

## Activated Carbons for Direct Air Capture: Adsorption Mechanisms, Material Design and Performance Optimization

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### ABSTRACT

Direct air capture (DAC) has emerged as a critical technology for mitigating atmospheric CO<sub>2</sub> emissions, offering a pathway toward negative carbon emissions. Among various adsorbents, activated carbons (ACs) have gained significant attention due to their tunable porosity, chemical modifiability and cost-effectiveness. This review provides a comprehensive evaluation of AC-based DAC, focusing on material synthesis, functionalization strategies, adsorption mechanisms and regeneration processes. The influence of precursor selection, activation methods and surface modifications on CO<sub>2</sub> uptake efficiency is discussed in detail. Additionally, the challenges associated with adsorption under ultra-dilute conditions, energy-intensive regeneration and long-term stability are critically analyzed. Future research directions are highlighted, emphasizing the need for advanced hybrid materials, low-energy desorption techniques and large-scale deployment strategies. The findings underscore the potential of activated carbons as a viable and scalable solution for DAC, contributing to global climate mitigation efforts.

**Keywords:** Direct air capture; Activated carbon; CO<sub>2</sub> adsorption; Functionalization; Regeneration; Carbon capture; Adsorption kinetics; Sustainable materials

### Introduction

The increasing concentration of CO<sub>2</sub> in the atmosphere, primarily due to fossil fuel combustion, industrial emissions and deforestation, has led to an urgent need for carbon mitigation strategies. Climate models predict that without significant reductions in CO<sub>2</sub> emissions, global temperatures will continue to rise, exacerbating climate change effects such as extreme weather events, ocean acidification and loss of biodiversity<sup>1</sup>. Carbon capture technologies, particularly DAC, have gained attention as a necessary complement to emission reduction efforts, as they offer a means to directly remove CO<sub>2</sub> from the ambient air, regardless of its source. Unlike point-source carbon

capture, which targets emissions from industrial facilities and power plants, DAC can address dispersed CO<sub>2</sub> emissions that are otherwise challenging to mitigate<sup>2</sup>.

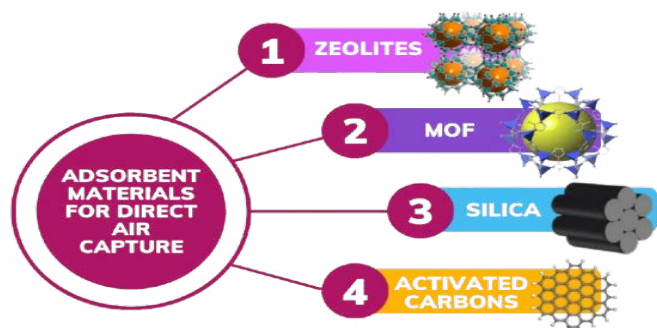
DAC technologies rely on adsorbent materials with high CO<sub>2</sub> capture efficiency, excellent selectivity and energy-efficient regeneration. Various classes of adsorbents, including metal-organic frameworks (MOFs), zeolites, covalent organic frameworks (COFs) and functionalized polymers, have been extensively studied for DAC applications<sup>3-5</sup> (**Figure 1**). MOFs and COFs exhibit high CO<sub>2</sub> adsorption capacities due to their well-defined pore structures and tunable surface chemistry, but their synthesis complexity, high cost and stability limitations

present challenges for large-scale deployment<sup>6</sup>. Zeolites, known for their strong CO<sub>2</sub> affinity and structural rigidity, often suffer from lower adsorption capacity under ultra-dilute conditions and high regeneration energy demands<sup>7,8</sup>. Functionalized polymers provide versatility in tailoring adsorption properties, but their scalability and durability remain significant concerns<sup>9</sup>.

Among these materials, activated carbons stand out due to their cost-effectiveness, availability and tunability. Unlike crystalline adsorbents, activated carbons offer a more flexible and scalable solution due to their diverse precursor sources, ease of synthesis and adjustable surface properties. Activated carbons are produced from abundant and renewable sources such as biomass, coal and synthetic polymers, making them economically viable for large-scale applications. Their intrinsic high surface area and well-developed microporosity enable efficient CO<sub>2</sub> capture even at low partial pressures, a critical requirement for DAC applications<sup>10</sup>. Furthermore, activated carbons exhibit excellent chemical and thermal stability, ensuring prolonged operational lifetimes and resistance to degradation over multiple adsorption-desorption cycles<sup>11</sup>.

Another significant advantage of activated carbons lies in their modifiable surface chemistry. Through functionalization techniques such as nitrogen doping, amine grafting<sup>12</sup> or oxidation treatments, the CO<sub>2</sub> affinity and selectivity of activated carbons can be significantly enhanced. These modifications introduce additional adsorption sites that facilitate stronger CO<sub>2</sub> interactions while minimizing competitive adsorption of other atmospheric gases like N<sub>2</sub><sup>13</sup>. Additionally, the relatively low regeneration energy required for desorbing CO<sub>2</sub> from activated carbons further strengthens their feasibility for DAC applications, reducing the overall energy footprint compared to alternative adsorbents.

This review provides a comprehensive assessment of the current advancements in activated carbon-based DAC materials. It discusses key factors influencing adsorption performance, including pore structure, surface chemistry and regeneration efficiency. Additionally, various synthesis and functionalization strategies are examined to identify optimal material properties for large-scale deployment. The review also highlights challenges in cost-effective production, long-term stability and energy-efficient desorption cycles, which must be addressed to make activated carbon-based DAC a commercially viable solution.



**Figure 1:** Various types of adsorbent materials utilized for Direct air capture.

## Fundamentals of CO<sub>2</sub> Adsorption on Activated Carbons

Understanding the mechanisms of CO<sub>2</sub> adsorption on activated carbons is essential for optimizing their performance in DAC applications. The adsorption behavior of CO<sub>2</sub> is governed by several key factors, including the textural properties of the

material, surface chemistry and thermodynamic parameters such as pressure and temperature. Activated carbons, due to their high surface area and tunable porosity, primarily capture CO<sub>2</sub> through physical adsorption mechanisms. However, chemical interactions can also play a significant role, especially when surface functionalization is introduced. This section discusses the primary modes of CO<sub>2</sub> capture on activated carbons and highlights how different structural and chemical modifications influence adsorption capacity and selectivity.

### Physisorption vs Chemisorption in activated carbons

CO<sub>2</sub> adsorption on activated carbons occurs via two primary mechanisms: physisorption and chemisorption. Physisorption is a process driven by weak van der Waals forces, where CO<sub>2</sub> molecules are physically adsorbed onto the carbon surface without undergoing chemical bonding. This interaction is highly dependent on surface area, pore structure and gas pressure. Activated carbons with a well-developed microporous network provide confinement effects that enhance CO<sub>2</sub> physisorption, making them highly effective in DAC applications. The adsorption energy in physisorption is typically in the range of 20–40 kJ/mol, allowing for easy desorption and low-energy regeneration cycles<sup>14</sup>. Due to the reversible nature of physisorption, activated carbons can undergo multiple adsorption-desorption cycles without significant structural degradation.

Chemisorption, on the other hand, involves stronger interactions where CO<sub>2</sub> molecules form covalent or ionic bonds with active sites on the carbon surface. This process is typically induced by functionalization with basic groups such as amines, nitrogen species or metal oxides. Unlike physisorption, chemisorption results in higher adsorption enthalpies, making desorption more energy intensive. However, chemisorption significantly enhances CO<sub>2</sub> selectivity, particularly under ultra-dilute conditions like those encountered in DAC applications<sup>14,15</sup>. The phenomenon of chemisorption and physisorption are depicted graphically in (Figure 2).



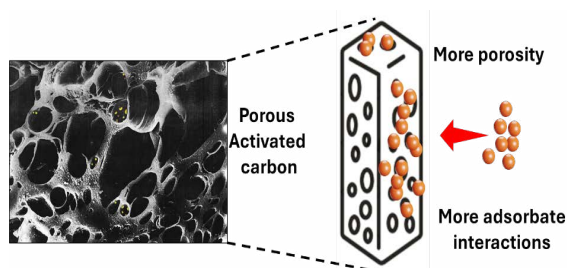
**Figure 2:** Graphical depiction of the difference in mechanism between physisorption and chemisorption.

### Impact of pore size Distribution and surface chemistry

The efficiency of CO<sub>2</sub> adsorption is dictated by the complex interplay between pore size distribution and surface chemistry. Activated carbons with a high concentration of ultra micropores (<0.7 nm) exhibit the strongest interactions with CO<sub>2</sub> molecules due to enhanced van der Waals forces and molecular sieving effects<sup>16</sup>. Micropores in the range of 0.5–1.0 nm contributes to higher CO<sub>2</sub> uptakes by increasing the available adsorption sites<sup>16,17</sup>. However, an overabundance of mesopores (>2 nm) may lead to reduced adsorption capacity due to lower confinement effects, though they can facilitate rapid mass transfer during adsorption and desorption cycles.

Beyond pore size, the surface chemistry of activated carbons plays a critical role in dictating CO<sub>2</sub> affinity and selectivity. The

introduction of heteroatoms such as nitrogen, oxygen and sulfur enhances surface basicity, creating stronger interactions with CO<sub>2</sub> molecules. Nitrogen-doped carbons, for instance, promote Lewis base-acid interactions, which favor CO<sub>2</sub> binding over competing gases like N<sub>2</sub><sup>18</sup>. Oxygen-containing functional groups (e.g., hydroxyls, carboxyl's) influence adsorption properties by modulating the hydrophobicity and electronic charge distribution of the carbon surface<sup>19</sup>. Meanwhile, sulfur-functionalized carbons have shown promise in improving CO<sub>2</sub> binding strength through electron donor-acceptor interactions<sup>20</sup>. **(Figure 3)** presents the pore size distributions and CO<sub>2</sub> adsorption capacities of AC, highlighting the relationship between pore characteristics and adsorption performance.



**Figure 3:** Graphical illustration of the relationship between porosity and adsorbent interactions in activated carbons.

### Role of surface functionalization

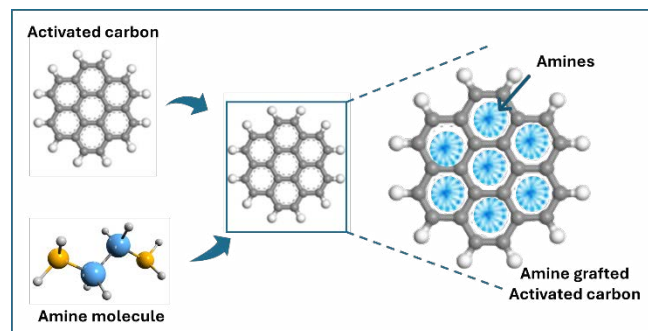
Surface functionalization is a key strategy for enhancing the CO<sub>2</sub> adsorption capacity of activated carbons. The introduction of heteroatoms such as nitrogen, oxygen and sulfur modify the surface charge distribution, creating basic sites that improve CO<sub>2</sub> affinity. These modifications influence the adsorption mechanisms, shifting the equilibrium towards higher CO<sub>2</sub> selectivity and uptake. Empirical studies have demonstrated that nitrogen-doped carbons exhibit increased CO<sub>2</sub> binding due to the formation of Lewis basic sites, improving the interaction strength between CO<sub>2</sub> molecules and the carbon surface.

Amination is one of the most extensively studied functionalization techniques for activated carbons, given its strong affinity for CO<sub>2</sub>. Amine-functionalized activated carbons leverage the nucleophilic nature of amine groups, which facilitates the formation of zwitterionic or carbamate intermediates upon CO<sub>2</sub> binding<sup>21</sup>. The mechanism of amine grafting onto activated carbon is presented graphically in **(Figure 4)**. A study by Girimonte et al. (2022) reported that TEPA-functionalized mesoporous SBA-15 exhibited a significantly improved CO<sub>2</sub> adsorption capacity due to the incorporation of amine groups. The study found that amine-functionalized materials enhanced CO<sub>2</sub> uptake by increasing the density of active adsorption sites and facilitating the formation of carbamate species. However, similar research has demonstrated the effectiveness of amine functionalization in enhancing CO<sub>2</sub> adsorption capacities of activated carbons under comparable conditions<sup>22</sup>. Polyethylenimine (PEI) impregnation has been shown to significantly enhance the CO<sub>2</sub> adsorption capacity of various porous materials. For instance, a study by Bai et al. (2019) reported that PEI-impregnated resin HPD450 exhibited an adsorption capacity of 4.44 mmol/g for pure CO<sub>2</sub> and 3.62 mmol/g for 15 vol% CO<sub>2</sub>. Moreover, the material retained an average capacity of 3.58 mmol/g under flue gas conditions over 90 consecutive adsorption cycles<sup>23</sup>. Similarly, research by Fatima et al. (2022) demonstrated that surface-functionalized

activated carbon impregnated with pyrrolidinium-based ionic liquid achieved a CO<sub>2</sub> adsorption capacity of 2.165 mmol/g at 25 °C<sup>24</sup>.

A study by González et al. (2018) investigated CO<sub>2</sub> adsorption on activated carbons derived from glucose and phosphoric acid. The findings revealed that the sample with the highest oxygen content exhibited a CO<sub>2</sub> uptake of 3.57 mmol/g at 25°C and 1 bar, highlighting the significant impact of oxygen functionalization on adsorption performance<sup>25</sup>. Oxygen-functionalized groups, including hydroxyl and carbonyl species, can serve as additional active sites for CO<sub>2</sub> interactions, though excessive oxidation can sometimes lead to pore blockage, reducing adsorption efficiency. Metal-impregnation techniques, such as introducing alkali metals like potassium or lithium, have also been employed to enhance adsorption capacity by increasing surface polarity and interaction strength<sup>26</sup>.

Surface functionalization of activated carbons is a pivotal strategy for enhancing CO<sub>2</sub> adsorption capacities, particularly in direct air capture (DAC) applications. Introducing sulfur-containing groups, such as thiol (-SH) functionalities, onto the carbon surface has been shown to improve CO<sub>2</sub> binding strength through electron donor-acceptor interactions. For instance, a study by Tang et al. (2018) demonstrated that activated carbons treated with sulfuric acid, which introduces thiol and sulfonic acid groups, exhibited increased reactivity towards pollutant removal, suggesting that these sulfur-containing functional groups play a significant role in enhancing adsorption performance<sup>27</sup>. Additionally, combining different functionalization strategies, such as amination with metal impregnation or oxygenation, has been explored to further optimize adsorption performance<sup>24</sup>. These mixed functionalization approaches aim to leverage the synergistic effects of various surface modifications to tailor activated carbons for improved CO<sub>2</sub> capture efficiency in DAC applications<sup>28</sup>.



**Figure 4:** Mechanism depicting the functionalization of activated carbons with amines.

### Adsorption kinetics and mass transfer limitations

The kinetics of CO<sub>2</sub> adsorption on activated carbons are influenced by factors such as pore accessibility, diffusion resistance and surface energy, which collectively determine the rate at which adsorption equilibrium is achieved. Microporous activated carbons often exhibit slower adsorption kinetics due to restricted diffusion pathways, whereas mesoporous structures can enhance mass transfer, leading to improved adsorption rates. Understanding these kinetics is essential for optimizing operational parameters in direct air capture (DAC) applications<sup>29</sup>.

Adsorption kinetics are commonly described using models such as the pseudo-first-order and pseudo-second-order

kinetic models. The pseudo-first-order model assumes that the adsorption rate is proportional to the number of available adsorption sites, while the pseudo-second-order model considers the adsorption rate to be dependent on both the adsorbate concentration and the available sites. Experimental studies on functionalized activated carbons have indicated that CO<sub>2</sub> adsorption often follows the pseudo-second-order model, suggesting a chemisorption-dominated process, especially in materials with amine or nitrogen functionalities. For instance, a study on CO<sub>2</sub> adsorption kinetics using NiO-modified activated carbon found that the pseudo-second-order model provided a better fit to the experimental data, indicating chemisorption as the rate-limiting step<sup>30</sup>.

A study by Bedia et al. (2021), investigated the adsorption kinetics of methylene blue on high surface area mesoporous-activated carbon derived from coconut shells. The study found that increasing the temperature from 35°C to 55°C enhanced the adsorption rate, suggesting that mesoporous carbons facilitate faster adsorption kinetics compared to microporous counterparts. The equilibrium adsorption capacity was measured at 312 mg/g, demonstrating the improved diffusion rates in mesoporous structures<sup>31</sup>. Additionally, A study by Sayari et al. (2012), investigated CO<sub>2</sub> adsorption on amine-functionalized mesoporous silica materials. The research found that amine-functionalized adsorbents achieved a maximum CO<sub>2</sub> adsorption capacity of 3.56 mmol/g at 75°C and 1 bar. The study highlighted that amine grafting significantly improved CO<sub>2</sub> uptake by increasing the availability of active adsorption sites for chemisorption<sup>32</sup>.

Mass transfer significantly influences adsorption efficiency in direct air capture (DAC) applications, particularly under ultra-dilute conditions (~400 ppm CO<sub>2</sub>). The process involves three primary stages: (1) bulk gas diffusion, (2) pore diffusion and (3) surface adsorption. Mesopores facilitate faster pore diffusion by reducing resistance, thereby enhancing adsorption rates. However, an excessive presence of mesopores can diminish adsorption capacity due to reduced confinement effects. Research indicates that the balance between micropores and mesopores is crucial for optimizing both adsorption capacity and kinetics. For instance, a study by Song et al. (2015) found that activated carbons with a higher mesopore volume exhibited improved CO<sub>2</sub> adsorption performance when the BET surface area was below 500 m<sup>2</sup>/g, while those with a higher micropore area performed better above this threshold. This suggests that an optimal micropore-to-mesopore ratio is essential for achieving efficient CO<sub>2</sub> capture<sup>33</sup>. Additionally, a study by Lawtae et al. (2021) demonstrated that high surface area mesoporous-activated carbons derived from coconut shells exhibited superior adsorption kinetics and capacity compared to microporous carbons. This underscores the importance of mesopore presence in facilitating rapid CO<sub>2</sub> uptake<sup>31</sup>.

Furthermore, the presence of surface functional groups, such as amines, can alter the energy barrier for CO<sub>2</sub> adsorption. A study by Wang et al. (2020), investigated CO<sub>2</sub> adsorption on amino-functionalized mesoporous silica. The results demonstrated that amine functionalization significantly improved adsorption performance due to the increased number of interaction sites for CO<sub>2</sub> molecules, leading to higher adsorption kinetics compared to unmodified adsorbents<sup>34</sup>. Similarly, a review by Li et al. (2022), analyzed the impact of amine-functionalized carbon-

based adsorbents on CO<sub>2</sub> capture. The study highlighted that these materials exhibited adsorption capacities of up to 4.5 mmol/g at 25 °C and 1 bar, owing to the strong nucleophilic interactions between amine groups and CO<sub>2</sub> molecules. The findings further emphasized that primary and secondary amines enhanced CO<sub>2</sub> uptake by facilitating the formation of carbamate species, thereby improving adsorption kinetics and selectivity<sup>14</sup>.

Optimizing adsorption kinetics is crucial for large-scale direct air capture (DAC) applications to minimize processing time and energy consumption. Techniques such as Temperature Swing Adsorption (TSA) and Pressure Swing Adsorption (PSA) are widely employed to enhance desorption efficiency. For instance, a study by Chen et al. (2021) investigated the use of internal heat exchangers within adsorption beds to improve heat and mass transfer during TSA processes. Their findings suggest that incorporating such heat exchangers can significantly enhance regeneration efficiency, though specific quantitative data on desorption time reduction were not provided<sup>35</sup>. Additionally, a comprehensive review on carbon dioxide separation and capture by Karimi et al. (2023) highlights the importance of optimizing process parameters in TSA and PSA methods to achieve efficient CO<sub>2</sub> desorption and adsorbent regeneration. The review emphasizes that careful thermal management and process design are essential to minimize energy consumption and enhance overall system performance<sup>36</sup>. **(Table 1)** provides a summary of adsorption rate constants and equilibrium times for various activated carbon materials under DAC conditions.

Activated Carbon Type	Adsorption Rate Constant (min <sup>-1</sup> )	Equilibrium Time (min)	Reference
Microporous AC	0.019	10–15	37
Mesoporous AC	0.030	5	37
Amine-Grafted AC	0.032	8	34
Primary Amine-Functionalized AC	0.032	7	14
TSA-Optimized AC	0.035	6	35

**Table 1:** Summary of adsorption rate constants and equilibrium times for various activated carbon material

### Thermodynamic influences on CO<sub>2</sub> adsorption

The adsorption of CO<sub>2</sub> onto activated carbons is significantly affected by thermodynamic parameters, particularly temperature and pressure. These factors dictate both the adsorption mechanism and the energy required for regeneration, which are critical for optimizing DAC performance.

Physisorption, the dominant mechanism for CO<sub>2</sub> uptake in most activated carbons, is an exothermic process and thus more efficient at lower temperatures. Elevated temperatures reduce the van der Waals forces between CO<sub>2</sub> molecules and the carbon surface, leading to a decrease in adsorption capacity. Empirical studies confirm this trend: for instance, A study by Suba et al. (2023) examined CO<sub>2</sub> adsorption on amine-functionalized KIT-6 materials. The findings revealed that the adsorption capacity decreased from 2.23 mmol/g at 40 °C to 0.95 mmol/g at 70 °C, indicating a significant reduction in performance at elevated temperatures<sup>38</sup>. Conversely, chemisorption-based adsorbents, which involve stronger CO<sub>2</sub>-sorbent interactions, exhibit less sensitivity to temperature fluctuations. Amine-functionalized activated carbons, for example, retain their adsorption efficiency over a wider temperature range due to the formation of stable carbamate species. In a study Wang et al. (2020) assessed CO<sub>2</sub>

uptake on amino-functionalized mesoporous silica. The study reported an increase in CO<sub>2</sub> adsorption capacity with rising aging temperatures during material preparation, achieving up to 2.24 mmol/g, suggesting that higher synthesis temperatures may enhance adsorption performance<sup>34</sup>. Furthermore, a study by Lotfinezhad et al. (2023) investigated the role of humidity in CO<sub>2</sub> adsorption using amine-functionalized carbon-based sorbents. The results indicated that the presence of water vapor facilitated chemisorption of CO<sub>2</sub>, enhancing the adsorption capacity of the sorbents<sup>39</sup>.

Adsorption pressure significantly influences CO<sub>2</sub> capture performance. In direct air capture (DAC) applications, which operate under ultra-dilute conditions (~400 ppm CO<sub>2</sub>), the effectiveness of adsorbents is contingent upon their pore structure and surface functionality. Research indicates that activated carbons with a higher proportion of ultra micropores (<0.7 nm) demonstrate enhanced CO<sub>2</sub> uptake under low partial pressure conditions. For instance, a study by Prauchner et al. (2020) reported that granular activated carbons derived from coconut shells achieved a CO<sub>2</sub> adsorption capacity of 1.17 mmol/g at 0.15 bar and 25°C, highlighting the importance of ultra microporosity in DAC applications<sup>40</sup>. Functionalization of activated carbons further enhances CO<sub>2</sub> adsorption performance under low-pressure conditions. A study by Zhao et al. (2023) demonstrated that potassium carbonate (K<sub>2</sub>CO<sub>3</sub>)-impregnated activated carbons exhibited a CO<sub>2</sub> adsorption capacity of 1.12 mmol/g at 298 K and 10% CO<sub>2</sub> concentration, outperforming unmodified carbons. The improved performance is attributed to the introduction of basic sites that facilitate stronger interactions with CO<sub>2</sub> molecules<sup>41</sup>.

The energy required for regenerating CO<sub>2</sub>-saturated activated carbons is a critical factor in the efficiency of direct air capture (DAC) systems. Physisorption-based materials, which rely on weaker van der Waals forces, typically necessitate mild heating (80–120°C) for regeneration. In contrast, chemisorption-based adsorbents, such as amine-functionalized carbons, often require higher temperatures, exceeding 150°C, to break the stronger chemical bonds formed during CO<sub>2</sub> capture. This increased energy demand can impact the overall efficiency and cost-effectiveness of DAC operations. Temperature Swing Adsorption (TSA) is a widely adopted method to facilitate desorption in DAC applications. Studies have shown that optimizing the desorption temperature can significantly reduce energy consumption. For instance, a study by Li et al. (2019) evaluated the entropy generation in a four-step TSA process and found that lowering the desorption temperature from 120°C to 100°C reduced energy dissipation, thereby enhancing the energy efficiency of the regeneration process<sup>42</sup>. Given the low partial pressures of CO<sub>2</sub> in DAC scenarios, it is essential to optimize adsorbent properties to maintain efficient capture rates. Activated carbons with a micropore-to-mesopore ratio of at least 3:1 have demonstrated superior adsorption performance under these conditions. Functionalization with nitrogen or alkali metals further enhances CO<sub>2</sub> affinity, improving capture efficiency. Future research should focus on fine-tuning porosity, increasing the density of functional groups and developing energy-efficient regeneration methods to enhance DAC performance while minimizing energy costs.

## Material Design And Functionalization Strategies

### Precursor selection and activation methods

Activated carbons can be synthesized from a variety of precursors, including biomass, coal and synthetic polymers. The choice of precursor significantly influences the pore structure, surface chemistry and adsorption performance of the resulting material. Biomass-derived activated carbons, such as those from coconut shells and wood, typically exhibit high microporosity, making them well-suited for direct air capture (DAC) applications. In contrast, synthetic polymer-based activated carbons offer more tunable porosity, allowing for tailored adsorption characteristics. Activation processes are generally categorized into physical and chemical methods. Physical activation involves high-temperature treatment in an oxidizing atmosphere (e.g., steam or CO<sub>2</sub>), selectively removing carbon and creating a well-developed pore network. Chemical activation, using agents such as KOH or ZnCl<sub>2</sub>, facilitates pore development at lower temperatures, leading to higher surface areas and improved CO<sub>2</sub> adsorption capacities.

Empirical studies have demonstrated the effectiveness of chemical activation. For instance, a study by Nandi et al. (2023) reported that KOH-activated carbons derived from rice husk exhibited CO<sub>2</sub> adsorption capacities of up to 6.3 mmol/g at 0 °C and 1 bar. At 25 °C and 1 bar, the adsorption capacity was 4.4 mmol/g<sup>43</sup>. In comparison, steam-activated carbons generally show lower CO<sub>2</sub> uptake. A study on walnut shell-derived activated carbons prepared via steam activation reported CO<sub>2</sub> adsorption capacities of approximately 1.9 mmol/g at 25 °C and 1 bar<sup>44</sup>. These findings highlight the significant impact of activation methods on the adsorption performance of activated carbons, with chemical activation, particularly using KOH, leading to materials with superior CO<sub>2</sub> capture capabilities.

### Hybrid and composite materials

Hybrid materials combining activated carbon with metal-organic frameworks (MOFs), covalent organic frameworks (COFs) or polymeric networks have been explored to synergistically enhance adsorption performance and regeneration stability. MOF-AC composites leverage the high surface area and tunable adsorption sites of MOFs while retaining stability and low cost of activated carbon. For instance, a study by Beygzadeh et al. (2023) developed composites of MOF-5 and Cu-BDC with activated carbon, achieving methane adsorption capacities of up to 7.3 mmol/g at room temperature and 35 bar. Although this study focused on methane, the significant adsorption capacity indicates the potential of such composites for CO<sub>2</sub> capture applications<sup>45</sup>.

COF-AC composites, which incorporate porous organic frameworks with high nitrogen content, have demonstrated superior adsorption performance at ultra-dilute CO<sub>2</sub> concentrations (400 ppm). These materials offer enhanced CO<sub>2</sub>-philic interactions while maintaining rapid adsorption/desorption kinetics. For example, a study by Green et al. (2024) reported that potassium carbonate-infused activated carbon fiber felt composites exhibited promising results for direct air capture applications, highlighting the potential of such hybrid materials<sup>10</sup>. Polymer-coated activated carbons, particularly those modified with ionic liquids, have been investigated for improving CO<sub>2</sub> selectivity under humid conditions. A comprehensive review by Latif et al. (2024) discusses various methods for the synthesis of carbon materials and modification techniques, including the use of polymeric networks, to enhance CO<sub>2</sub> capture performance<sup>46</sup>. These studies underscore the potential of hybrid materials

in advancing CO<sub>2</sub> capture technologies by combining the advantageous properties of different components to achieve superior performance.

### Performance Analysis of Various Activated Carbon-Based Materials At DAC Conditions

A comparative analysis of different activated carbon materials under DAC conditions is essential to identify optimal materials

for large-scale deployment. Table 2 presents a summary of CO<sub>2</sub> uptake, BET surface area and operational parameters for various activated carbon types.

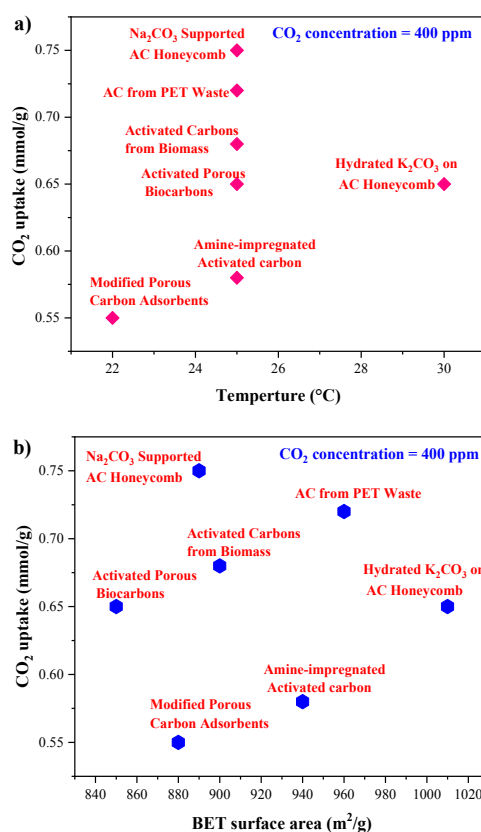
To further analyze the trends in CO<sub>2</sub> uptake across different activated carbons, Figures 5(a) and 5(b) illustrate the relationships between CO<sub>2</sub> uptake vs. temperature and CO<sub>2</sub> uptake vs. BET surface area, respectively.

**Table 2:** Summary of CO<sub>2</sub> uptake capacities, surface area and operational parameters of various activated carbon materials under direct air capture (DAC) conditions.

Activated Carbon Type	CO <sub>2</sub> Uptake (mmol/g)	Modification	BET Surface Area (m <sup>2</sup> /g)	CO <sub>2</sub> Feed Concentration (ppm)	Temperature (°C)	Humidity	Reference
Amine-impregnated AC from Jatropa	0.58	Amine Functionalization	940	400	25	Yes	47
Na <sub>2</sub> CO <sub>3</sub> Supported AC Honeycomb	0.75	Sodium Carbonate Grafting	890	400	25	Yes	48
Hydrated K <sub>2</sub> CO <sub>3</sub> on AC Honeycomb	0.65	Potassium Carbonate Hydration	850	400	25	Yes	49
Activated Porous Biocarbons	0.65	Nitrogen Functionalization	1010	400	30	No	50
AC from PET Waste	0.72	KOH Chemical Activation	960	400	25	No	51
Modified Porous Carbon Adsorbents	0.55	Various Activating Agents	880	400	22	Yes	52
Activated Carbons from Biomass	0.68	None	900	400	25	Yes	53

(Figure 5(a)) shows that Na<sub>2</sub>CO<sub>3</sub>-supported activated carbon honeycomb exhibits the highest CO<sub>2</sub> uptake (0.75 mmol/g) at 25°C, followed closely by AC from PET waste (0.72 mmol/g). In contrast, amine-impregnated activated carbon (0.58 mmol/g) and modified porous carbon adsorbents (0.55 mmol/g) demonstrate lower adsorption capacities. The trend indicates that temperature variations in the 22–30°C range do not drastically affect CO<sub>2</sub> uptake, suggesting that physisorption-based materials retain relatively stable adsorption under DAC conditions. However, amine-functionalized materials tend to experience a more pronounced decline in adsorption efficiency as temperature increases, likely due to weakened interactions between amine groups and CO<sub>2</sub> molecules.

(Figure 5(b)) presents the impact of BET surface area on CO<sub>2</sub> adsorption capacity. The highest BET surface area material, activated porous biocarbons (1010 m<sup>2</sup>/g), achieves a moderate CO<sub>2</sub> uptake (0.65 mmol/g), whereas AC from PET waste (960 m<sup>2</sup>/g) and Na<sub>2</sub>CO<sub>3</sub>-supported AC (890 m<sup>2</sup>/g) show higher adsorption capacities despite lower surface areas. This suggests that while surface area is an important factor, CO<sub>2</sub> uptake is also strongly influenced by chemical modifications. Notably, materials that incorporate alkali metal functionalization (Na<sub>2</sub>CO<sub>3</sub>, K<sub>2</sub>CO<sub>3</sub>) consistently outperform non-functionalized carbons, highlighting the role of surface chemistry in enhancing CO<sub>2</sub> affinity.



**Figure 5:** a) CO<sub>2</sub> uptake of various activated carbon adsorbents as a function of temperature, highlighting the impact of material composition on adsorption performance, b) CO<sub>2</sub> uptake of the same activated carbon adsorbents as a function of BET surface area, illustrating the correlation between surface properties and adsorption capacity.

## Key observations and implications for DAC applications

Functionalized activated carbons, particularly those incorporating alkali metals ( $\text{Na}_2\text{CO}_3$ ,  $\text{K}_2\text{CO}_3$ ), exhibit superior  $\text{CO}_2$  adsorption at 400 ppm  $\text{CO}_2$ . BET surface area alone does not dictate adsorption performance, chemical modifications, micropore volume and surface charge play crucial roles in determining  $\text{CO}_2$  uptake efficiency. Temperature effects are less pronounced for most physisorption-based activated carbons; however, amine-functionalized materials exhibit sensitivity to temperature fluctuations, requiring optimization for stable performance. Activated carbons from PET waste and biomass-derived materials provide high adsorption capacities with minimal functionalization, making them attractive candidates for low-cost DAC deployment.

## Challenges And Future Directions In Activated Carbon-Based Direct Air Capture

Activated carbon-based direct air capture (DAC) systems face several technical and economic challenges that impact their efficiency and scalability. One of the primary hurdles is the ultra-dilute concentration of  $\text{CO}_2$  in ambient air (~400 ppm), which necessitates adsorbents with high selectivity and strong interactions with  $\text{CO}_2$  molecules to effectively separate them from other atmospheric gases<sup>54</sup>.

Regenerating  $\text{CO}_2$ -saturated adsorbents is a major energy constraint in DAC systems. Physisorption-based activated carbons typically require mild heating (80–120°C) for  $\text{CO}_2$  desorption, whereas chemisorption-based materials, such as amine-functionalized carbons, demand significantly higher temperatures (>150°C) to break the chemical bonds formed during  $\text{CO}_2$  capture [54]. This high energy requirement makes DAC systems costly and limits their widespread adoption. Alternative regeneration strategies, such as electrothermal swing adsorption (ETSA) and pressure swing adsorption (PSA), have been explored to reduce energy consumption while preserving adsorbent integrity<sup>55</sup>.

Repeated adsorption-desorption cycles can lead to the structural degradation of adsorbents, further impacting DAC efficiency. Amine-functionalized activated carbons, while highly effective, suffer from oxidative degradation and leaching, reducing their long-term performance. Protective coatings or hybrid composites have been proposed to enhance stability and prolong material lifespan<sup>55</sup>. The cost-effectiveness of DAC remains a significant challenge, particularly concerning the production and regeneration of high-performance adsorbents. Biomass-derived activated carbons offer a sustainable and cost-efficient alternative; however, their variability in composition affects adsorption performance consistency. Scalable and low-cost activation and functionalization strategies must be developed to ensure economic viability at large scales<sup>54</sup>.

Aligning DAC operations with renewable energy sources can significantly lower the carbon footprint and operational costs. Utilizing solar or wind energy for energy-intensive  $\text{CO}_2$  regeneration processes can improve sustainability and make DAC more environmentally viable. Future research should focus on developing novel precursor materials to enhance the adsorption properties of activated carbons while optimizing their pore structure and surface chemistry for improved  $\text{CO}_2$  capture. Designing hybrid adsorbents, such as activated carbon-metal-organic framework (MOF) composites, can further enhance

adsorption efficiency by combining the advantages of both materials. Additionally, optimizing regeneration strategies is crucial to minimizing energy consumption while maintaining the stability and reusability of adsorbents over multiple cycles. Scaling up production methods is essential to ensure the feasibility of large-scale deployment, making activated carbon-based direct air capture (DAC) more economically viable. Enhancing operational conditions, such as fine-tuning adsorption kinetics and selectivity under ultra-dilute  $\text{CO}_2$  concentrations, can further improve efficiency while reducing energy input. Addressing these challenges will help establish activated carbon-based DAC as a scalable and effective solution for atmospheric  $\text{CO}_2$  removal and climate change mitigation.

## Conclusion

Activated carbons have emerged as a promising class of adsorbents for direct air capture due to their tunable porosity, functionalization ability and cost-effectiveness. Advances in activation methods, surface modifications and composite materials have significantly improved  $\text{CO}_2$  uptake and selectivity. However, key challenges remain in optimizing adsorption under ultra-dilute conditions, minimizing regeneration energy and ensuring long-term stability.

Future efforts should focus on refining material synthesis techniques, developing energy-efficient regeneration methods and integrating DAC processes with sustainable energy sources. Addressing these challenges will be essential to making activated carbon-based DAC a scalable and economically viable solution for  $\text{CO}_2$  removal, ultimately contributing to global climate mitigation strategies.

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