1st INTERNATIONAL CONFERENCE ON
Climate Change & Sustainable Development
"Shaping a Sustainable Future: Global Solutions for Climate Change"
25th to 26th Feb 2025
SINES, NUST Islamabad

A Sustainable Pathway for Scalable Carbon Capture and Climate Mitigation

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Abstract

The increasing concentration of atmospheric greenhouse gases, particularly carbon dioxide (CO_2), has intensified the global climate crisis, necessitating the development of efficient, scalable, and sustainable carbon capture technologies. In this study, aluminum formate ($Al(HCOO)_3$, ALF), a metal-organic framework (MOF), was evaluated as a candidate for CO_2 capture through detailed computational investigations. Although ALF exhibited promising properties, its potential for gas separation remained underexplored. To address this gap, Grand Canonical Monte Carlo (GCMC) simulations were employed to systematically assess its adsorption behavior, selectivity, and interaction mechanisms with CO_2, N_2, and H_2O. The CO_2 adsorption capacity of ALF was determined to be 4.8 mmol/g at 298 K and 1 bar, with an adsorption energy of −32.916 kcal/mol, indicating strong electrostatic interactions with Al–OH functional groups. Comparative analysis with conventional adsorbents, including zeolites, activated carbon and amine-based sorbents, revealed that ALF exhibited superior adsorption capacity and energy efficiency under identical conditions. Selectivity simulations demonstrated preferential CO_2 uptake over N_2 and H_2O, with significantly lower adsorption energies of −8.000 kcal/mol and −5.845 kcal/mol, respectively. The material's humidity tolerance was computationally evaluated, showing stable 70% CO_2 adsorption performance 30% relative humidity beyond which competitive water adsorption reduced efficiency. While this study was limited to computational modeling, the results provided valuable predictive insights and established a foundation for future experimental validation. These findings contributed to advancing Sustainable Development Goals (SDG) 13 (Climate Action) and SDG 9 (Industry, Innovation, and Infrastructure), highlighting the importance of computational screening in identifying next-generation materials for low-carbon technologies.

Keywords: ALF, CO_2 Capturing, MC Simulations, Adsorption Energy

1. INTRODUCTION

The increasing concentration of greenhouse gases (GHGs) in the atmosphere has accelerated climate change, posing severe environmental and economic challenges worldwide. Carbon dioxide (CO_2), the most prevalent anthropogenic GHG, is primarily emitted from fossil fuel combustion, industrial processes, and deforestation [1]. Globally, CO_2 emissions have reached unprecedented levels, necessitating urgent mitigation strategies. In Pakistan, the rising CO_2 emissions present significant concerns, with the country emitting approximately 223.6 million metric tons of CO_2 in 2021, showing an annual growth rate of 3.9% due to increasing industrialization and energy demands [2]. The energy sector is responsible for around 46% of these emissions, followed by transportation (28%) and industry (18%) [3]. These emissions contribute to severe environmental degradation, including worsening air pollution, increased frequency of extreme weather events, and reduced agricultural productivity. Thus, the development of efficient carbon capture technologies is imperative to mitigate the impact of CO_2 emissions [4].

Several materials have been extensively investigated for CO_2 capture, including zeolites, activated carbons, metal oxides and amine-based sorbents. Zeolites, characterized by their well-defined microporous structures, exhibit high CO_2 adsorption capacities; however, their performance is often compromised by competitive adsorption in the presence of water vapor and their limited tunability for selective gas capture [5, 6]. Activated carbons, derived from both biomass and synthetic precursors, offered a cost-effective option owing to their high surface area, yet they typically lack sufficient selectivity toward CO_2 over other gas species such as N_2 and CH_4 [7, 8]. Metal oxides, including calcium oxide (CaO) and magnesium oxide (MgO), function via reversible chemisorption mechanisms but are hindered by high regeneration energy demands which constrain their practical implementation at industrial scale [9]. Amine-functionalized materials, such as porous polymers and mesoporous silica, demonstrate excellent CO_2 selectivity through strong chemical interactions but their long-term viability is challenged by oxidative degradation, volatility and toxicity concerns [10]. In contrast, MOFs have emerged as next-generation sorbents for carbon capture, owing to their exceptionally high porosity, modular design and tunable surface functionality that enables precise control over gas adsorption behavior. MOFs are widely studied for gas adsorption due to their tunable porosity; however, many exhibit poor hydrothermal stability under humid conditions, which limits their practical deployment [11]. Frameworks like MOF-5 and HKUST-1, despite their high surface areas, suffer from structural degradation in the presence of water vapor due to labile metal-ligand bonds [12]. In contrast, Aluminum Formate (ALF), composed of strong Al–O bonds and devoid of large organic linkers, offers enhanced stability in humid environments [13]. This hydrolytic robustness makes ALF a promising candidate for real-world carbon capture applications, especially in settings where moisture is unavoidable. Structurally, ALF crystallizes in a ReO_3-type framework topology, characterized by a three-dimensional network of corner-sharing AlO_6 octahedra connected via bidentate formate ligands. This open and highly symmetrical structure not only contributes to its inherent thermal and mechanical stability but also facilitates the formation of uniform and accessible adsorption sites for CO_2 molecules.

This study evaluates ALF's CO_2 adsorption capabilities through advanced computational techniques. Computational simulations are conducted to examine the electronic structure, bonding interactions, and adsorption energies of ALF, providing valuable insights into its affinity for CO_2 molecules. Furthermore, the adsorption capacity, selectivity, and interaction energies

are evaluated for CO_2 in comparison with other gases, including N_2 and water vapor. Despite ALF's promise as a sustainable sorbent, no prior computational study has systematically modeled its CO_2 adsorption energetics under competitive hydration conditions. This work fills that critical gap by incorporating water vapor effects into the simulation framework, allowing for a more realistic assessment of adsorption performance. This thorough computational analysis offers a comprehensive evaluation of ALF's potential as a CO_2 adsorbent, thereby supporting its viability for large-scale application in industrial carbon capture processes.

2. COMPUTATIONAL METHODS

The computational investigation of the ALF material involved a multi-step approach encompassing structural optimization, Grand Canonical Monte Carlo (GCMC) simulations for gas adsorption and subsequent calculation of adsorption energies. All simulations were performed using the BIOVIA Materials Studio 2020 software suite.

2.1 Structural Optimization

The initial three-dimensional atomic coordinates of the ALF unit cell were constructed from their constituent molecular building blocks and subsequently assembled into a periodic framework using the graphical user interface of Materials Studio. Geometry optimization was then performed using the Forcite module within Materials Studio. The Universal Force Field (UFF), developed by Rappe et al. [14], was selected for this optimization. UFF was chosen due to its broad applicability across the periodic table, making it suitable for systems containing both the metal centers and organic linker components typical MOFs thereby providing a consistent description of interatomic interactions [15].

To accurately simulate the bulk behavior of the crystalline ALF material and eliminate surface effects, periodic boundary conditions (PBCs) were rigorously applied in all three spatial dimensions. This effectively replicated the unit cell infinitely, allowing for the calculation of properties representative of a macroscopic crystal. The optimization process employed a sequential combination of energy minimization algorithms: initially, the steepest descent method was used for initial coarse optimization, followed by the more efficient conjugate gradient method, and finally, the highly precise Newton–Raphson method was employed to achieve fine convergence. Convergence thresholds were stringently set at an energy tolerance of 1.0×10^{-5} kcal/mol, a maximum force tolerance of 0.005 kcal/mol/Å, and a maximum displacement tolerance of 5.0×10^{-5} Å. During the optimization, all atomic coordinates and lattice parameters of the ALF unit cell were allowed to relax over a total of 5000 iterations to ensure the attainment of the global minimum energy configuration.

2.2 Grand Canonical Monte Carlo (GCMC) Simulations for CO_2 Adsorption

Grand Canonical Monte Carlo (GCMC) simulations were conducted to model the adsorption behavior of CO_2 within the optimized ALF framework. These simulations were performed using the Adsorption Locator tool in Materials Studio, which facilitates the calculation of interaction sites and adsorption energies. Interactions within the system were described by a combination of force fields. The interactions within the ALF framework and between the framework and adsorbed gas molecules were modeled using the Dreiding force field [16]. The Dreiding force field was specifically selected for its proven accuracy and general applicability to a wide range of molecular and crystalline systems, particularly in MOF simulations where it has been validated to provide reliable predictions of structural and adsorption properties [15]. A cutoff radius of 12.8 Å was applied for all Lennard-Jones interactions, beyond which interactions were truncated. CO_2 was modeled as a rigid, linear triatomic molecule with a fixed C=O bond

length of 1.16 Å. The parameters for the CO_2 molecule, including its partial charges and LJ parameters, were specifically derived from the TraPPE (Transferable Potentials for Phase Equilibria) force field [17]. Partial charges of +0.70e were assigned to the carbon atom and −0.35e to each oxygen atom, accurately representing the quadrupole moment of the CO_2 molecule.

Throughout the GCMC simulations, the ALF framework was treated as a rigid structure with fixed atomic positions. This approximation was justified by the known high structural rigidity conferred by its ReO_3-like topology, which ensures that framework flexibility effects are negligible under typical low-pressure adsorption conditions for small guest molecules such as CO_2. As with structural optimization, periodic boundary conditions were consistently maintained in all directions to simulate the adsorption within a continuous, extended porous material.

2.3. Competitive Adsorption and Selectivity

To thoroughly assess the competitive adsorption behavior of CO_2 in the presence of other common gases, the GCMC simulations were extended to include binary and ternary gas mixtures. Specifically, competitive adsorption studies were conducted for the following mixtures: CO_2/N_2, CO_2/H_2O, and $CO_2/H_2O/N_2$. The relative adsorption selectivity was subsequently evaluated by analyzing the calculated interaction energies and the corresponding uptake ratios of the different gas species within the ALF framework under 1 bar pressure and 298K temperature conditions.

2.4. Adsorption Energy Calculation

The adsorption energy (E_{ads}) for each gas molecule interacting with the ALF framework was computed based on the total energies obtained from the simulations. The E_{ads} was calculated using the following equation:

$$E_{ads} = \frac{E_{system} - E_{framework} - nE_{gas}}{n}$$

Where, E_{system} is the energy of the system with adsorbed gases, $E_{framework}$ is the energy of the empty framework and n is the number of gas molecules adsorbed in the framework. A more negative E_{ads} value quantitatively indicates a stronger interaction between the gas molecule and the ALF material, and consequently, a more favorable adsorption [18].

3. RESULTS & DISCUSSIONS

Metal(III) formates, $MIII(HCOO)_3$ (M = Al, Fe, Ga, In, Mn), represented an underexplored class of materials with potential applications in gas capture and small molecule separations, particularly for CO_2 adsorption [19]. These compounds adopt a ReO_3-type structural framework, known for its adaptability and porosity, making them promising candidates for adsorption-based technologies [20]. Their three-dimensional structure, where metal ions are octahedrally coordinated with formate ligands, creates cavities that can accommodate guest molecules such as CO_2. While existing studies focus on them adduct formation with CO_2 and water, their practical use in gas separation remains largely unexplored. In this study, ($Al(HCOO)_3$) has been identified as a promising material due to its abundance, environmental sustainability, and scalability [21].

3.1 Geometry Optimization of ALF

Using the Forcite module in Materials Studio, a molecular structure was constructed consisting of a central carbon atom bonded to two hydrogen atoms and two oxygen atoms, characteristic of the formic acid (methanoic acid) moiety (Figure 1a). The optimized geometry exhibited features resembling to a metal carbonyl complex, specifically an aluminum tricarbonyl-like coordination environment [22]. This resemblance was attributed to the spatial arrangement of the aluminum center coordinated with oxygen

atoms from formate ligands, which exhibited a geometry similar to the coordination observed in typical carbonyl complexes [23]. The molecular unit was subsequently replicated to generate a three-dimensional periodic structure, as illustrated in Figure 1b. Following energy minimization, the final lattice parameters were determined to be **a = b = c = 6.564 Å** and **α = β = γ = 90°**, indicating a cubic symmetry. These parameters were found to be in good agreement with previously reported crystallographic data for aluminum formate metal-organic frameworks (MOFs), thereby validating the accuracy of the modeled structure [24].

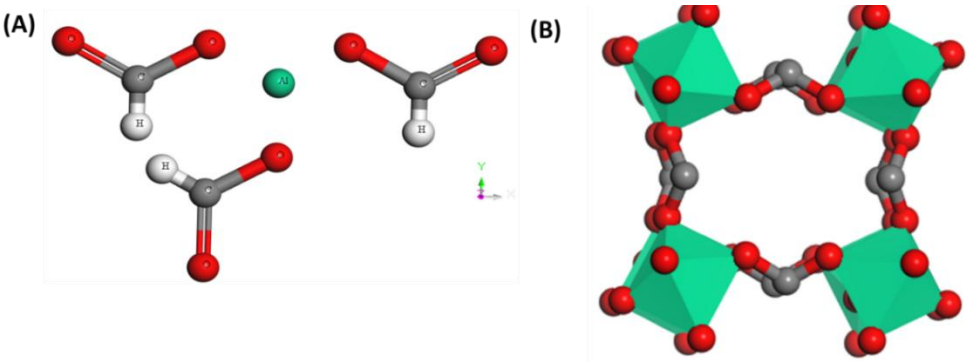

Figure 1: (a) Molecular structure of formic acid and aluminum tricarbonyl complex. **(b)** 3D unit cell showing the periodic arrangement of aluminum-carbonyl units.

The geometry optimization was performed using the Forcite module in Materials Studio with the Universal Force Field (UFF), employing the Smart algorithm that combines steepest descent, conjugate gradient and Newton-Raphson methods for efficient convergence [25]. The optimization was conducted with rigorous convergence criteria, including energy (0.001 kcal/mol), force (0.5 kcal/mol/Å) and displacement (0.005 Å) thresholds. As shown in Figure 2(A), the initial optimization phase (first 100 steps) exhibited significant fluctuations in energy (ΔE up to 2727 kcal/mol) and forces (>15 kcal/mol/Å), corresponding to substantial structural rearrangements. The system subsequently achieved stable convergence, with final energy variations below 0.01 kcal/mol/step and maximum forces reduced to <0.3 kcal/mol/Å, confirming attainment of a minimum-energy configuration.

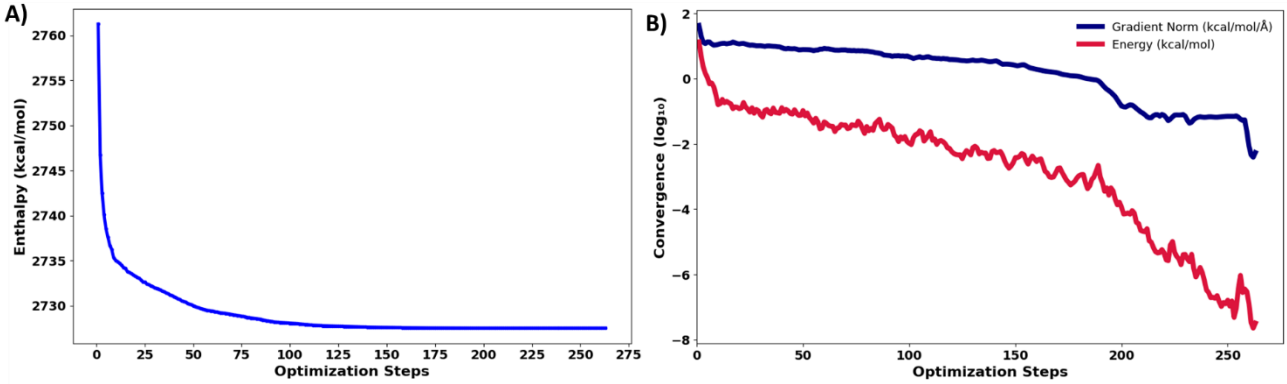

Figure 2: Geometry optimization convergence profile for aluminum formate (ALF) from Forcite simulations: **(a)** Energy and gradient norm trends across optimization steps; **(b)** Logarithmic convergence plot demonstrating stabilization.

3.2. Monte Carlo Simulations

Using Materials Studio's Adsorption Locator module, Monte Carlo simulations investigated the adsorption of CO_2, N_2, and H_2O within ALF MOF [26]. The simulations evaluated adsorption feasibility (via interaction energies and system stability), calculated adsorption energies and identified stable adsorption configurations. These simulations provide insights into the interactions between these gases and ALF, assessing its potential for gas adsorption applications like decarbonization and environmental remediation, and informing its suitability for gas separation and storage.

3.3 Optimized structures of Gases

Using Materials Studio's Forcite module, optimized molecular structures were obtained for CO_2, H_2O, and N_2. CO_2 exhibits a linear configuration (C=O double bonds), H_2O a bent geometry (O-H single bonds), and N_2 a diatomic structure with a strong N≡N triple bond as depicted in Figure 3 [27]. These optimized structures inform further computational analysis of their properties.

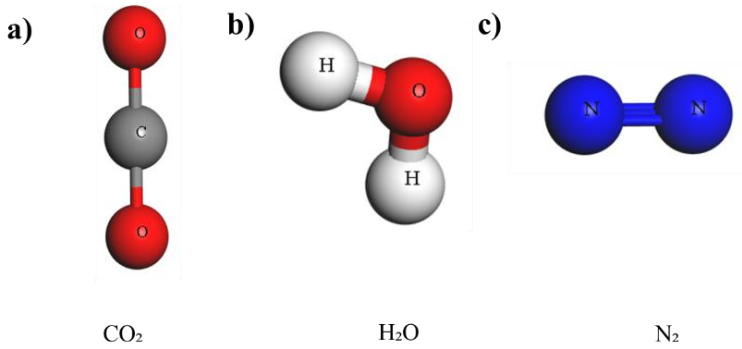

Figure 3: Optimized molecular structures of **(a)** carbon dioxide (CO_2), **(b)** water (H_2O), and **(c)** nitrogen (N_2)

3.4. Adsorption Analysis of CO_2, N_2, and H_2O in ALF MOF

The adsorption characteristics of CO_2, N_2 and H_2O in the ALF MOF was analyzed via MC simulations to identify energetically favorable adsorption sites, quantify binding energies, and assess selectivity. GCMC simulations were conducted with 1×10^5 equilibration steps followed by 1×10^5 production steps, under 298 K in the NVT ensemble. The Universal Force Field (UFF) was used and validated against DREIDING for reliability. Electrostatic interactions were treated using the Ewald summation method and fully periodic boundary conditions were applied in all three spatial dimensions. The ALF framework was modeled as rigid, supported by prior validation of its structural stability under these operational conditions. Results revealed that CO_2 interacts strongly with Al-OH functional groups through electrostatic forces, leading to enhanced adsorption as shown in Figure 4. In contrast, N_2 exhibited weak physisorption with a binding energy of -8 kcal/mol while H_2O adsorption was moderate. These findings underscore ALF MOF's promising selectivity for CO_2 capture applications, particularly in gas separation processes where preferential adsorption of carbon dioxide over nitrogen and water vapor is critical.

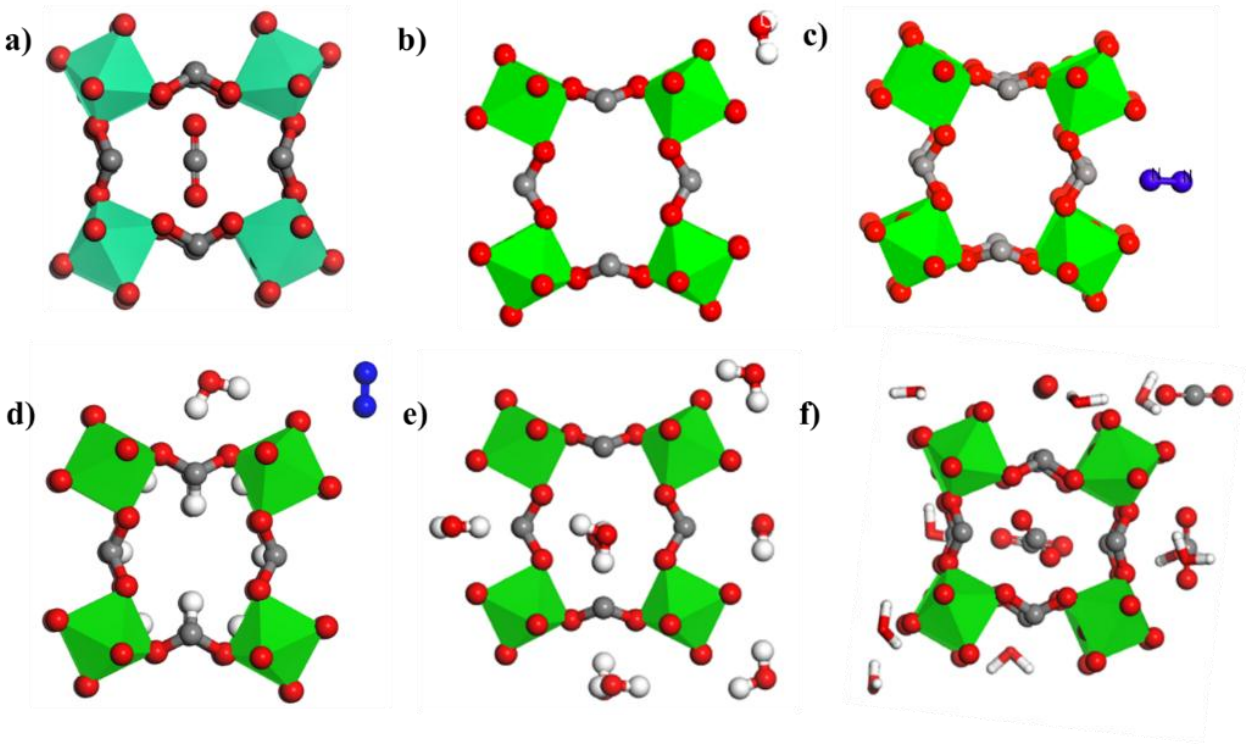

Figure 4: Competitive adsorption configurations of CO_2, N_2, and H_2O in ALF MOF. **(a)** CO_2 preferentially adsorbed within the pore; **(b–c)** H_2O and N_2 exhibit weak interactions with the framework; **(d)** Co-adsorption of H_2O and N_2 indicates preferential H_2O interaction; **(e)** High H_2O concentration forms hydrogen-bonded networks; **(f)** Competitive CO_2/H_2O adsorption within the ALF.

Molecular simulations offer detailed insights into the adsorption behavior of CO_2, N_2 and H_2O within the ALF elucidating the mechanisms underlying selective CO_2 capture. MC simulations revealed that CO_2 adsorption is predominantly driven by physisorption, characterized by a significant adsorption energy of -32.916 kcal/mol and an isosteric heat of adsorption of -28.861 kcal/mol. This strong interaction stems from electrostatic attractions between CO_2 molecules and the Al-OH functional groups within the ALF framework which also contribute to its high CO_2 selectivity. In contrast, N_2 exhibits weak physisorption on ALF with a considerably lower adsorption energy of -8.000 kcal/mol. The limited interaction of N_2 with ALF's active sites is primarily due to weak van der Waals forces, which are insufficient to facilitate significant N_2 adsorption. The marked difference in adsorption strength between CO_2 and N_2 underscores ALF's potential for selective CO_2 capture in mixed-gas environments. Water molecules interact with ALF through physisorption as well, albeit with a distinct energetic profile. The simulations indicate a less negative adsorption energy for water (-5.845 kcal/mol), suggesting a different binding mechanism. Strong hydrogen bonding between water molecules and the ALF framework is likely responsible for this interaction. Under high-humidity conditions, water molecules can compete with CO_2 for adsorption sites, potentially hindering CO_2 uptake. However, under carefully controlled moisture levels, CO_2 adsorption remains the dominant process, highlighting ALF's viability for carbon capture applications even in the presence of moderate humidity [28]. A summary of the adsorption energies and mechanisms is presented in Table 1.

Table 1: Adsorption Energies and Mechanisms of CO_2, N_2, and H_2O in ALF MOF

Sr no.	Gas Molecule	Adsorption Energy (kcal/mol)	Adsorption Mechanism
1	CO_2	-32.916	Physisorption (Electrostatic Interaction with Al-OH)
2	N_2	-8.000	Physisorption (Weak van der Waals Forces)
3	H_2O	-5.845	Physisorption (Hydrogen Bonding)

These findings demonstrate the potential of ALF MOF for effective CO_2 capture, with minimal interference from nitrogen and, under controlled humidity, water. The

3.5 Selectivity and Efficiency of ALF in CO_2 Adsorption

To further elucidate the competitive adsorption behavior of ALF under realistic multicomponent conditions, GCMC simulations were conducted using ternary gas mixtures of CO_2, N_2, and H_2O. As illustrated in Figure 5, systems such as $2H_2O$–$2N_2$–$1CO_2$ and $1H_2O$–$8N_2$–$1CO_2$ exhibited strong preferential adsorption of CO_2 within the ALF cavities. This selectivity arises primarily from favorable quadrupole framework interactions, van der Waals forces and pore confinement effects, which stabilize CO_2 within the pore environment. In contrast, N_2 and H_2O, despite their respective quadrupole and hydrogen-bonding capabilities, showed limited interaction with the pore interior and remained largely confined to the external surfaces or pore openings.

To evaluate the influence of elevated moisture content on adsorption behavior, an additional simulation using a $4H_2O$–$4N_2$–$1CO_2$ mixture was performed (Figure 5d).

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selectivity and performance of ALF make it a promising material for industrial gas separation and carbon capture applications.

Under these conditions, a notable reduction in CO_2 occupancy was observed within the cavities. The increase in H_2O concentration enhanced hydrogen bonding interactions with the framework, enabling H_2O molecules to partially displace CO_2 from the adsorption sites. Despite this displacement, CO_2 still exhibited measurable retention within the pore, indicating a competitive balance between hydrogen bonding (favoring H_2O) and quadrupole–framework interactions (favoring CO_2). These findings highlight the dynamic adsorption behavior of ALF in mixed-gas environments. While CO_2 consistently exhibits the strongest interaction with the MOF under most conditions, the adsorption profile can shift in the presence of elevated H_2O levels due to intermolecular competition and framework–adsorbate affinity. This underscores the importance of considering moisture interference when evaluating MOF performance for gas separation, particularly in humid or post-combustion flue gas scenarios, where water vapor is abundant.

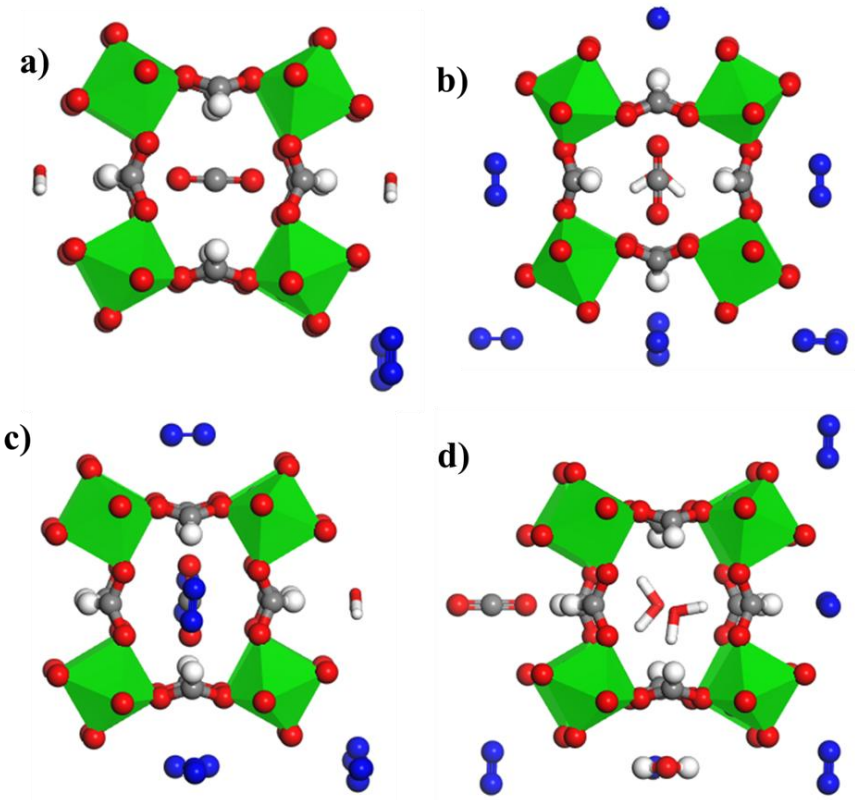

Figure 5: Competitive adsorption of CO_2, N_2 and H_2O in ALF. (a) $2H_2O$–$2N_2$–1CO (b) front view and (c) lateral view of $1H_2O$–$8N_2$–$1CO_2$, (d) $4H_2O$–$4N_2$–$1CO_2$. CO_2 consistently dominates cavity adsorption. At higher H_2O levels, partial displacement of CO_2 is observed.

MC simulations showed a consistent CO_2 adsorption within ALF pores across varying concentrations, while N_2 and H_2O remain at box boundaries. Simulations with equimolar N_2/H_2O/CO_2 and even excess N_2/limited CO_2 confirmed preferential CO_2 adsorption as demonstrated in Figure 5.

3.6 Comparative Study of ALF with Existing CO_2 Capture Materials

The ALF Metal-Organic Framework exhibited impressive CO_2 adsorption capacity (4.8 mmol/g), surpassing activated carbon, though slightly lower than HKUST-1. Its high selectivity made it effective for flue gas separation. The adsorption energy of ALF (-32.916 kcal/mol) indicated stronger interactions with CO_2 compared to activated carbon (5–8 kcal/mol) and amine-based sorbents (15–20 kcal/mol), establishing it as a highly efficient CO_2 capture material. However, its adsorption strength remained higher than zeolites (25–30 kcal/mol) and HKUST-1 (12–15 kcal/mol), offering a balance between adsorption strength and regeneration efficiency. In contrast to zeolites and amine-based sorbents, which experience significant moisture interference, ALF maintained CO_2 uptake even in humid conditions, improving its practical applicability. Its moderate hydrophobicity further supported its stability across various environments.

Table 2: Comparative Performance of ALF MOF and Other CO_2 Capture Materials

Parameter	ALF MOF	Zeolites	HKUST-1	Activated Carbon	Amine-Based Sorbents
Adsorption Capacity	Very High	High	Very High	Low	Very High
Selectivity	High	Moderate	Very High	Low	Moderate
Adsorption Energy(kcal/mol)	-32.916	-25–30	-12–15	-5–8	-15–20
Thermal Stability	~450°C	~600°C	~400°C	>800°C	~200–250°C
Moisture Resistance	Good	Poor	Moderate	High	Poor
Cost	Moderate	Low	High	Low	High
Scalability	High	Very High	Moderate	Very High	Low
Environmental Impact	Low	Low	Moderate	Low	High

With low-cost synthesis, scalability, and minimal environmental impact, ALF proves to be a more feasible alternative compared to expensive MOFs like HKUST-1 or amine-based sorbents that generate harmful byproducts [29]. While its adsorption capacity does not exceed that of high-performance MOFs, ALF's superior cost-effectiveness, moisture resistance, and ease of regeneration position it as a competitive candidate for sustainable CO_2 capture technologies.

4. CONCLUSION

The escalating atmospheric CO_2 concentration necessitates advanced carbon capture technologies. This computational study identifies aluminum formate (ALF), as a promising CO_2 adsorbent, owing to its distinct ReO_3-type structure. Geometry optimization confirmed ALF's cubic symmetry (a=b=c=6.564 Å, α=β=γ=90∘), consistent with prior crystallographic data. Grand Canonical Monte Carlo (GCMC) simulations revealed ALF's significant CO_2 adsorption capacity of 4.8 mmol/g. CO_2 adsorption, primarily physisorption, exhibited a strong adsorption energy of –32.916 kcal/mol and an isosteric heat of –28.861 kcal/mol, driven by electrostatic interactions with intrinsic Al–OH groups. In contrast, N_2 showed weak physisorption (–8.000 kcal/mol, van der Waals forces), and H_2O displayed moderate physisorption (–5.845 kcal/mol, hydrogen bonding). Competitive adsorption studies consistently demonstrated ALF's preferential CO_2 selectivity due to favorable quadrupole–framework interactions and pore confinement. Even at high H_2O concentrations, CO_2 retention was measurable, confirming its viability in humid environments. Comparatively, ALF's CO_2 adsorption performance is impressive. Its 4.8 mmol/g capacity surpasses activated carbon, and its high selectivity (~70%) is promising for flue gas separation. The adsorption energy of –32.916 kcal/mol indicates stronger CO_2

interactions than activated carbon and amine-based sorbents, while offering a balanced adsorption strength relative to zeolites and HKUST-1. ALF also exhibited good moisture resistance, a significant advantage over moisture-sensitive materials. These findings highlight ALF MOF's promising selectivity and performance for industrial gas separation and carbon capture. Future efforts should focus on experimental validation under realistic flue gas conditions, including contaminant assessment (SO_2, NO_x) and comprehensive evaluation of dynamic operational parameters (regeneration, cyclic stability) to bridge the gap between theoretical insights and practical deployment.

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Author Contributions

F.P.M. served as the principal investigator (PI) of the project providing overall supervision and guidance. H.N. carried out all simulations, data analysis, and interpretation, and was responsible for preparing the original manuscript draft and compilation of results.

6. ACKNOWLEDGEMENTS

The authors gratefully acknowledge the Research & Innovation Center (RIC), National University of Sciences and Technology (NUST), for funding this project. The School of Interdisciplinary Engineering & Sciences (SINES), Islamabad, NUST, is also sincerely acknowledged for providing the computational resources and facilities that made this work possible.

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