Study on CO$_2$ Adsorption and Permeance of Porous Carbon and Nitrogen Membranes Co-regulated by Charge and Strain

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Abstract. In order to capture and separate CO$_2$ effectively, a novel method of controlling gas permeance by charge and strain is proposed, which has the superiority of controlled dynamic. The effects of porous C$_3$N$_7$ nanosheets on CO$_2$ capture and permeability under different charge quantities and strains were analysed by molecular dynamics (MD) simulations and first-principles density function (DFT) calculations. The molecular permeability of CO$_2$ can be as high as 5.9 × 10$^7$ GPU (CO$_2$/CH$_4$ separation) through 5 e$^-$ charge regulation. In addition, CO$_2$ permeability increased with the increase of tensile strain, and the maximum permeability of 9% stretched C$_3$N$_7$ membrane is 3.6 × 10$^7$ GPU. On this basis, the method of combining negative charge and tensile strain was adopted to study the synergic effect. Under the condition of negative charge of 1 e$^-$ and tensile strain of 3%, CO$_2$ permeability (CO$_2$/CH$_4$ separation) reached 3.2 × 10$^7$ GPU, which was 8 times of CO$_2$ permeability when only 3% strain was added and 9 times of CO$_2$ permeability when only 1 e$^-$ was added. Additionally, under the circumstance of negative charge of 5 e$^-$, the CO$_2$ obtained extra electrons -0.0666 e compared with natural C$_3$N$_7$ membrane. These results provide theoretical guidance for the development of highly controllable materials with CO$_2$ capture and separation.

Keywords. CO$_2$ separation; permeability; combined effect; nanosheet.

1. Introduction

The fossil fuel-based energy consumption structure which leading to high CO$_2$ emissions in the atmosphere, and the increase of CO$_2$ gas content will induce seriously environmental problems [1-4]. Therefore, in order to protect the environment and achieve carbon neutrality, China has repeatedly proposed the development strategy of “carbon peak and carbon neutrality” in the Government report of the State Council in 2021 to achieve efficient capture and separation of CO$_2$ gas by optimizing the industrial structure and energy process. In the chemical industry, organic amine solution is mostly used to absorb CO$_2$, but this method has low efficiency, high pollution and difficulty in adsorbent regeneration [5-7]. With the development of polymer materials, membrane separation technology depended on energy saving, efficiently and easily regenerative, which was considered as a great potential gas separation technology [8].

Membrane separation method is a method to separate mixed gases by using the different permeation rates and capacities of various gases in membrane materials [9-10]. To improve the gas separation efficiency is the difficulty of using membrane separation method to capture CO$_2$ [11]. In order to solve the problem of “trade-off” between permeability and selectivity in the commercial application of polymer membranes, some scholars proposed that reducing the membrane thickness can improve the
permeability of gas, but also reduce the selectivity of membrane materials. The emergence of two-dimensional material membrane breaks the “trade-off” effect [12]. At present, a variety of new membrane materials have been used for the separation and adsorption of CO$_2$ gas, such as molecular sieve, metal-organic frameworks, carbon-based nanosheets and graphene. Inorganic carbon materials such as graphene are regarded as ideal adsorption materials due to their advantages of high specific surface area, corrosion resistance, high chemical and thermal stability [13-17]. Studies have found that graphene membranes can still maintain high selectivity at ultra-thin thickness due to their different gas separation mechanisms [18]. Subsequent studies have shown that the introduction of N-containing groups on the carbon surface can significantly improve the CO$_2$ adsorption performance, and the Lewis acid-base interaction between CN nanosheets and CO$_2$ gas was an important reason for the enhancement of CO$_2$ capture capacity of carbon and nitrogen materials [18-21]. Therefore, a variety of porous carbon-nitrogen membranes with uniform pore sizes have been used to study gas separation [22-24]. This method can not only regulate the CO$_2$ separation process, but realize the CO$_2$ capture process reversibly. Li et al. found that 3 e$^-$ applied to the C$_3$N nanosheet can increase the CO$_2$ adsorption capacity which increased 20 times compared with neutral C$_3$N [25]. In addition, the strain-regulated membrane has also attracted the attention of scholars. Liu et al. improved the selectivity and separation efficiency of carbon and nitrogen membrane for helium by applying compressive strain on C$_6$N$_7$ membrane [26]. C$_9$N$_7$ as a new carbon and nitrogen material, has an effective pore size of 0.333 nm, which is equal to the CO$_2$ molecule kinetic diameter. However, there are relatively few studies on C$_9$N$_7$ membrane separation under charge and stress regulation, and the specific adsorption characteristics and mechanism are still unclear. In order to investigate the membrane separation technology for CO$_2$ adsorption, we research the CO$_2$ gas adsorption characteristics on porous carbon and nitrogen membrane (C$_9$N$_7$) by MD simulations and DFT calculations, and propose a new method of improving the CO$_2$ permeability (charge and strain synergistically regulated C$_9$N$_7$). This method has the advantages of reversibility and controllable dynamics, which can provide theoretical guidance for the development of new gas separation membrane.

2. Model and Methods

2.1. Model

Figure 1 presented the optimized C$_9$N$_7$ nanosheet construction in a 2 × 2 supercell. The side length of the parallelogram was 1.61 nm, which was the length of C$_9$N$_7$ lattice constant (a). The C$_9$N$_7$ nanosheet pores are evenly distributed. The distance between C–C atoms ($d_1$) and N–N atoms ($d_3$) are 0.142 and 0.254 nm, respectively. At the same time, the C–N bond ($d_2$ and $d_4$) are optimized to be 0.132 and 0.137 nm, respectively. Additionally, figure 1 showed that the initial structure of interaction energy between gas molecules (CO$_2$, CH$_4$ and C$_2$H$_2$) and porous C$_9$N$_7$ membrane. In order to figure out the mechanism of gas adsorption, the interaction energy of gas molecules and C$_9$N$_7$ membrane was investigated by DFT calculations. Additionally, the adsorption height of CO$_2$, CH$_4$ and C$_2$H$_2$ molecules with C$_9$N$_7$ membrane were changed from 0 to 4 Å, which can investigate the interaction energy at various position.

![Figure 1. The optimized C$_9$N$_7$ nanosheet structure in a 2 × 2 supercell and calculated model of interaction structure between gas molecule (a) CO$_2$, (b) CH$_4$, (c) C$_2$H$_2$.](image)
2.2. Molecular Dynamics Simulations

To study the separation and capture performance of carbon dioxide on C₃N₇ nanosheets by charge and strain controlling, the simulation study was carried out using the Forcite module in Material Studio (MS) software, and the atomic simulated force field was described for the condensed matter optimization molecular potential of atomic interaction. [27] and the NVT synthesis was selected for the series,[28] and the simulation temperature was kept constant. The cutoff distance between van der Waals and static electricity was 1.25 nm. The time step in MD simulation was 1 ps, data acquisition time was 1 fs, and the total simulation time was 5 ns, which was enough to detect and record the movement of gas molecules.

2.3. Density Functional Theory Calculations

Based on the first principle, DFT calculation was carried out by using the DMol³ module of MS software [29] to calculate the adsorption energy of gas through C₃N₇ membrane and optimize the adsorption membrane structure. All configurations are fully optimized by the Generalized Gradient Approximation (GGA) [30] method and handle the Perdew-Burke-Ernzerhof Exchange Correlation Potential (PBE), which is corrected for long-range variance by the Grimme scheme.[31] The base set of the system is a fully electron bi-numbered atomic orbital enhanced by the d polarization function (DNP). The DFT+D (D represents variance) method is used to achieve Green’s vDW correction. In addition, at convergence standards of 10⁻⁶ au, a self-consistent field calculation of the total energy is performed. To ensure accurate electron convergence, real-space global orbital cutoff radius was 0.6nm, smearing point was 0.002 Ha (1 Ha = 27.2114 eV). In order to display the Brillouin zone for all slab models, we used the Monkhorst-Pack special k-points of 6 × 6 × 2 meshes. To reduce the nonphysical interaction between periodic interlayers, vacuum space was set to 40 Å in the X direction. The surface gas molecular interaction energy (E_{int}) of C₃N₇ is calculated by the following formula:

\[ E_{int} = E_{C₃N₇+gas} - E_{gas} - E_{C₃N₇} \]  

where \( E_{gas} \) is the energy of isolated gas molecules, \( E_{C₃N₇} \) is the energy of isolated C₃N₇ surface, and \( E_{C₃N₇+gas} \) is the energy of surface with gas molecules.

3. The CO₂/CH₄, CO₂/C₂H₂ Separation Capability of Porous C₃N₇ Membrane

3.1. The CO₂ Permeance Changed with Charged and Strained C₃N₇ Membrane

3.1.1. The CO₂/CH₄ Separation Capability with Different Charges ad Strains. Good conductivity and high electron mobility are the basic characteristics of charge-regulated CO₂ adsorption. Due to the fact that CO₂ is a Lewis acid molecule, it is easy to obtain electrons. The C atom in CO₂ is positively charged, and the N in the CN membrane regulated by negative charges is electronegativity. Thus, the CO₂ molecule has strong interaction with the negatively charged C₃N₇ nanosheets. Therefore, we first studied the CO₂ adsorption behavior of C₃N₇ membrane regulated by negative charge after 5 ns MD simulation time at 298K. According to MD simulations, the number of CO₂ molecule which through C₃N₇ membrane pores was calculated to investigate the CO₂ permeance. CO₂ permeability as the significant parameter to estimate the carbon dioxide and methane separation capacity with charged C₃N₇ nanosheet, and the calculation equation as follows:

\[ F = \frac{N}{S \Delta P \cdot T} \]  

where \( F \) is permeance (mol·s⁻¹·Pa⁻¹·m⁻²), \( N \) and \( S \) are the moles of gas molecules outside the gas box and the area of the C₃N₇ nanosheet (2.34 × 10⁻¹⁷ m²), respectively. \( T \) is the total simulation time, \( \Delta P \) is the pressure drop to put the gas molecules across the pore. As shown in table 1, the CO₂ permeability increase with the negative charges changed from 1 to 5 e⁻, nevertheless, the CO₂ permeability decreased
when negative charge was 6 e\textsuperscript{−}. The CO\textsubscript{2} permeability up to peak when the charge number is 5 e\textsuperscript{−}, which displayed the excellent adsorption and separation performance.

Table 1. The relationship of CO\textsubscript{2} permeance with different charge quantities.

| Negative charge number | 0   | 1 e\textsuperscript{−} | 2 e\textsuperscript{−} | 3 e\textsuperscript{−} | 4 e\textsuperscript{−} | 5 e\textsuperscript{−} | 6 e\textsuperscript{−} |
|------------------------|-----|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| Permeance (× 10\textsuperscript{7} GPU) | 0.04 | 0.34                   | 3.31                   | 4.75                   | 5.51                   | 5.94                   | 3.99                   |

Considering the carbon dioxide and methane molecules possess different kinetic diameter (carbon dioxide: 0.33 nm, methane: 0.38 nm), the tensile strains were applied on the C\textsubscript{9}N\textsubscript{7} membrane to testify the CO\textsubscript{2} permeance. Table 2 demonstrated that the strain increasing from 0 to 9%, the permeability of carbon dioxide on the C\textsubscript{9}N\textsubscript{7} nanosheet also extremely enhanced and the homologous permeability were changed from 0.04 × 10\textsuperscript{7} to 3.56 × 10\textsuperscript{7} GPU. Because carbon dioxide molecule was less than the effective pore size of the C\textsubscript{9}N\textsubscript{7} nanosheet under the strain regulation. Otherwise, the methane kinetic diameter was bigger than the C\textsubscript{9}N\textsubscript{7} pore size with 0-9% tensile strain engineering. Therefore, compared with CH\textsubscript{4}, the carbon dioxide molecules were easier to penetrate through the C\textsubscript{9}N\textsubscript{7} nanopores.

Table 2. The relationship of CO\textsubscript{2} permeance with different strains.

| Strain  | 0   | 1.5% | 3%  | 4.5% | 6%   | 7.5% | 9%   |
|---------|-----|------|-----|------|------|------|------|
| Permeance (× 10\textsuperscript{7} GPU) | 0.04 | 0.08 | 0.38 | 1.78 | 2.33 | 3.61 | 3.56 |

Based on the influence of charge and strain regulation on the CO\textsubscript{2} adsorption characteristics, a new regulation method was proposed in this manuscript: the synergistic negative charge and strain regulation were applied on C\textsubscript{9}N\textsubscript{7} nanosheets, and the CO\textsubscript{2}/CH\textsubscript{4} separation behaviours on the C\textsubscript{9}N\textsubscript{7} nanosheet were observed. As described in table 3, under the condition of 1 e\textsuperscript{−} and 3%, CO\textsubscript{2} permeability (CO\textsubscript{2}/CH\textsubscript{4} separation) can up to 3.2 × 10\textsuperscript{7} GPU, which was 9 times of CO\textsubscript{2} permeability when only 1 e\textsuperscript{−} was added and 8 times of CO\textsubscript{2} permeability when only 3% strain was added. However, the CO\textsubscript{2} permeability decreased with the charge number was 5 e\textsuperscript{−}, the higher strain has negligible effect on CO\textsubscript{2} permeability. Due to the replaced N element in the C\textsubscript{9}N\textsubscript{7} structure, the electrostatic interaction was enhanced to adsorb more carbon dioxide molecules on the surface and pore centre. Thus, the penetrated quantities of carbon dioxide molecules decreased with the charge number reach 6 e\textsuperscript{−}. Moreover, the strain engineering can reduce energy barriers of carbon dioxide pass through nanopores.

Table 3. The relationship of carbon dioxide permeance with different charge numbers and strains.

| Charge number | Strain | Permeance (× 10\textsuperscript{7} GPU) |
|---------------|-------|----------------------------------------|
| 0             |       | 0.04                                   |
| 1 e\textsuperscript{−} | 0   | 0.34                                   |
|               | 1.5% | 1.57                                   |
|               | 3%   | 3.18                                   |
| 5 e\textsuperscript{−} | 0   | 5.94                                   |
|               | 1.5% | 5.26                                   |
|               | 3%   | 4.11                                   |
3.1.2. *The CO\(_2\)/C\(_2\)H\(_2\) Separation Capability with Different Charges and Strains.* At the same time, the CO\(_2\)/C\(_2\)H\(_2\) separation capability with different charges and strains was investigated by the same method as CO\(_2\)/CH\(_4\) separation. Due to the fact that acetylene (C\(_2\)H\(_2\)) and carbon dioxide have the same linear molecular shapes and kinetic diameters (0.33 nm), as well as extremely similar character (boiling points: acetylene: 189.3 K; carbon dioxide: 194.7 K), the discrimination and separation between C\(_2\)H\(_2\) and CO\(_2\) become one of the most challenging and complex industrial processes under ambient conditions. The charged and strained C\(_9\)N\(_7\) nanosheets separated CO\(_2\) and C\(_2\)H\(_2\) efficiently. As shown in table 4, the CO\(_2\) permeance gradually increased with the synergistic regulation, the CO\(_2\) permeance of 2 e\(^-\) and 3% strain controlled membrane can reach to 4.24 × 10\(^7\) GPU. Above all, the combined regulation was a superior method to develop stable materials with excellent carbon dioxide separation performance. Simulation results show that the permeance of CO\(_2\) molecules improved remarkably under charge and strain.

| Charge number | Strain  | Permeance (× 10\(^7\) GPU) |
|--------------|--------|-----------------------------|
| 0            | 0      | 0                           |
|              | 1.5 %  | 0.17                        |
|              | 3 %    | 0.42                        |
| 1 e\(^-\)    | 0      | 0.72                        |
|              | 1.5 %  | 0.89                        |
|              | 3 %    | 2.55                        |
| 2 e\(^-\)    | 0      | 2.63                        |
|              | 1.5 %  | 3.73                        |
|              | 3 %    | 4.24                        |

3.2. Interaction of Gas Molecules and C\(_9\)N\(_7\) Membrane Regulated by Charge and Strain

To further examine the mechanism of gas separation capability, the interaction energy between carbon dioxide, methane, acetylene molecules and charged and strained C\(_9\)N\(_7\) nanosheet. The negative value of interaction energy is more attractive. The distance was defined as the length between the mass centre of gas molecules and centroid of C\(_9\)N\(_7\) nanopore. As demonstrated in figure 2, the interattraction between carbon dioxide molecules and C\(_9\)N\(_7\) nanosheet becomes stronger and the mutual repulsion between carbon dioxide molecules and C\(_9\)N\(_7\) nanosheet becomes weaker with increasing the strains, and the interaction energy curve first rises and then tends to flatten. Compared figures 2a, 2b and 2c, applying different charge numbers on the C\(_9\)N\(_7\) can increase the attraction interaction between carbon dioxide molecules and nanosheet. More importantly, when carbon dioxide molecules penetrate through the nanopores of C\(_9\)N\(_7\) (adsorption height < 1.5 Å), the interattraction dramatically increases due to the acid-base interactions between carbon dioxide molecule and C\(_9\)N\(_7\) nanosheet.

![Figure 2](image-url)
In contrast, when CH$_4$ molecule adsorption height was lower than 2.5 Å, the mutual repulsion between CH$_4$ molecule and C$_9$N$_7$ nanosheet became weaker with increasing adsorption height in figure 3a. The reason why CH$_4$ cannot permeate membrane pores was that both C atoms in CH$_4$ molecule and C$_9$N$_7$ nanosheet possess electronegativity. As demonstrated in figures 3b and 3c, with the negative quantities changed 1 e$^-$ and 5 e$^-$, the interaction energy of CH$_4$ molecule and C$_9$N$_7$ membrane increased but the CH$_4$ molecule still distributed in the inner of C$_9$N$_7$ nanosheet.

![Figure 3](image)

**Figure 3.** The interaction energy between methane molecules and charged and strained C$_9$N$_7$ nanosheet as a function of adsorption height (a) 0, 1.5%, 3%, (b) 1 e$^-$, 1 e$^-$ and 1.5%, 1 e$^-$ and 3%, (c) 5 e$^-$, 5 e$^-$ and 1.5%, 5 e$^-$ and 3%.

Similarly, the adsorption height of C$_2$H$_2$ molecule was under 2.5 Å, the repulsive interaction gradually decreased with the adsorption height decreased, as shown in figure 4. Due to its gradually interaction energy, C$_2$H$_2$ molecules were hard to penetrate through the combined controlled C$_9$N$_7$ membrane although its physics properties were similar with CO$_2$ molecules.

![Figure 4](image)

**Figure 4.** The interaction energy between C$_2$H$_2$ molecules and charged and strained C$_9$N$_7$ membrane as a function of adsorption height (a) 0, 1.5%, 3%, (b) 1 e$^-$, 1 e$^-$ and 1.5%, 1 e$^-$ and 3%, (c) 2 e$^-$, 2 e$^-$ and 1.5%, 2 e$^-$ and 3%.

### 3.3. The CO$_2$ Adsorption Height and Energy with C$_9$N$_7$ Membrane Regulated by Charge and Strain

The adsorption configuration and adsorption energy of CO$_2$ molecule on C$_9$N$_7$ surface were calculated by DFT. The adsorption energy between carbon dioxide and neutral and strain-free nanosheet can be calculated (-0.26 eV). As shown in figure 5, the adsorption energy gradually increased from -5.99 eV to -6.13 eV with the strain increasement from 0 to 3%. Compared figures 5a, 6a and 7a, the adsorption heights were 2.44, 2.41 and 2.01 Å with the negative charge quantities 1, 2 and 5 e$^-$, and the adsorption energy changed -10.77 and -19.21 eV when the charge numbers were 2 and 5 e$^-$. Therefore, negatively charged C$_9$N$_7$ membrane can donate electrons to CO$_2$ molecules, resulting in a strongly attractive interaction between CO$_2$ molecule and the surface, which can well explain why the negatively charged C$_9$N$_7$ membrane can adsorb and permeate the CO$_2$ molecules.
Figure 5. The adsorption height and energy between CO\textsubscript{2} molecule and charged and strained C\textsubscript{9}N\textsubscript{7} membrane (a) 1 e\textsuperscript{-}, (b) 1 e\textsuperscript{-} and 1.5\%, (c) 1 e\textsuperscript{-} and 3\%.

Figure 6. The adsorption height and energy between CO\textsubscript{2} molecule and charged and strained C\textsubscript{9}N\textsubscript{7} membrane (a) 2 e\textsuperscript{-}, (b) 2 e\textsuperscript{-} and 1.5\%, (c) 2 e\textsuperscript{-} and 3\%.

Figure 7. The adsorption height and energy between CO\textsubscript{2} molecule and charged and strained C\textsubscript{9}N\textsubscript{7} membrane (a) 5 e\textsuperscript{-}, (b) 5 e\textsuperscript{-} and 1.5\%, (c) 5 e\textsuperscript{-} and 3\%.

Moreover, the Hirshfeld charge of carbon dioxide and acetylene molecules were calculated to better understand the interaction mechanism as described in figure 8. When CO\textsubscript{2} molecular adsorbed on natural g-C\textsubscript{9}N\textsubscript{7} membrane, the O, C1, C2 charge of CO\textsubscript{2} was 0.2863 e, -0.1396 e and -0.1516 e, respectively. With respect to CO\textsubscript{2} molecules adsorbed on 5 e\textsuperscript{-} charged C\textsubscript{9}N\textsubscript{7} membrane, the total amount of CO\textsubscript{2} charge was -0.0715 e, which obtained extra electrons -0.0666 e compared with natural C\textsubscript{9}N\textsubscript{7} membrane. However, the Hirshfeld charge analysis of C\textsubscript{2}H\textsubscript{2} molecule illustrated that 5 e\textsuperscript{-} charged C\textsubscript{9}N\textsubscript{7} membrane can donate more electrons (-0.1676 e) to C\textsubscript{2}H\textsubscript{2} molecules, which leading to C\textsubscript{2}H\textsubscript{2} molecule tightly adsorbed on C\textsubscript{9}N\textsubscript{7} surface and cannot break through the barrier to penetrate membrane pores.

Figure 8. The Hirshfeld Charge distribution of the gas molecules which adsorbed on (a) CO\textsubscript{2} on the neutral, (b) CO\textsubscript{2} on the 5 e\textsuperscript{-} charged, (c) C\textsubscript{2}H\textsubscript{2} on the neutral, (b) C\textsubscript{2}H\textsubscript{2} on the 5 e\textsuperscript{-} charged g-C\textsubscript{9}N\textsubscript{7} membrane.

4. Conclusion
In summary, we mainly studied the adsorption characteristics of porous C\textsubscript{9}N\textsubscript{7} nanosheets to capture CO\textsubscript{2} through charge and strain regulation. It was found that the CO\textsubscript{2} permeance increased with the increase of charge and strain. Under the simulation conditions, with the numbers of charge increased from 1 to 5 e\textsuperscript{-}, the carbon dioxide permeability increasingly. The CO\textsubscript{2} permeability can up to maximum when charge
number was 5 e', however, the CO$_2$ permeability decreases significantly when charge number increased 6 e'. It may be that the pores of C$_{3}N$_7 nanosheet are blocked by carbon dioxide molecules, leading to the decrease of the permeability of CO$_2$ molecules. Meanwhile, the permeance of CO$_2$ increases with the increase of strain. When the strain was 7.5%, the CO$_2$ permeance reached 3.6 $\times 10^5$ GPU. Additionally, the synergetic effect of negative charge and tensile strain on the adsorption characteristics of CO$_2$ adsorb on C$_{3}N$_7 nanosheet was tested. The adsorption energy of CO$_2$ molecule was as high as -11.11 eV when the C$_{3}N$_7 membrane was controlled by 2 e' and 3%. It is much higher than the adsorption energy of neutral and strain-free membrane (-0.26 eV), and the permeability is significantly improved than that of single control. Therefore, C$_{3}N$_7 membrane has adjustable negative charge and strain adsorption capacity for CO$_2$, which can be used to reduce greenhouse gases and produce clean energy.

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