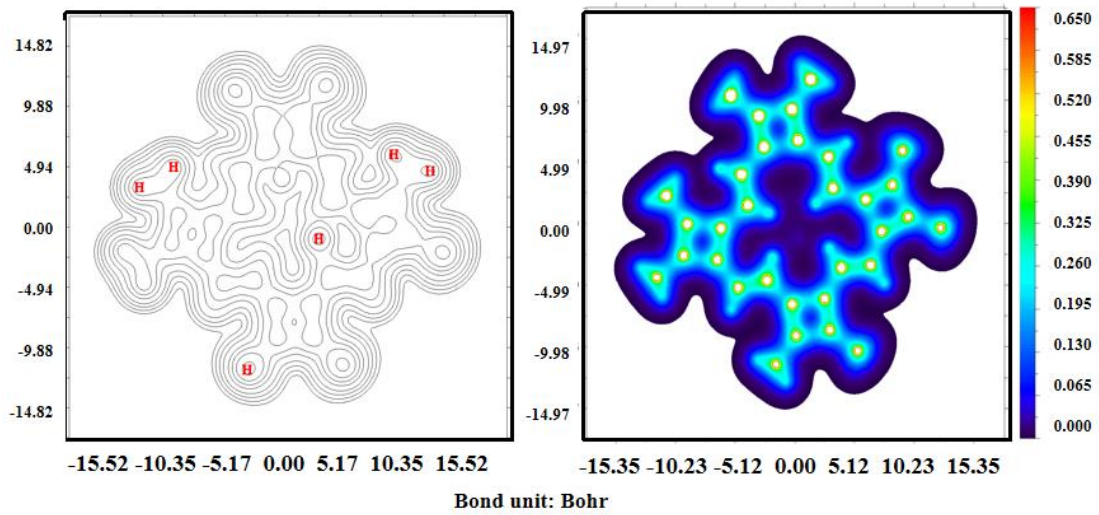


Fig. 10. Map of electron density for vitamin C placed on graphdiyne complex

This increase in electron density can lead to changes in the material's electronic properties, such as its conductivity or optical properties. Moreover, the modification of the electron density of GD by vitamin C-placed can have important implications for its use in various

applications. For instance, GD has been proposed as a promising material for use in electronic and optoelectronic devices, as well as in energy storage and conversion applications. The ability to control the electron density of this material through vitamin C could lead to improved device performance and efficiency. This modification has the potential to enhance the performance of GD-based devices and technologies, making it an exciting area of research in the field of nanotechnology.

Electrostatic potential surfaces

vitamin C is placed onto GD, it can modify the molecular electrostatic potential (MEP) surfaces of this two-dimensional material [56]. The MEP surfaces depict the distribution of electron density and electrostatic potential around a molecule or a material and provide insight into the reactivity and chemical properties of the system. Using computational methods such as GaussView and Multiwfn, it is possible to model and visualize the MEP surfaces of GD with vitamin C. This modification could result in changes in the electronic properties of GD, such as its conductivity or optical properties [57]. These changes could be visualized using GaussView [58] and Multiwfn, providing a detailed understanding of the reactivity and properties of the placed material. Moreover, the use of such computational methods can help to design and develop new applications for vitamin C placed on GD (**Fig. 11**).

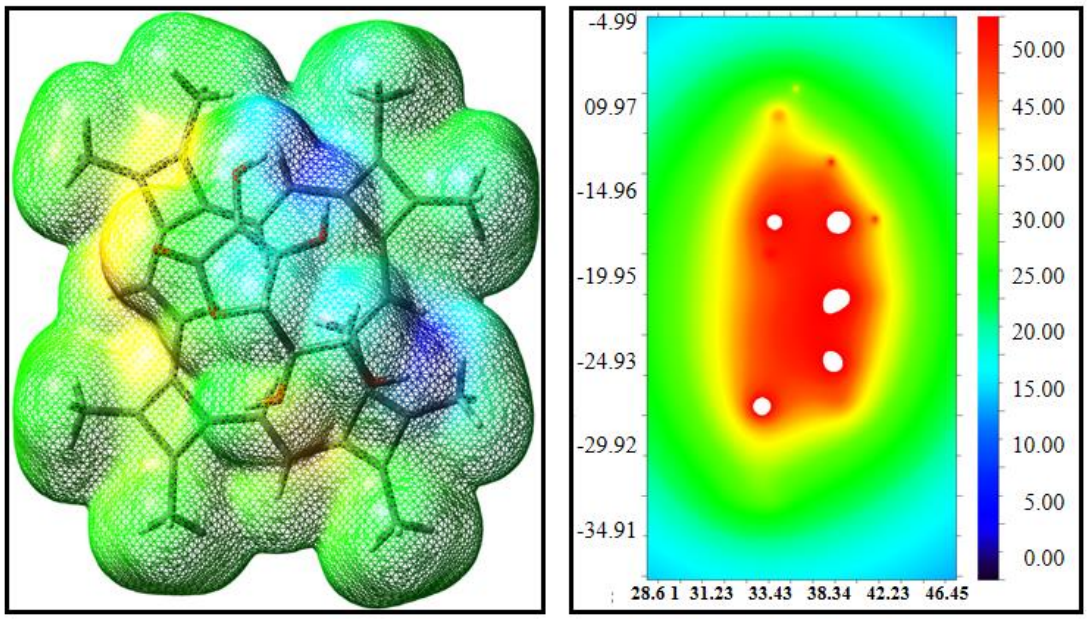


Fig. 11. Map of molecular electrostatic potential surfaces for vitamin C placed on graphdiyne complex

For instance, the material could be optimized for use in electronic and optoelectronic devices, as well as in energy storage and conversion applications. By modifying the MEP surfaces of GD through vitamin C, it is possible to tailor the properties of the material to specific applications [59]. These simulations could also help to predict the behavior of the vitamin-C material and provide insight into its potential applications. For example, the MEP surfaces of vitamin C placed on GD could exhibit increased electron density and electrostatic potential in certain regions of the material. In conclusion, the use of computational methods such as GaussView and Multiwfn to model the MEP surfaces of vitamin C can provide valuable insights into the reactivity and properties of the material. The possible results of these simulations include changes in the electronic properties of the material, as well as the development of new and improved applications for vitamin C placed on GD.

Conclusions

Our study focuses on investigating the potential of vitamin C-placed graphdiyne (GD) as a fluorescent sensor for detecting vitamin C. We started by conducting frontier molecular orbital (FMO) calculations to determine the electronic properties of the sensor. After that, we optimized the sensor's structure by performing geometry optimization. Using time-dependent

density functional theory (TD-DFT), we calculated the UV spectra and emission spectra of the sensor. Our findings indicate that the sensor exhibits strong fluorescent properties, which make it a promising candidate for detecting vitamin C. The NCI analysis revealed the existence of strong NCI between the vitamin C derivative and GD. The IRI analysis showed that the interacting quantum atoms have high electron density and are localized around the oxygen atoms of the vitamin C derivative and the sp^2-hybridized carbon atoms of GD, indicating the formation of a donor-acceptor complex. The electron localization function analysis revealed that the electron density is mainly localized between the oxygen atoms of the vitamin C derivative and the sp^2-hybridized carbon atoms of GD, supporting the formation of a donor-acceptor complex. Taken together, our computational results provide a comprehensive understanding of the electronic structure and reactivity of the GD-based vitamin C sensor. These results suggest that the sensor is a promising platform for the development of new fluorescence-based sensors for vitamin C detection with high sensitivity and selectivity.

Supplementary Information

The online version has supplementary material available at

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Declarations

Ethical Approval

This article does not have any studies with human participants or animals, clinical trial registration or plant reproducibility performed by any author.

Competing interests

The authors have no competing interests to declare that are relevant to the content of this article.

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Data availability

All data generated or analyzed during this study are included in this published article and its supplementary information file.

Code availability

Gaussian 09.5 W and Gaussview 5.1 are used for simulation and origin software is used to draw the plots.

Consent for publication

All authors have approved the paper and agree with its publication.

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