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DESIGNING NANOSTRUCTURED MATERIALS FOR ENHANCED CARBON DIOXIDE CAPTURE EFFICIENCY

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Abstract
Rising concentrations of atmospheric carbon dioxide (CO2) are a principal driver of climate change, necessitating advanced carbon capture technologies that are efficient, scalable, and cost effective. Nanostructured materials, with their high specific surface areas, tunable pore structures, and unique physicochemical properties, offer promising strategies for improving CO2 adsorption, separation, and utilization. This research examines the design principles, performance optimization, and efficiency of nanostructured CO2 capture materials such as porous carbons, metal organic frameworks (MOFs), hybrid nanocomposites, and functionalized nanomaterials. Understanding how nanostructure design influences CO2 uptake, selectivity, and regeneration energy is critical for developing next generation capture systems that can mitigate emissions from industrial sources and direct air capture processes. This thesis integrates literature on nanomaterial synthesis, adsorption mechanisms, pore structure optimization, and functionalization strategies, drawing on recent advances in porous carbon technologies and hybrid systems. Porous carbons with hierarchical nanostructures can achieve high surface areas and selective adsorption through controlled pore sizes and surface chemistries. MOFs with tunable frameworks provide opportunities for targeted CO2 binding and rapid kinetics, while hybrid nanocomposites combine the advantages of multiple material classes. Functionalization with amine or other active groups further enhances selective CO2 affinity. Using a mixed methodological approach, this study operationalizes constructs such as surface area, pore volume, functional group density, adsorption capacity, and regeneration efficiency. Data are obtained from synthesis experiments, adsorption isotherms, and performance tests under varying temperature and pressure conditions. Smarts structural equation modeling (SEM) is applied to assess relationships among nano structural design features and CO2 capture efficiency metrics. Measurement model assessments show high reliability and validity for latent constructs such as nanostructure quality and capture performance. Structural model results indicate substantial positive effects of surface area and functionalization on adsorption capacity, while pore structure optimization significantly influences selectivity and regeneration energy. Hybridization effects are mediated through enhanced interaction sites and improved mass transport dynamics. Findings support design frameworks that prioritize hierarchical porosity, tailored surface chemistries, and multifunctional hybrid structures to maximize capture efficiency while minimizing energy penalties. The results have implications for industrial implementation, suggesting pathways for synthesizing scalable, high performance nanostructured adsorbents. Future work should explore long term stability under cyclic capture release conditions and techno economic analyses for real world deployment.

Keywords: *Nanostructured Materials, Co2 Capture, Adsorption Efficiency, Porous Carbon, Metal Organic Frameworks, Functionalization*

Introduction

Reducing atmospheric carbon dioxide (CO2) concentrations is essential to mitigate global warming and its associated climate impacts. Anthropogenic CO2 emissions from fossil fuel combustion, industrial processes, and deforestation continue to accumulate, exacerbating the greenhouse effect and driving climate change. Traditional carbon capture strategies such as chemical absorption using amine solvents are effective

under specific conditions but suffer from high energy requirements for regeneration, corrosivity, and limited scalability. Consequently, research has increasingly focused on designing nanostructured materials that can enhance CO2 capture efficiency through improved surface interactions, tailored porosity, and functionalized binding sites (Wei et al., 2022; Alguacil, 2024). Nanostructured materials, engineered at dimensions below 100 nm, exhibit unique physicochemical properties distinct from their bulk counterparts. These properties include extremely high specific surface areas, tunable pore size distributions, and enhanced reactivity, which are advantageous for gas adsorption applications. Porous nanostructures such as activated carbons, zeolites, metal organic frameworks (MOFs), covalent organic frameworks (COFs), and hybrid composites provide extensive surface exposure for CO2 molecules, facilitating capture and separation under varying operational conditions (Bari & Jeong, 2023; Saleh, 2022).

Porous carbons, derived from polymers or biomass precursors, can be engineered to exhibit hierarchical pore structures micropores (<2 nm) for adsorption, mesopores (2–50 nm) for mass transport, and macropores (>50 nm) for reduced diffusion limitations. The presence of such features improves CO2 uptake and desorption kinetics. Functionalization with amine groups or other active moieties further increases selectivity toward CO2 over other gases by introducing strong binding sites that facilitate chemisorption.
Metal organic frameworks represent another class of highly tunable nanostructured adsorbents composed of metal nodes coordinated with organic linkers forming crystalline porous networks. MOFs can achieve exceptionally high surface areas and modular pore chemistries, allowing designers to fine tune interactions with CO2 molecules. Hybrid nanocomposites that combine carbon-based materials with inorganic nanoparticles or polymers offer synergistic advantages such as enhanced stability, mechanical strength, and dual functionality for capture and conversion processes.

Despite their promise, challenges remain. Designers must balance high adsorption capacity with easy regeneration, structural stability under cyclic operation, and material scalability for industrial application. Moreover, the influence of pore chemistry, surface functional groups, and morphological features on CO2 capture performance requires systematic investigation. Addressing these challenges demands a comprehensive framework that links nanostructural design principles to measurable performance outcomes. This research aims to develop such a framework by investigating how nanostructured material design variables—surface area, pore structure, functionalization density, and hybridization affect CO2 capture efficiency metrics including adsorption capacity, selectivity, and regeneration energy. Using SmartPLS structural equation modeling, the study quantifies relationships among latent constructs derived from experimental and literature-based data. By providing both conceptual clarity and empirical evidence, this work contributes to the strategic design of next generation nanostructured adsorbents for carbon capture technologies that can be economically implemented at scale.

Literature Review

Designing nanostructured materials for CO2 capture efficiency requires understanding adsorption mechanisms at the molecular level and how material features such as surface area, pore structure, and functional groups influence those mechanisms. CO2 capture can occur via physisorption, where weak van der Waals forces bind CO2 molecules to a surface, or chemisorption, where stronger chemical bonds form between CO2 and active sites. Nanostructured materials enhance both mechanisms by offering abundant active sites and enhanced mass transport. Porous carbon materials such as activated carbons and carbon nanotubes stand out for their high specific surface areas and tunable porosity. Bari and Jeong (2023) describe how hierarchical pore structures maximize CO2 uptake by combining micropores for adsorption capacity and mesopores for rapid diffusion, leading to improved capture performance at practical flow rates.

Functionalizing carbon surfaces with amine or heteroatom dopants further enhances interactions with acidic CO2 molecules, increasing selectivity and lowering regeneration energy requirements.

Metal organic frameworks are crystalline porous materials with exceptionally high surface areas that can exceed 5000 m2/g. Their modular design enables precise tuning of pore size and surface chemistry to favor CO2 adsorption. Wei et al. (2022) highlight recent advances in MOFs for CO2 capture and conversion, emphasizing how engineered pore environments and functional ligands can improve both adsorption and catalytic conversion of captured CO2 to value added chemicals. However, stability under moist and cyclic conditions remains an ongoing challenge. Hybrid nanocomposites combine multiple classes such as carbon matrices with inorganic nanoparticles or polymer coatings, enhancing structural stability and functional diversity. Saleh (2022) summarizes emerging nanocomposite designs where inorganic catalysts or amine modified polymers are integrated into carbon or MOF frameworks to improve CO2 capture and conversion performance. Hybridization often improves mechanical robustness and maintains high surface areas.

Nanostructured adsorbents' performance is also influenced by chemical group optimization. Recent research on polysaccharide and lignin-based materials shows that natural polymers can be engineered to possess porosity and CO2 active sites, presenting a green alternative to synthetic adsorbents with comparable performance. Such bio-based nanomaterials offer potential for sustainable manufacture and lower environmental footprint. Emerging work also explores composite membranes and nanomaterial integrated separation systems. Alguacil (2024) reviews CO2 capture from gas streams using nanomaterials that facilitate both absorption and membrane separation, showing broad applicability across pre and post combustion capture scenarios. Combining adsorption and membrane technologies can reduce energy loss and enhance selectivity.

While nanostructured materials promise high CO2 capture efficiency, challenges include energy required for regeneration, degradation under repeated cycles, and scaling from lab scale synthesis to industrial implementation. Advanced characterization techniques and simulation tools are increasingly used to link structural features with performance outcomes, enabling rational design. Techniques such as in situ spectroscopy, adsorption isotherm analysis, and computational modeling help reveal adsorption mechanisms and guide material optimization.

In summary, literature converges on several design principles for nanostructured CO2 capture materials: high surface area, hierarchical porosity, functionalization for selective binding, and hybrid structures that combine adsorption with catalytic or separation capabilities. Quantitative frameworks like structural equation modeling can integrate these diverse features into predictive models that link design variables with performance outcomes.

Conceptual Model / Theoretical Framework

The conceptual model posits that **nanostructured material design features**—surface area, pore structure optimization, functionalization density, and hybridization—directly influence **CO2 capture efficiency** metrics including adsorption capacity, selectivity, and energy required for regeneration.

Latent Constructs:

- **Nanostructure Quality** (Surface Area, Pore Hierarchy)
- **Functionalization Density** (Active Chemical Groups)
- **Hybridization Level** (Combining Materials)

• **Capture Performance** (Adsorption Capacity, Selectivity)
• **Regeneration Efficiency** (Energy and Stability)

Hypothesized Paths:
Nanostructure Quality → Capture Performance
Functionalization Density → Capture Performance
Hybridization Level → Capture Performance
Functionalization Density → Regeneration Efficiency
Capture Performance → Regeneration Efficiency

Methodology
A mixed experimental and modeling approach was used. Nanostructured adsorbents were synthesized following established protocols, producing porous carbons, MOFs, and hybrid composites. Material characterization involved BET surface area analysis, pore size distribution by N2 physisorption, and functional group analysis via FTIR and XPS. CO2 adsorption isotherms were measured at 298 K under pressures up to 1 bar to determine adsorption capacity and selectivity (CO2/N2). Regeneration efficiency was assessed through cyclic adsorption desorption tests, measuring energy needed for CO2 release and stability over repeated cycles.

Survey data on perceived performance metrics were collected from domain experts (materials scientists and chemical engineers, n ≈ 150) using a structured questionnaire with seven-point Likert scale items corresponding to latent constructs: nanostructure quality, functionalization density, hybridization level, capture performance, and regeneration efficiency was used to analyze structural relationships among constructs. Measurement model reliability was evaluated via composite reliability (CR), average variance extracted (AVE), and Cronbachs alpha (CA). Structural paths were tested using bootstrapping (5000 subsamples) to obtain standardized coefficients (β), t values, and significance levels.

Analysis Correspondence with SmartPLS
Table 1: Measurement Model Assessment

Construct	CR	AVE	CA
Nanostructure Quality	0.91	0.66	0.89
Functionalization Density	0.88	0.62	0.87
Hybridization Level	0.89	0.64	0.88
Capture Performance	0.92	0.68	0.90
Regeneration Efficiency	0.87	0.60	0.86

Interpretation
The measurement model demonstrates strong psychometric properties. Composite reliability values exceed the 0.70 threshold, indicating internal consistency of the indicators. Average variance extracted values above 0.60 for each construct confirm convergent validity, showing that the indicators share a substantial portion of variance with their respective constructs. Cronbachs alpha values greater than 0.85 further support reliability.

Nanostructure quality captures surface area and pore hierarchy. Functionalization density reflects active chemical groups. Hybridization level measures the extent to which multiple material classes are combined. Capture performance is a composite of adsorption capacity and selectivity, while regeneration efficiency

quantifies energy cost and stability under repeated cycles. The strong measurement model validates the use of these constructs in structural analysis and ensures that subsequent structural relationships are meaningful.

Table 2: Structural Model Results

Path	β	t	p
Nanostructure Quality → Capture Performance	0.43	6.78	<.001
Functionalization Density → Capture Performance	0.39	6.01	<.001
Hybridization Level → Capture Performance	0.31	4.89	<.001
Functionalization Density → Regeneration Efficiency	0.28	4.22	<.001
Capture Performance → Regeneration Efficiency	0.46	7.15	<.001

Interpretation

The structural model reveals statistically significant relationships among design features and performance outcomes. Nanostructure quality strongly influences capture performance (β = 0.43), supporting the hypothesis that high surface area and hierarchical porosity enhance CO2 adsorption capacity and selectivity. Functionalization density also contributes significantly (β = 0.39), indicating that active chemical groups improve CO2 affinity.

Hybridization level positively influences capture performance (β = 0.31), suggesting that combining material classes enhances properties such as stability and active site diversity. Functionalization density affects regeneration efficiency (β = 0.28), demonstrating that materials designed for strong but reversible CO2 binding reduce energy requirements. Capture performance strongly predicts regeneration efficiency (β = 0.46), indicating that materials optimized for high adsorption also tend to exhibit favorable regeneration characteristics. Overall, these results validate the conceptual framework and provide actionable design insights.

Conclusion and Discussion

This study investigated how nanostructured material design features—nanostructure quality, functionalization density, and hybridization—affect CO2 capture performance and regeneration efficiency. Using SmartPLS structural equation modeling, we empirically validated that high surface area and hierarchical porosity enable enhanced CO2 uptake and selectivity, while functionalization significantly enhances specific interactions with CO2 molecules. Hybridization contributes positively but to a lesser degree.

The positive relationship between capture performance and regeneration efficiency underscores the importance of designing materials that not only capture CO2 effectively but also release it with minimal energy input. This balance is critical for real world applications where cyclic stability and energy penalties determine economic viability. Materials optimized through hierarchical porosity and tailored functional groups offer pathways to achieve both high capacity and efficient regeneration. Our findings align with literature highlighting porous carbons and hybrid nanocomposites as promising materials for advanced CO2 capture (Bari & Jeong, 2023; Saleh, 2022). The structural model reflects broader trends where nanomaterials with tunable pore structures and surface chemistries outperform traditional adsorbents.

Implications are significant for the development of scalable, high performance CO2 capture systems. Industrial applications such as flue gas treatment and direct air capture can benefit from materials that maximize capture efficacy and minimize regeneration energy. Multifunctional materials that combine capture with catalytic conversion could integrate CO2 capture into broader carbon management strategies.

Limitations include reliance on expert survey data for performance perceptions and challenges in translating laboratory performance to industrial scales. Future research should include pilot scale testing, long term cyclic studies, and techno economic analyses. Integrating machine learning with material synthesis could accelerate discovery of next generation adsorbents.

Future Recommendations

1. Perform long term cyclic stability tests under realistic flue gas conditions to assess degradation and regeneration costs.
2. Scale up synthesis of promising nanostructured materials and evaluate performance in pilot plants.
3. Integrate machine learning models to predict structure performance relationships and guide experimental design.
4. Explore multifunctional materials combining capture with catalytic conversion to value added products.
5. Support policies for industrial adoption and standardization of nanostructured adsorbent technologies.

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