Theoretical Investigations of CO_2-N_2 Separation on γ-Graphyne Membranes: A Classical Molecular Dynamics Study

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Abstract. γ-graphynes recently emerged as promising candidates for molecular sieving applications due to their intrinsic and tunable nanoporosity. The possibility to modulate the dimension of the pore is, therefore, a key aspect for the design of new-generation nano-materials for carbon-neutrality techniques. In the present contribution, a preliminary analysis on graphtetrayne has been performed in order to characterize the main morphological properties and underline the most important adsorption processes. In details, classical molecular dynamics simulations have been performed, in order to investigate the interaction of a single graphtetrayne layer with CO_2 and N_2 molecules. Preliminary results indicate a stronger interaction of carbon dioxide compared to molecular nitrogen leading to a higher selectivity toward CO_2 over N_2, driven by a combination of energy contributions and morphological aspects. Overall, the present study represents a preliminary investigation aimed at characterizing the adsorption and selectivity properties of graphtetrayne as candidates for the design of membranes for CO_2 - N_2 separation under post-combustion conditions. These findings provide a basis for a more comprehensive study, which will be extended to multilayer configurations in order to better assess their potential for carbon capture applications.

Keywords: Carbon-based nanomaterials · CO_2 Adsorption · Classical Molecular Dynamics · Force Field

1 Introduction

The development of new techniques aimed at removing and reducing the concentration of greenhouse gases became a primary issue in the context of a transition toward sustainable technologies. The increasing level of carbon dioxide (CO_2) in the atmosphere, mainly coming from antropic effects, such as fossil fuels combustion, has been directly linked to climate change and its related environmental impacts. As a consequence, one of the main focuses of modern

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technologies is the development of efficient strategies for CO_2 capture and separation. In this context, various approaches have been proposed as promising techniques for the selective removal of CO_2 from gas mixtures, in particular those containing molecular nitrogen (N_2) which is the main component of the atmosphere. Within this framework, the achievement of high selectivity and adsorption capacity, as well as low energy requirements, is essential for practical development. The use of porous materials [1–5], including zeolites, metal–organic frameworks (MOFs), and covalent organic frameworks (COFs), have been extensively studied for gas adsorption and separation. The main advantages of these structures are related to tunable pore sizes, high surface areas, and different possibilities of chemical functionalization, leading to a high impact on adsorption properties. Together with a series of advantages, several challenges remain open, including high cost of synthesis, limited structural stability under operative conditions and potential degradation over time. These limitations, together with energy requirements, challenge the continuous search for alternative materials. Recently, two-dimensional (2D) carbon-based nanomaterials have emerged as promising candidates for the development of new-generation membranes for gas adsorption and separation [6,7]. Their unique properties, including atomic-scale thickness, high surface-to-volume ratios, and tunable chemical characteristics, enable strong and tunable interactions with gas molecules. The prototypical 2D carbon material is represented by Graphene and it has been widely investigated due to its exceptional mechanical, thermal and chemical properties [8]. However, pristine graphene exhibits limited gas permeability and weak physisorption interactions with many gas species, which reduces its range of applicability. Different strategies have been developed to overcome this issue, including functionalization, introduction of vacancies and defects [9,10]. Another alternative is represented by the use of similar materials, Graphynes, which represent a versatile family of 2D carbon allotropes composed of both sp and sp^2 hybridized carbon atoms, whose structure is characterized by benzene rings interconnected via acetylenic links, which provides intrinsic porosity and tunable structural features. The number of consecutive acetylenic units can be modulated and determines the size and shape of the pores, as well as the mechanical flexibility and electronic properties of the material. A series of computational investigations have been already performed to identify the adsorption properties of different structures, including graph-tryine [11,12] and graph-dyine [13–15], revealing intriguing effects, depending on the nature of the interacting molecules. Among the various graphyne allotropes, graphtetrayne (G4)-defined by four consecutive acetylenic linkages connecting adjacent carbon rings-remains relatively unexplored. The recent syntesys of cristalline graphtetrayne [16], triggered the interest in this peculiar structure. In particular, the expanded pore network and the morphological properties suggest unique adsorption behavior, particularly for small molecules such as CO_2 and N_2. While recent studies have investigated the structural, electronic, and stacking properties of multilayer graphyne systems, the fundamental mechanisms governing adsorption at the single-layer level remain poorly understood. Within this framework, a computational investiga-

tion appears to be extremely important. Atomistic simulations, indeed, provide a powerful framework to investigate these interactions at a molecular level. In details, Classical molecular dynamics (MD), based on a correct description of the intermolecular force fields, allows for systematic exploration of configurational space, enabling the identification of energetically favorable adsorption sites, preferred orientations of adsorbates, and selectivity trends between different gas species. In this work, we performed a preliminary analysis of the interaction of CO_2 and N_2 molecules with a single layer of graphtetrayne, using classical molecular dynamic simulations to analyze the adsorption properties. By establishing these fundamental insights, this study sets the stage for future investigations into more complex systems, including multilayer graphyne assemblies, functionalized derivatives, and hybrid materials. Ultimately, our work contributes to the ongoing effort to design efficient, scalable, and sustainable materials for CO_2 capture and separation technologies, offering potential pathways toward environmentally friendly and economically viable solutions.

2 Theoretical Methods

2.1 *Ab Initio* calculations

An initial analysis on the monomeric structure was performed at the DFT level, in order to characterize the morphological properties of the pore and compare the size of the available site in different types of graphynes (namely graphdiyne, graphtriyne anf graphtetrayne). As already reported in several cases before [17–22], *ab initio* calculations based on DFT theory represent a good compromise between chemical accuracy and computational cost, especially in the case of big systems, which needs a high computational power. For this purpose, geometry optimization and frequency analysis were performed at the B3LYP [23,24] level of theory, in conjunction with the 6-31G [25,26] basis set. The *Gaussian09* [27] was used for electronic structure calculatons, while the visulaization of the frequencies was performed using Avogadro.

2.2 Molecular Dynamics

In order to understand the adsorption properties of a graphtetrayne layer, molecular dynamics simulations were performed to analyze the interaction between the structure and a mixture of CO_2 and N_2 molecules. The DL_POLY [28] simulation package was used, considering the NVT ensemble, where the number of particles (N), volume (V) and temperature (T) are kept constant and using a Hoover-Nose thermostat [29] with a relaxation constant of 0.5 ps. After an initial equilibration period of 1 ns, all the simulations were performed for a total time of 5 ns, considering a temperature of 300 K, while the pressure was calculated using the Peng - Robinson equation of state, and resulting in 5.2 atm. It must be noticed that the reference pressure reported in this work was not used only as an input parameter in the MD runs, but rather to determine the initial density of the gas mixture. In particular, the Peng–Robinson equation of state was

employed to estimate the equilibrium density of the equimolar CO_2/N_2 mixture at the chosen temperature and pressure conditions. This density was then used to define the simulation box size, which remains fixed throughout the NVT simulations. During the simulations, the graphtetrayne membrane structure was kept frozen, and the gas molecules were treated as rigid bodies. The force field was built on the basis of previous works [11,30], where the electrostatic contribution was developed considering a three charge model for N_2 and five charge model for CO_2. The non-electrostatic component of the interaction was described using the Improved Lennard–Jones (ILJ) potential, as detailed in the next section.

Non-electrostatic Long Range Interactions: the ILJ Model. As already reported, the force field built for the MD analysis is composed by two contributions: the electrostatic potential (V_{elec}) and the non-electrostatic contribution (V_{nelec}). In details, V_{nelec}, was evaluated considering the *Improved Lennard-Jones (ILJ)* model [31–35], in which each pair of interacting atoms (or particles) is treated considering the following formulation:

$$V_{nelec} = V_{ILJ} = \varepsilon \left[\frac{m}{n(r) - m} \left(\frac{r_m}{r} \right)^{n(r)} - \frac{n(r)}{n(r) - m} \left(\frac{r_m}{r} \right)^{m} \right] \tag{1}$$

where ε and r_m are, for each interacting pair, the well depth and its position. The ε and r_m values are estimated on the basis of the molecular polarizabilty, partitioned in different components and assigned to each interaction center.

The *n(r)* term is described as:

$$n(r) = \beta + 4 \left(\frac{r}{r_m} \right)^2 \tag{2}$$

where the β parameter represents the hardness of the two interacting species. In particular, the values of the parameters inserted in equation (1) are linked to fundamental quantities that control the strength and the range of the intermolecular potential, including the dipole moment (μ) and the quadrupole moment (Q) and the atomic/molecular polarizability (α). For a comprehensive explanation and a detailed analysis of how these parameters are calculated, see [30,36].

A complete list of the parameters used to build the force field can be found in [11], while the values for the main interacting centers are reported in Table 1

Table 1. List of the main ILJ parameters describing the interaction of CO_2 and N_2 with a layer of graphtetrayne (indicated as G4). The value of β is considered in the range between 6 and 8.

Interaction	ε (meV)	r_m (Å)
N_{N_2}-C_{G4}	3.97	3.83
C_{CO_2}-C_{G4}	3.55	3.56
O_{CO_2}-C_{G4}	5.01	3.67

3 Results and Discussion

3.1 Electronic Structure Calculations

A first geometry optimization was performed in order to characterize the morphological properties of the G4 structure, considering a monomer, composed of three benzene rings linked by four acetylenic units. The resulting geometry is characterized by a triangular-shaped pore with a geometric diameter of around 8 Å. In order to compare the geometrical features of the pore, a comparison were performed considering the optimized structure of G2 and G3. In Fig. 1 are reported the geometries of the three monomers obtained through DTF calculations.

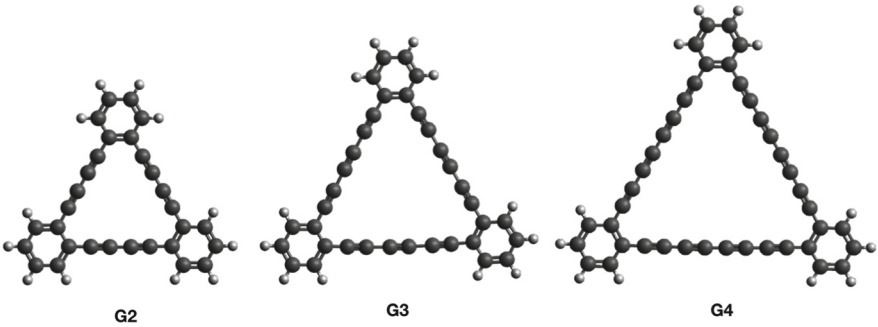


Fig. 1. Schematic representation of the monomeric structure of G2, G3 and G4, obtained through DFT calculations.

As can be seen, the morphology of the structure remains the same, whith a clear modification of the dimension of the pore. The accessible pore diameters of the considered graphyne structures (G2, G3, and G4) were estimated based on the interatomic arrangement and the van der Waals radius of carbon (1.7 Å). As expected, the value of the accessible pore shows an increase of the number of acetilenic units, with G2 showing a relatively small accessible diameter of 2.8 Å, G3 increases to 3.7 Å(as reported also in [11]), and G4 reaches values around 5.0 Å. The differences in the value of the pore diameter can be used to rationalize the possible effects of the structures as material for selective adsorption. The small pore of G2, in fact, can reduce the accessibility to CO_2 and other small molecules, such as N_2, suggesting intrinsic selectivity. G3 provides larger pores that allow both CO_2 and N_2 to penetrate the pore, while G4 may present pores that are too large to sustain strong size-based selectivity, as suggested also in some previous works [37]. These observations highlight the delicate balance between pore size and selective adsorption in graphyne-based materials.

3.2 Classical Molecular Dynamics Analysis

In order to characterize the main adsorption properties and gain insights on the potential selective role of G4 layer, classical MD calculations were performed

considering an equimolar gas mixture of CO_2 and N_2. An appropriate equilibration period of 2 ns was considered in order to allow a fluctuation of the temperature below a factor of 5% and leading the simulations useful to predict and characterize adsorption properties. In Fig. 2 are reported the plots of the radial distribution function in order to characterize the interaction of CO_2 and N_2 with the C atoms of the graphyne layer.

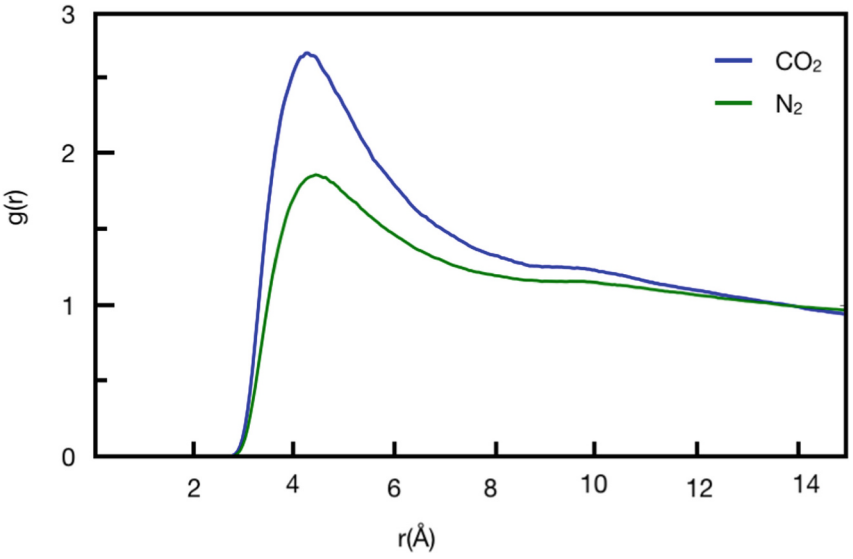


Fig. 2. Radial distribution funtion, g(r), of CO_2 and N_2 molecules interaction with one the C atoms of the G4 layer.

As can be seen, both CO_2 and N_2 show a peak at a distance of around 4.2 Åfrom the surface of the layer. However, a key difference emerges in the intensity of the peak: CO_2 shows a significantly higher and sharper peak compared to N_2. This indicates a higher probability of finding CO_2 molecules at that preferred distance, with respect to N_2. In contrast, the lower peak observed for N_2 reflects weaker correlations and a less pronounced interfacial ordering. This behavior can be rationalized considering the lower intensity of van der Waals forces established between N_2 and the graphyne layer with respect to the case of CO_2 (as already noted also for the case of graph-triyne [11]). At larger distances, both plots smoothly decay toward unity, although CO_2 maintains slightly higher values over an extended range, suggesting a more persistent influence of the surface.

Further insight is provided by the Z-density profiles along the surface-normal direction (z-axis), reported in Figs. 3 and 4.

As can be seen in Fig. 3, the CO_2 density profile is characterized by two peaks located on both sides of the membrane (indicated by the dashed vertical line), revealing the formation of well-defined adsorption layers. The high intensity

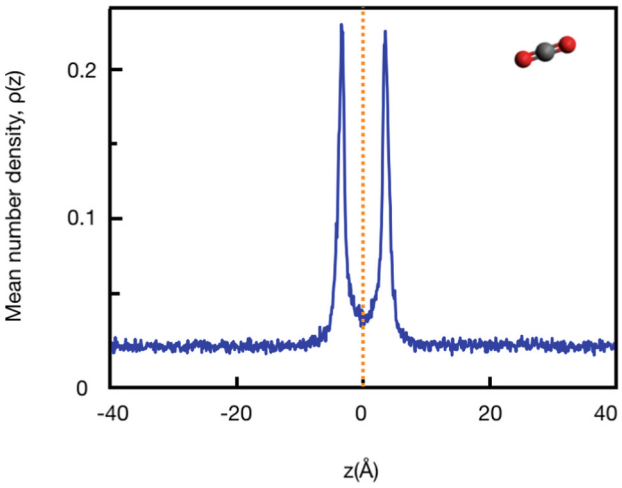


Fig. 3. Z-density profile of CO_2 molecules interacting with the G4 layer, indicated with the orange line.

and narrow width of these peaks reflects the high interaction potential of CO_2 with the graphtetrayne layer. Similarly, the N_2 density profile shows the same behavior but is characterized by less intense peaks, indicating (as expected), that N_2 molecules are less confined near the surface and more uniformly distributed throughout the simulation box. Additionally, the positions of the peaks for both species are comparable, in agreement with the g(r) analysis.

In order to have more consistent initial data and quantify the adsorption process, the number of molecules in the interfacial region was obtained by integrating the z-density profiles over the adsorption domain. In details, the adsorption selectivity was quantified by integrating the number density profiles in the interfacial region corresponding to the pore vicinity and the selectivity was then defined as the ratio between the adsorbed amounts of CO_2 and N_2. This process leads to a value of selectivity of around 1.6, inidcating modest but clear preferential adsorption of CO_2 over N_2. The moderate value of the selectivity suggests that the separation mechanism is governed by weak differences in adsorption strength rather than strong chemical specificity.

Finally, Fig. 5 reports a representative snapshot of the simulation box, obtained from the final step of the calculations, providing a qualitative visualization of the molecular arrangement of the system.

As can be seen, the graphtetrayne layer is located at the center of the simulation box, with both gas species distributed around it. In particular, it's easy to notice that CO_2 molecules are more frequently observed in close proximity to the surface with respect to N_2 molecules, which predominantly occupy the bulk-like regions further away. This visual evidence is consistent with the quantitative observations derived from both the radial distribution functions and the density profiles and can help to highlight the preferential interaction of CO_2

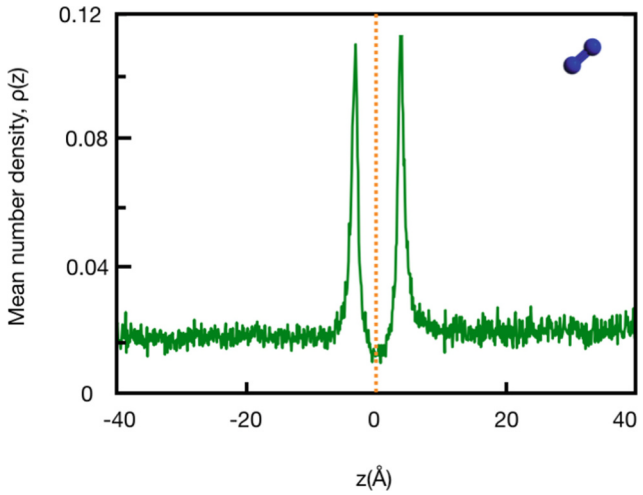


Fig. 4. Z-density profile of N_2 molecules interacting with the G4 layer, indicated with the orange line. (Color figure online)

with the G4 layer. Overall, the combined analysis highlights a clear difference in the effective adsorption strength of the two species. Although both CO_2 and N_2 share the same preferred adsorption distance from the surface, CO_2 exhibits a higher probability of occupying these energetically favorable positions, reflecting stronger intermolecular interactions with the graphyne framework. This behavior can be attributed to the larger quadrupole moment and higher polarizability of CO_2, which enhance its interaction with the carbon-based surface.

Despite this preferential adsorption, which reflects the results of a similar analysis already performed considering G3 systems [11], the overall selectivity can be influenced by the shape of the pore. The relatively large pore size of the G4 graphyne can indeed represent a limitation of the degree of confinement and does not impose a strong steric or energetic discrimination between the two species. As a result, both CO_2 and N_2 can access the vicinity of the surface without significant restriction, and the difference in adsorption strength alone can not be sufficient to achieve highly efficient separation. While pore size and confinement effects play a role in the adsorption behavior, they are not the sole determinant of the observed selectivity. The results indicate indeed that the separation is governed by a combination of geometric confinement and molecule–surface interactions within the G4 layer, where the stronger adsorption of CO_2 can be attributed to its larger quadrupole moment and stronger electrostatic interactions with the graphyne-based pore environment, especially in proximity to the acetylene-rich regions. For this reason, while the G4 monolayer exhibits a measurable preference for CO_2 adsorption, its performance as a selective membrane must be analyszed in details. Future developments will therefore focus on more complex architectures, such as bilayer systems, where the interlayer

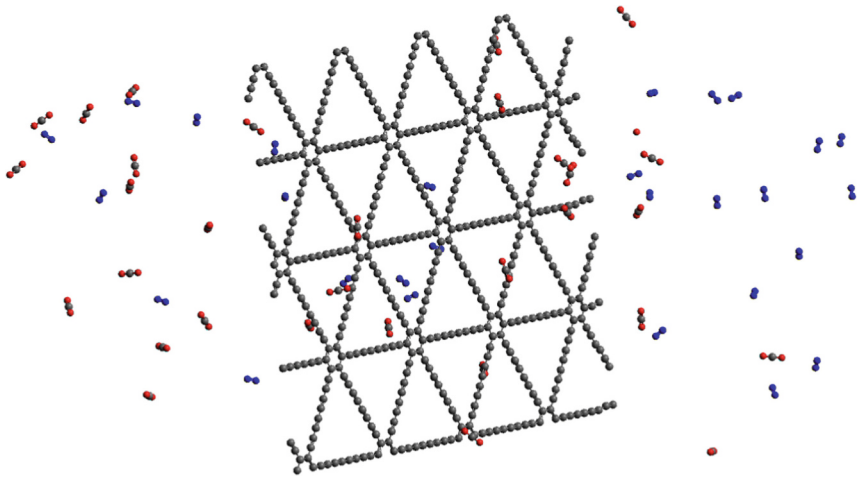


Fig. 5. Snapshot of the final configuration of the system coming from MD calculations.

space can act as a confined adsorption region. In such configurations, enhanced confinement and cooperative interactions between the two layers are expected to increase both the residence time and the selectivity of CO_2, potentially overcoming the limitations coming from the single-layer system and providing a more effective pathway toward gas separation applications.

4 Conclusions

In the present contribution, we performed a preliminary analysis of the adsorption properties of a new generation of carbon-based nanomaterial, composed by graphtetrayne layers, taking into account a gas mixture formed by 50% CO_2 and 50% N_2 molecules, in order to gain useful insights on the potential use of this architectures to remove atmospheric CO_2 molecules in post-combustion environments. Classical MD simulations were performed considering a NVT ensamble to derive structural and physico-chemical information on the system. The analysis of the radial distribution functions (evaluated considering the interaction of C atoms of the G4 structure and CO_2 and N_2 molecules, respectively), corroborated by the plot of the Z-density profiles for both species, clearly show a preferential interaction of CO_2 with the surface of the material, with respect to N_2. This behavior is consistent with the analysis of the strenght of long-range interactions between the selected molecules and the G4 layer. An important parameter to be taken into account for the study of adsorption processes is represented also by the dimension of the pore in the layered structure. In conclusion, although the G4 monolayer exhibits a measurable affinity for CO_2 adsorption, the pore dimensions can affect its properties. The results set the stage for the analysis of more complex architectures, such as bilayer systems, offering a promising strategy to significantly enhance both selectivity and efficiency in gas separation processes.

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