Supporting Information

Waste wool derived nitrogen-doped hierarchical porous carbon for selective CO$_2$ capture

Yao Li,$^{ac}$ Ran Xu,$^a$ Xin Wang,$^b$ Binbin Wang,*$^b$ Jianliang Cao,$^d$ Juan Yang*$_{ac}$ and Jianping Wei*$_{ac}$

$^a$ School of Safety Science and Engineering, Henan Polytechnic University, Jiaozuo, Henan 454000, China.

$^b$ School of Materials Science and Engineering, Henan Polytechnic University, Jiaozuo, Henan 454000, China.

$^c$ State Key Laboratory Cultivation Base for Gas Geology and Gas Control, Henan Polytechnic University, Jiaozuo 454000, China.

$^d$ School of Chemistry and Chemical Engineering, Henan Polytechnic University, Jiaozuo 454000, China.

* Corresponding authors.

-E-mail address: wangbb580@aliyun.com (B. Wang), yangjuanhpu@163.com (J. Yang), hpuwjp@163.com (J. Wei).
Fig. S1 The CO$_2$ adsorption isotherm of the WNPC-3 measured under high pressure at 0 °C.

Fig. S2 The initial slopes are calculated from CO$_2$ and N$_2$ adsorption isotherms at 25 °C for WPC-3. The CO$_2$/N$_2$ selectivity ratio is 23.
The ideal adsorption solution theory (IAST) calculation

The pure adsorption isotherms of CO\textsubscript{2} and N\textsubscript{2} on the WNPC-3 at 25 °C and 1 bar are given in Fig. 6c.

The CO\textsubscript{2} and N\textsubscript{2} experimental adsorption isotherms were fitted to the dual-site Langmuir model (DL) and single site Langmuir model (L), respectively, as following:

Dual site Langmuir model = q\textsubscript{A} + q\textsubscript{B}; Single site Langmuir model = q\textsubscript{A}

\[ q = q\textsubscript{A} + q\textsubscript{B} = \frac{q_{\text{sat},A} b\textsubscript{A} p}{1 + b\textsubscript{A} p} + \frac{q_{\text{sat},B} b\textsubscript{B} p}{1 + b\textsubscript{B} p} \]

Where A and B are two distinct adsorption sites, \( q \) is the amount of gas adsorbed (mmol/g), \( p \) is the pressure (bar), \( q_{\text{sat},i} \) is the saturation capacity (mmol/g), \( b\) is the dual-site Langmuir parameter (bar\textsuperscript{-1}).
Fig. S3 CO\textsubscript{2} and N\textsubscript{2} 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.\textsuperscript{S4-S6} Adsorption selectivity ($S_{\text{ads}}$) for binary mixtures is defined as following:

$$S_{\text{ads}} = \left[\frac{q_1}{q_2}\right] / \left[\frac{p_1}{p_2}\right]$$

Where $S_{\text{ads}}$ 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 CO\textsubscript{2}/N\textsubscript{2} selectivity, partial pressures of CO\textsubscript{2} and N\textsubscript{2} 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 CO$_2$ 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:\textsuperscript{56-58}

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

Where $P_1$ and $P_2$ are the pressures, for the same of CO$_2$ adsorbed amount, at different temperatures of $T_1$ and $T_2$, respectively. $\Delta H_{\text{ads}}$ gives the isosteric heat of adsorption.
Table S1 The comparison of CO$_2$ uptake and CO$_2$/N$_2$ 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 ºC) | Reference |
|--------------|-------------------------------|----------------------------------|-----------|
|              | 0 ºC  | 25 ºC  | 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 ºC;

$^c$Selectivity was calculated from IAST for 15/85 gas mixtures for CO$_2$/N$_2$ at 25 ºC.

References

S1  X. Ma, Y. Li, M. Cao and C. Hu, *J. Mater. Chem. A*, 2014, 2, 4819-4826.

S2  J. Kou and L. B. Sun, *Ind. Eng. Chem. Res.*, 2016, 55, 10916-10925.

S3  T. Islamoglu, S. Behera, Z. Kahveci, T. D. Tessema, P. Jena and H. M. El-Kaderi, *ACS Appl. Mater. Interfaces*, 2016, 8, 14648-14655.
S4 R. Li, X. Ren, X. Feng, X. Li, C. Hu and B. Wang, *Chem. Commun.*, 2014, **50**, 6894-6897.

S5 Y. Shi, J. Zhu, X. Liu, G. Geng and L. Sun, *Acs Appl. Mater. Interfaces*, 2014, **6**, 20340-20349.

S6 S. Bandyopadhyay, A.G. Anil, A. James and A. Patra, *Acs Appl. Mater. Interfaces*, 2016, **8**, 27669-27678.

S7 S. M. Mahurin, J. Gorka, K. M. Nelson, R. T. Mayes and S. Dai, *Carbon*, 2014, **67**, 457-464.

S8 M. Dinca and J. Long, *J. Am. Chem. Soc.*, 2005, **127**, 9376-9377.

S9 H. Wei, W. Qian, N. Fu, H. Chen, J. Liu, X. Jiang, G. Lan, H. Lin and S. Han, *J. Mater. Sci.*, 2017, **52**, 10308-10320.

S10 J. Wei, D. Zhou, Z. Sun, Y. Deng, Y. Xia and D. Zhao, *Adv. Funct. Mater.*, 2013, **23**, 2322-2328.

S11 D. L. Sivadas, R. Narasimman, R. Rajeev, K. Prabhakaran and K. N. Ninan, *J. Mater. Chem. A*, 2015, **3**, 16213-16221.

S12 R. Narasimman, S. Vijayan and K. Prabhakaran, *Rsc. Adv.*, 2014, **4**, 578-582.

S13 L. Wang and R. T. Yang, *J. Phys. Chem. C*, 2012, **116**, 1099-1106.

S14 J. Wang, I. Senkovska, M. Oschatz, M. R. Lohe, L. Borchardt, A. Heerwig, Q. Liu and S. Kaskel, *Acs Appl. Mater. Interfaces*, 2013, **5**, 3160-3167.

S15 S. Gadipelli and Z. X. Guo, *ChemSusChem*, 2015, **8**, 2123-2132.

S16 J. W. F. To, J. He, J. Mei, R. Haghpanah, Z. Chen, T. Kurotsawa, S. Chen, W. G. Bae, L. Pan, J. B. H. Tok, J. Wilcox and Z. Bao, *J. Am. Chem. Soc.*, 2016, **138**, 1001-1009.

S17 D. Lee, C. Z. Zhang, C. Wei, B. L. Ashfeld and H. Gao, *J. Mater. Chem.*, 2013, **1**, 14862-14867.

S18 S. Khalili, B. Khoshhandam and M. Jahanshahi, *RSC Adv.*, 2016, **6**, 35692-35704.