

Single-step dry synthesis of biomass-derived porous carbon for sustainable CO₂ capture: Experimental and simulation study

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ABSTRACT

The utilization of bio-based affordable adsorbents is crucial for developing sustainable solutions for CO₂ capture. In this work, an in-situ nitrogen-doped low-temperature CO₂ adsorbent is synthesized via single-step dry pyrolysis of biomass (cow dung) and melamine mixtures (1:0, 1:1, 1:2) using KHCO₃ as a green activating agent. The developed nitrogen-doped activated porous carbon (NDPC) is investigated using FE-SEM, XRD, BET, XPS and Raman spectroscopy. The optimized sample (NDPC-1) produced at a 1:1 ratio of cow dung to melamine, exhibits a nitrogen content of 2.95% and a high surface area (1153 m²/g) with the finely tuned micro- and mesoporous structure. These features result in an excellent CO₂ adsorption capacity of 3.7 mol/kg at 1.013 bar and 303 K over 10 cycles. It shows 28% higher sorption capacity than pristine carbon without N-doping (CDAC) and 58% higher than pyrolyzed CD (CDC). The adsorption kinetics is studied using various adsorption models, and the Avrami model best fits the adsorption isotherm with a rate constant of 0.125 min⁻¹. Furthermore, atomistic simulations (ReaxFF-MD) of CDAC and NDPC-1 frameworks were performed, using a force field parameterized for C/H/O/N chemistry. The simulation isotherms for CO₂ adsorption computed using grand-canonical Monte Carlo (GCMC) show strong agreement with experimental data. Overall, the cow dung-derived N-doped porous activated carbon shows significant CO₂ capture capacity over multiple cycles at 303 K. Results highlights its potential to be used as scalable materials for CO₂ capture at low temperature.

1. Introduction

The substantial increase in anthropogenic CO₂ concentration (~428 ppm) leads to global warming and climate change [1]. The Carbon capture, utilization and storage (CCUS) technology is one of the key approach to control CO₂ concentration in the atmosphere [2]. The CO₂ concentration in flue gas varies depending on the fuel type and industrial process. For instance, coal combustion results in 12–15 mol % CO₂, while natural gas combustion produces 3–4 mol % CO₂. In industrial plants, CO₂ levels also depend on the specific process, such as oil refining (8–9 mol % CO₂), cement production (14–33 mol % CO₂), and iron and steel manufacturing (20–44 mol %) [3] and the flue gas temperature is comparatively high (less than 200 °C) [4].

The CO₂ capture is generally accomplished through aqueous amine solutions absorption [5], membrane separation [6], and adsorption [7]. In absorption, mainly liquid amine absorption remains the primary technology used in industry. However, it faces several challenges, including high energy consumption, equipment corrosion, solvent

degradation, and the generation of potentially hazardous waste [8]. Membrane separation technology faces challenges, including high development costs and underdeveloped process technology [9]. To address these challenges, solid adsorbents gain significant attention for selectively CO₂ adsorption under high and intermediate temperatures (400–700 °C) [10,11] and ambient conditions (25 °C, 1 bar) [12]. However, high temperature CO₂ capture requires energy. In contrast, low temperature CO₂ capture includes solid adsorbents such as zeolite [13], metal-organic frameworks (MOFs) [14], porous organic polymers (POPs) [15] and carbon nanotubes (CNTs), and the adsorption capacity spans 0.4–2.97 mol/kg [16]. These are expensive and involve several complex preparation processes compared to waste biomass-derived porous carbon materials.

Porous carbons with hierarchical pore structures and heteroatom doping are regarded as ideal adsorbents for CO₂. The typical synthesis process for porous using palm kernel, ion-exchange resin, sucrose, pomelo peel and lotus stalks carbon involves pre-carbonization and activation using highly corrosive and toxic agents like KOH and ZnCl₂,

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which present significant handling and disposal challenges [17–20]. After pyrolysis, the resulting carbon materials are usually washed with dilute HCl to remove residual inorganic minerals and activating agents. Thus, the after-pyrolysis washing step also generates wastewater and requires careful management to prevent secondary pollutants that cause environmental risks and further complicate large-scale applications and sustainability [21,22]. Additionally, some of these processes are very costly and not easily scalable.

Therefore, a growing interest is in developing low-cost, sustainable, and scalable porous carbons derived from abundant biomass sources such as cow dung. Porous carbon utilizes its extensive pore structure for CO₂ adsorption, primarily by the physical adsorption process influenced by CO₂ concentration and temperature. However, pore structure alone is insufficient, limits its high-performance capture and typically adsorbs CO₂ only 1.5–2.5 mol/kg at 25 °C [23]. This disadvantage is sometimes reduced by incorporating heteroatoms into the carbon matrix [24,25]. In fact, functionalization of heteroatom such as nitrogen shows higher CO₂ capture capacity (~ 2.5–6 mol/kg at 25 °C [26]) due to the Lewis acid-base interaction [27,28] and enhanced hydrogen-bonding interactions along with electrostatic forces [29]. Most reported syntheses of N-doped porous carbon use multiple activation steps followed by N-doping, typically employing KOH and ZnCl₂ as an activating agents [30,31]. Also, some of this synthesis process involves wet process which requires acid wash after pyrolysis.

To overcome these limitations, there is need for single step dry process synthesis route to develop efficient low temperature CO₂ capture materials using green activating agents. Several studies have explored greener activation strategies that employ mild salts, such as KHCO₃, or molten eutectic systems [32,33]. For example, Li et al. demonstrated that KHCO₃ activation of biomass precursors can generate hierarchical pore networks through in-situ release of CO₂ and H₂O gases during pyrolysis [34]. More recently, Wang et al. employed a NaCl/Na₂CO₃ binary molten-salt system to prepare rice-husk-derived porous carbon, demonstrating simultaneous carbonization, activation, and silica removal within a single pyrolysis step highlighting the potential of salt-mediated activation for sustainable CO₂ adsorbents [35]. Similarly, Li et al. [36] and Zhao et al. [37] demonstrated that KHCO₃ and other mild alkaline salts can act as efficient in-situ pore formers, promoting micropore generation and surface basicity while avoiding corrosive waste.

In addition to experimental progress, computational modeling has emerged as a powerful tool to unravel the atomistic mechanisms governing CO₂ adsorption in heteroatom-doped porous carbons. Recent studies have provided valuable insights into how nitrogen functionalities and pore topology influence adsorption behaviour. For instance, Morales-Ospino et al. demonstrated through molecular simulations that nitrogen doping enhances CO₂ binding via Lewis base interactions, though overall performance remains strongly dependent on pore connectivity [38]. Khosrowshahi et al. combined experiments with molecular dynamics to correlate nitrogen configuration (pyridinic vs. graphitic) with adsorption trends in biomass-derived carbons [39]. However, most of these computational efforts employ static or non-reactive models and thus fail to capture the dynamic structural evolution that occurs during carbonization and repeated adsorption-desorption cycles [38]. In this context, the present study employs reactive force-field molecular dynamics (ReaxFF-MD) [40] in conjunction with experimental validation to provide a deeper mechanistic understanding of how nitrogen configuration, defect formation, and hierarchical pore evolution collectively dictate CO₂ adsorption thermodynamics and kinetics. This integrative approach bridges experimental observation and atomistic simulation, offering a holistic view of the structure-property relationships essential for designing next-generation sustainable sorbents. To address the sustainability and mechanistic gaps, the present study develops cow dung-derived high-surface-area, nitrogen-doped porous carbon for efficient low-temperature CO₂ capture. The above discussion highlights the need

for precursors that are both environmentally benign and naturally suited to interact with mild activating salts to form hierarchical pores.

With high availability and rich organic content, cow dung is a low-cost, sustainable feedstock for nitrogen-doped porous carbons. Particularly in India, which has ~110 million cows producing 9–15 kg of dung per day each [41]. Presently, cow dung is widely used for cooking fuel, biogas production, and rural construction. Its versatility spans traditional practices such as agriculture, energy, and advanced materials [42, 43]. In fact, cow dung has been linked to energy production through biogas plants, addressing environmental concerns and reducing reliance on non-renewable resources [44]. Moreover, the recent research programs like Scientific Utilization through Research Augmentation-Prime Products from Indigenous Cows (SUTRA-PIC India) are also working to explore its components for sustainable products like personal care items [45]. Thus, the diverse applications highlight the role of cow dung in India's sustainable development and cultural heritage. However, to the best of our knowledge, there has been no reported work on converting cow dung into in-situ nitrogen-doped activated porous carbon (NDPC) materials for low-temperature CO₂ capture, representing a significant opportunity to integrate circular economy strategies for environmental and resource sustainability.

The present work develops cow dung-derived high surface area, nitrogen-doped porous carbon for efficient low-temperature CO₂ capture. It is synthesized via single-step dry method using KHCO₃/KCl as an eco-friendly activating agent and melamine as the nitrogen source, eliminating the need for separate activation steps. This sustainable, scalable approach effectively integrates waste valorization and green chemistry to meet the urgent need for sustainable solution for carbon capture. The synthesized N-doped porous carbon (NDPC) was thoroughly characterized using various techniques, including Field Emission Scanning Electron Microscopy (FE-SEM), Brunauer-Emmett-Teller (BET) surface area analysis, X-ray Photoelectron Spectroscopy (XPS), Raman spectroscopy, and Thermogravimetric Analysis (TGA). Experimental and characterization results reveal that nitrogen doping significantly enhances CO₂ adsorption affinity and capacity. To understand the insight of adsorption mechanism, various adsorption models are also fitted with the experimental results. Further atomistic insights into the interactions among carbon atoms and nitrogen functionalities during carbonization were obtained from reactive force-field molecular dynamics (ReaxFF-MD) simulations performed on liquid quench-generated amorphous carbon models (0.6 g/cm³ density). The Structural insights obtained via Voronoi decomposition and ring statistics analysis through the Interactive Structure Analysis of Amorphous and Crystalline Systems (ISAACS) framework revealed defect-rich morphologies and micropore-dominant architectures. The CO₂ capture performance of amorphous carbon models developed from MD simulations was also validated using experimental adsorption data. Overall, these findings demonstrate a green and scalable route to produce high-performance N-doped porous carbons for CO₂ capture and CCUS, thereby promoting sustainable biomass waste valorization for climate change mitigation.

2. Materials and methods

2.1. Materials

Dry cow dung was collected from a village near IIT Gandhinagar, Gujarat, India. The reagents used to prepared Nitrogen-doped porous carbon are all analytical pure. Potassium bicarbonate, potassium chloride and melamine are purchased from TCI chemicals. Ultra-high purity grade (UHP > 99 %) nitrogen gas used during pyrolysis.

2.2. Preparation of nitrogen-doped porous carbon

Firstly, cow dung was washed with deionized (DI) water and ethanol to remove contaminants and then dried in an oven before use. For the synthesis of nitrogen-doped porous carbon (NDPC), 3 g of the dried cow

dung were mixed with potassium bicarbonate (KHCO_3), potassium chloride (KCl), and melamine (3 g or 6 g, depending on the intended nitrogen content). The mixture was ground thoroughly for 30 min to ensure uniform mixing, transferred to a porcelain boat, and pyrolyzed in a tube furnace at 800°C for 1 h under a nitrogen flow of 50 mL min^{-1} . After cooling, the resulting carbon material was repeatedly washed with DI water to remove residual salts and impurities, followed by oven drying. The obtained samples were denoted as NDPC-X, where X corresponds to the mass ratio of cow dung to melamine. The material produced without melamine was labeled cow dung derived activated carbon (CDAC), while direct carbonization of cow dung at 800°C without any additives yielded the pristine sample referred to as CDC. To optimize the activation conditions, 3 g of washed and dried cow dung were combined with two different salt loadings: 9 g KHCO_3 + 9 g KCl (denoted CADC-0) and 12 g KHCO_3 + 12 g KCl (denoted CDAC). Among these, the 12 g KHCO_3 + 12 g KCl formulation exhibited the highest BET surface area and was selected as the optimal activation system. Subsequently, 3 g and 6 g of melamine were added to this optimized mixture (CDAC) to develop NDPC-1 and NDPC-2 respectively (Scheme 1).

2.3. Characterization

The morphology of N-doped porous carbon was observed by field emission scanning electron microscope (FE-SEM, JEOL JSM-7900F, Japan) operated at an accelerating voltage of 5–10 kV. The pore-size distribution and BET surface area of the synthesized porous carbon were calculated using a BET surface area analyzer based on N_2 adsorption-desorption isotherms at -77 K (Quantachrome, NOVA 2000, United States). Before measurement, the samples were degassed at 150°C for 6 h. The chemical states of the elements in the sample were analyzed using X-ray photoelectron spectroscopy (XPS, Thermo Scientific K-Alpha and ESCALAB QXi instruments, USA) equipped with a monochromatic Al $\text{K}\alpha$ X-ray source (photon energy = 1486.7 eV) operated at 15 kV and 10 mA. Survey spectra were recorded with a pass energy of 50 eV, while high-resolution spectra were acquired with a pass energy of 20 eV. Data processing and peak deconvolution were performed using OriginPro (OriginLab, USA) with a Shirley background and Gaussian-Lorentzian peak fitting under consistent full-width-at-half-maximum (FWHM) constraints. Raman spectroscopy of N-doped porous carbon was carried out using a Raman RXN1 system (Kaiser Optical Systems, USA). The Raman probe was equipped with a 450 mW diode laser operating at an excitation wavelength of 785 nm to record the Raman spectra of the carbon samples. The elemental contents were detected by an elemental analyzer (Elementar Analysensysteme GmbH). The thermal stability of the materials was tested using a simultaneous

thermal analyzer (STA 449 F3 Jupiter, Netzsch Germany) under nitrogen flow (50 mL min^{-1}) with a heating rate of $10^\circ\text{C min}^{-1}$.

2.4. CO_2 adsorption experiment

The CO_2 adsorption properties of materials are measured by using simultaneous thermal analyzer (STA 449 F3 Jupiter, Germany). The experimental procedure is as follows - 5 mg of material was added in alumina crucible and first degassed at 200°C in N_2 atmosphere (50 mL/min , 5°C/min) for 1 hour to remove moisture and impurities in the sample. The temperature was then reduced to the desired adsorption temperature and held constant for 20 min. Finally the N_2 gas was shifted by CO_2 , and maintained constant temperature (30°C) for 1 h. The adsorption capacity (mol/kg) and kinetic of CO_2 at the corresponding temperature were obtained by changing the mass. The desorption experiment was carried out by heating the materials after the completion of adsorption by shifting CO_2 with N_2 . The cyclic adsorption-desorption behavior of the materials was evaluated by continuously repeating the adsorption-desorption cycles.

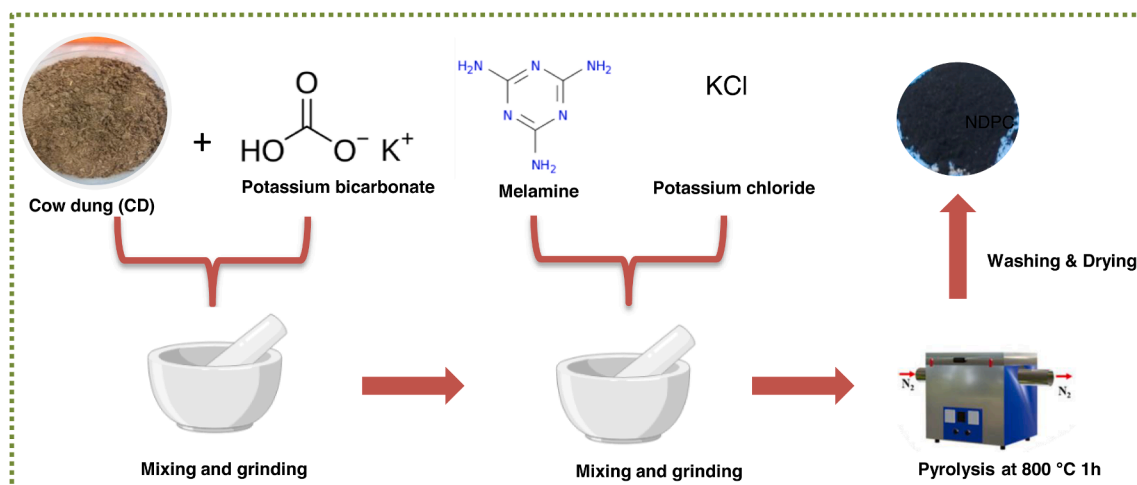
2.5. Adsorption kinetics study

To investigate the CO_2 adsorption kinetics of the synthesized NDPC, three different kinetic models shown in Table-1 were applied: pseudo-first-order, pseudo-second-order, and Avrami models. The pseudo-first-order model is typically used to describe gas-solid adsorption processes dominated by surface diffusion and is well-suited for predicting CO_2 adsorption behavior in physical adsorbents. On the other hand, the pseudo-second-order model assumes that the adsorption process at the

Table-1
Adsorption kinetic models.

Kinetic model	Equation	Differential form	Reference
Pseudo-first order	$q_t = q_e[1 - \exp(-k_1 t)]$	$\frac{dq_t}{dt} = k_1 (q_e - q_t)$	[46]
Pseudo-second order	$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$	$\frac{dq_t}{dt} = k_2 (q_e - q_t)^2$	[46]
Avrami's fractional-order	$q_t = q_e[1 - \exp(-k_A t^{n_A})]$	$\frac{dq_t}{dt} = k^n t^{n-1} (q_e - q_t)$	[47]

Where q_e and q_t : amount of CO_2 adsorbed (mol/kg) at equilibrium and time t . k_1 [=] min^{-1} ; k_2 [=] $\text{kg (mol}^{-1} \cdot \text{min}^{-1})$ and k_A [=] min^{-1} : The adsorption rate constants corresponding to the pseudo-first-order, pseudo-second-order, and Avrami kinetic models, respectively.
 n_A : Avrami fractional exponent.



Scheme 1. Schematic illustration for synthesis of NDPC.

gas–solid interface is governed by chemical reactions, making it more appropriate for systems where chemical interactions play a significant role in CO₂ adsorption [46]. Avrami's fractional kinetic model considers various adsorption mechanisms, such as surface diffusion, intraparticle diffusion, and both physical and chemical interactions between CO₂ molecules and active sites. The Avrami index (*n*) is linked to the nucleation process and the nature of the adsorption growth mechanism [47]. The all the kinetics models are expressed in Table-1.

The validity of adsorption isotherms is confirmed by two key metrics: the correlation coefficient (*R*²) and the normalized standard deviation (ΔQ). The ΔQ is calculated using the following equation (Eq-1):[48]

$$\Delta Q(\%) = \sqrt{\frac{\sum_{i=1}^n (Q_{exp} - Q_{cal}/Q_{exp})^2}{n}} \times 100 \quad (\text{Eq.-1})$$

Here, *Q*_{exp} is the amount of adsorption measured in experiments, *Q*_{cal} is the amount predicted by the model, and *n* is the number of data points.

2.6. Simulation methodology:

The liquid quench method has been successfully used to generate realistic models of amorphous carbon across a wide density range (0.5–3.2 g/cm³), accurately capturing key structural features such as pore size distribution and carbon hybridization. The choice of the liquid quench method is due to its widespread use in modelling amorphous carbon with varying densities [49–51] and its excellent agreement with reproducing structural and functional features reported experimentally. This approach enables systematic tuning of simulation parameters and produces models in good agreement with experimental and other computational studies, making it a robust method for investigating disordered carbon materials [50,51]. First, we have modelled the final product after the pyrolysis of cow dung (CDAC), which is devoid of volatile content, and hence an amorphous carbon is a good surrogate model for this purpose. Atomistic models for amorphous carbon-based frameworks CDAC and NDPC-1 were constructed using reactive molecular dynamics (ReaxFF-MD) with the ReaxFF force field parametrized for C/H/O/N chemistry [52], which was specifically developed to model nitrogen incorporation and carbonization processes in polymers such as polyacrylonitrile (PAN) and polybenzoxazole (PBO). The initial pristine amorphous carbon structures were generated by the liquid quench method [49,50] by placing a desired number of carbon atoms randomly in a simulation box at a target density of 0.6 g/cm³. The system was equilibrated at 3000 K for 500 ps under the NVT ensemble using a Langevin thermostat (damping constant: 25 fs, time step: 0.2 fs), followed by cooling to 300 K with a cooling rate of 5K/ps under the NVT ensemble and subsequent equilibration for 1 ns under the NPT ensemble (1 bar, Langevin thermostat) to stabilize the density. Hydrogen, oxygen, and nitrogen atoms were introduced at stoichiometric ratios matching the experimental compositions (Supplementary Table S2). For NDPC-1, the chosen composition facilitated pyridinic nitrogen site formation via ring-opening mechanisms, while CDAC underwent identical thermal treatment to ensure structural consistency. All molecular dynamics simulations were performed using the LAMMPS [51] package with the ReaxFF force field. Structural visualization using the OVITO software [11] confirmed dopant integration and bond stability (Fig. 10a, b). Ring statistics were quantified using the ISAACS (Interactive Structure Analysis of Amorphous and Crystalline Systems) code [53], and pore architectures were analyzed via Voronoi decomposition built in the Zeo++ code [54] (using a probe radius of 1.2 Å). These structural characterizations provide valuable information on the nanoscale structures of the amorphous carbon models. CO₂ adsorption isotherms were computed using grand-canonical Monte Carlo (GCMC) simulations in RASPA2 code [55] at 300 K over a pressure range of 0 to 1 bar in intervals of 0.1 bar. The TraPPE force field [56,57] was used to model interactions within CO₂ molecules, while the framework interactions were described using the DREIDING [58] potential. Cross-interactions

between CO₂ and the framework were handled using Lorentz–Berthelot mixing rules. The force fields DREIDING and TraPPE have been validated for gas adsorption in frameworks as cited in literature [59,60]. The calculation of isotherm at each pressure included 50,000 Monte Carlo steps under periodic boundary conditions. This comprehensive simulation methodology enabled a direct comparison of the role of nitrogen in adsorbate–framework interactions between the undoped (CDAC) and nitrogen-doped (NDPC-1) models.

3. Result and discussion

3.1. Morphological analysis

Field-emission scanning electron microscopy (FE-SEM) is used to observe the surface morphology of samples. The images of pristine carbon, activated carbon and N-doped porous carbon are shown in Fig. 1. The modified carbon samples exhibit lower density and increased porosity, consistent with the BET surface area analysis. Also, SEM images show the pores developed after the activation compared to the pristine carbon, and the surface morphology of N-doped porous carbon shows the formation of flakes. The formation of a porous structure is attributed to the pyrolysis of melamine at high temperatures, releasing organic volatiles that create additional voids within the material, enhancing its porosity [61]. CDAC as shown in Fig. 1 (b) without N-doping possess a dense three-dimensional porous framework with uneven pores. Additionally, as shown in Table 2, the surface area of NDPC-1 is 1153 m²/g more than the NDPC synthesis by Adio et al. using sugarcane bagasse, KOH and melamine, which is 1000 m²/g [30]. As the ratio of CD/melamine is increased from 1 to 2, the surface area reduces from 1153 m²/g to 390 m²/g, which is approximately 3 times lower than the NDPC-1. It can be inferred that excessive melamine may lead to pore collapse [62]. A layer-like structure was clearly observed in the melamine-modified samples, indicating successful polymerization of melamine. The nitrogen content, quantified by CHNSO analysis (Table S1), increased progressively with higher melamine incorporation into the pristine carbon framework, as shown in Table 2.

3.2. Pore textural characteristics

The pore characteristics and surface area of the materials are compared using N₂ adsorption and desorption isotherms. As shown in Fig. 2, all the isotherms observed mainly present type IV isotherms, indicating that the pore structures in the materials are mixtures of micropores and mesopores [17,63,64]. A monolayer-multilayer with capillary condensation is considered in this type of adsorption isotherm. Also, the slope typically shows an increased adsorbate uptake as the pores are filled at higher pressures, with an inflection point occurring near the completion of the first monolayer. The entire samples exhibit an H3-type hysteresis loop in their adsorption–desorption isotherms, indicating the presence of mesoporous structures. This loop is attributed to the difference between pore filling and emptying during capillary condensation. The textural properties, including BET surface area, total pore volume, average pore diameter, and micropore volume, are summarized in Table 2, among them; NDPC-1 shows the highest BET surface area. All the modified materials exhibit higher BET surface areas than the unmodified cow dung-derived carbon (CDC). Notably, incorporating melamine at a lower ratio (1:1) followed by thermal treatment significantly enhances the surface area of the sorbents. However, a further increase in melamine content leads to a reduction in surface area, likely due to excessive surface coverage by melamine at higher loadings. This suggests that an optimal melamine-to-biomass ratio of 1:1 provides the most favorable textural properties. The pore size distribution curves, presented in Fig. 3, show that all samples predominantly possess pores with diameters around 3 nm. The comparison of pore size distribution in Fig. 3 indicates that NDPC-1 has the highest pore volume in the mesoporous range, followed by NDPC-2 and CDAC, while CDC has the lowest

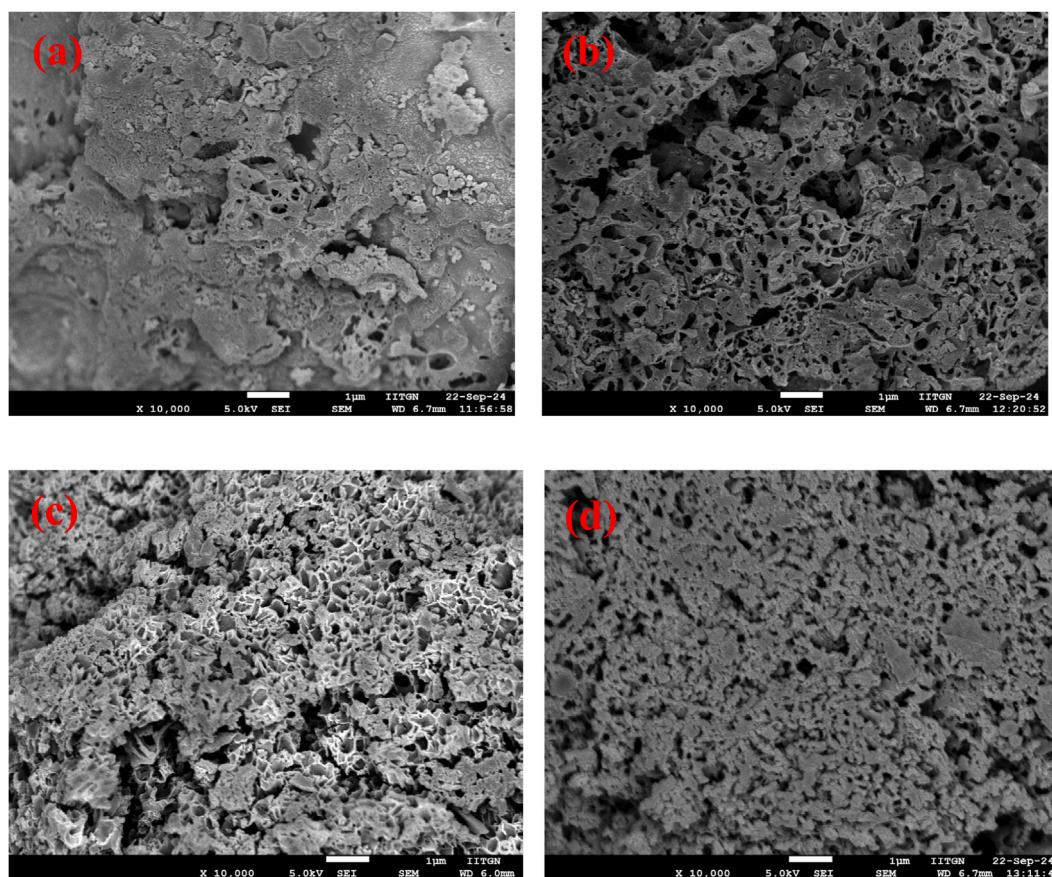


Fig. 1. SEM images of materials: (a) CDC, (b) CDAC, (c) NDPC-1, and (d) NDPC-2. The micrographs reveal distinct surface morphologies and pore structures for each sample, highlighting variations in porosity and texture.

Table 2

The specific pore structure parameters of samples.

Sample	BET Surface Area (m ² /g)	Total pore volume (cm ³ /g)	Average pore diameter (nm)	N- content by Elemental analysis	V _{micro} (cm ³ /g)
CDC	165	0.14	3.35	1.60	0.053
CDAC	983	0.73	2.97	0.61	0.389
NDPC-1	1153	0.86	2.98	2.95	0.430
NDPC-2	390	0.36	3.62	11.93	0.125

porosity. These results confirm that modifying cow dung-derived carbon with nitrogen-doped porous structures effectively enhances the surface area and pore characteristics, making them suitable candidates for applications in gas adsorption and separation processes.

Table 2 illustrates a clear relationship between nitrogen content obtained by CHNSO analysis (Supplementary Table S1) and surface area in nitrogen-doped porous carbons: as the nitrogen content increases from 2.95 wt. % in NDPC-1 to 11.93 wt. % in NDPC-2, the BET surface area sharply decreases from 1153 m²/g to 390 m²/g, and the micropore volume drops from 0.430 to 0.125 cm³/g, indicating that excessive nitrogen doping—often achieved by increasing melamine content—leads to significant pore blockage and collapse of the microporous structure [65]. This trend is consistent with recent studies showing that while moderate nitrogen incorporation can enhance surface functionalities and adsorption properties, its excessive amount, especially when introduced via high melamine ratios—compromises the porous architecture by filling or blocking pores, thus reducing accessible surface area and pore

volume [65,66]. These findings highlight the necessity of optimizing the nitrogen doping level to balance surface area and functional group introduction for applications like gas adsorption.

3.3. XRD analysis

The crystal structures of CDC, CDAC, and NDPC carbon samples were examined using XRD, as illustrated in Fig. 4.

The diffraction patterns of all samples exhibit broad peaks in the 2θ range of 20°–30°, corresponding to the (002) plane of disordered graphitic carbon, which is a characteristic signature of partially graphitized amorphous carbons derived from biomass precursors [67]. The peak (002) depicts a feature of unstructured carbon due to the Activation and doping in the carbon surface [68]. This broad diffraction feature indicates short-range ordering of stacked graphene-like layers within an overall amorphous carbon matrix, suggesting a balance between graphitic ordering and structural disorder that enhances textural stability and facilitates electron and gas transport during CO₂ adsorption [69]. In addition, a weaker peak observed around 42°–45° corresponds to the (100) plane, associated with in-plane graphitic order [70]. Such broad and low-intensity reflections confirm the amorphous nature of the carbon framework, typical of activated porous carbons prepared via heteroatom doping and chemical activation. Furthermore, the interlayer spacing (*d*₀₀₂) and crystallite size (*L*_c) were estimated using Bragg's law and the Scherrer equation, confirming the presence of disordered graphitic domains embedded within an amorphous matrix, consistent with previous reports on biomass-derived porous carbons [71]. With these parameters and standard XRD methodology, the interlayer distance (*d*₀₀₂) is estimated at approximately 0.37 nm larger than pristine graphite (*d*₀₀₂ ≈ 0.335) demonstrating increased turbostratic disorder

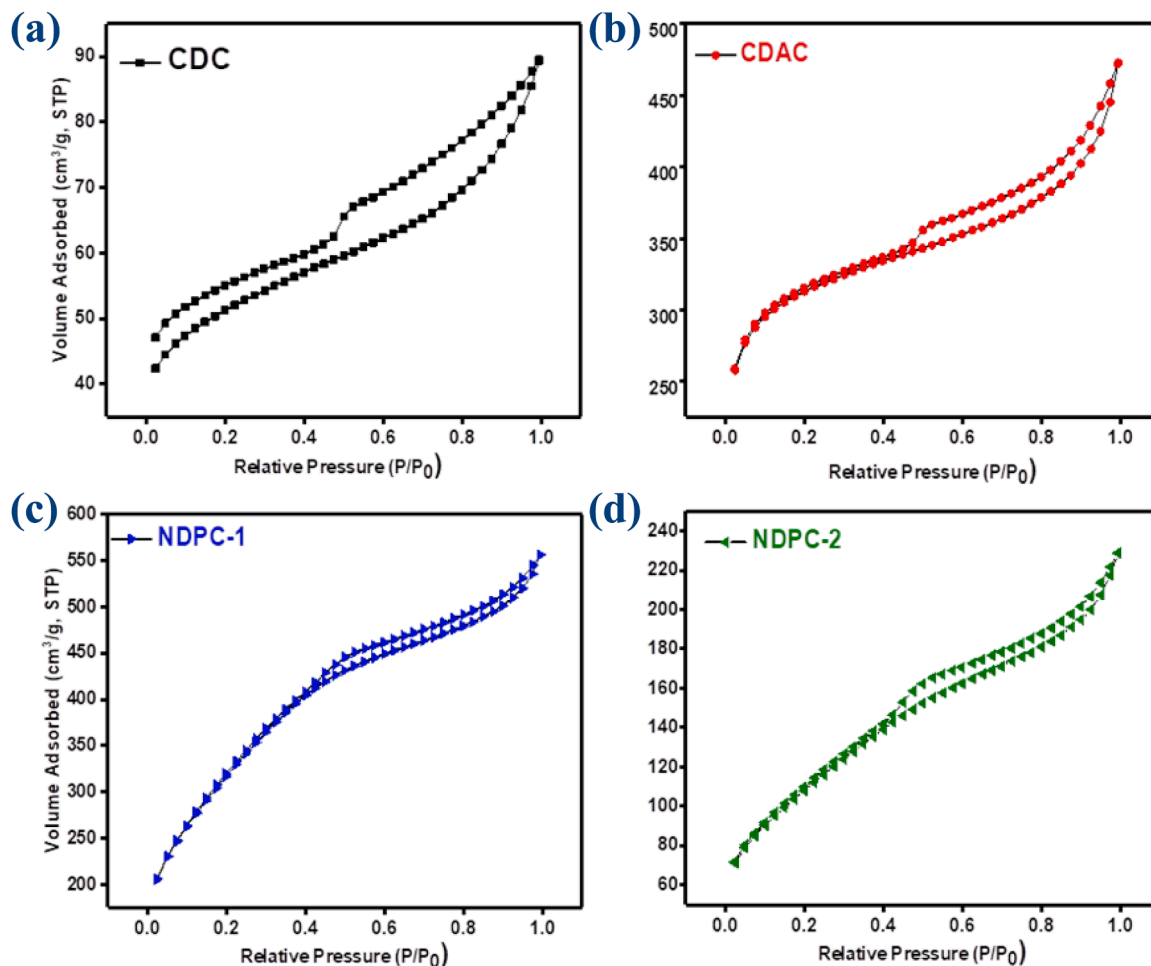


Fig. 2. Nitrogen adsorption-desorption isotherms at 77 K of four different carbon materials: (a) CDC, (b) CDAC, (c) NDPC-1, and (d) NDPC-2. The plot shows the relationship between volume of nitrogen adsorb (cm^3/g , STP) and the relative pressure (P/P_0).

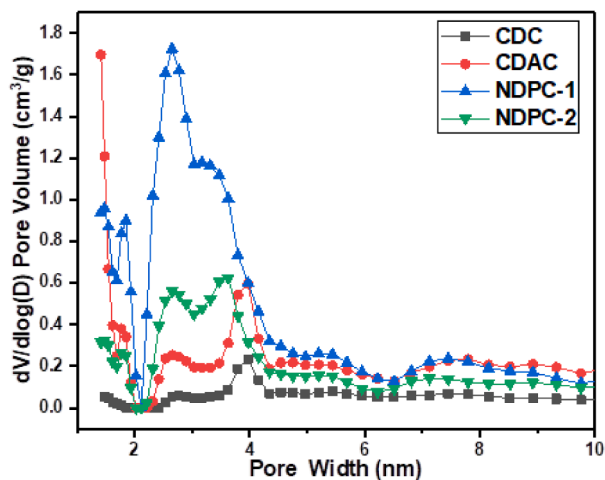


Fig. 3. Pore size distribution curves of four different carbon materials: CDC, CDAC, NDPC-1, and NDPC-2. The plot shows the differential pore volume ($dV/d\log(D)$), in cm^3/g as a function of pore width (nm).

and effects of activation and possible nitrogen doping in the carbon framework [72]. The crystallite size (L_c) for such carbons, calculated using the Scherrer equation, is frequently in the range of 1–3 nm for the (002) peak, and increases with higher temperature treatments but remains well below the values for bulk graphite [73].

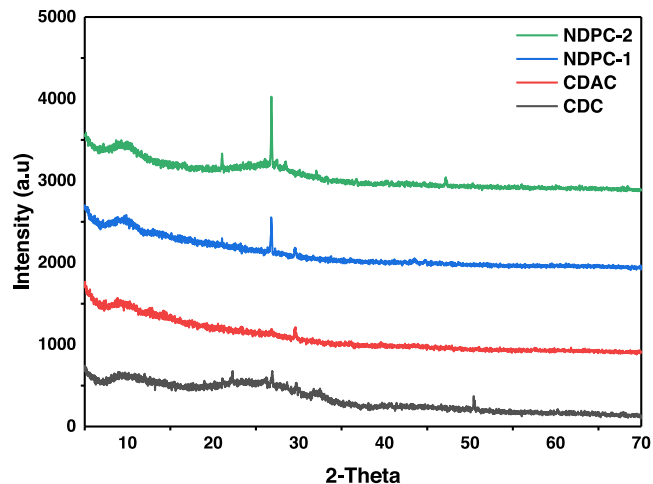


Fig. 4. XRD spectra of four different carbon materials: CDC, CDAC, NDPC-1, and NDPC-2. The intensity (a.u.) is plotted against the 2-Theta angle ($^\circ$). The broad peaks observed in all samples indicate their predominantly amorphous carbon structure.

3.4. Raman spectroscopy analysis

Raman spectroscopy is employed to analyze the defects created in carbon materials after N-doping. As shown in Fig. 5 in each sample two

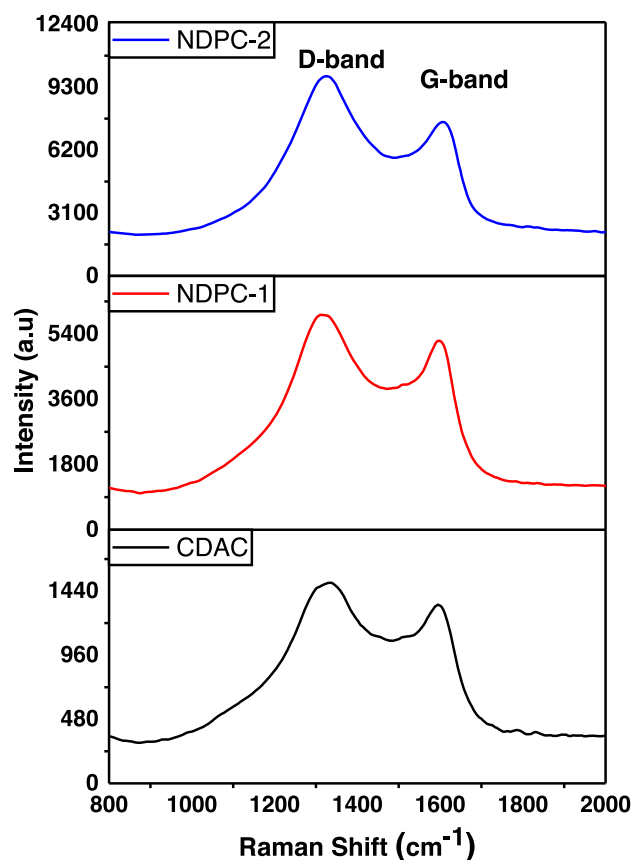


Fig. 5. Raman spectra of three different carbon materials: CDAC, NDPC-1, and NDPC-2. Each spectrum displays two important peaks: the D-band (around 1350 cm^{-1}), associated with structural disorder and defects in the carbon lattice, and the G-band (around 1580 cm^{-1}), which corresponds to the graphitic (sp^2) carbon structure.

characteristic bands were observed approximately at 1350 cm^{-1} and 1580 cm^{-1} , corresponding to D and G band respectively. The D and G bands are closely associated with disordered carbon structures and sp^2 -bonded carbon, respectively. An increase in the I_D/I_G ratio indicates a more significant disorder and reduced graphitization [62,74]. A higher I_D/I_G ratio suggests increased defect density and a more amorphous nature [75].

As shown in Table 3, the I_D/I_G ratio increases after nitrogen doping, signifying the introduction of additional defects into the carbon framework. This increase confirms that nitrogen doping disrupts the graphitic ordering, leading to a higher degree of disorder and reduced graphitization in all NDPC samples. Thus, the Raman analysis confirms that nitrogen doping effectively introduces structural defects, enhances porosity, and forms amorphous nitrogen-doped porous carbon materials with a disordered carbon network.

3.5. X-ray photoelectron spectroscopy (XPS)

X-ray photoelectron spectroscopy (XPS) was performed on the adsorbent to analyze the surface elemental composition and the chemical states of carbon and nitrogen within the material (Fig. 6). The C1s

spectra of all the adsorbents show carbon species bind around 283 eV . The C1 spectrum was deconvoluted to gain insight into chemical bonding between carbon and nitrogen atoms. The peaks appear at 284.8 , 286 and 288 , representing C-C , C-N , and C=O , respectively [76,77]. After deconvolution of N1s spectra, four peaks were observed at 398.3 eV , 400 eV , 402 eV and 404.6 eV , representing pyridinic, pyrrolic, quaternary and oxidized N species are present in N-doped porous carbon as shown in Fig. 6 [76,78]. The XPS spectra confirmed the incorporation of nitrogen elements into the carbon frameworks using melamine as the precursor. Therefore, the high surface area, extensive porosity and heteroatom-doped frameworks highlight their potential applications in gas adsorption and storage.

3.6. CO_2 adsorption study

After successfully synthesis of nitrogen-doped porous carbons (NDPC) with well-developed pore size distribution (PSD), we subsequently evaluate their CO_2 adsorption performance. The CO_2 adsorption-desorption isotherms are shown in Fig. 7 at 303 K , along with a detailed summary of the calculated performance parameters in Table 4. The developed materials exhibit significant variations in CO_2 adsorption capacities, strongly influenced by their surface areas, pore structures, and nitrogen contents. NDPC-1 shows the highest CO_2 uptake of 3.70 mol/kg , attributed to its highest BET surface area ($1153\text{ m}^2/\text{g}$), high total pore volume ($0.86\text{ cm}^3/\text{g}$), and nitrogen content 2.90% . CDAC, with a surface area of $983\text{ m}^2/\text{g}$ and nitrogen content of 0.60% , achieves a CO_2 uptake of 2.85 mol/kg , supported by its substantial micropore volume ($0.389\text{ cm}^3/\text{g}$). Interestingly, NDPC-2, despite its lower surface area ($390\text{ m}^2/\text{g}$), exhibits CO_2 uptake of 2.71 mol/kg due to the highest nitrogen content (11.93%), emphasizing the critical role of nitrogen doping in enhancing CO_2 affinity. Recent studies have demonstrated that the synergistic effects of hierarchical porosity and heteroatom doping are crucial for achieving high CO_2 capture performance in sustainable carbon materials. For instance, Du et al. [20] synthesized pomelo peel-derived N-doped porous carbon through in-situ activation, reporting a CO_2 uptake of 2.8 mol kg^{-1} at 298 K and 1 bar , primarily attributed to the formation of microporous networks enriched with pyridinic and pyrrolic nitrogen. Similarly, Adio et al. [30] developed melamine-modified sugarcane bagasse-derived porous carbon using KOH activation, achieving 3.34 mol kg^{-1} under comparable conditions, where moderate nitrogen incorporation enhanced CO_2 affinity through Lewis acid–base interactions. Tian et al. [31] reported a highly porous carbon derived from melamine–formaldehyde resin with a CO_2 uptake of 3.52 mol kg^{-1} at 298 K , showing that controlled polymerization and subsequent activation could tailor nitrogen functionalities for improved adsorption. In another recent study, Wu et al. [79] utilized bamboo shoot biomass and K_2CO_3 activation to prepare magnetic porous carbon with a CO_2 adsorption capacity of 3.44 mol kg^{-1} at 298 K , attributing the performance to well-developed micropores and surface basic sites. Most of these reported synthesis routes employ conventional activating agents such as KOH or ZnCl_2 , which, despite producing high surface area carbons, involve corrosive chemicals and generate acidic wastewater during post-treatment. More recently (2024), Liu et al. [80] presented a route to convert e-waste into nitrogen-doped porous carbons and reported markedly improved CO_2 uptake and surface basicity due to well-dispersed N-sites that promote Lewis acid–base interactions, achieving a CO_2 adsorption capacity of 3.14 mmol g^{-1} at 25°C and 1 bar , further emphasizing the importance of optimizing both activation and nitrogen incorporation strategies for enhanced CO_2 capture. To ensure transparency and completeness, all temperature-dependent calculations, extended adsorption data at $298\text{--}323\text{ K}$, and the full comparative dataset referenced herein are included in the Supplementary Information (Table S5).

In contrast, CDC has the lowest surface area ($165\text{ m}^2/\text{g}$) and nitrogen content (1.75%), resulting in the lowest CO_2 uptake (1.51 mol/kg). Compared to other N-doped carbons, our material NDPC-1 (3.70 mol/kg

Table 3

The peak intensity of RAMAN spectra.

Sample	D-band (cm^{-1})	G-band (cm^{-1})	I_D/I_G
CDAC	1345	1578	1.02
NDPC-1	1348	1580	1.20
NDPC-2	1350	1584	1.31

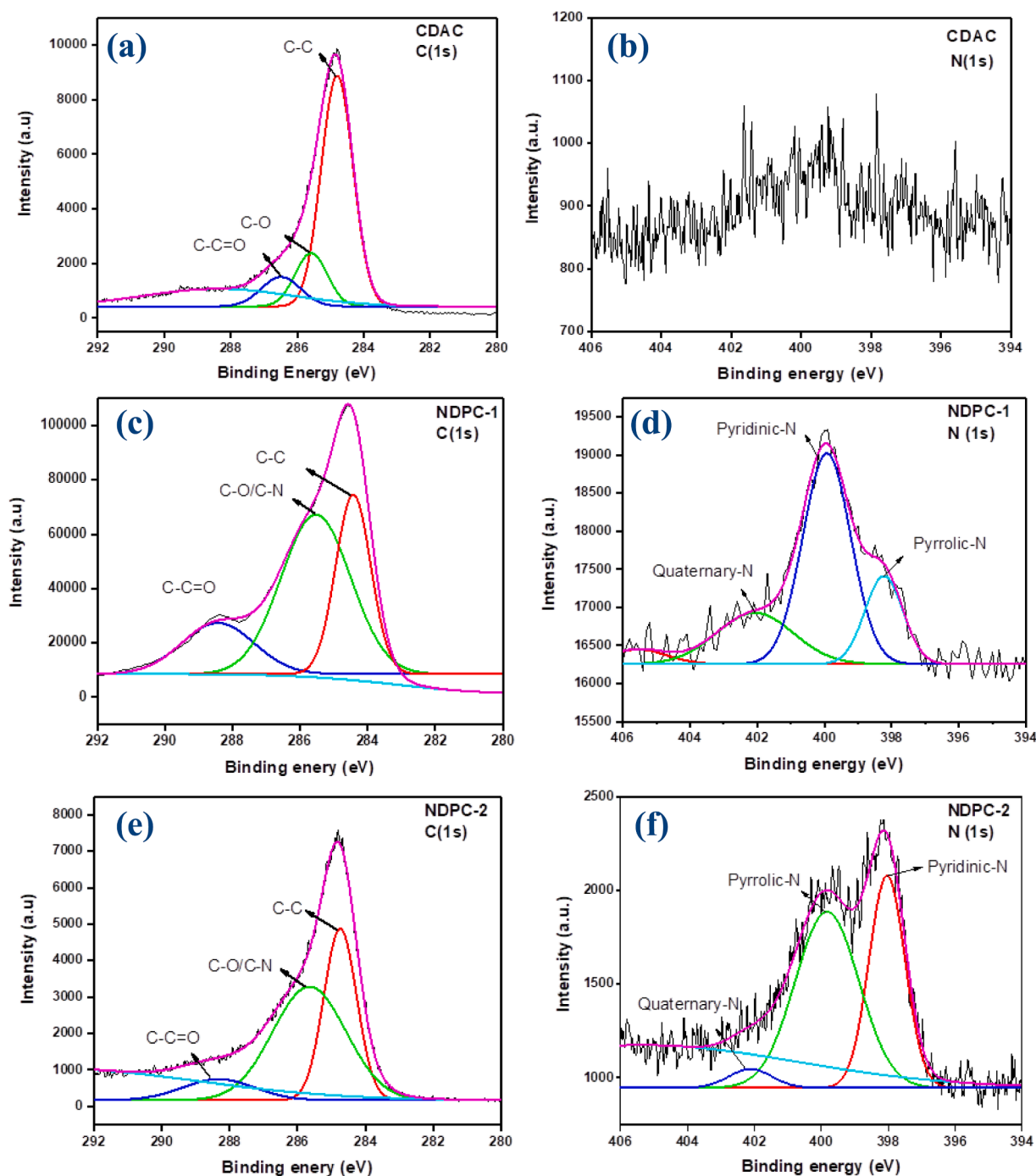


Fig. 6. XPS spectra of three different carbon materials. (a, b) CDAC: (a) C 1 s and (b) N 1 s spectra; (c, d) NDPC-1: (c) C 1 s and (d) N 1 s spectra; (e, f) NDPC-2: (e) C 1 s and (f) N 1 s spectra. The deconvoluted C 1 s spectra show the presence of various carbon bonding environments, while the N 1 s spectra for NDPC-1 and NDPC-2 confirm the presence of pyridinic, pyrrolic, and quaternary nitrogen species.

at 303 K) outperforms many biomass-derived N-doped carbons materials such as pine wood (2.53 mol/kg, 0.52 wt. % N) and walnut shell (2.57 mol/kg, 0.74 wt. % N) based materials, primarily due to its higher nitrogen content and optimized pore structure. These findings highlight that high surface area and optimized pore structures enhance CO₂ adsorption, while nitrogen doping significantly improves CO₂ affinity even in samples with moderate porosity. Overall, a synergistic combination of tailored pore architecture and surface chemistry is essential for developing efficient CO₂ adsorbents.

As shown in Table 4, NDPC-1 outperformed similar carbon–nitrogen-based materials prepared from different precursors, owing to its

optimized nitrogen functionalities, hierarchical porosity, and sustainable, readily available feedstocks such as cow dung and melamine. These features enhance its CO₂ adsorption capacity and make the synthesis process more environmentally and economically favourable. As also discussed in Supplementary Information Section 1, surface characterisations, such as FE-SEM, FTIR, XPS, and TGA, carried out before and after CO₂ exposure, indicate that NDPC-1 retains a stable porous framework, enabling reversible CO₂ uptake mainly via physisorption on oxygen- and nitrogen-containing surface sites. Building on this outstanding performance, NDPC-1 is subsequently subjected to regeneration studies, demonstrating remarkable stability and consistency of

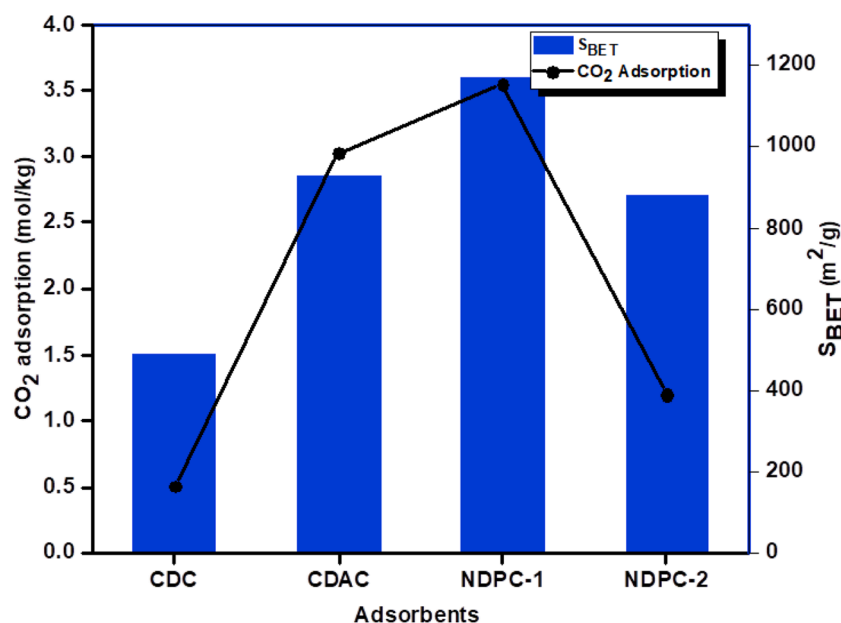


Fig. 7. CO₂ adsorption capacity of CDAC and NDPC at 303 K for 1hr obtained from TGA vs. SBET (BET Surface area in m²/g).

Table 4
Comparison data with the reported literature.

Carbon Source	Activating & doping agent	Temperature & Pressure	CO ₂ uptake (mol/kg)	References
Palm kernel shell	CO ₂ & Diethanolamine	298 K, 1 bar	2.13	[17]
Ion-exchange resins	KOH	298 K, 1bar	2.38	[18]
Sucrose	ZnCl ₂	298 K, 1bar	2	[19]
pomelo peel	ZnCl ₂	298 K, 1bar	2.8	[20]
Bamboo	K ₂ CO ₃	298 K, 1bar	3.44	[79]
Lotus stalk	KOH	298 K, 1bar	3.68	[81]
sugarcane bagasse	Zinc-acetate and Melamine	298 K, 1bar	3.34	[30]
Melamine-formaldehyde resin	KOH, melamine	298 K, 1bar	3.52	[31]
Corn stalk	KHCO ₃ /KCl	298 K, 1bar	3.6	[82]
Microporous carbon foam	MEA, DEA and TEA	298 and 323 K, 1bar	3.22 and 1.93	[83]
polybenzoxazine	TEPA	298 and 323 K, 1bar	1.96 and 1.41	[84]
Cellulose carbon	KOH/Urea	298 and 303 K, 1 bar	3.26 and 2.05	[85]
Chitosan/ZIF-8	-	298 and 303 K, 1 bar	2.50 and 1.29	[86]
PET waste	KOH	303 K, 1bar	2.31	[87]
Cow dung	KHCO ₃ /KCl, melamine	303 K, 1bar	3.7	This work
Cow dung	KHCO ₃ /KCl, melamine	313 K, 1bar	3.1	This work

its initial CO₂ capture capacity after 10 adsorption-desorption cycles (Fig. 8). This combination of high efficiency, sustainability, and excellent regenerative performance underscores NDPC-1 substantial potential for practical and scalable CO₂ capture applications.

3.7. CO₂ adsorption kinetics

The adsorption kinetics of an adsorbent directly reflects its material properties, such as adsorption rate, which is a major factor in determining its suitability for industrial applications. Three kinetic models

were employed to analyze the adsorption data to evaluate the adsorption rate and elucidate the underlying reaction mechanism.

Table S3 and Fig. 9 present the kinetic parameters and fitting curves for CO₂ adsorption on CDAC and NDPC (NDPC-1 and NDPC-2) at 303 K, analyzed using three different models. NDPC-1 shows the highest CO₂ adsorption capacity (3.7 mol/kg), followed by CDAC (2.85 mol/kg) and NDPC-2 (2.71 mol/kg), indicating the positive effect of nitrogen doping on adsorption performance. The pseudo-first-order model gives low R² values (0.823–0.896), suggesting a poor fit, while the pseudo-second-order model gives higher R² values (0.906–0.967), indicating that the interaction between adsorbent and adsorbate is due to strong CO₂ binding on the adsorbent surface, which controls the rate. This model is suitable for describing CO₂ adsorption behaviour involving chemical interaction [88]. Avrami's model was initially developed to analyze phase transition and crystal growth rates in materials, but it has recently been shown to effectively predict the adsorption kinetics of CO₂ on modified activated carbon adsorbents [89]. The Avrami model is an excellent fit for the CO₂ adsorption of all the materials, showing the highest R² values (0.948–0.995). Additionally, the equilibrium adsorption capacities derived from the model closely align with the experimentally measured values with only slight differences [90]. As shown in Table S3, *k*, value of NDPC-2 is lower compared to others, such as 0.107 min⁻¹, which signifies slower CO₂ adsorption kinetics due to fewer accessible active sites, often resulting from a lower surface area, which reduces the rate and efficiency of adsorption [48]. This relationship is well established, as a high surface area typically provides more adsorption sites, enhancing both capacity and kinetic rates for CO₂ capture [48]. In conclusion, these results confirm that Avrami's model best describes the CO₂ adsorption kinetics, suggesting multi-step adsorption mechanisms. It also highlights NDPC-1 as a promising material for industrial CO₂ capture due to its high adsorption capacity and favourable kinetics.

3.8. Simulation results

The atomistic structure of carbon-based amorphous carbon (CDAC) is shown in Fig. 10 (a), highlighting its disordered network and pore connectivity as visualized with OVITO. Fig. 10(b) presents the nitrogen-doped amorphous carbon (NDAC-1) model, where nitrogen incorporation subtly alters the local structure while maintaining the amorphous and porous character. The amorphous carbon frameworks generated

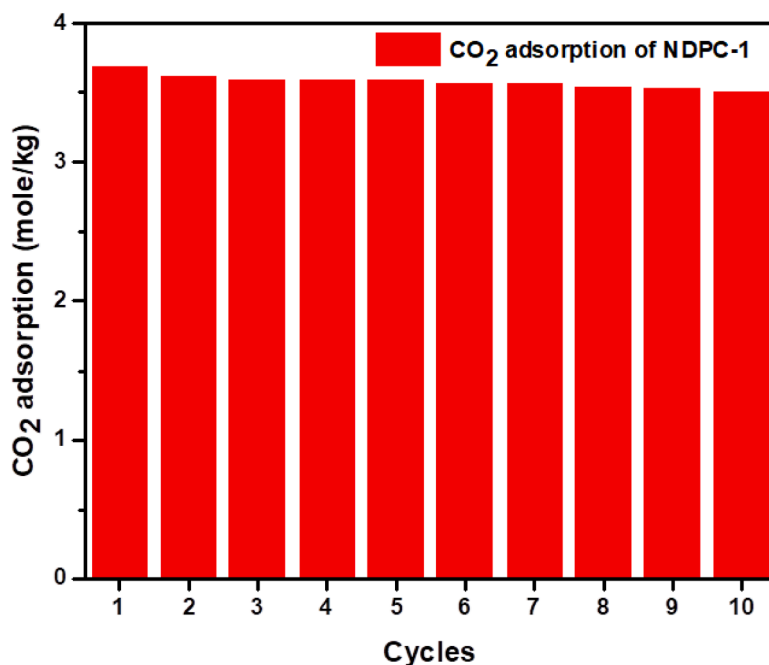


Fig. 8. Cyclic CO₂ adsorption (303 K) and desorption (473 K) isotherm obtained from TGA.

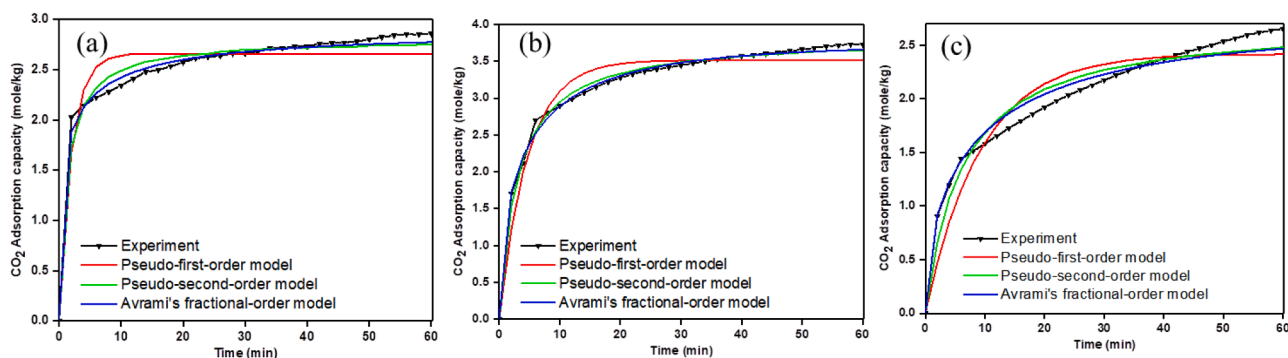


Fig. 9. Kinetics of CO₂ adsorption on (a) CDAC, (b) NDPC-1 and (c) NDPC-2 as represented by Pseudo-first order, Pseudo-second order and Avrami's fractional-order model.

through the liquid quench method exhibit pyridinic nitrogen features upon nitrogen doping. Pore size distribution analysis using Zeo++ (refer to Fig. 10(d)) demonstrates that the amorphous carbon models develop narrow micropore structures with pore widths predominantly below 15 Å. The sharp peak around 50–70 Å (5–7 nm, mesopores) in the pore size distribution indicates structural heterogeneity, while the presence of smaller micropores (<2 nm) enhances CO₂ adsorption through strong adsorbate-framework interactions, further supported by the BET-derived average pore diameter (2.98 nm). As reported by Presser et al., pores smaller than 0.8 nm (<8 Å, ultra-micropores) dominate CO₂ uptake at ambient pressure, underscoring the critical role of sub-nanometer pores in efficient carbon capture [91].

Nitrogen doping led to moderate reductions in the accessible surface area (~15 %) and volume fraction (~7 %) compared to the pristine carbon framework (refer SI Table 4). Despite these changes, both structures retained highly disordered morphologies, characterized by wrinkled graphitic fragments and the presence of topological defects such as 4-membered rings and fused 5/7-membered rings. These high-energy features are known to arise from rapid quenching and the presence of heteroatoms, and they were observed in both the pristine and N-doped structures with comparable frequency. We also performed characterization of the hybridization environment and ring size distribution

in both NDPC-1 and CDAC amorphous carbon-based models. As shown in the hybridization plots in (refer Fig. 10, e), both models display nearly identical distributions, with sp²-hybridized carbon atoms being predominant, followed by a smaller fraction of sp, and minimal sp³ content. This indicates that both models capture a similar graphitic character with limited diamond-like bonding in the amorphous carbon matrix. The high-temperature pyrolytic process within the liquid quench framework induces the sp² content; nonetheless, it is dependent on the density [49,50]. Since the model we created has a low density of 0.6 g/cc, the sp² content dominates, as can be inferred from relevant studies [49,50]. Ring size distribution analysis using the ISAACS tool revealed that both CDAC and NDPC-1 models predominantly contained 5 and 6-membered rings, consistent with typical amorphous carbon structures, with a slight excess of 3-membered rings for NDPC-1 model (refer to Fig. 10(f)). Radial distribution function (RDF) analysis for the pair-wise separation between the C from adsorbed CO₂ and the elements of the framework (C/N/O/H) is presented in Fig. 10 (g). A few important adsorption characteristics can be gleaned from the Figure: N plays a pivotal role in adsorbing CO₂ in NDPC-1 as seen from the C-N peaks which are comparable with the peaks obtained for the CDAC structure. In fact, the intensity of the first C-N peak for NDPC-1 (occurring at 4.2 Å) exceeds the first peak intensity for other C-framework atoms in NDPC-1,

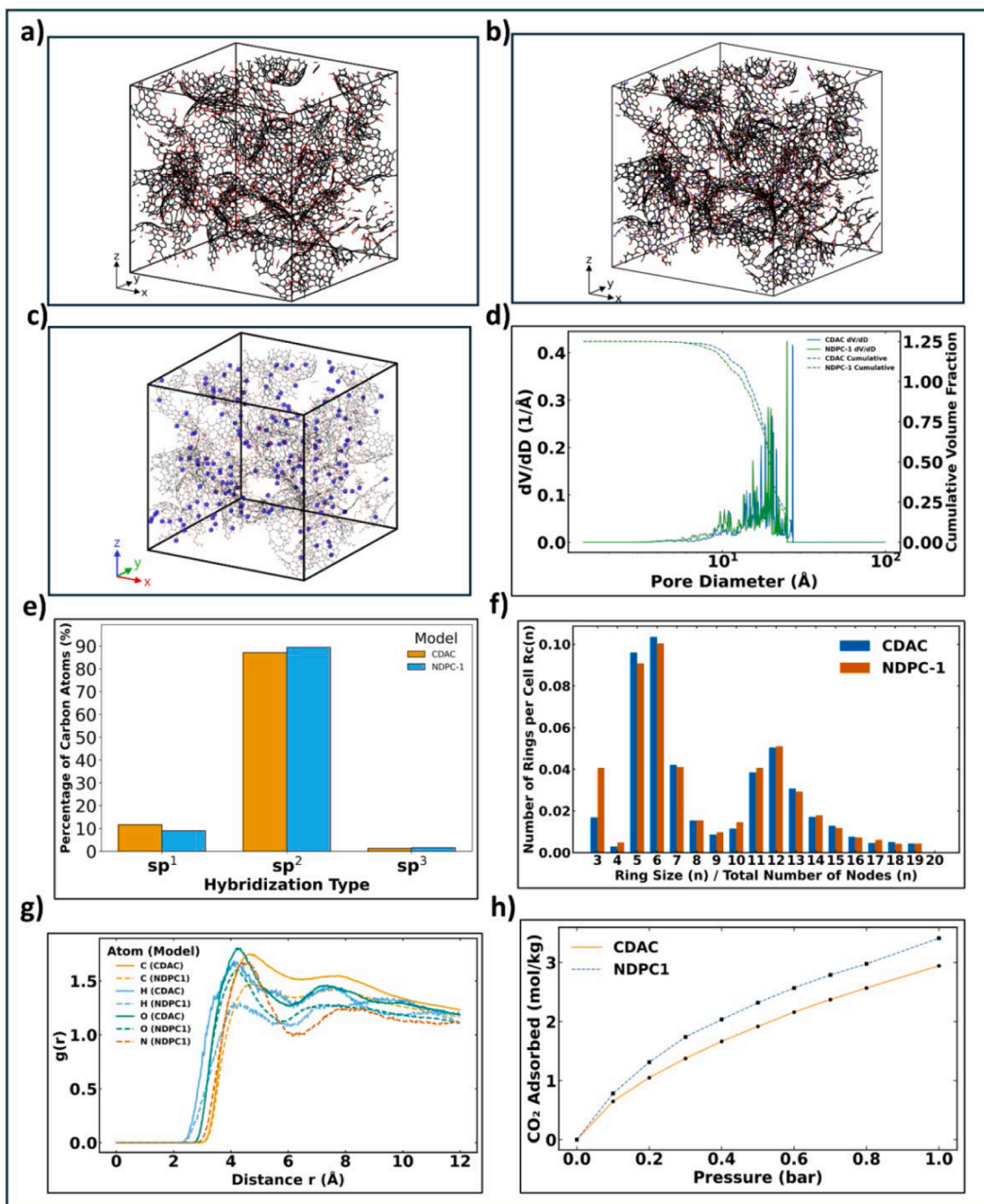


Fig. 10. Structural and adsorption analysis of undoped (CDAC) and nitrogen-doped (NDPC-1) amorphous carbon. (a,b) 3D pore network visualizations for CDAC and NDPC-1. (c) Illustration of CO₂ adsorption in NDPC-1 pores and on surface sites. (d) Pore size distributions and cumulative pore volume fractions. (e) Ring size distributions showing increased small-ring content in NDPC-1. (f) Radial distribution functions highlight local atomic environments. (g) CO₂ adsorption isotherms at 300 K, with NDPC-1 showing higher uptake than CDAC across all pressures.

indicating a strong preference for C to adsorb close to N sites. Additionally, the similarity in peak positions between N-N, N-C and C-C peaks in NDPC-1 (refer supplementary figure 2) shows a well-dispersed distribution of N in the framework as shown in Fig. 10(c).

The radial distribution function (RDF) in Fig. 10(g) also exhibits a clear secondary peak around 7.5 Å, indicating the presence of medium-range structural correlations in both CDAC and NDPC-1 amorphous carbon models. GCMC simulations revealed distinct adsorption behaviors between the undoped (CDAC) and nitrogen-doped (NDPC-1) models

(refer to Fig. 10(h)). At 300 K and 1 bar pressure, the nitrogen-doped NDPC-1 framework demonstrated a CO₂ uptake of 3.75 mol/kg, representing a 28 % increase over the CDAC model (2.93 mol/kg). The simulations exhibited excellent agreement with experimental adsorption models, showing deviations of CO₂ uptake within ± 0.15 mol/kg across the studied pressure range. The results demonstrate that controlled nitrogen doping represents an effective strategy for enhancing CO₂ adsorption performance in amorphous carbon materials, where surface chemistry modifications provide the dominant contribution to improved

performance

4. Conclusions

In summary, the current work presents a single step dry process to synthesis highly porous in-situ N-doped activated carbon from cow dung for low-temperature CO₂ using a green activator. Notably, the material prepared from a 1:1 ratio of cow dung to melamine (NDPC-1), containing 2.95 % nitrogen doping, exhibits a CO₂ uptake of 3.7 mol/kg at 303 K and 1 bar which is 28 % higher than undoped activated carbon (CDAC) and 58 % higher than pristine carbon (simple pyrolyzed cow dung without any activation) along with excellent cyclic stability. The superior performance of activated nitrogen-doped porous carbon derived from cow dung is attributed to the optimal balance of a high BET surface area (1153 m²/g) and a micropore-rich structure with an average pore diameter of less than 15 Å. Additionally, the presence of nitrogen functionalities, especially pyridinic nitrogen, enhances the material's affinity for CO₂. The material's facile single-step synthesis and the use of green activators indicate its strong potential for industrial applications. Kinetic analysis indicated rapid adsorption, best described by Avrami's model. The synergy between green synthesis protocols and atomistic modelling (via liquid quench methods and grand-canonical Monte Carlo simulations) provides a rational approach for designing carbon capture materials from biomass. This integrated approach enables the development of high-performance, nitrogen-enriched porous carbons with optimized textural and chemical properties. These materials demonstrate enhanced CO₂ adsorption capacity and regeneration stability, highlighting their potential for sustainable and scalable carbon capture applications.

Declaration of generative AI and AI-assisted technologies

During the preparation of this work, the author(s) used Perplexity AI (a generative AI language tool) to assist with English language polishing and phrasing suggestions. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the published article.

Author statement

The authors confirm that this manuscript is original, not under consideration elsewhere, and approved by all authors. The authors declare no conflict of interest.

CRediT authorship contribution statement

Ranjeet Kumar: Writing – original draft, Validation, Methodology, Data curation, Conceptualization. **Sree Harsha Bharadwaj H:** Software, Methodology. **Raghavan Ranganathan:** Writing – review & editing, Software, Resources. **Chinmay Ghoroi:** Writing – review & editing, Validation, Supervision, Resources, Funding acquisition, Formal analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.surfin.2026.108833](https://doi.org/10.1016/j.surfin.2026.108833).

Data availability

All the data associated with this work will be made available on request.

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