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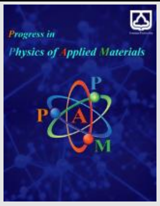

Investigation of CO2 and N2 adsorption on pristine and oxidized γ-graphyne using density functional theory (DFT): A First-principles analysis

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ABSTRACT

Graphyne is of great interest to researchers due to its unique electronic and mechanical properties, which make it a potentially valuable material for a wide range of applications. The importance of graphyne lies in its potential to enable new technologies and applications in a variety of fields, from electronics to materials science. In this paper, the density functional theory (DFT) calculation was used to investigate CO_2 and N_2 adsorption on pristine and oxidized γ-graphyne in both two horizontal and vertical directions at hollow and bridge sites. Based on the results, the highest stability was observed when the CO_2 and N_2 molecules approached the γ-graphyne sheet in a hollow space. Oxygenation of γ-graphyne led to increased CO_2 adsorption capacity compared to pristine γ-graphyne. This can be attributed to the interaction between the Pπ electrons of the carbon in graphyne and carbonyl groups with the unbonded electron pair of the oxygen in CO_2, leading to a more significant interaction of CO_2 with the γ-graphyne surface. Furthermore, no significant N_2 absorption was observed for oxygenated γ-graphyne.

1. Introduction

The increase in CO_2 concentration in the atmosphere due to fossil fuel usage has caused environmental pollution, which is the main source of global warming. Several theoretical and experimental studies have been conducted on reducing and controlling CO_2 in the atmosphere to decrease greenhouse gases' harmful effects on the environment [1]. The use of carbon dioxide absorption on a solid adsorbent is considered an effective method due to low operating costs and energy requirements [1, 2]. Recently, many adsorbent materials have been widely considered. Several studies have suggested carbon-based adsorbents as potential candidates to remove or reduce atmospheric CO_2 concentration due to their elasticity, high surface area, and low weight [3–7]. On the other hand, by introducing selectivity and permeability as two important factors in evaluating the performance of absorbent materials and knowing the inverse ratio of permeability to thickness [8, 9], it can be concluded that one-atom-thick materials can be evaluated as a successful candidate for reducing CO_2 concentration. Among the different carbon allotropes, graphyne has attracted much scientific attention. Graphyne as an actively predicted graphene analog was first proposed by Baughman et al [10–14]. This structure, with 12 carbon atoms per unit cell, may be described as an *sp* and *sp²* hybridized lattice in which hexagonal graphyne is formed by *sp²* hybridized carbon atoms that are connected to each other through acetylene bonds (−C≡C−) [3, 4, 6, 8, 9, 15]. By substituting some carbon-carbon bonds with

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acetylenic linkages, various carbon allotropes, including graphdiyne and graphyne, are formed [16]. Several theoretical and experimental studies have focused on the properties of these novel graphyne analogues, which future nanoelectronic devices may benefit from [3, 4, 17, 18]. Among several different graphyne geometries, α-graphyne and β-graphyne are predicted to be semimetals with a zero gap. At the same time, γ-graphene is a semiconductor with a band gap of about 0.45 eV [17]. The semiconducting property of γ-graphyne allows it to find possible applications in sensors, transistors, and energy storage materials such as electrodes in fuel cells, etc. In a study, the physical adsorption of H_2 on graphyne and graphene monolayers using DFT calculations was investigated by Bartolomei et al [19]. The results showed more favorable H_2 adsorption on graphyne, which can be attributed to higher binding energies at equilibrium distances of graphene. In another study, molecular dynamics simulations were used to study the adsorption and separation of CO_2 and N_2 molecules on graphtriyne multilayers [10]. It was found that the CO_2 adsorption average increases linearly with increasing initial pressure, which can be compared with other carbon-based adsorbents. On the other hand, the first principle calculations on the adsorption of CO_2 and N_2 on single-walled aluminum nitride nanotubes showed strong chemical binding of CO_2 to AlN nanotubes [11]. Inspired by the dominant properties of oxygenated graphyne on adsorption techniques, we were motivated to study the pristine and oxygenated γ-graphyne's adsorption ability of CO_2 and N_2 gas molecules. Based on the results, oxidized graphyne improves gas adsorption capacity compared to pristine graphyne. Furthermore, oxygenated graphyne showed a high absorption capacity for carbon dioxide. However, it does not affect the N_2 molecule's energy absorption rate.

The calculations were performed based on density functional theory (DFT) using the $DMOL_3$ package embedded in Material Studio software for condensed matter systems and different types of carbon allotropes [12, 13, 20]. The generalized gradient approximation (GGA) method with Perdew-Burke-Ernzerhof (PBE) correlation and a double plus polarization (DNP) numerical basis was used. The GGA-PBE functional was applied to describe the interaction between organic molecules and a carbon-based substrate, which has been widely utilized in the physics of materials science [21, 22]. A supercell of γ-graphyne consisting of 144 carbon atoms in a graphyne's surface of 23.849A°× 23.800 A° is designed with the positions of atoms related to meet the convergence criteria of 10^{-6} Hartree in a 3×2 monkhorst-Pack k-Point mesh. In order to simulate an infinitely large system, periodic boundary conditions (PBC) with a vacuum of 30 A° were chosen in the space between the two adjacent planes [14, 17, 18]. The adsorption energy (E_{ad}) of CO_2 and N_2 molecules on the surfaces of the pristine and functionalized graphyne was obtained using the following equations, respectively:

$$E_{ad} = E_{total} - E_{graphyne} - E_{co_2 orN2} \quad (1)$$

$$E_{ad} = E_{total} - E_{graphyne} - E_{O} - E_{co_2 orN2} \quad (2)$$

Where E_{ad} is the adsorption energy, E_{total} describes the total energy, $E_{graphyne}$ is the isolated graphyne energy, and E_0 represents the isolated oxygen energy. Based on the above equations, lower adsorption energy indicates greater stability. Since dispersion interactions play an important role in the interaction between gas molecules and graphyne surfaces, the developed DFT method with dispersion correction (DFT-D_3) was employed for a better description [23].

2. Computational Details

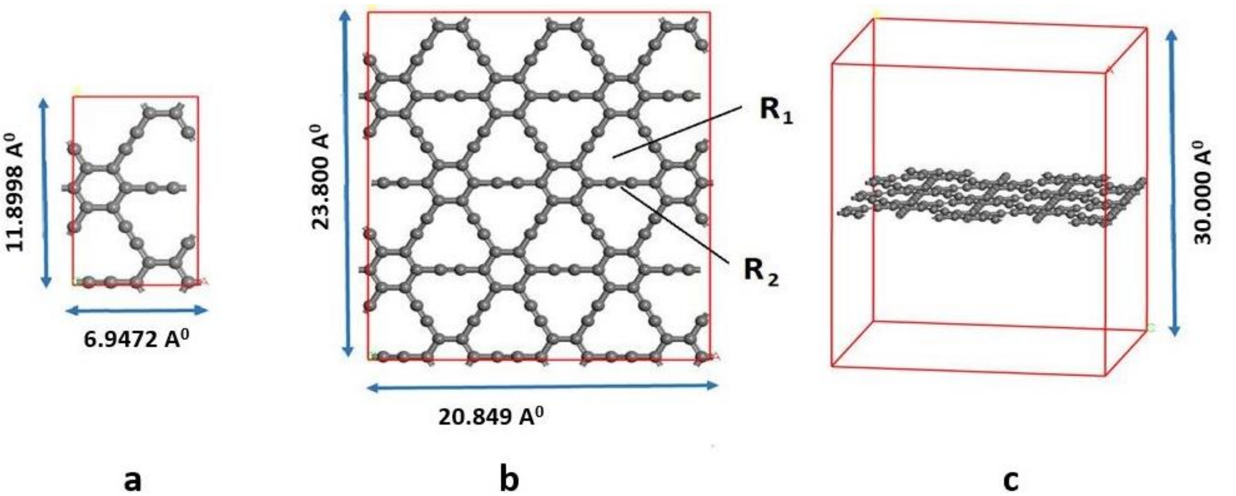

Fig. 1. Geometries of graphyne (a) a unit cell of the 3×2 supercell structure of graphyne and surface of the unit cell 6.9472 A°×11.8998 A°. (b) Structure of the unit cell a graphyne sheet. And the surface of the unit cell 20.849 A°×23.800 A°×30.000 A° with coexisting hybridized sp and sp^2 atoms. (c) The height required to keep the thickness was determined at 30.000 A°

3. Results and discussion

At first, the geometry optimization of the graphyne cells was performed based on the GGA (PBE) method. Graphyne lattice constants were calculated to be 20.849

A°×20.849 A°×23.800 A°. To simplify the calculations, it is useful to represent them as 3×2 supercells as shown in Figures 1a-b. Figures 1a-b show the structure of a graphyne sheet in a unit cell consisting of 24 carbon atoms with their sp and sp^2 hybridization of atoms. The optimized lattice parameter of a graphyne unit cell was calculated to be 20.849 A°×20.849 A°, which is half of the supercell lattice parameter, and in reasonable agreement with previously reported results [16, 19, 24, 25], approximately 23.800 A°. Electrostatic interaction was carried out by atomic charges during adsorption. Therefore, to estimate the charge distribution of the graphyne's surface, a Mulliken charge analysis was performed. This was done by calculating the charge difference of each adsorbent atom, ΔQ, before and after the adsorption process, denoted by Q_i and Q_f, respectively (equation 3).

$$\Delta Q_n = Q_{in} - Q_{fn} \tag{3}$$

Where the subscript n specifies the n-th atom of graphyne (CO_2 or N_2). The adsorption behavior of single CO_2 and N_2 molecules on the graphyne surface is investigated at two different adsorption sites R_1 (hollow site) and R_2 (bridge site) and two different adsorption directions, parallel and perpendicular to the graphyne surface.

3.1. Adsorption of single molecules of CO_2 and N_2 parallel to graphyne

To study the adsorption of CO_2 and N_2 molecules on the surface of graphyne, two different sites of adsorption, hollow sites and bridge sites, are investigated on the surface of graphyne through geometry optimization. First, the adsorption characteristics of a single CO_2 molecule on the graphyne's surface were investigated (Figure 2a). As can be seen in Figures 2a and 2b, the adsorption energies and their corresponding bond length of the molecules to the graphyne plane in two adsorption sites were calculated as -0.341 eV and 3.14 A° at the hollow site and -0.397 eV and 3.08 A° at the bridge site, respectively. The results of the calculations showed that the bridge site is a more favorable site for CO_2 adsorption compared to the hollow site.

The adsorptive properties of the N_2 molecule on the graphyne surface for two different bridge and hollow sites were analyzed, as shown in Figure 3. The adsorption energies of a single N_2 molecule and their corresponding bond lengths in the above two adsorption sites were calculated to be -0.360 eV and 3.43 A° in the hollow site and -0.347 eV and 3.63 A° in the bridge site, respectively. DFT calculations showed that the hollow site of R1 is the most preferable site for the adsorption of N_2 molecules. In contrast, the most adsorption site for CO_2 molecule adsorption was observed at the bridge site. Table 1 shows the charge transfer of single CO_2 and N_2 horizontal molecules on graphyne.

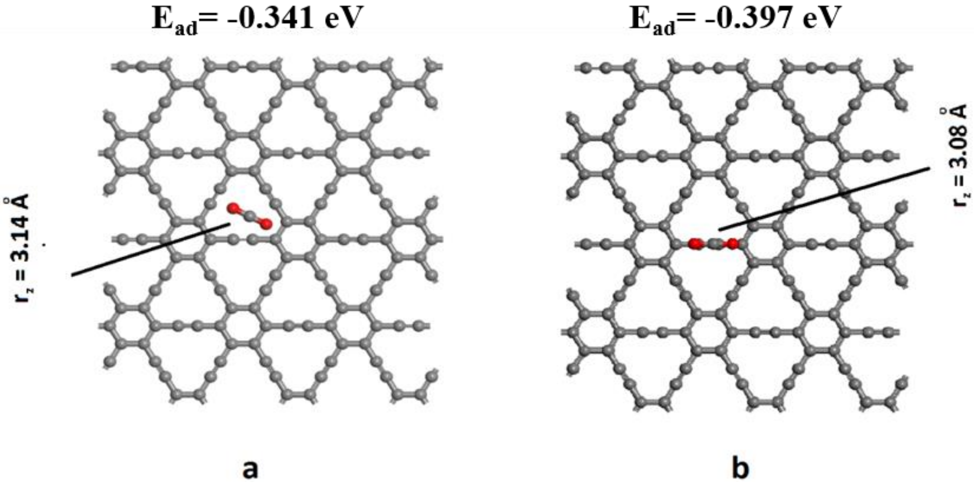

Fig. 2. Adsorptive configurations of horizontal CO_2 on graphyne using DFT calculation. CO_2 adsorption at (a) the hollow site between the acetylene links on R_1, and (b) the bridge site on R_2.

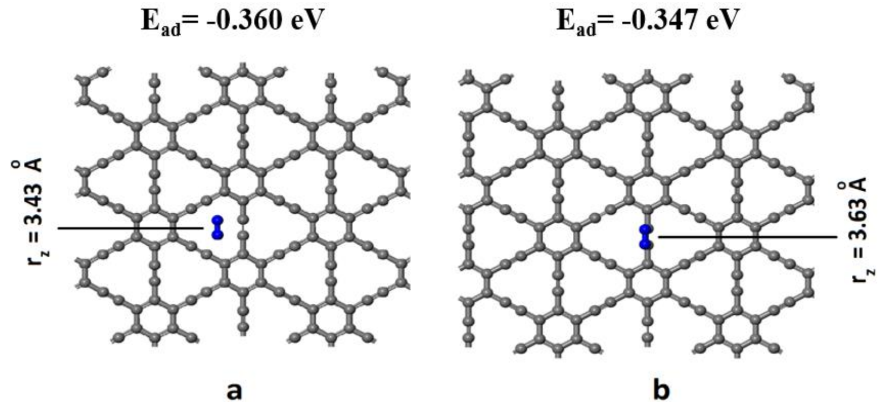

Fig. 3. Adsorptive configurations of horizontal N_2 on graphyne using DFT calculation. N_2 adsorption-(a) the hollow site between acetylene links R_1. (b) the bridge site on R_2.

Table 1. Charge transfer of single CO_2 and N_2 horizontal molecules on graphyne by DFT calculation.

Site		Charge transfer for CO_2(-e)	Charge transfer for N_2(-e)
Graphyne	Hallow	0.006	-0.002
Graphyne	Bridge	0.013	-0.001

3.2. Adsorption of CO_2 and N_2 single molecules perpendicular to graphyne

The results of geometry optimization showed several favorable sites for the adsorption of single molecule CO_2 vertically on the graphyne's surface. The adsorption energies and the corresponding bond lengths are calculated to be - 0.310 eV and 3.32 A° at the hollow sites on R_1 (Figure 4b) and - 0.287 eV and 3.49 A° at the bridge site on R_2 (Figure 4a), where the bonding length, r, showed the distance between the oxygen atom in CO_2 molecule and the yellow carbon with triple bond on the surface of graphyne. The adsorption characteristics of the N_2 molecule are shown in Figure 5. The geometry optimization of the structure revealed that the single N_2 molecule in rotated form was adsorbed near carbon triple bonds. The adsorption energies and bond lengths are -0.321 eV and 3.92 A° at the bridge site on R_2, and -0.357 eV and 3.57 A° at the hollow site on R_1, respectively. DFT calculations showed that the hollow site between acetylene bonds is the most favorable adsorption site for CO_2 and N_2 single molecules. Charge transfer of single CO_2 and N_2 vertical molecules on graphyne were shown in Table 2.

Table 3 represents the bond lengths, adsorption energies, and charge transfer for CO_2 and N_2 adsorption, parallel and perpendicular to graphyne (at the bridge site on (R_2) and the hollow site between acetylene bonds (R_1)).

Fig. 6 briefly summarizes the results of sections 3.1 and 3.2. The 3D schematic of adsorption energy and charge transfer (Figures 6a and b) vs rz and adsorption type, was shown for CO_2 and N_2 single molecules, parallel and perpendicular to graphyne, respectively.

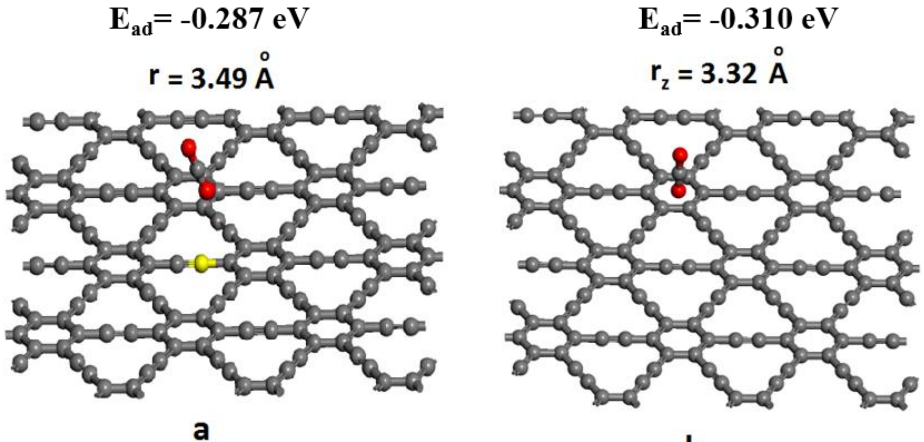

Fig. 4. Adsorptive configurations of vertical CO_2 on graphyne using DFT calculation. CO_2 adsorption at (a) the bridge site on (R_2), and (b) the hollow site between the acetylene links on (R_1).

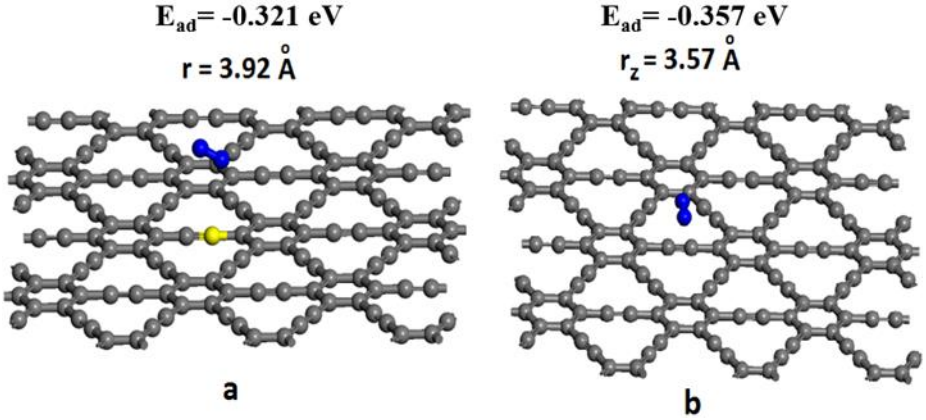

Fig. 5. Adsorptive configurations of vertical N_2 on graphyne using DFT calculation. N_2 adsorption at (a) the bridge site on (R_2), and (b) the hollow site between acetylene links (R_1)

Table 2. Charge transfer of single CO_2 and N_2 vertical molecules on graphyne by DFT calculation.

Site		Charge transfer CO_2(-e)	Charge transfer N_2(-e)
Graphyne	Hallow	0.005	-0.003
Graphyne	Bridge	0.003	-0.002

Table 3. Results of the bonding length, adsorption energy, and charge transfer of CO_2 and N_2 adsorption, parallel and perpendicular to graphyne.

Materials and types of adsorptions	**rz (A)** ***rz denotes r and rz.**	**E_{ad} (eV)**	**Charge transfer (-e)**
CO_2 horizontal on graphyne/hollow site between links R_1 (CO_2_HHR_1)	3.14	-0.341	0.006
CO_2 horizontal on graphyne/the bridge site on R_2 (CO_2_HBR_2)	3.08	-0.397	0.013
N_2 horizontal on graphyne/the hollow site between acetylene links R_1. (N_2_HHR_1)	3.43	-0.360	-0.002
N_2 horizontal on graphyne/the bridge site on R_2 (N_2_HBR_2)	3.63	-0.347	-0.001
CO_2 vertical on graphyne/the hollow site between acetylene links R_1. (CO_2_VHR_1)	3.49	-0.287	0.005
CO_2 vertical on graphyne/the bridge site on R_2 (CO_2_VBR_2)	3.32	-0.310	0.003
N_2 vertical on graphyne/the hollow site between acetylene links R_1 (N_2_VHR_1)	3.92	-0.321	-0.003
N_2 vertical on graphyne/the bridge site on R_2 (N_2_VBR_2)	3.57	-0.357	-0.002

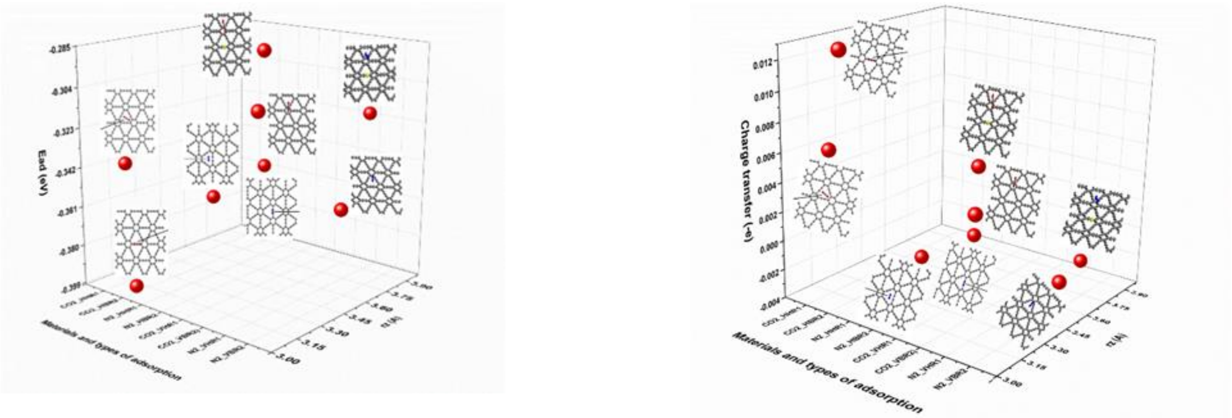

Fig.6. 3D schematic of (a) adsorption energy (z direction), and (b) charge transfer (z direction) vs rz (x direction) and materials and type of adsorption (y direction), respectively for CO_2 and N_2 single molecules adsorption, parallel and perpendicular to graphyne.

3.3 Formation of a functional group on the triple bond of graphyne

In the oxidation of graphyne (Figure 7a), the highest occupied molecular orbital (HOMO) of the triple bonded carbon atom with the lowest unoccupied molecular orbital (LUMO) of the oxygen atom are used. The triangle epoxide structure is formed by a positively charged carbon atom and a negatively charged oxygen atom [26]. The double bond of the epoxide ring creates high angular pressure, which breaks one of the epoxide ring bonds. Therefore, the oxygen atom gains an additional negative charge, and the carbon atom gains an additional positive charge. Due to its lack of five-bond capacity, the carbon atom resonates on the triple bond to form the ketone functional group. This is ultimately the most stable configuration for the ketone functional group on the surface of graphyne (Figure 7b) [27].

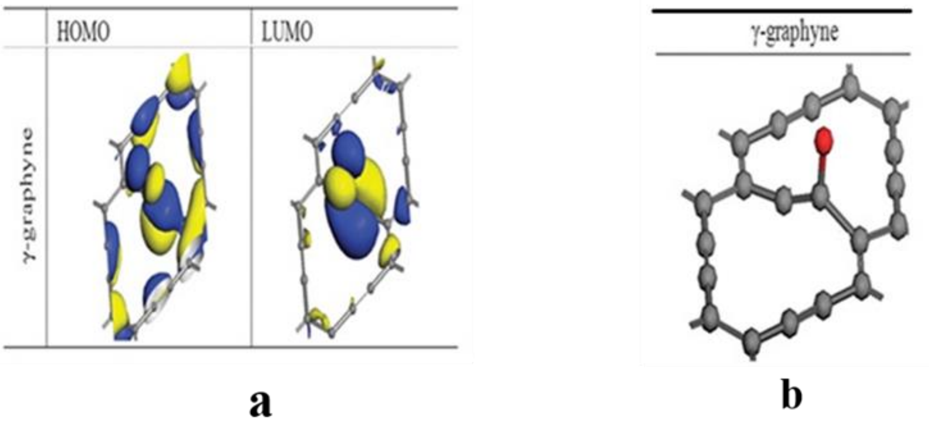

Fig 7. (a) HOMO and LUMO of oxygenated γ-graphyne, and (b) the most stable structure of oxygenated γ-graphyne.

3.4. The analysis of CO_2 molecule adsorption on graphyne functionalized surface

In the carbon dioxide molecule, the polarity of the covalent bonds and the increased electronegativity of the oxygen atom led to a partial positive charge on the carbon atom. So, when the CO_2 molecule approaches horizontally to the graphyne functionalized side (up) (Figure 8a) the interaction of the P_π carbon atom of the graphyne and oxygen electron pair of CO_2 is more effective than the other opposite side of the functionalized group (down) (Figure 8-b) which is exhibited in the calculation results. Graphyne oxidation leads to increased interactions on the graphyne surface. Therefore, the adsorption energy increases when the CO_2 molecule approaches horizontally from the functionalized surface of graphyne. Charge transfer results corresponded to the amount of absorbed energy. Table 4 shows the adsorption energy E_{ad} (eV), bond length, and charge transfer of CO_2 adsorption on the surface of oxygenated graphyne.

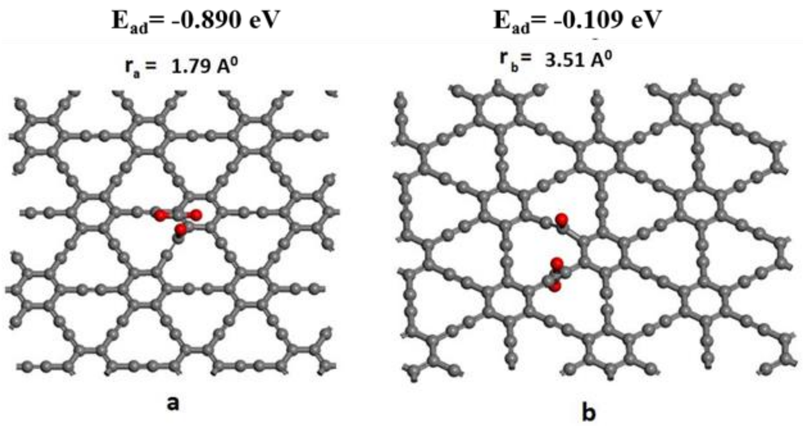

Fig. 8. Adsorptive configurations of CO_2 on oxygenated graphyne using DFT calculation.

Table 4. Adsorption energy E_{ad} (eV), bond length, and charge transfer of CO_2 adsorption on the surface of oxygenated graphyne by DFT calculation.

position	direction	**E_{ad} (eV)**	d($\mathring{A}$)	$\Delta q(-e)$
$CO_2 - down$	V	-0.109	3.51	-0.003
$CO_2 - up$	h	-0.890	1.79	-0.017

3.5. The analysis of N_2 molecule absorption on graphyne functionalized surface

A study of the adsorption of nitrogen molecules under the same conditions as the CO_2 molecule was conducted to assess the selectivity of the functionalized graphyne surface. Figures 9a and b show that modifying the graphyne configuration did not affect the adsorption of N_2 molecules on the surface when approached horizontally (up and down). This result indicates that the adsorption capability depends strongly on the adsorbent's physical properties. Adsorption energy and bonding distance confirmed the interaction. The energy of E_{ad} bond length and charge transfer of N_2 single molecule adsorption on the surface of oxygenated graphyne were shown in Table 5. Summary of the bonding length, adsorption energy, and charge transfer for CO_2 and N_2 adsorption, parallel and perpendicular to graphyne are available in Table 6.

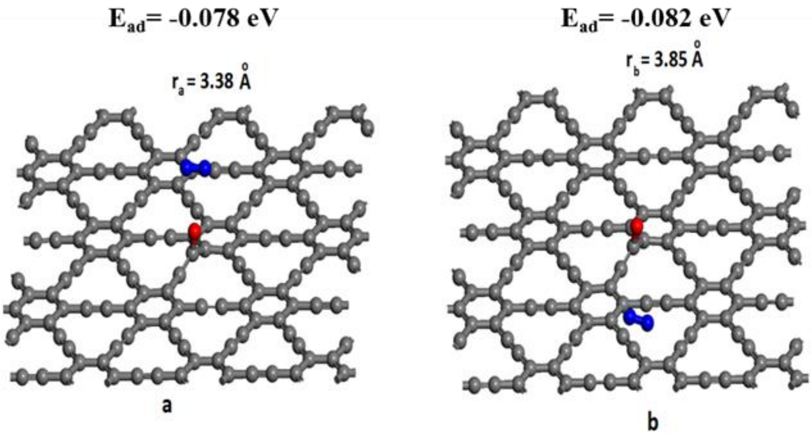

Fig. 9. Adsorptive configurations of N_2 on oxygenated graphyne using DFT calculation.

Table 5. Adsorption energy E_{ad} (eV), bond length and charge transfer of N_2 single molecule adsorption on the surface of oxygenated graphyne by DFT calculation.

Position	Direction	**E_{ad} (eV)**	d($\mathring{A}$)	$\Delta q(-e)$
$N_2 - down$	H	-0.082	3.85	-0.003
$N_2 - up$	H	-0.078	3.38	-0.002

Table 6. Summary of the bonding length, adsorption energy, and charge transfer for CO_2 and N_2 adsorption, parallel and perpendicular to graphyne.

Materials and types of adsorptions	**d (A)**	**Ead (eV)**	$\Delta \boldsymbol{q}(-\boldsymbol{e})$
Co$_2$ molecule approaches the surface horizontally from the graphyne functionalized side (up) (CO$_2$_HFU)	3.51	-0.109	-0.003
Co$_2$ molecule approaches the surface horizontally from the graphyne functionalized side (down) (CO$_2$_HFD)	1.79	-0.890	-0.017
N$_2$ molecule approaches the surface horizontally from the graphyne functionalized side (up) (N$_2$_HFU)	3.85	-0.082	-0.003
N$_2$ molecule approaches the surface horizontally from the graphyne functionalized side (down) (N$_2$_HFD)	3.38	-0.078	-0.002

4. Conclusion

The adsorption of CO_2 and N_2 single molecules on γ-graphyne is competitively investigated to clarify the adsorptive properties of this carbon allotrope. Comparatively, with other graphyne forms, this form has higher site diversity and higher chemical stability. In this study, DFT quantum calculations and optimization of graphyne geometry were performed to investigate the sorption of CO_2 and N_2 single molecules through hollow and bridge positions in horizontal and vertical directions. Based on the results, adsorption of CO_2 and N_2 molecules occurred physically when these molecules approached the graphyne surface horizontally, which is due to the low charge transfer and bonding distance. The highest stable geometry for CO_2 and N_2 molecules is found in a hollow position when they approach vertically the graphyne surface. Both CO_2 and N_2 molecules showed high stability and affinity for adsorbing in hollow sites. To improve the adsorption of carbon dioxide and nitrogen molecules on the surface, an oxidized γ-graphyne sheet was employed. Calculations showed that functionalizing graphyne increases the surface selectivity for carbon dioxide without affecting the rate of nitrogen molecule adsorption. Therefore, functionalizing graphyne may be a complementary strategy for adsorbing and separating carbon dioxide from the atmosphere.

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