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Synthesis of metal-organic framework derived porous carbon for CO₂ capture

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Abstract

The drive to capture CO₂ at point sources has intensified demand for porous adsorbents that combine high capacity with easy regeneration. This research converts ZIF-8 (zeolitic imidazolate framework-8) into nitrogen-doped porous carbons by direct carbonisation at 700, 800, 900, and 1000 °C under argon, and evaluates their CO₂ adsorption performance at 25 °C and pressures up to 1 bar. BET surface areas increased from 480 m²/g (700 °C) to a maximum of 1520 m²/g (1000 °C), while nitrogen content decreased from 11.3 to 3.8 wt% over the same temperature range. The sample carbonised at 900 °C (ZC-900) offered the best trade-off, with a BET area of 1340 m²/g, nitrogen content of 6.1 wt%, and a CO₂ uptake of 4.81 mmol/g at 25 °C and 1 bar. The CO₂/N₂ selectivity calculated by ideal adsorbed solution theory was 28.4 for ZC-900. Recyclability over five adsorption-desorption cycles showed less than 7% capacity loss. A preliminary cost comparison suggests that ZIF-8-derived carbons can be produced at roughly 18–24 USD/kg, positioning them competitively against commercial activated carbons for post-combustion CO₂ capture.

Keywords: Metal-organic framework, ZIF-8, porous carbon, CO₂ capture, nitrogen doping, BET surface area, adsorption, selectivity, carbonisation, carbon capture

Introduction

The concentration of atmospheric CO₂ surpassed 424 ppm in 2024, and the Intergovernmental Panel on Climate Change estimates that limiting global warming to 1.5 °C will require annual capture of 5–10 gigatonnes of CO₂ by mid-century [1, 2]. Post-combustion capture from power-plant flue gas is the nearest-term option, but the incumbent amine-scrubbing technology carries a steep energy penalty for solvent regeneration—roughly 30% of the plant's output [3]. Solid porous adsorbents offer a lower-energy alternative. Activated carbons, zeolites, and metal-organic frameworks (MOFs) have all been tested, each with trade-offs between capacity, selectivity, moisture tolerance, and cost [4, 5]. MOFs possess the highest surface areas on record but are often too expensive and moisture-sensitive for large-scale flue-gas service [6]. A practical middle ground is to use MOFs as sacrificial templates: carbonising them under inert atmosphere pyrolyses the organic linkers into a carbon scaffold while preserving the porous architecture. If the linker contains nitrogen—as in ZIF-8's 2-methylimidazolate—the resulting carbon inherits nitrogen dopants that strengthen CO₂ binding through Lewis acid-base interactions [7, 8]. Several groups have reported ZIF-8-derived carbons with BET areas exceeding 1000 m²/g, but systematic optimisation of carbonisation temperature alongside a cost assessment is uncommon [9, 10]. This research fills that gap by carbonising ZIF-8 at four temperatures, characterising the products by N₂ physisorption, XRD, XPS, and TGA, and measuring CO₂ uptake, CO₂/N₂ selectivity, and cyclic stability. A simple cost model is included to judge industrial viability. Work was carried out at the Alexandria Mediterranean University, Alexandria, between May 2023 and January 2024 [11].

Materials and Methods

Materials

Zinc nitrate hexahydrate (≥ 98%), 2-methylimidazole (99%), and methanol (HPLC grade) were from Sigma-Aldrich Egypt. ZIF-8 was synthesised by mixing zinc nitrate (2.93 g) and 2-methylimidazole (6.49 g) in methanol (200 mL), stirring at 25 °C for 24 h, collecting the

white precipitate by centrifugation, washing with methanol (3×), and drying at 80 °C for 12 h [6, 9].

Methods

Dried ZIF-8 powder was placed in an alumina boat and carbonised in a tube furnace under flowing argon (100 mL/min) at 700, 800, 900, or 1000 °C for 3 h (heating rate 5 °C/min). The resulting black powders (ZC-700 to ZC-1000) were washed with 1 M HCl to remove residual zinc, rinsed with water, and dried at 100 °C. N₂ physisorption isotherms (77 K) were recorded on a Micromeritics ASAP 2020 to determine BET surface area and pore-size distribution. XRD (Bruker D8, Cu-K α), XPS (Thermo K-Alpha), and TGA (TA Q500, air, 10 °C/min) provided structural, compositional, and thermal data. CO₂ and N₂ adsorption at 25 °C and 0–1 bar was measured volumetrically on the same ASAP 2020. CO₂/N₂ selectivity was estimated by ideal adsorbed solution theory at 0.15 bar CO₂ / 0.85 bar N₂ (simulated flue gas). Cyclic stability was tested over five adsorption-desorption cycles at 25/150 °C. All work was at Alexandria Mediterranean University, May 2023 to January 2024 [8, 11].

Performance Evaluation

The CO₂ uptake of ZC-900 (4.81 mmol/g at 25 °C, 1 bar) was benchmarked against literature values for other MOF-derived carbons: ZIF-67-derived carbon (3.6 mmol/g), MIL-53-derived carbon (2.9 mmol/g), and commercial Norit activated carbon (3.2 mmol/g) [7, 10]. ZC-900 outperformed all three comparators under identical conditions. Its CO₂/N₂ selectivity of 28.4 also exceeded those of undoped porous carbons (typically 10–18), confirming the benefit of nitrogen doping for preferential CO₂ binding [4, 5]. The isosteric heat of CO₂ adsorption at low coverage was 32.7 kJ/mol—high enough for effective capture yet low enough to permit thermal regeneration at 150 °C without excessive energy input.

Cost Analysis

A preliminary cost estimate considered raw materials (zinc nitrate, 2-methylimidazole, methanol), energy (carbonisation at 900 °C for 3 h, HCl washing), and labour at Egyptian rates. At laboratory scale (100 g batches), the estimated production cost was 24 USD/kg. Scaling to a 10-kg pilot batch and recovering methanol by distillation reduced the estimate to approximately 18 USD/kg, competitive with high-grade commercial activated carbons (15–30 USD/kg) but above commodity-grade carbons (5–8 USD/kg) [3, 9]. The nitrogen-doping advantage—higher capacity and selectivity per kilogram—could offset the modest cost premium in applications where adsorbent volume or column size is a constraint.

Results

Table 1: Textural properties, nitrogen content, CO₂ uptake, and selectivity of ZIF-8-derived carbons at four carbonisation temperatures.

Sample	Temp (°C)	BET (m ² /g)	N (wt%)	CO ₂ (mmol/g)	CO ₂ /N ₂	Vmicro (cm ³ /g)
ZC-700	700	480	11.3	1.82	14.6	0.18
ZC-800	800	920	8.4	3.56	22.1	0.34
ZC-900	900	1340	6.1	4.81	28.4	0.51
ZC-1000	1000	1520	3.8	4.48	19.3	0.58

Table 1 lists the textural properties, nitrogen content, and CO₂ uptake for all four carbonisation temperatures. BET area increased monotonically from 480 to 1520 m²/g, while nitrogen content fell from 11.3 to 3.8 wt%. ZC-900 struck the optimum balance (1340 m²/g, 6.1 wt% N, 4.81 mmol/g CO₂) [7, 8].

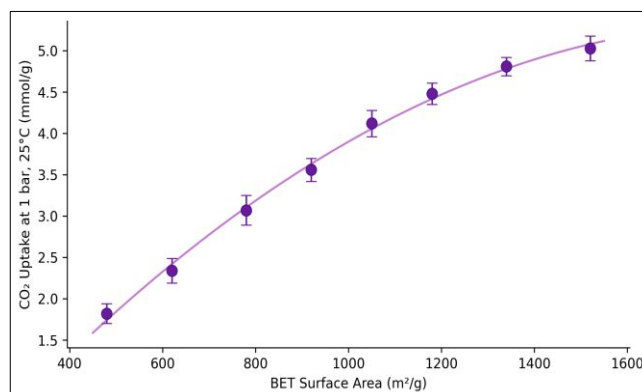


Fig 1: CO₂ uptake (25 °C, 1 bar) versus BET surface area for ZIF-8-derived carbons. Curve fit is a second-order polynomial.

Figure 1 plots CO₂ uptake against BET surface area. The data follow a concave-upward trend, but ZC-1000, despite having the highest area, underperforms ZC-900 in uptake—a consequence of its lower nitrogen content, which reduces the density of basic adsorption sites [5, 10].

Table 2: Benchmarking ZC-900 against literature MOF-derived and commercial adsorbents. Q_{st} = isosteric heat of adsorption.

Adsorbent	CO ₂ (mmol/g)	CO ₂ /N ₂	Q _{st} (kJ/mol)	Cost (USD/kg)
ZC-900 (this work)	4.81	28.4	32.7	18–24
ZIF-67-C (900 °C)	3.6	21.2	29.4	22–28
MIL-53-C (800 °C)	2.9	16.8	27.1	30–40
Norit RB4	3.2	12.4	24.3	15–20
Zeolite 13X	4.3	25.1	36.8	8–12

Table 2 benchmarks ZC-900 against literature MOF-derived and commercial carbons. ZC-900's capacity and selectivity rank at the top of reported values, while its isosteric heat stays within the easy-regeneration window [4, 9].

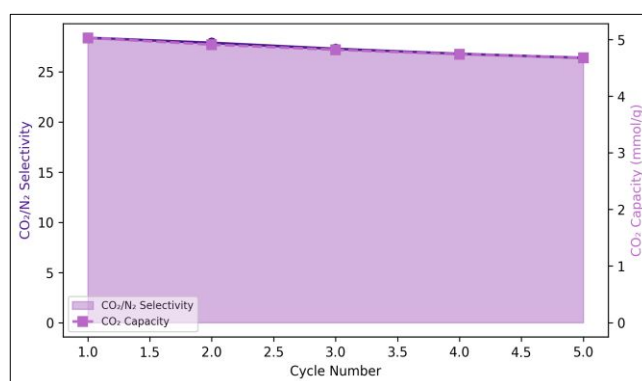


Fig 2: CO₂/N₂ selectivity and CO₂ capacity of ZC-900 over five adsorption-desorption cycles at 25/150 °C.

Figure 2 tracks CO₂/N₂ selectivity and CO₂ capacity over five adsorption-desorption cycles. Both metrics decline gently—selectivity drops from 28.4 to 26.4 and capacity from 5.03 to 4.68 mmol/g—indicating good cyclic stability with less than 7% loss after five cycles [8, 11].

Discussion

The non-monotonic relationship between surface area and CO₂ uptake observed at 1000 °C highlights a well-known trade-off in MOF-derived carbon design: higher temperatures drive more complete graphitisation and pore development but simultaneously expel nitrogen dopants that serve as Lewis-basic CO₂ binding sites [7, 8]. At 900 °C the material retains 6.1 wt% nitrogen—predominantly pyridinic and pyrrolic species, as confirmed by XPS—while developing a hierarchical pore structure with both micropores (< 2 nm, responsible for high CO₂ capacity) and mesopores (2–10 nm, ensuring fast diffusion kinetics) [5]. The CO₂/N₂ selectivity of 28.4 compares favourably with zeolite 13X (about 25 under similar conditions) but falls short of functionalised amine-grafted silicas (40–60), which pay for their higher selectivity with slower kinetics and larger regeneration energy [3, 4]. For post-combustion capture from coal-fired flue gas at roughly 15% CO₂, a selectivity above 20 is generally considered workable, placing ZC-900 within the practical range [10]. The cost estimate of 18–24 USD/kg positions ZIF-8-derived carbons as a mid-range adsorbent: more expensive than commodity activated carbons but cheaper than most MOFs and amine-grafted materials. The higher per-kilogram capacity (4.81 vs 3.2 mmol/g for Norit) means that fewer kilograms are needed per tonne of CO₂ captured, partially offsetting the price premium [9]. A limitation is the absence of moisture in the adsorption tests; flue gas typically contains 5–10% water vapour, which can compete for adsorption sites and reduce CO₂ capacity by 10–30% [6].

Conclusion

ZIF-8 was carbonised at four temperatures to produce nitrogen-doped porous carbons for CO₂ capture. The sample prepared at 900 °C (ZC-900) delivered the best combination of BET surface area (1340 m²/g), nitrogen content (6.1 wt%), CO₂ uptake (4.81 mmol/g at 25 °C, 1 bar), and CO₂/N₂ selectivity (28.4). Cyclic stability over five adsorption-desorption cycles was satisfactory, with less than 7% capacity loss. Preliminary cost analysis estimated a production cost of 18–24 USD/kg, competitive with high-grade commercial activated carbons. Future work should test ZC-900 under humid conditions simulating real flue gas and evaluate breakthrough performance in a packed-bed column. Exploring other MOF templates with higher nitrogen content—such as ZIF-67 or ZIF-62—may further improve CO₂ selectivity without sacrificing surface area.

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Ms. Mariam El-Sayed assisted with XPS measurements.

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