# Efficient $CO_2$ adsorption on nitrogen-doped porous carbons derived from D-glucose

**(Supporting Information)**

Limin Yue[a], Linli Rao[a], Linlin Wang[b], Liying An[a], Chunyun Hou[a], Changdan Ma[a], Herbert DaCosta[c], Xin Hu*[,a],

[a]College of Chemistry and Life Sciences, Zhejiang Normal University, 688 Yingbin Ave. Jinhua 321004, PR China

[b]College of Engineering, Zhejiang Normal University, 688 Yingbin Ave. Jinhua 321004, PR China

[c]Math, Science, and Engineering Division, Illinois Central College, 1 College Drive East Peoria, IL 61635, USA

*Corresponding author's e-mail: huxin@zjnu.cn; phone: 86-151-0579-0257; fax: 86-579-8228-8269

## Urea modification

A mixture of GC and urea (weight ratio 1:1) was heated in air at 350 °C for 2 hours. The collected samples were rinsed with hot distilled water a few times to get rid of any unreacted urea. Finally, the resulting products were put into the oven to dry at 120 °C overnight. The resulting sample was denoted as NGC.

## $K_2CO_3$ activation

In a typical preparation, 2 g NGC were first mixed with a solution containing 8 g $K_2CO_3$. This mixture was stirred with a magnetic stirrer at room temperature for 24 h.

The resulting mixture was then dried overnight at 120℃ in an oven and placed in a horizontal quartz pipe reactor for activation. The activation process was as follows: (i) flowing $N_2$ through the reactor at a constant rate of 400 ml/min throughout the entire activation process, (ii) heating the reactor to the final activation temperature of 650℃ at a rate of 5°C/min, (iii) holding at the activation temperature for 60 min, and then (iv) cooling to room temperature. The resulting samples were washed with distilled water until the filtrate appears neutral. After being heated at 150℃ under vacuum for 24 h, the final product is obtained.

**Characterization**

Powdered X-ray diffraction (XRD) patterns were carried out on a PHILIPS PW3040/60 powder diffractometer using CuKα radiation (λ =0.15406nm). Scanning electron microscopy (SEM Hitachi S-4800) was used to observe the morphology of the samples of carbon materials. Further details of the pore structure were determined by transmission electron microscopy (TEM, JEOL-2100F) operated at 200 kV. The CHN elements were analyzed using a VarioEL III Elemental Analyzer. Nitrogen adsorption and desorption isotherms were measured on a Beshide 3H-2000PS2 sorption analyzer at -196$^{o}$C. Ultrahigh-purity $N_2$ (99.999%, Shanghai Pujiang Gas Co., Ltd) was used for measurement. Before measurement, the samples were degassed in a vacuum at 200$^{o}$C for at least 12h. The specific surface area ($S_{BET}$) was calculated according to the multipoint Brunauer-Emmett-Teller (BET) method from the adsorption data in the relative pressure range between 0.005 and 0.05. The total micropore volume ($V_t$) was deduced from the $N_2$ adsorption data by the t-plot method,

and the total pore volume ($V_0$) was estimated from the adsorbed amount of liquid nitrogen at a relative pressure of 0.99. The pore size distribution was calculated using the density functional theory (DFT) method. In addition, X-ray photoelectron (XPS) measurements were performed using an AXIS Nova spectrometer (Kratos Inc., NY, USA) equipped with a monochromatic Al Kα X-ray source (1486.6 eV). XPS survey spectra were recorded with a pass energy of 160 eV, and high-resolution spectra with a pass energy of 40 eV.

The $CO_2$ adsorption isotherms were measured using the Beshide 3H-2000PS2 sorption analyzer at 0$^{o}$C and 25$^{o}$C, respectively. Pure $CO_2$ (99.99%, Shanghai Pujiang Gas Co., Ltd) was used for adsorption. Prior to each adsorption experiment, the sample was degassed for 12 h at 200$^{o}$C to remove the guest molecules from the pores. The volume of narrow micropores (with sizes <1 nm), $V_n$, was calculated from $CO_2$ adsorption at 0°C using the Dubinin–Radushkevich (D-R) equation. The measurements were repeated for each sample, until the values fell within ± 2% of each other.

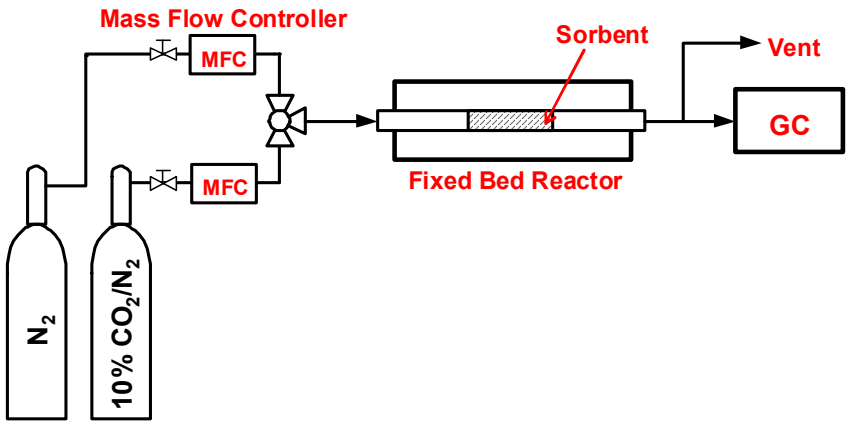
**Measurement of dynamic $CO_2$ uptake of the sorbents**

The dynamic $CO_2$ uptake of the sorbents was tested on a fixed-bed reactor schematically illustrated in Scheme S1 at 1 bar and 25 °C. First, the sample was heated at 100°C for 1 h under $N_2$ at a flow rate of 20 mL/min. The gas flow was shifted from nitrogen to a 10% mixture of $CO_2$ in $N_2$ at a flow rate of 10 mL/min, when the sample temperature was lowered to 25°C. The effluent gases were monitored online using an Agilent 7820A gas chromatograph with a thermal

conductivity detector (TCD). From the breakthrough curves, the dynamic $CO_2$ capture capacity on an adsorbent was calculated.

**Measurement of $CO_2$ adsorption kinetics**

The adsorption kinetics of $CO_2$ was measured in a thermogravimetric analyzer (NETZSCH STA 449C). In the kinetic analysis, the sample (~5 mg) was degassed under a He stream at 200°C for 1 h. Next, the temperature was cooled to the experimental temperature of 25°C. Then the $CO_2$ gas was fed into the test chamber with a flow rate of 50 mL/min and the weight variation with time was recorded.




Scheme S1. Schematic of the fixed-bed reactor system.

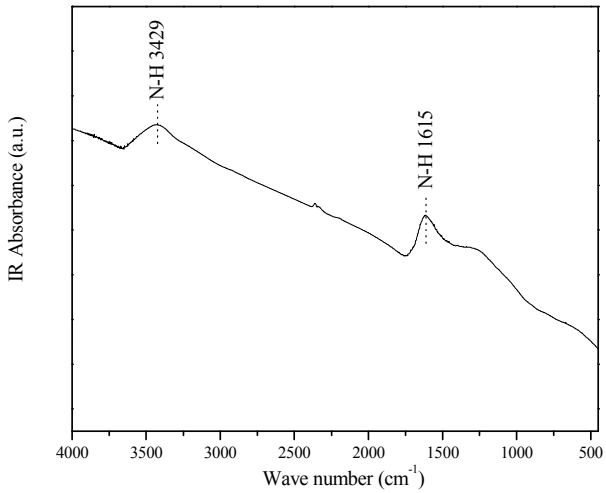



Figure S1. FT-IR spectrum of NGC-650-4.

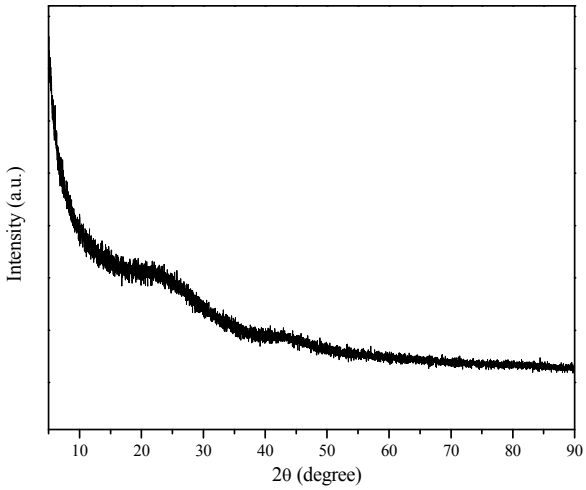



Figure S2. XRD pattern of NGC-650-4.

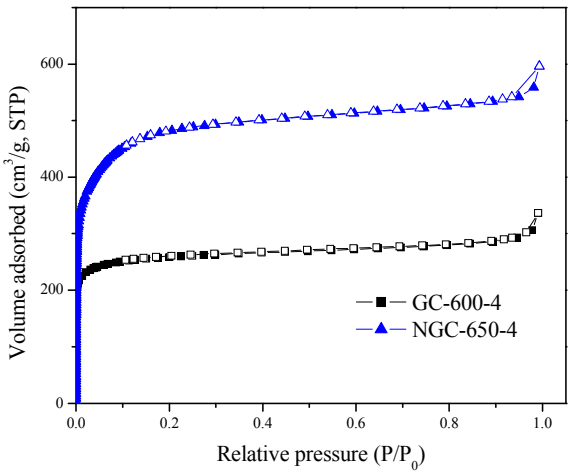



Figure S3. The $N_2$ sorption isotherms of GC-650-4 and NGC-650-4. Filled and empty symbols represent adsorption and desorption branches, respectively.

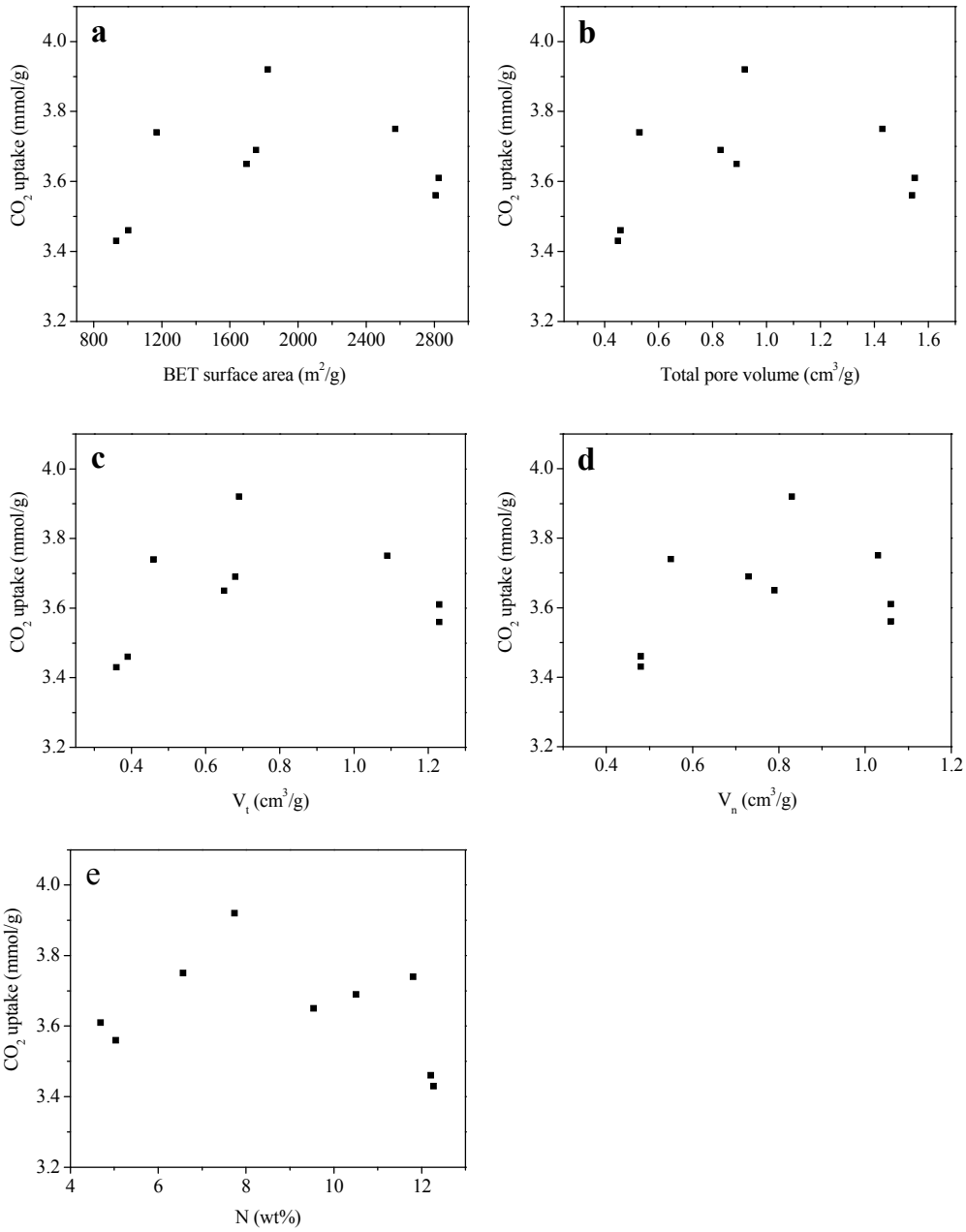



Figure S4. Plot of each porous properties characteristics (a) $S_{BET}$, (b) $V_o$, (c) $V_t$ (d) $V_n$ and (e) nitrogen content versus $CO_2$ uptake.

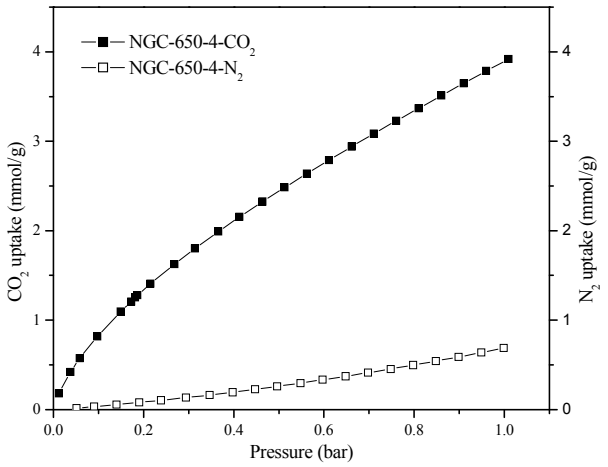



Figure S5. $CO_2$ (filled symbols) and $N_2$ (empty symbols) adsorption isotherms of NGC-650-4 at 25 °C.

Table S1. Comparison of the $CO_2$ adsorption (25 °C and 1 bar) for different sorbents

| Sample | $CO_2$ uptake (mmol/g) | Ref. |
|---|---|---|
| PC-2 | 3.5 | 32 |
| CP-2-600 | 3.9 | 54 |
| H250-800 | 3.7 | 52 |
| N-TC-EMC | 4.0 | 55 |
| MOF-2 | 0.6 | 10 |
| MOF-505 | 3.3 | 10 |
| ZIF-78 | 2.7 | 58 |
| COF-102 | 3.5 | 57 |
| NGC-650-4 | 3.9 | This study |