

Supporting Information

Waste wool derived nitrogen-doped hierarchical porous carbon for selective CO₂ capture

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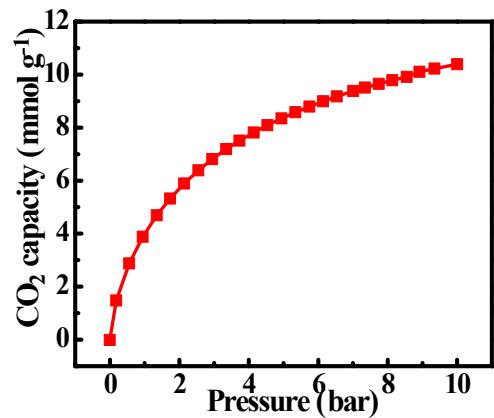


Fig. S1 The CO₂ adsorption isotherm of the WNPC-3 measured under high pressure at 0 °C.

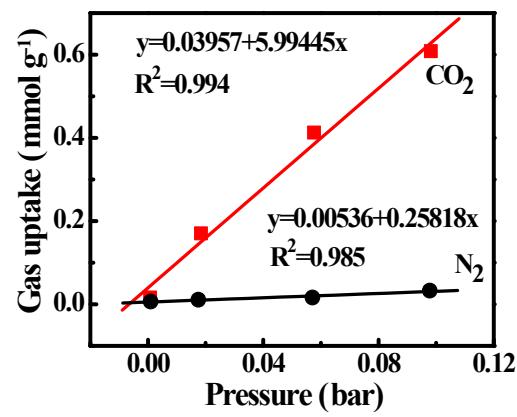


Fig. S2 The initial slopes are calculated from CO₂ and N₂ adsorption isotherms at 25 °C for WPC-3. The CO₂/N₂ selectivity ratio is 23.

The ideal adsorption solution theory (IAST) calculation

The pure adsorption isotherms of CO₂ and N₂ on the WNPC-3 at 25 °C and 1 bar are given in Fig. 6c.

The CO₂ and N₂ experimental adsorption isotherms were fitted to the dual-site Langmuir model (DL) and single site Langmuir model (L), respectively, as following.^{S1-S3}

Dual site Langmuir model = q_A + q_B; Single site Langmuir model = q_A

$$q = q_A + q_B = \frac{q_{\text{sat},A} b_A p}{1 + b_A p} + \frac{q_{\text{sat},B} b_B p}{1 + b_B p}$$

Where A and B are two distinct adsorption sites, q is the amount of gas adsorbed (mmol/g), p is the pressure (bar), q_{sat,i} is the saturation capacity (mmol/g), b_i is the dual-site Langmuir parameter (bar⁻¹).

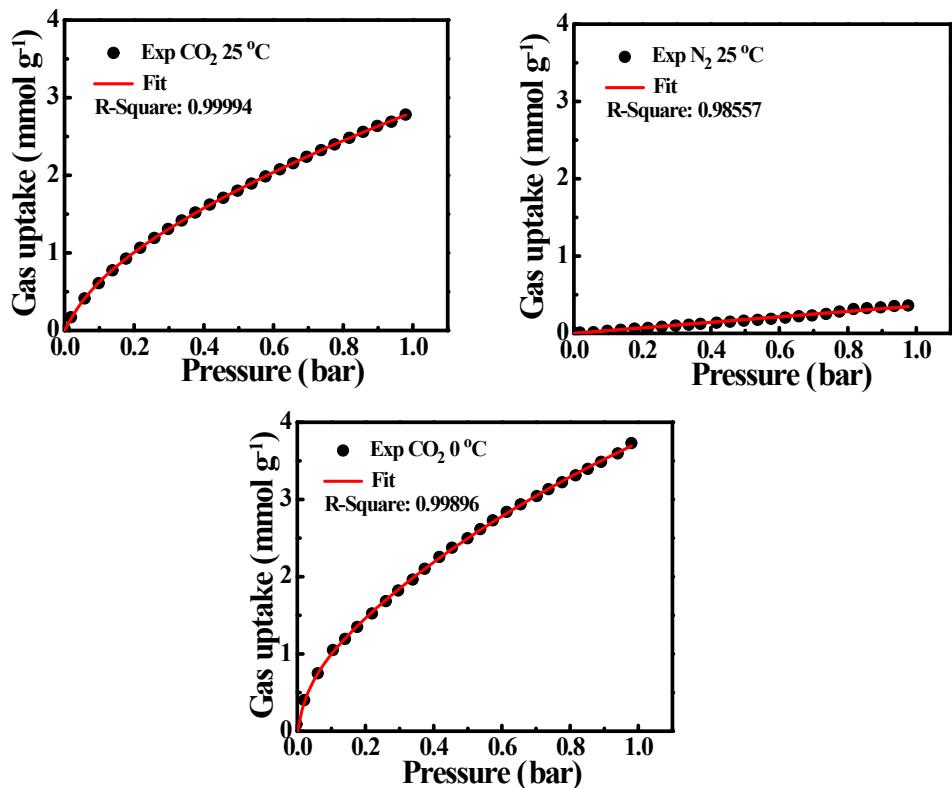


Fig. S3 CO₂ and N₂ gas adsorption isotherms for WPC-3 (black dot). The red lines correspond to DL and L equation fits.

The ideal adsorption solution theory (IAST) of developed by Myers and Prausnitz has been reported to predict binary gas mixture adsorption on porous materials.^{S4-S6} Adsorption selectivity (S_{ads}) for binary mixtures is defined as following:

$$S_{ads} = [q_1/q_2] / [p_1/p_2]$$

Where S_{ads} is the selectivity factor, q_i is the amount adsorbed at partial pressure p_i of the gas i in the binary mixture. Generally, to estimate the CO₂/N₂selectivity, partial pressures of CO₂ and N₂ are taken as 0.15 and 0.85, respectively, which is a typical composition of flue gas.

The isosteric heat of adsorption (Qst) calculation

Isosteric heat of adsorption (Qst) is the standard enthalpy of adsorption at a fixed surface coverage. The Qst of CO₂ adsorption on the WNPC-3 was calculated at two different temperatures (0 °C and 25 °C) considering the same adsorbed amount obtained at two different pressures using a modified version of the Clausius-Clapeyron equation:^{S6-S8}

$$\ln \left(P_1/P_2 \right) = \Delta H_{\text{ads}} \left(\frac{T_2 - T_1}{R \cdot T_1 \cdot T_2} \right)$$

Where P₁ and P₂ are the pressures, for the same of CO₂ adsorbed amount, at different temperatures of T₁ and T₂, respectively. ΔH_{ads} gives the isosteric heat of adsorption.

Table S1 The comparison of CO₂ uptake and CO₂/N₂ selectivity for **WNPC-3 in this work** with several other reported porous carbons.

Sample	CO ₂ uptake (mmol·g ⁻¹)		CO ₂ /N ₂ selectivity (25 °C)		Reference
	0 °C	25 °C	Initial slope ^a	IAST ^b	
aC-AO1	4.237	2.489	22.4	----	[S7]
NPCs-2-500	4.0	2.5	----	21.5	[S9]
H-NMC-2.5	----	2.8	37	----	[S10]
STC-2.5	2.3	1.3	17	----	[S11]
4 AN	3.37	2.4	14	----	[S12]
N-TC-EMC	----	4.0	14	----	[S13]
NC-800	2.65	1.95	----	----	[S14]
700 ^c	----	3.51	----	79	[S15]
SU-MAC-600	----	4.18	32	----	[S16]
500-2	4.8	3.5	----	41.6	[S17]
AC-PAIN-F	----	2.69	----	18.97	[S18]
WNPC-3	3.72	2.78	23	16	This work

^a Selectivity was calculated from initial slope calculations at 25 °C;

^c Selectivity was calculated from IAST for 15/85 gas mixtures for CO₂/N₂ at 25 °C.

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