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Density Functional Theory (DFT) Study on Molecular Interaction Between H_2O and Graphene

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ABSTRACT

Graphene has attracted significant attention as an anode material due to its high surface area and unique electronic properties. This study explores the adsorption behavior of H_2O molecules on graphene using Density Functional Theory (DFT) with the van der Waals density functional (vdW-DF). Various molecular orientations (zero-leg, one-leg, and two-leg) and adsorption sites (top, bridge, hollow) were analyzed. The results show that the most stable configuration is the two-leg orientation at the hollow site, with an adsorption energy of -0.123 eV. The findings suggest that the stability of the adsorbed system is governed more by the interaction between hydrogen atoms and the carbon surface than by the oxygen atom. All stable structures are characterized by adsorption distances between 2.8 and 3.2 Å. The interaction is classified as physisorption due to its low energy and minimal charge transfer. These results are consistent with previous studies, confirming the key role of molecular orientation and adsorption site in determining the adsorption behavior of H_2O on graphene.

Keywords: *DFT; Graphene; Adsorption;* H_2O*.*

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ABSTRACT

Graphene telah menarik perhatian sebagai material anoda karena luas permukaan yang tinggi dan sifat elektroniknya. Studi ini meneliti perilaku adsorpsi molekul H_2O *pada graphene menggunakan metode Density Functional Theory (DFT) dengan pendekatan van der Waals density functional (vdW-DF). Berbagai orientasi molekul (zero-leg, one-leg, dan two-leg) serta posisi adsorpsi (top, bridge, hollow) dianalisis. Hasil menunjukkan bahwa konfigurasi paling stabil adalah orientasi two-leg pada situs hollow, dengan energi adsorpsi sebesar -0,123 eV. Stabilitas sistem lebih dipengaruhi oleh interaksi antara atom hidrogen dengan permukaan karbon dibandingkan dengan atom oksigen. Semua struktur stabil memiliki jarak adsorpsi antara 2.8 hingga 3.2 Å. Interaksi diklasifikasikan sebagai fisisorpsi karena energi yang rendah dan transfer muatan yang minimal. Hasil ini konsisten dengan penelitian sebelumnya, menegaskan pentingnya orientasi molekul dan lokasi adsorpsi dalam menentukan perilaku adsorpsi* H_2O *pada graphene.*

Keywords: *DFT; Graphene; Adsorption;* H_2O*.*

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INTRODUCTION

Carbon is widely utilized as an anode material, particularly in the forms of graphene, graphite, or hard carbon [1], due to its cost-effectiveness and abundant availability [2][3]. These carbon variants differ structurally: graphene is a single, hexagonal carbon layer [4][5] with exceptional electrical conductivity and a large specific surface area [6]. It also exhibits remarkable adsorption capabilities for both organic and inorganic molecules [7][8] and high optical transparency [9]. These properties make graphene suitable for applications such as fuel cells [10], gas sensors [11], and sodium-ion batteries [3]. Graphene's reactivity, particularly with oxygen-containing species like O_2, H_2O, and CO_2 [12] is significant. Studying the adsorption and desorption of H_2O molecules on graphene sheets is essential for understanding critical aspects of the carbon gasification reaction. However, the precise reaction mechanisms and interactions between carbon and water at the molecular level remain poorly understood.

Graphene has attracted considerable attention in recent years due to its exceptional physical and chemical properties, including high electrical conductivity, large specific surface area, and excellent mechanical stability. These characteristics make graphene a promising material for a wide range of technological applications such as energy storage devices, gas sensors, catalysis, and electrochemical systems. In particular, graphene-based materials have been widely explored as electrode materials in lithium-ion and sodium-ion batteries because their two-dimensional structure enables efficient charge transport and provides abundant active surface sites for molecular interactions [3][10].

The interaction between graphene surfaces and small molecules plays a critical role in determining the performance of graphene-based devices. Among various molecules, water (H_2O) is of particular interest because it is commonly present in ambient environments and can significantly influence the electronic properties and surface chemistry of graphene. Water adsorption may affect charge transfer processes, modify surface reactivity, and influence the stability of graphene-based materials in electrochemical systems [14][16]. Therefore, understanding the adsorption behavior of water molecules on graphene surfaces is essential for predicting the performance and reliability of graphene-based technologies.

At the atomic scale, the interaction between water molecules and graphene surfaces is typically dominated by weak intermolecular forces, particularly van der Waals interactions. These interactions are difficult to analyze experimentally due to their small energy scale and the complexity of surface processes. Computational approaches, especially Density Functional Theory (DFT), provide an effective framework for investigating such interactions by enabling detailed atomistic analysis of adsorption structures, adsorption energies, and molecular configurations. Furthermore, Density Functional Theory (DFT) is a widely adopted computational method in physics and chemistry for analyzing the quantum properties of complex multi-electron systems, such as molecules and solids. DFT has been effectively used to study atomic adsorption on graphene [13][14][15]. However, accurately describing weak intermolecular interactions remains challenging because conventional exchange–correlation functionals may underestimate long-range dispersion forces. To address this limitation, dispersion-corrected Density Functional Theory methods have been developed. One widely used approach is the DFT-D3 dispersion correction proposed by Grimme, which introduces an empirical correction to account for long-range van der Waals interactions and significantly improves the accuracy of adsorption energy calculations for weakly interacting systems

In this study, the interaction between water and graphene is investigated using the van der Waals density functional (vdW-DF). This functional is promising as it seamlessly captures both weak van der Waals (vdW) interactions and covalent interactions, while also providing reasonable accuracy in describing hydrogen bonding [16]. Motivated by these considerations, this study investigates the adsorption behavior of H_2O molecules on graphene using Density Functional Theory calculations with the DFT-D3 dispersion correction. By systematically evaluating severeal configurations, this study aims to identify the most stable adsorption structure and to analyze the role of molecular orientation in determining adsorption stability by the presence of DFT-D3 dispersion correction. The findings of this work provide further insight into the interaction mechanisms between water molecules and graphene surfaces, which is important for improving the design and performance of graphene-based materials in practical applications.

LITERATURE REVIEW

DFT is grounded in the Hohenberg-Kohn theorems, which establish that the ground-state properties of a many-electron system are uniquely determined by its electron density, $\rho(r)$ The first theorem proves that the external potential (and thus the total energy) is a unique functional of the electron density. The second theorem states that the ground-state energy is obtained by minimizing the energy functional $E[\rho]$. The total energy functional can be written as:

$$[\rho] = T[\rho] + V_{\text{ext}}[\rho] + E_{\text{H}}[\rho] + E_{\text{xc}}[\rho] \tag{1}$$

where $T[\rho]$ is the kinetic energy, $V_{\text{ext}}[\rho]$ is the external potential energy, $E_{\text{H}}[\rho]$ is the Hartree (Coulomb) energy, and $E_{\text{xc}}[\rho]$ is the exchange-correlation energy, which accounts for quantum mechanical effects.

The practical implementation of DFT relies on the Kohn-Sham (KS) formalism, which maps the interacting many-electron system onto a fictitious system of non-interacting electrons with the same electron density. The Kohn-Sham equations are:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{eff}}(\boldsymbol{r})\right)\psi_i(\boldsymbol{r}) = \epsilon_i\psi_i(\boldsymbol{r}) \tag{2}$$

where $V_{\text{eff}}(\boldsymbol{r})$ is the effective potential, including contributions from the external potential, Hartree potential, and exchange-correlation potential, and $\psi_i(\boldsymbol{r})$ are the Kohn-Sham orbitals. The electron density is computed as

$$\rho(\boldsymbol{r}) = \sum_i |\psi_i(\boldsymbol{r})|^2 \tag{3}$$

METHOD

First-principles calculations were performed using Density Functional Theory (DFT) as implemented in the Quantum ESPRESSO package [17]. Ultrasoft pseudopotentials (USPP) were employed to describe electron–ion interactions. The plane-wave kinetic energy cutoff was set to 60 Ry, and the charge density cutoff was 600 Ry. Brillouin zone sampling was performed using a 16 × 16 × 1 Monkhorst–Pack k-point mesh. To accurately capture weak intermolecular interactions between H_2O molecules and the graphene surface, the DFT-D3 dispersion correction proposed by Grimme was applied. Structural optimization was performed until the total energy convergence threshold reached 10^{-8} Ry and the residual forces acting on each atom were smaller than 10^{-3} Ry/Bohr.

A 3 × 3 graphene supercell containing 18 carbon atoms was used in the simulations. A vacuum spacing of 20 Å was introduced along the z-direction to eliminate interactions between periodic images. The adsorption distance was defined as the vertical distance between the oxygen atom of the water molecule and the average z-position of the carbon atoms in the graphene plane. The adsorption energy was calculated as a function of the distance between the water molecule and the graphene structure, defined by,

$$E_{ads} = E_{H_2O+graphene} - E_{graphene} - E_{H_2O}$$

where $E_{H_2O+graphene}$represents the total energy of the adsorption system, $E_{graphene}$is the energy of the isolated graphene surface, and $E_{H_2O}$is the energy of the isolated water molecule. The distance between the water molecule and the graphene structure was defined as the difference in z-coordinates between the oxygen (O) atom of the water molecule and the graphene plane. Additionally, structure optimization was carried out for the most stable adsorption configurations.

RESULTS AND DISCUSSION

Adsorption Configuration

The adsorption behavior of H_2O molecules on graphene was investigated by considering three molecular orientations (zero-leg, one-leg, and two-leg) combined with three adsorption sites on the graphene surface, namely the top, bridge, and hollow positions, as seen in Figure 1. These configurations allow a systematic evaluation of how molecular orientation and adsorption site influence the stability of the adsorption system. The calculated adsorption energies and adsorption distances for all configurations are summarized in Table 1. The results show that the adsorption energies range from −0.074 eV to −0.123 eV, indicating relatively weak interactions between the water molecule and the graphene surface. Such small adsorption energies suggest that the interaction is dominated by van der Waals forces, which is characteristic of physisorption processes.

Among the nine configurations examined, the two-leg orientation at the hollow site exhibits the lowest adsorption energy (−0.123 eV), indicating the most stable adsorption configuration. In this configuration, both hydrogen atoms of the water molecule are oriented toward the graphene surface, allowing stronger interaction between the partially positive hydrogen atoms and the π-electron system of graphene. This orientation enhances electrostatic attraction between the hydrogen atoms and the carbon surface.

In contrast, the zero-leg configuration, where the oxygen atom is oriented toward the graphene surface, shows comparatively higher adsorption energies. This indicates that the interaction between the oxygen atom and the graphene surface is weaker than the interaction involving hydrogen atoms. These results suggest that the adsorption stability is primarily governed by the interaction between hydrogen atoms and the graphene surface rather than oxygen–carbon interactions.

The adsorption distances obtained in this study range between 2.8 Å and 3.2 Å, which is consistent with typical adsorption distances reported for weakly adsorbed molecular systems on graphene surfaces. These distances further support the classification of the interaction as physisorption, where the molecule is weakly bound to the surface without forming strong chemical bonds.

The results obtained in this study are consistent with previous theoretical studies on water adsorption on graphene. For instance, Abidin *et al.* [14] and Liang *et al.* [19] also reported that the two-leg configuration at the hollow site is the most stable adsorption structure. The adsorption energy obtained in the present study (−0.123 eV) falls within the range reported in the literature, confirming the reliability of the computational approach used in this work.

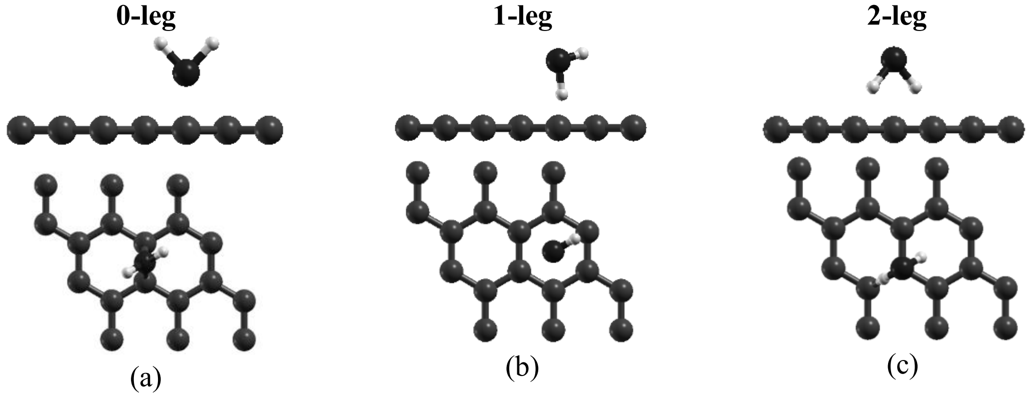

Figure. 1. Side (upper panel) and top (lower panel) views of the water adsorption configuration on pristine graphene for (a) 0-leg, (b) 1-leg, and (c) 2-leg configurations. The variation positions of H_2O on graphene are bridge, hollow, and top in all H_2O configurations. H, C, and O atoms are represented by white, navy, and red spheres, respectively.

The adsorption energies corresponding to various configurations at different adsorption sites are summarized in Table 1. Analysis indicates that the orientation of the H_2O molecule plays a crucial role in influencing its adsorption behavior on the carbon surface. This finding is consistent with previous studies in the literature [14][16][18].

Table 1. Energy and Distance of Adsorption of H_2O and Graphene

Configuration	Position	Energy (*eV*)	Distance (Å)
0-leg	Bridge	-0.111	3.2
	Hollow	-0.080	2.9
	Top	-0.074	2.9
1-leg	Bridge	-0.117	3.1
	Hollow	-0.122	3.1
	Top	-0.116	3.1
2-leg	Bridge	-0.113	3.1
	Hollow	**-0.123**	3
	Top	-0.115	3.1

The zero-leg configuration has the lowest energy compared to other configurations. At the top and bridge sites, the most stable configuration is one-leg (-0.117 *eV* and -0.116 *eV*, respectively), while at the hollow site, it is two-leg (-0.123 *eV*). The interaction between H_2O and graphene is stronger at the hollow site compared to the bridge and top sites because the hollow site allows more atoms of H_2O to interact directly with the carbon surface, leading to a more stable configuration and lowest energy. All stable structures have a distance between 2.8 and 3.2 Å (measured from the position of the O atom). The zero-leg configuration at the hollow and top sites has the shortest distance, while at the bridge site it has the longest. But even with a short distance, the energy is still higher compared to the two-leg configuration at the hollow site, which means it is less stable. Based on this, distance doesn't determine the most stable structure. However, among all positions and H_2O configurations, the most stable is the two-leg configuration at the hollow site with an adsorption energy of -0.123 *eV*.

The adsorption energies of H_2O molecules with different orientations on different active sites were found to be more affected by the orientation of the H_2O molecule. A shared characteristic among the three orientations is that the hydrogen atoms tend to be attracted to the carbon surface. Orientation two leg on hollow site is more stable than the other orientations and positions. This suggests that the key factor driving the adsorption of H_2O molecules onto the carbon surface is the interaction involving the hydrogen atoms rather than the oxygen atom. The interaction between H_2O and graphene is classified as physisorption because it has a low adsorption energy and involves minimal charge transfer [14][18].

Table 2. Comparison of adsorption energies of H_2O on graphene reported in previous studies

Study	Method	E_{ads} (eV)
Leenaerts *et al.* (2008) [18]	DFT-PBE	−0.120
Hamada (2012) [16]	vdW-DF	−0.140
Liang *et al.* (2021) [19]	DFT	−0.116
Abidin *et al.* (2022) [14]	DFT	−0.126
A. O. Santos et al. (2026) [20]	DFT (vdW-C09)	−0.093 to −0.145
This study	**DFT-D3**	**−0.123**

Previous studies by Abidin *et al.* and Zeng Liang *et al.* also reported similar findings, stating that the two-leg configuration at the hollow site is the most stable structure, but with differing adsorption energies of -0.126 *eV* and -0.116 *eV* [14][19]. These differences arise due to variations in the graphene size used, calculation methods, pseudopotential files, and versions of the Quantum ESPRESSO software.

Role of Molecular Orientation in Adsorption Stability

The results obtained in this study indicate that the molecular orientation of the H_2O molecule plays a crucial role in determining the adsorption stability on the graphene surface. Although the adsorption site influences the interaction strength, the orientation of the water molecule relative to the graphene plane appears to have a more significant effect on the adsorption energy. In the two-leg configuration, both hydrogen atoms of the water molecule are directed toward the graphene surface. This orientation allows the partially positive hydrogen atoms to interact more effectively with the delocalized π-electron system of graphene. As a result, this configuration produces the lowest adsorption energy, particularly at the hollow site, indicating a more stable adsorption structure.

In contrast, the zero-leg configuration, where the oxygen atom faces the graphene surface, results in weaker interactions. This behavior can be explained by considering the charge distribution within the water molecule. The oxygen atom carries a partial negative charge, while the hydrogen atoms are partially positive. Since graphene surfaces possess delocalized electron density, the interaction between hydrogen atoms and the graphene surface is energetically more favorable than interactions involving the oxygen atom. The one-leg configuration represents an intermediate case where only one hydrogen atom interacts directly with the graphene surface. Consequently, the adsorption energies for this configuration fall between those of the zero-leg and two-leg configurations. These findings demonstrate that the orientation of the water molecule significantly influences the strength of the adsorption interaction.

Similar observations have been reported in previous theoretical studies. For example, Leenaerts *et al.* [18] reported that adsorption configurations where hydrogen atoms point toward the graphene surface tend to be energetically more stable due to favorable electrostatic interactions. Likewise, Hamada [16] showed that dispersion interactions play a significant role in stabilizing water adsorption on graphene when hydrogen atoms are oriented toward the surface. Overall, the results indicate that the adsorption of water on pristine graphene is governed by a combination of weak electrostatic interactions and van der Waals forces, rather than strong chemical bonding. This explains the relatively low adsorption energies obtained in the present study and further supports the classification of the adsorption mechanism as physisorption.

CONCLUSION

This study investigated the adsorption behavior of H_2O molecules on a graphene surface using Density Functional Theory (DFT) with the DFT-D3 dispersion correction to account for van der Waals interactions. The results demonstrate that both the molecular orientation of the water molecule and the adsorption site on graphene significantly influence the stability of the adsorption system. Among the nine adsorption configurations analyzed, the two-leg orientation at the hollow site was found to be the most stable structure, exhibiting the lowest adsorption energy of −0.123 eV. The results indicate that the adsorption stability is mainly governed by the interaction between the hydrogen atoms of the H_2O molecule and the graphene surface, rather than interactions involving the oxygen atom. The adsorption distances obtained in this study range between 2.8 Å and 3.2 Å, which are consistent with typical values reported for weakly adsorbed molecular systems.

The relatively small adsorption energies observed for all configurations indicate that the interaction between H_2O molecules and graphene is dominated by weak van der Waals forces, confirming that the adsorption mechanism can be classified as physisorption. The calculated adsorption energy is also in good agreement with values reported in previous theoretical studies, further supporting the reliability of the computational approach employed in this work. From a broader perspective, understanding the adsorption behavior of water molecules on graphene surfaces is important for the development of graphene-based technologies, including gas sensors, energy storage systems, and catalytic materials. Since water molecules are commonly present in practical environments, their interaction with graphene can significantly influence the surface properties and performance of these devices. Future work will focus on a more detailed investigation of the electronic properties of the adsorption system, including charge transfer analysis and electronic structure characterization, in order to further elucidate the interaction mechanisms between water molecules and graphene surfaces.

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