



MOLECULAR INSIGHTS INTO CO₂ SEQUESTRATION IN MOF-74

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ABSTRACT

Advancements in materials for efficient carbon sequestration are crucial in addressing the rising levels of CO₂. Metal Organic Frameworks (MOFs) have emerged as a key focus due to their high CO₂ adsorption capacity and versatility. This study focuses on evaluating the equilibrium CO₂ adsorption properties of Mg-MOF-74 using hybrid MD / GCMC simulation in LAMMPS. The simulations were conducted at a temperature of 313 K with pressure variations ranging from 1 to 40 bar. The resulting CO₂ uptake was 10.185 mmol/g even at a low pressure of 1 bar. As pressure increases, CO₂ adsorption steadily rises, reaching 12.810 mmol/g at 40 bar. The Radial Distribution Function (RDF) analysis of CO₂ molecules within Mg-MOF-74 clarified the significant role of ligands in CO₂ adsorption. The observed decrease in the diffusion coefficient with increasing pressure suggests slower diffusion and indicates a strong interaction between CO₂ and the MOF at higher pressures. Moreover, the increasingly negative trend of interaction energy with rising pressure indicates enhanced adsorption at higher pressures, with van der Waals interactions contributing predominantly to the total interaction energy between adsorbate and adsorbent. This research sheds light on the potential of Mg-MOF-74 as an effective material for CO₂ capture and sequestration.

Keywords: Diffusion, interaction energy, metal organic frameworks, molecular dynamics, sequestration

INTRODUCTION

The rapidly growing global population and industrialization result in explosive energy consumption (Liu *et al.*, 2012). Since the industrial revolution, more than 85% of global society's energy demand has been met largely by the combustion of fossil fuels, including coal, petroleum, and natural gas (Birdi, 2019). Carbon dioxide (CO₂) is a major byproduct of such combustion (Liu *et al.*, 2012). The steep and continuous increase in CO₂ concentration was observed since the early 19th century (Birdi, 2019). CO₂ concentration in the early 1800s was found to be 280 parts per million (ppm), which in 2021 increased to 415 ppm (IPCC, 2023). According to the IPCC, atmospheric CO₂ concentration could reach up to 950 ppm by 2100 (Ding *et al.*, 2019). The massive emission of CO₂ has resulted in serious environmental issues, such as global warming, ocean acidification, extreme weather, and species extinction (Ding *et al.*, 2019). In this scenario, it is crucial to implement effective strategies for reducing CO₂ emissions across various sectors of society to safeguard the global climate and protect our environment. One highly efficient method for lowering the concentration of CO₂ in the atmosphere is through a process known as Carbon Capture and Storage (CCS) (Smit *et al.*, 2014).

CCS involves the separation of CO₂ from industrial and energy-related sources, its transportation to a storage location, and long-term isolation from the

atmosphere. This process is considered as part of the mitigation actions aimed at stabilizing atmospheric greenhouse gas concentrations (Metz *et al.*, 2005). Various adsorbents, including microporous and mesoporous materials (such as activated carbon, carbon molecular sieves, zeolites, and chemically functionalized mesoporous materials), as well as metal oxides, are actively researched for CO₂ separation and capture (Bae & Snurr, 2011). In the traditional landscape, zeolites and activated carbons have been extensively employed as CO₂ adsorbents (Díaz *et al.*, 2008). Zeolites, characterized by their porous aluminosilicate structure, face limitations in CO₂ adsorption capacity and stability in the presence of water (Zhang *et al.*, 2008). Even though activated carbon exhibits a higher capacity to adsorb carbon dioxide, they suffer from low CO₂/N₂ selectivity at higher pressure. Metal-Organic Frameworks (MOFs) emerge as promising alternatives, boasting superior surface areas compared to traditional adsorbents (Park *et al.*, 2020). Thus, among the array of adsorbents, MOFs are recognized as potential candidates for efficient carbon capture (H.-H. Wang *et al.*, 2017).

MOFs are three-dimensional coordination networks consisting of inorganic nodes (either single metal-based nodes or clusters) surrounded by specific organic ligands such as carboxylate, tribenzoate, imidazolate, and pyridyl (Elsaidi *et al.*, 2018; Maurin *et al.*, 2017). With advancements in advanced synthesis processes, many thousands of MOFs have been synthesized to

date. MOFs exhibit diverse framework structures (Jiang *et al.*, 2020), high porosity up to 90% (Z. Li *et al.*, 2020), large BET (Brunauer Emmett Teller) surface areas (Rezaei *et al.*, 2017), and adjustable pore structures (H. Li *et al.*, 2019), low crystal density as well as high thermal and chemical stability (Bae & Snurr, 2011). MOFs have accumulated growing attention in a variety of applications like gas separation and storage, catalysis, drug delivery, purification, water harvesting, catalysis, and enzyme immobility (Yu *et al.*, 2017; X. Zhang *et al.*, 2020). Additionally, the presence of open metal sites makes MOFs promising candidates for applications in CO₂ capture, showcasing their potential in addressing environmental challenges (Elhenawy *et al.*, 2020).

MOF-74 is a honeycomb-like material formed by combining divalent metal ions (Zn, Mg, Co, Ni, etc.) and 2,5-dioxido-1,4-benzene-dicarboxylate (dobdc) linker (Pham *et al.*, 2015). Among several MOFs, MOF-74 exhibits high CO₂ adsorption performance as there is a presence of open metal sites (OMSs) in hexagonal channels aligned along the c-axis (Ding *et al.*, 2019). Mg-MOF-74, possessing a pore width of 10.2 Å and a BET surface area of 1174 m²/g, was experimentally documented to achieve CO₂ adsorption of 8.61 mmol/g (37.8%) at 298 K and 1 bar pressure (Bao *et al.*, 2011).

Molecular dynamics is a simulation method analyzing the physical movements of atoms and molecules by numerically integrating Newton's equations of motion over time (Lee, 2016). MD simulations, which commenced in the late 1950's with the study of simple

gases, have become a foundational computational technique for analyzing particle dynamics across diverse systems (Hollingsworth & Dror, 2018). To understand how effectively CO₂ bonds to MOF, researchers use a molecular force field method, which proves to be more practical than other approaches (Tian *et al.*, 2016). Once a good potential is selected, MD offers comparable results at a lower cost compared to expensive electronic structure methods such as Hartree Fock and Density Functional Theory (DFT) (Mao *et al.*, 2023).

In this study, we conducted an in-depth investigation of Mg-MOF-74 to assess its capacity for CO₂ capture. Through a hybrid GCMC/MD simulation, we introduced CO₂ into the MOF structure and analyzed its adsorption and diffusion characteristics. We further identified the specific binding sites for CO₂ molecules and evaluated the strength of their interactions. This distinctive application of a combined Grand Canonical Monte Carlo (GCMC) and Molecular Dynamics (MD) approach in the LAMMPS environment offers a more comprehensive understanding, encompassing both the equilibrium properties of CO₂ adsorption and its dynamic behavior within Mg-MOF-74.

MATERIALS AND METHODS

A triclinic structure of Mg-MOF-74 was taken (Adhikari *et al.*, 2024) which contain 54 atoms in its unit cell. The unit cell was replicated $4 \times 4 \times 4$ times, resulting in a total of 3456 atoms comprising magnesium, hydrogen, carbon, and oxygen.

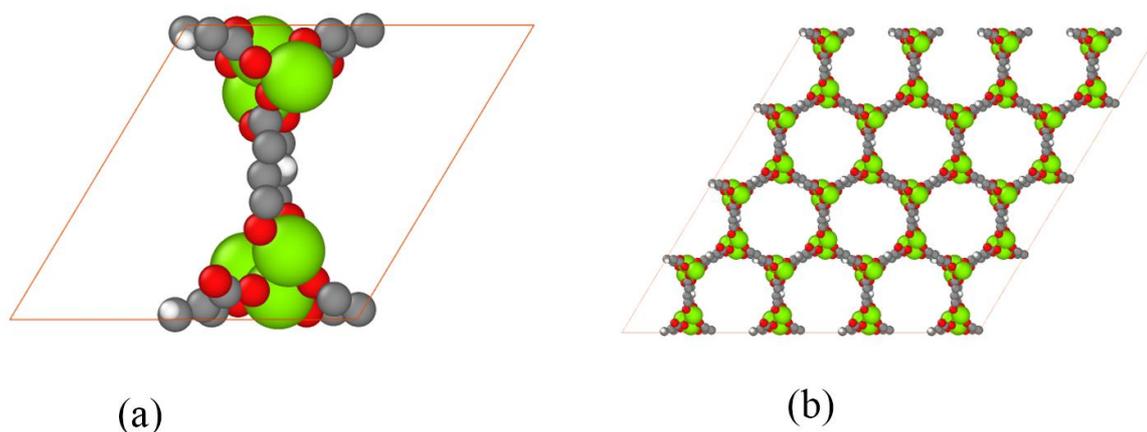


Figure 1. (a) Unit cell structure of Mg-MOF-74 where green = Mg, red = O, grey = C and white = H, (b) $4 \times 4 \times 4$ super cell structure of Mg-MOF-74

The bounded interactions between Mg-MOF-74 atoms were determined using universal force field (UFF) (G. Zhang *et al.*, 2023) whereas CO₂ molecule was represented in TraPPE model developed by Potoff and Siepmann (Potoff & Siepmann, 2001). The force field

parameters are shown in table 1. A combination of Lennard Jones (LJ) and Coulombic potentials were applied to illustrate interaction between adsorbate - adsorbate and adsorbate-adsorbent (equation (1)) (Du *et al.*, 2020). Lorentz-Berthelot mixing rules shown in equations (2) and (3) were utilized to assess interactions

between diverse atoms in CO₂ adsorption isotherms, enhancing insights into intermolecular forces (Putra *et al.*, 2022). A cutoff radius of 12 Å was used for the force field. The PPPM method with a precision of 10⁻⁴ was employed to compute long-range electrostatic

interactions. The partial charges of the atoms were computed using Gaussian09, for which B3LYP hybrid functional along with the 6-311g(2d,2p) basis set was applied.

$$U_{ij}(r) = 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \quad (1)$$

$$\sigma_{ij} = \frac{\sigma_{ii} + \sigma_{jj}}{2} \quad (2)$$

$$\epsilon = \sqrt{\epsilon_{ii}\epsilon_{jj}} \quad (3)$$

Table 1. Parameters used in the simulation (Potoff & Siepmann, 2001, Zhang *et al.*, 2023)

Atoms	$\epsilon/K_B(\text{K})$	σ (Å)	q(e)
Mg	55.8574	3.0210	1.1151
H	7.6489	3.1950	0.1267
C1	73.8224	3.9830	-0.1681
C2	73.8224	3.9830	0.1873
C3	73.8224	3.9830	-0.9870
C4	73.8224	3.9830	0.6469
O1	47.8562	3.8983	-0.6521
O2	47.8562	3.8983	-0.5320
O3	47.8562	3.8983	-0.6251
C(CO ₂)	27	2.8000	0.7
O(CO ₂)	79	3.0500	-0.35

To simulate CO₂ adsorption at molecular level, Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software was used (Thompson *et al.*, 2022). The Peng - Robinson equation of state was employed for the calculation of fugacity coefficient at different pressure (Peng & Robinson, 1976). We employed an NVT ensemble to maintain a stable temperature of 313 K, facilitating quicker attainment of equilibrium. Temperature control was managed by a Nosé-Hoover thermostat with a temperature damping parameter of 100 fs, while the entire simulation utilized a time integration step of 1 fs. The MOF structure was kept rigid to reduce computational costs. The Metropolis sampling technique was utilized to study the insertion and deletion of CO₂ molecules within the MOF. A single cycle of GCMC comprising of 20 GCMC exchanges were performed every 100 timesteps of the simulation. GCMC simulations were carried out for up to 500,000 steps (fs). To elucidate the structure and dynamics characteristics of the system, MD analysis was performed for a total of 1×10^6 steps after completing GCMC. The CO₂ adsorption properties of

the MOF were investigated by performing simulations in a pressure range of 1-40 bar.

RESULT AND DISCUSSION

Adsorption isotherm

The GCMC adsorption process is a crucial aspect for investigating the properties and performance of MOFs. In our study, we conducted GCMC simulations to examine the introduction of CO₂ molecules into the MOF structure. Initially, the injection rate of CO₂ was observed to rapidly increase (figure 2a), leading to a swift rise in adsorption within the MOF. However, as the process progressed, the adsorption of CO₂ molecules within the MOF reached a saturation level after a certain number of time steps. To ensure a thorough understanding of the adsorption behavior, we extended the GCMC simulation to 500,000 timesteps, allowing the system to reach equilibrium and capture the full range of adsorption phenomena. Additionally, our analysis revealed a direct correlation between pressure and adsorption, with higher pressures resulting in increased adsorption of CO₂ molecules within the MOF.

To further analyze the adsorption data, we employed the Langmuir adsorption isotherm, as illustrated in figure 2b. This mathematical model allowed us to fit the experimental data and gain insights into the adsorption process. By computing the average amount of CO₂ molecules adsorbed during the saturation period (after 300,000 timesteps), we quantified the extent of adsorption within the MOF. At 1 bar

pressure, we noted an adsorption of 10.185 mmol/g of CO₂, which increased to 12.810 mmol/g at 40 bar pressure. This trend suggests that higher pressures enhance adsorption within the MOF. However, it's important to highlight that further increases in pressure do not yield significant changes in adsorption capacity. Instead, a saturation point is evident, as depicted by the plateau observed in the figure 2b.

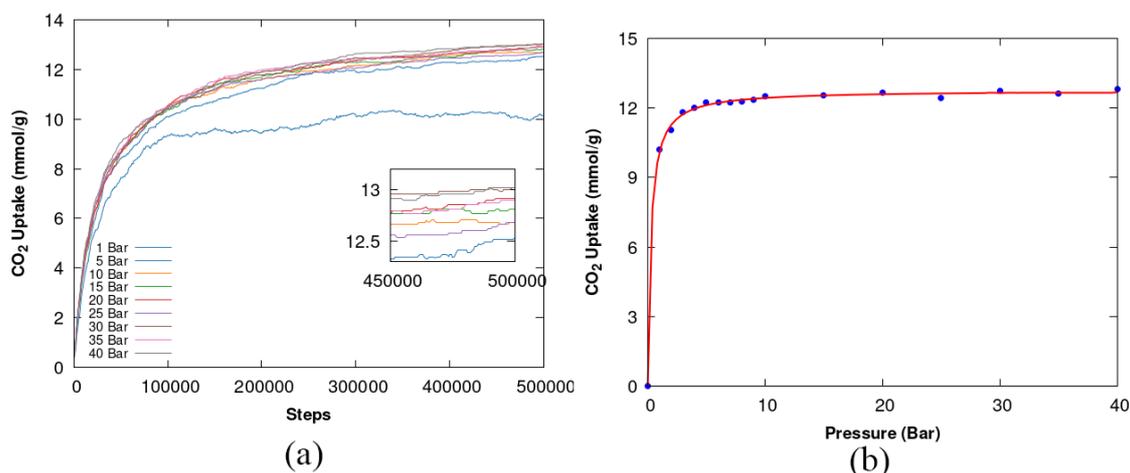


Figure 2. (a) Fluctuation in CO₂ uptake at different pressure (b) CO₂ adsorption isotherm of MOF-74 at 313 K

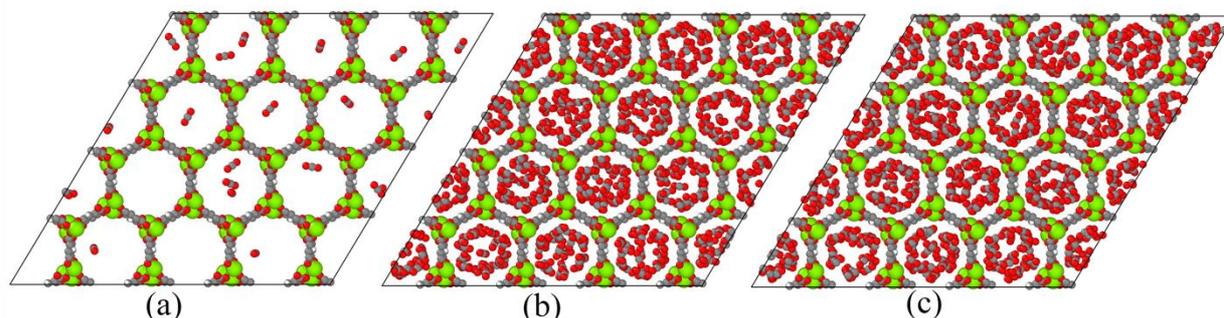


Figure 3. (a) Initial configuration with limited CO₂ molecules; (b) 300,000 timesteps, showing increased adsorption; (c) 500,000 timesteps, CO₂ densely occupies MOF-74 pores, nearing equilibrium.

Figure 3 presents a sequential visualization of CO₂ adsorption within Mg-MOF-74 at 1 bar pressure, captured through Grand Canonical Monte Carlo (GCMC) simulations over the course of 500,000 timesteps. In subfigure (a), representing the initial state, only a limited distribution of CO₂ molecules is observed within the MOF framework, indicating the starting point of the adsorption process. By 300,000 timesteps, as shown in subfigure (b), a significant increase in CO₂ density within the pores of MOF-74 is evident, reflecting the onset of adsorption saturation as the material approaches its capacity for CO₂ uptake. Finally, subfigure (c) at 500,000 timesteps illustrates the system nearing equilibrium, with CO₂ molecules densely populating the pore spaces and reaching near-saturation levels. This progression highlights the

adsorption dynamics in Mg-MOF-74, showcasing its potential for CO₂ capture under the simulated conditions and demonstrating the framework's ability to accommodate a substantial amount of CO₂ over time.

We also compared our simulation results with experimental results reported by Herm *et al.* at similar experimental conditions (Herm *et al.*, 2011). This comparison, shown in figure 4, reveals a similar adsorption trend, validating our simulation's reliability and alignment with previously established experimental findings. Thus, while our study is simulation-based, this cross-validation with Herm *et al.*'s experimental data provides confidence in the accuracy and relevance of our results.

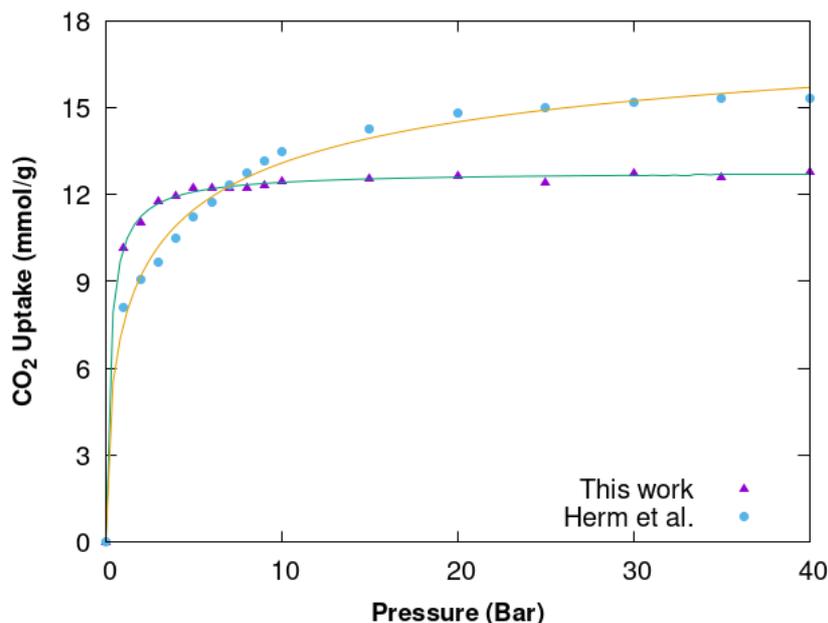


Figure 4. Comparison of simulation data with experimental data

Adsorption sites of CO₂

The Radial Distribution Function (RDF) is a statistical measure indicating the likelihood of finding particles at various distances from a reference particle, providing insights into the spatial arrangement and packing density of atoms or particles within a system. RDF can be expressed by the equation (4) (Yang, 2018).

$$g(r) = \frac{n(r)}{8\pi\rho r^2 dr} \quad (4)$$

where $g(r)$ is the RDF; $n(r)$ is the mean number of

atoms in a shell of width dr at distance r and ρ is the mean atom density.

The RDF was computed to analyze the gas adsorption mechanism and determine the predominant attractive sites for CO₂. The RDF illustrates the distribution of CO₂ molecules relative to all atoms (Mg, H, C1, C2, C3, C4, O1, O2, and O3) within Mg-MOF-74 at 1 bar, providing valuable insights into the interaction between CO₂ and the material.

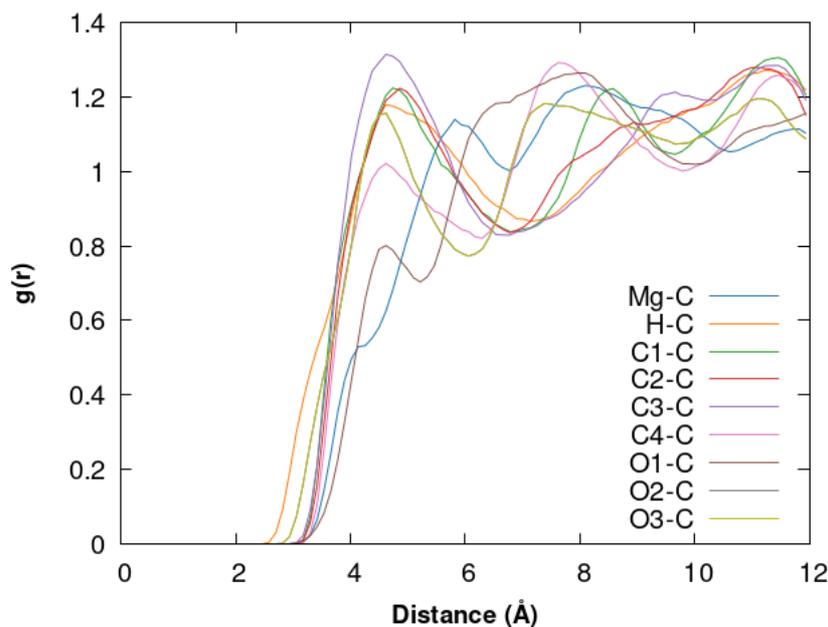


Figure 5. RDF of CO₂ molecules around MOF-74 framework at 1 bar pressure

The RDF plot reveals intricate details about the nature of their interaction. One notable observation from the RDF is the absence of peaks below 2.57 Å, indicating a

significant repulsion between CO₂ molecules and the MOF material at very close distances. This suggests the presence of a substantial energetic barrier that impedes

the proximity of CO₂ molecules to the MOF surface within this range.

Despite the observed repulsion, there is a distinct pattern of CO₂ adsorption closer to the hydrogen atoms of the MOF. This intriguing finding suggests the potential formation of hydrogen bonds between CO₂ molecules and the hydrogen atoms of the MOF-74. Such hydrogen bonding represents a form of chemical adsorption, indicating a dual mechanism of adsorption involving both physical and chemical interactions between CO₂ and the MOF material.

Further analysis of the RDF data reveals three prominent peaks between CO₂ and specific atoms of the MOF (C3, C4, and C1) at distances of 4.41 Å, 7.9 Å, and 11.36 Å, respectively. These peaks signify favored distances for interaction between CO₂ molecules and these particular atoms of the MOF, suggesting the presence of specific binding sites within the MOF framework.

Interestingly, the RDF also shows the appearance of the first peak for the Mg atom (metal site) at a relatively longer distance of 5.80 Å compared to peaks for other atoms of the MOF. This indicates that the Mg atom may play a role in CO₂ adsorption at greater distances from the MOF surface. Thus, while hydrogen atoms are involved in close-range interactions, the metal site appears to contribute to CO₂ adsorption dynamics at relatively longer distances within the MOF structure.

In brief, the RDF peaks observed at shorter distances (< 4 Å) primarily correspond to intramolecular interactions within CO₂ molecules and short-range intermolecular interactions with the MOF-74 framework. These shorter peaks highlight direct interactions crucial for adsorption initiation. For the longer-distance peaks (4-12 Å), these represent intermolecular correlations within the adsorbed CO₂ phase and between CO₂ molecules and more distant framework atoms within MOF-74. Such longer-range interactions are significant as they indicate the arrangement of CO₂ molecules within the pore network and help illustrate the spatial distribution within the MOF at higher CO₂ loadings. These peaks are important for understanding the clustering and arrangement patterns, which affect adsorption capacity, diffusion properties, and ultimately the material's efficiency for CO₂ capture (Barpaga *et al.*, 2019; Pathak *et al.*, 2019).

Interaction energy

The interaction energy is calculated to obtain insight into the interaction strength between the adsorbent and adsorbate (Yang, 2018). Figure 6 illustrates a histogram plot depicting the interaction energy between CO₂ and MOF-74 at various pressure levels. Notably, the negative values of interaction energy indicate the attractive force between the CO₂ molecules and the

MOF-74 framework (Wang *et al.*, 2021). Our analysis also shows that the van der Waals interactions dominate, accounting for the majority of the total interaction energy between CO₂ and Mg-MOF-74 across the pressure range studied. As pressure increases, both the total interaction energy and the vdW component indicate a strengthening of adsorption, with a gradual increase in the magnitude of energy values. In contrast, the contribution of electrostatic interactions remains relatively small and shows only slight changes with increasing pressure.

Self-diffusion coefficient of CO₂

The diffusion behavior of adsorbed CO₂ molecules was studied using mean-squared displacement (MSD) analysis technique. In MD simulation MSD determines the particle average displacement (Yang, 2018). The Einstein equation, expressed in equation (5), establishes a relationship between the diffusion coefficients (D) and the average Mean Squared Displacement (MSD) of molecules (Wang *et al.*, 2021).

$$D = \frac{1}{6} \frac{d \langle |r(t) - r(0)|^2 \rangle}{dt} = \frac{1}{6} \frac{d \langle |r(t) - r(0)|^2 \rangle}{t} \quad (5)$$

where $\langle \dots \rangle$ denotes ensemble average, $r(t)$ is the position vector of molecule j at time t , and N corresponds to the number of molecule j in the simulation system.

The pressure dependence of the diffusion coefficient is shown in figure 7. It is observed that the diffusion coefficient decreases with an increase in pressure, indicating slower diffusion of CO₂ at higher pressures. Additionally, it indicates an increase in adsorption capacity or strong interaction between the MOF and CO₂ with an increase in pressure. This is an expected result and can be explained by the increase in adsorbed CO₂, followed by the steric hindrance of movement for adsorbed CO₂ molecules within MOFs structures (Yang, 2018).

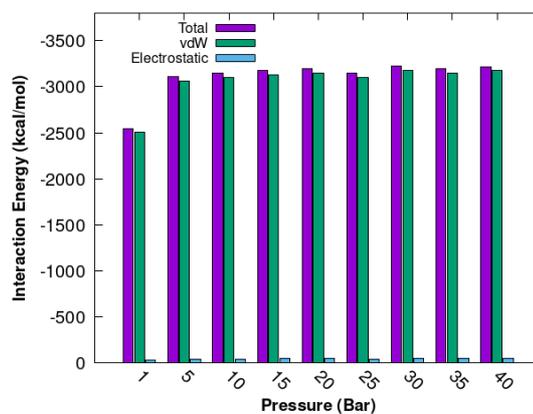


Figure 6. Variation of CO₂-MOF interaction energy with pressure, highlighting the contributions from vdW and electrostatic interactions.

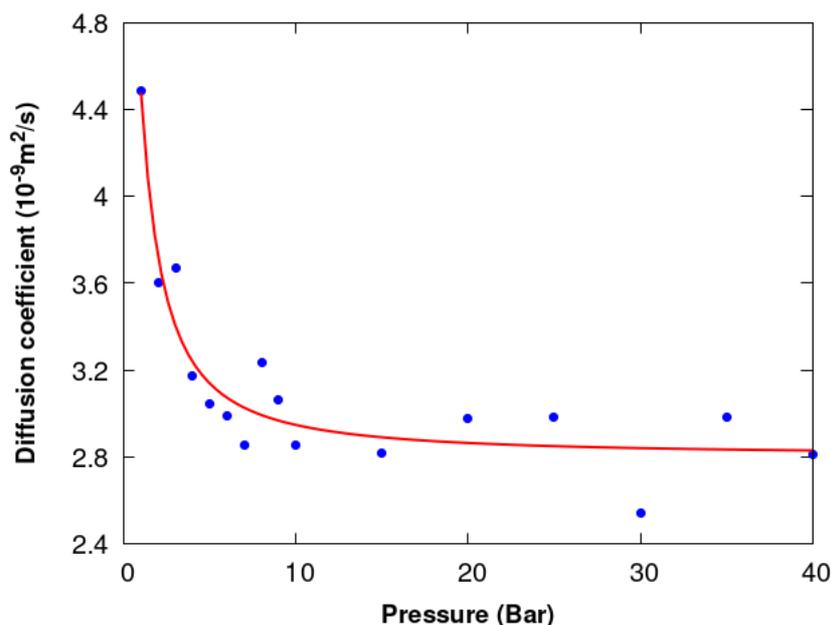


Figure 7. Relationship between the diffusion coefficient and pressure

CONCLUSIONS

A hybrid GCMC and MD simulation method using LAMMPS was adopted to investigate the CO₂ adsorption performance of Mg-MOF-74. Initially, the Langmuir adsorption fitting technique was done to explore the pressure dependence of CO₂ uptake within the framework. It was found that CO₂ uptake increases with an increase in pressure. The RDF analysis shows that organic ligands of Mg-MOF-74 play a crucial role in carbon capture. The interaction energy analysis proved that van der Waals interactions accounts for the majority of the total interaction energy between CO₂ and Mg-MOF-74 and the increasingly negative trend of interaction energy with an increase in pressure signifies enhanced adsorption at higher pressure. The diffusion coefficient decreases with increasing pressure, indicating slower diffusion and a strong interaction of CO₂ molecules in Mg-MOF-74. The increasingly negative trend of interaction energy with an increase in pressure signifies enhanced adsorption at higher pressure.

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AUTHOR CONTRIBUTIONS

Subedi A: software, data analysis, writing – original draft, visualization; Adhikari B: software, data analysis, writing – review and editing, visualization; Bhusal A: methodology / study design, writing – review and

editing, supervision; Adhikari K: conceptualization, methodology / study design, writing – review and editing, supervision.

CONFLICT OF INTEREST

The authors declare that they have no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author, upon reasonable request.

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