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Advanced Carbon Capture Materials: Innovation Pathways for Industrial Decarbonization

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Abstract

Industrial decarbonisation requires technological solutions capable of reducing carbon dioxide emissions from sectors where direct electrification and renewable energy substitution alone may be insufficient. Advanced carbon capture materials have emerged as a critical component of this transition because they can selectively capture carbon dioxide from industrial gas streams while potentially reducing the energy and environmental penalties associated with conventional capture technologies. This paper examines emerging materials and innovation pathways for industrial carbon capture, focusing on solid sorbents, metal–organic frameworks, covalent organic frameworks, porous polymers, advanced activated carbons, zeolites, amine-functionalised materials, membranes and hybrid capture systems. The paper evaluates how material properties—including adsorption capacity, selectivity, regeneration energy, chemical stability, moisture tolerance, thermal stability, mechanical durability and scalability—determine practical performance. Particular attention is given to the integration of computational materials discovery, artificial intelligence, molecular engineering and process optimisation to accelerate the development of next-generation capture materials. Applications across cement, steel, chemicals, refining, natural-gas processing and other hard-to-abate industries are considered. A multi-stage innovation framework is proposed linking material discovery, computational screening, laboratory validation, process integration, pilot-scale demonstration and lifecycle assessment. The paper argues that future progress will depend not simply on maximising laboratory adsorption capacity, but on designing materials for realistic industrial conditions, long-term durability, low regeneration energy, manufacturability and complete lifecycle sustainability. Advanced carbon capture materials therefore represent an interdisciplinary innovation opportunity connecting materials science, chemical engineering, artificial intelligence, industrial systems and climate technology.

Keywords: Carbon Capture, Advanced Materials, Industrial Decarbonisation, CO_2 Capture, Adsorbents, Metal–Organic Frameworks, Membranes, Porous Materials, Carbon Capture and Storage, Sustainable Materials.

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1. Introduction

Carbon dioxide emissions from industrial activity remain one of the most significant challenges in the global transition towards low-carbon production.

Industries such as:

- Cement.
- Steel.
- Chemicals.
- Refining.
- Fertiliser.
- Pulp and paper.
- Waste processing.

often produce emissions through a combination of fuel combustion and chemical processes.

Some of these emissions cannot be eliminated simply by replacing fossil-fuel energy with renewable electricity.

Carbon capture therefore provides an additional pathway for reducing industrial emissions.

The effectiveness of carbon capture, however, depends heavily on the materials used to separate CO_2 from other gases.

Conventional solvent-based capture technologies can involve substantial energy consumption, corrosion, solvent degradation and complex process requirements.

This has stimulated research into advanced materials capable of achieving:

- Higher CO_2 selectivity.
- Greater adsorption capacity.
- Faster mass transfer.
- Lower regeneration energy.
- Improved stability.
- Longer operating lifetimes.

The central research challenge is consequently shifting from:

"Can CO_2 be captured?"

to:

"Can CO_2 be captured efficiently, economically and sustainably under real industrial conditions?"

2. Industrial Carbon Capture

Industrial carbon capture generally involves separating CO_2 from a gas stream before it is released into the atmosphere.

The captured CO_2 can subsequently be:

- Stored underground.
- Used as an industrial feedstock.
- Converted into fuels or chemicals.

- Mineralised.
- Transported for long-term storage.

The capture material is therefore the first major technological interface between industrial emissions and carbon management.

3. Major Carbon Capture Approaches

Carbon capture can broadly be categorised as:

1. Post-combustion capture.
2. Pre-combustion capture.
3. Oxyfuel combustion.
4. Direct air capture.

For many existing industrial facilities, post-combustion capture is particularly relevant because it can potentially be integrated with existing production systems.

4. Importance of Capture Materials

A capture material must interact selectively with CO_2 while allowing other gases to pass through or remain relatively unaffected.

Important performance characteristics include:

Property	Importance
CO_2 capacity	Determines amount captured
Selectivity	Determines separation quality
Regeneration energy	Determines operating cost
Kinetics	Determines capture rate
Stability	Determines lifetime
Moisture tolerance	Important for industrial gases
Mechanical strength	Supports industrial deployment
Scalability	Determines manufacturing feasibility

5. Solid Sorbents

Solid sorbents are among the most extensively studied alternatives to conventional liquid solvents.

They capture CO_2 through:

- Physical adsorption.
- Chemical adsorption.
- Reversible surface interactions.

Potential advantages include:

- Lower corrosion.
- Reduced solvent loss.
- Compact equipment.
- Potentially lower regeneration energy.

6. Activated Carbon

Activated carbon contains a highly developed porous structure.

Its performance can be enhanced through:

- Surface modification.
- Heteroatom doping.
- Pore-size engineering.
- Functionalisation.

However, moisture and relatively low CO_2 selectivity under certain conditions can limit its industrial performance.

7. Zeolites

Zeolites are crystalline microporous materials with well-defined pore structures.

They can offer:

- High surface area.
- Molecular sieving.
- Good thermal stability.
- Strong adsorption selectivity.

However, water sensitivity can be problematic for certain zeolite structures.

8. Amine-Functionalised Sorbents

Amines can interact strongly with CO_2.

Functionalising porous materials with amine groups can combine:

High Surface Area + Chemical CO_2 Affinity

This can improve capture under relatively low CO_2 concentrations.

However, excessive chemical binding may increase regeneration energy.

9. Metal–Organic Frameworks

Metal–organic frameworks (MOFs) are crystalline porous materials constructed from metal centres and organic linkers.

Their structures can be engineered to provide:

- High surface areas.
- Tunable pore sizes.
- Selective adsorption.

- Functionalised chemical environments.

MOFs have therefore become an important platform for advanced CO_2 capture research.

10. MOF Design

The flexibility of MOF chemistry enables researchers to modify:

- Metal centres.
- Organic linkers.
- Pore dimensions.
- Functional groups.
- Surface chemistry.

This creates opportunities for molecular-level optimisation.

11. Covalent Organic Frameworks

Covalent organic frameworks (COFs) are porous crystalline materials constructed primarily from organic building blocks.

Their advantages may include:

- Low density.
- High surface area.
- Structural tunability.
- Functionalisation opportunities.

COFs are increasingly being investigated for gas separation and carbon capture.

12. Porous Organic Polymers

Porous organic polymers offer another class of tunable materials.

Their structures can be designed for:

- High porosity.
- Selective adsorption.
- Chemical stability.
- Functional group incorporation.

Their relatively flexible chemistry provides significant opportunities for materials engineering.

13. Carbon Molecular Sieves

Carbon molecular sieves use controlled pore structures to separate gases according to molecular size and interaction.

Their potential advantages include:

- Thermal stability.
- Chemical resistance.
- Tunable porosity.

14. Membrane-Based CO_2 Capture

Membranes separate gases through differences in:

- Permeability.
- Selectivity.
- Solubility.
- Diffusion.

A membrane-based system can potentially reduce the energy requirements associated with phase-change-intensive separation processes.

15. Advanced Polymer Membranes

Polymeric membranes can be engineered through:

- Polymer chemistry.
- Cross-linking.
- Functionalisation.
- Mixed-matrix structures.

The challenge is balancing:

Permeability ↔ Selectivity ↔ Stability

16. Mixed-Matrix Membranes

Mixed-matrix membranes combine a polymer matrix with inorganic or porous fillers.

Potential fillers include:

- MOFs.
- Zeolites.
- Nanoparticles.
- Porous carbons.

The objective is to combine the processability of polymers with the separation properties of advanced porous materials.

17. Inorganic Membranes

Inorganic membranes can offer strong thermal and chemical stability.

Examples include:

- Ceramic membranes.
- Silica-based membranes.
- Carbon molecular-sieve membranes.

Their wider deployment can be constrained by manufacturing complexity and mechanical considerations.

18. Nanomaterials

Nanostructured materials provide opportunities to manipulate:

- Surface chemistry.

- Diffusion pathways.
- Active sites.
- Pore structures.

Nanotechnology can therefore support the development of high-performance capture systems.

19. Biomass-Derived Carbon Materials

Waste biomass can be converted into porous carbon materials.

Potential feedstocks include:

- Agricultural residues.
- Forestry waste.
- Food-processing residues.
- Other biomass resources.

This creates a potential connection between:

Waste Valorisation + Carbon Capture + Circular Economy

20. Industrial Conditions

Laboratory testing often uses simplified gas streams.

Industrial gases may contain:

- Water vapour.
- Sulphur compounds.
- Nitrogen oxides.
- Oxygen.
- Particulates.
- Other contaminants.

A material that performs exceptionally well under dry laboratory conditions may perform poorly in an industrial environment.

21. Moisture Stability

Water can significantly influence CO_2 adsorption.

Depending on the material, moisture can:

- Compete for adsorption sites.
- Block pores.
- Modify surface chemistry.
- Improve or reduce CO_2 uptake.

Therefore, moisture tolerance must be considered during material design.

22. Regeneration Energy

After CO_2 is captured, the material must generally be regenerated.

This requires energy.

The objective is therefore not simply to maximise CO_2 adsorption.

A more useful metric is:

High Capture Performance + Low Regeneration Energy

23. Adsorption–Desorption Cycling

Industrial materials must withstand repeated capture and regeneration cycles.
A material may demonstrate excellent initial performance but degrade after repeated use.
Important parameters include:

- Capacity retention.
- Structural stability.
- Chemical stability.
- Mechanical stability.

24. Material Durability

Long operating lifetimes are essential for industrial economics.
Degradation can result from:

- Thermal stress.
- Chemical reactions.
- Moisture.
- Contaminants.
- Mechanical abrasion.

Durability should therefore be considered during early-stage material development rather than after discovery.

25. Artificial Intelligence for Materials Discovery

AI can accelerate carbon-capture materials research by identifying relationships between:

- Molecular structure.
- Pore characteristics.
- Surface chemistry.
- Adsorption behaviour.

Machine-learning models can screen large material databases before laboratory synthesis.

26. Computational Materials Discovery

A potential workflow is:

Material Database
↓
Molecular Simulation
↓
Machine Learning
↓
Candidate Screening

↓

Laboratory Validation

↓

Process Testing

This can reduce the number of materials requiring experimental investigation.

27. Molecular Simulation

Computational techniques can estimate:

- Adsorption energies.
- Molecular interactions.
- Diffusion.
- Pore accessibility.
- CO_2 selectivity.

These methods can provide insight into why particular materials capture CO_2 effectively.

28. Machine Learning-Based Prediction

AI models can predict material performance using descriptors such as:

- Surface area.
- Pore volume.
- Functional-group density.
- Heat of adsorption.
- Chemical composition.

Potential models include:

- Random forests.
- Gradient boosting.
- Neural networks.
- Graph neural networks.

29. Generative Materials Design

Generative AI may eventually assist in designing new materials rather than merely screening existing ones.

The workflow can become:

Desired Performance → AI-Generated Structures → Simulation → Experimental Validation

This represents a transition from:

Discovery → Prediction → Design

30. High-Throughput Materials Screening

Automated experimentation can test large numbers of candidate materials.
Combining robotics with AI can create:

Self-Driving Materials Laboratories

where computational predictions guide experiments and experimental results update predictive models.

31. Digital Twins for Carbon Capture

Digital twins can model the interaction between capture materials and industrial processes.
They can integrate:

- Material performance.
- Gas composition.
- Temperature.
- Pressure.
- Energy consumption.
- Regeneration behaviour.

This can help optimise capture operations.

32. Process Integration

A material cannot be evaluated independently of the capture process.
Material properties influence:

- Reactor design.
- Pressure requirements.
- Temperature requirements.
- Cycle time.
- Regeneration strategy.

Therefore:

Materials Engineering + Process Engineering

must be integrated.

33. Cement Industry

Cement production generates substantial CO_2 emissions through both fuel combustion and limestone calcination.
Carbon capture is particularly relevant because process emissions cannot be eliminated completely through renewable electricity alone.

Advanced capture materials may help reduce the energy penalty associated with cement-sector capture.

34. Steel Industry

Steel production can involve significant carbon emissions.

Potential applications for advanced capture materials include:

- Blast furnace gases.
- Direct reduction systems.
- Gas treatment.
- Hydrogen-related industrial processes.

35. Chemical Industry

Chemical plants generate diverse CO_2-containing streams.

Advanced materials could potentially be tailored to specific:

- Gas compositions.
- Pressures.
- Temperatures.
- CO_2 concentrations.

This highlights the importance of application-specific materials design.

36. Refining and Petrochemicals

Refineries and petrochemical facilities contain multiple gas streams suitable for carbon capture.

Material selection must consider contaminants and operating conditions.

37. Natural Gas Processing

CO_2 removal is already an important component of natural gas processing.

Advanced materials may improve:

- Selectivity.
- Energy efficiency.
- Processing throughput.

38. Carbon Capture and Utilisation

Captured CO_2 can potentially become a feedstock for:

- Synthetic fuels.
- Chemicals.
- Building materials.
- Carbonates.
- Algae and biological processes.

However, utilisation does not automatically guarantee permanent carbon removal; the complete carbon lifecycle must be considered.

39. Carbon Capture and Storage
Captured CO_2 can also be transported and stored in suitable geological formations.
The overall system therefore involves:

Capture → Compression → Transport → Storage
Capture materials influence the first stage and consequently affect the energy and cost of the complete system.

40. Lifecycle Assessment
Material performance should be evaluated over its entire lifecycle.
Important factors include:

- Raw-material extraction.
- Manufacturing energy.
- Material toxicity.
- Transport.
- Operational lifetime.
- Regeneration energy.
- End-of-life treatment.

A material with excellent adsorption capacity may not necessarily provide the lowest overall environmental impact.

41. Techno-Economic Analysis
Industrial deployment requires economic evaluation.
Important parameters include:

- Material cost.
- Capture capacity.
- Regeneration energy.
- Equipment cost.
- Replacement frequency.
- Operating cost.
- CO_2 captured per unit cost.

42. Proposed Innovation Framework
A comprehensive innovation pathway can be structured into seven stages:

Stage 1 — Molecular Design
Identify promising chemical structures.

Stage 2 — Computational Screening
Predict adsorption and selectivity.

Stage 3 — Laboratory Synthesis
Produce candidate materials.

Stage 4 — Realistic Gas Testing
Test under industrial conditions.

Stage 5 — Process Integration
Evaluate capture performance within a complete process.

Stage 6 — Pilot Demonstration
Validate performance at larger scale.

Stage 7 — Lifecycle and Economic Assessment
Determine environmental and commercial viability.

43. Integrated Materials Innovation Architecture

AI + Molecular Simulation
↓
Candidate Material Generation
↓
High-Throughput Screening
↓
Laboratory Validation
↓
Industrial Gas Testing
↓
Process Simulation
↓
Pilot Demonstration
↓
Lifecycle Assessment
↓
Commercial Deployment

44. Performance Metrics

Future studies should report multiple performance indicators rather than relying only on adsorption capacity.

Metric	Purpose
CO_2 capacity	Capture potential
Selectivity	Separation efficiency
Regeneration energy	Energy requirement
Kinetics	Capture speed
Cycle stability	Long-term performance
Moisture tolerance	Real-world suitability
Mechanical strength	Industrial durability
Material cost	Economic feasibility
Lifecycle impact	Environmental sustainability

45. Research Questions

1. Which advanced materials offer the best balance between CO_2 capacity and regeneration energy?
2. How can AI accelerate discovery of industrially viable capture materials?
3. How can materials be designed for humid and contaminated gas streams?
4. Can MOFs and COFs achieve economically competitive large-scale deployment?
5. How can membrane materials overcome the permeability–selectivity trade-off?
6. What role can biomass-derived materials play in low-cost carbon capture?
7. How can digital twins optimise material–process integration?
8. How should lifecycle impacts be incorporated into material discovery?
9. Which materials are best suited to specific industrial sectors?
10. How can advanced carbon capture materials be scaled from laboratory experiments to commercial systems?

46. Future Research Directions

Future research should emphasise:

- AI-guided materials discovery.
- Generative materials design.
- High-throughput experimentation.
- MOF and COF optimisation.
- Advanced amine-functionalised sorbents.
- Mixed-matrix membranes.
- Biomass-derived carbon materials.
- Low-temperature regeneration.

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- Moisture-resistant materials.
- Industrial contaminant tolerance.
- Digital-twin-enabled process optimisation.

47. Strategic Recommendations
Researchers and industry should:
1. Move beyond maximum adsorption capacity as the primary performance metric.
2. Test materials under realistic industrial conditions.
3. Integrate materials and process engineering from the beginning.
4. Use AI to accelerate candidate screening.
5. Develop scalable manufacturing methods.
6. Evaluate material durability over thousands of cycles.
7. Include lifecycle assessment during material development.
8. Prioritise low regeneration energy.
9. Develop sector-specific capture materials.
10. Establish standardised performance benchmarks.

48. Discussion
Advanced carbon capture materials represent an important pathway for reducing emissions from hard-to-abate industries.
However, the central challenge is not discovering a material with the highest theoretical CO_2 uptake.
The real challenge is developing a material that simultaneously provides:
High Selectivity + High Capacity + Low Regeneration Energy + Long-Term Stability + Low Cost + Scalability
This requires an interdisciplinary approach.
Materials scientists can design molecular structures.
Chemical engineers can optimise processes.
AI researchers can accelerate discovery.
Industrial organisations can provide realistic operating conditions.
Lifecycle researchers can evaluate environmental consequences.
Together, these disciplines can transform carbon capture from a laboratory materials challenge into an industrial decarbonisation technology.

49. Towards Application-Specific Carbon Capture Materials
A major future direction is moving away from the assumption that one material should serve every industrial application.
Different sectors have different:
- CO_2 concentrations.
- Temperatures.

- Pressures.
- Contaminants.
- Gas compositions.

Therefore, future materials may be designed specifically for:

Cement + Steel + Chemicals + Refining + Waste + Gas Processing
rather than attempting to create one universal sorbent.

50. Conclusion

Advanced carbon capture materials are becoming an increasingly important component of industrial decarbonisation strategies.

Emerging material platforms—including MOFs, COFs, porous polymers, zeolites, activated carbons, amine-functionalised sorbents and advanced membranes—provide opportunities to improve CO_2 separation while potentially reducing energy consumption and environmental impacts.

Artificial intelligence and computational materials science can significantly accelerate this development by enabling rapid screening, molecular-level prediction and generative design. However, laboratory-scale adsorption performance must be complemented by realistic testing, durability analysis, process integration, techno-economic assessment and lifecycle evaluation.

The future innovation pathway can therefore be represented as:

Molecular Engineering → AI Discovery → Experimental Validation → Process Integration → Industrial Demonstration → Sustainable Deployment

Ultimately, the most valuable carbon capture material will not necessarily be the material with the highest theoretical CO_2 capacity. It will be the material that can operate reliably, economically and sustainably under real industrial conditions.

Advanced carbon capture materials therefore have the potential to become a critical technological bridge between existing industrial infrastructure and a lower-carbon industrial economy.

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