

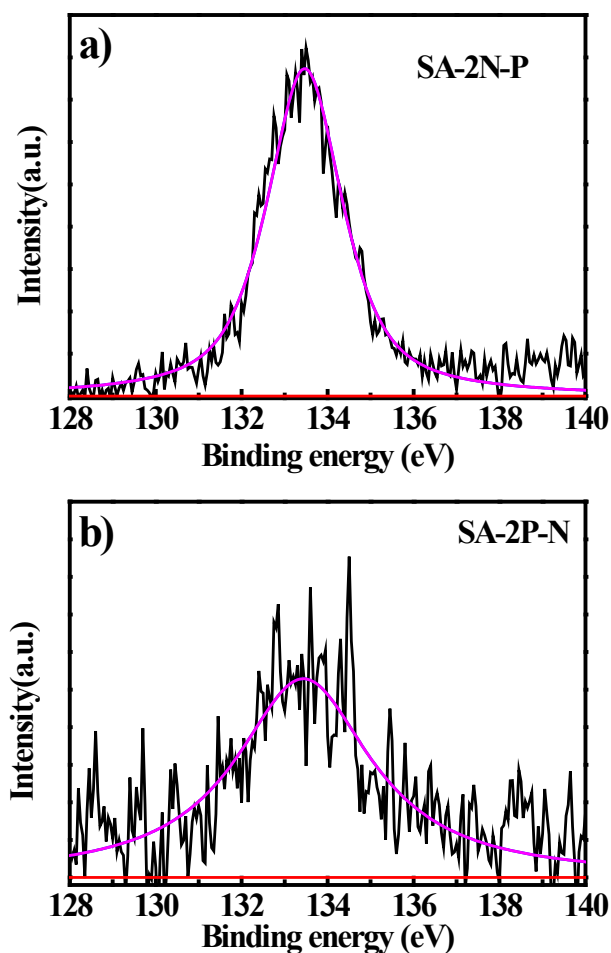
Electronic supplementary information (ESI)

A novel activating strategy to achieve highly porous carbon monolith for CO₂ capture

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Fig. S1 XPS P2p spectra of the samples (a) SA-2N-P and (b) SA-N-2P, respectively.



The high-resolution P2p XPS spectra of the samples (a) SA-2N-P and (b) SA-N-2P are shown in Figure S1. Two samples both display only one peak of P2p at 133.3 eV, which can be assigned to P-O bonding. However, the peak of P2p of P-C centered at 130.6 eV cannot be found, indicating that the P species exhibit in the form of PO_4^{3-} .

The Ideal Adsorption Solution Theory (IAST) calculations.

1. Pure component isotherm fitting

The pure component adsorption isotherms of CO₂ and N₂ on the SA-2N-P at 298 K and pressure up to 1 atm are given in Fig. 6a.

The experimental adsorption isotherms were fitted with a dual-site Langmuir model as follows:^{S4-S7}

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

where we have two distinct adsorption sites A and B; b_i dual-Langmuir constant (Pa⁻¹); q_i molar loading of species i , mmol g⁻¹; $q_{sat,i}$ saturation capacity of species i , mmol g⁻¹.

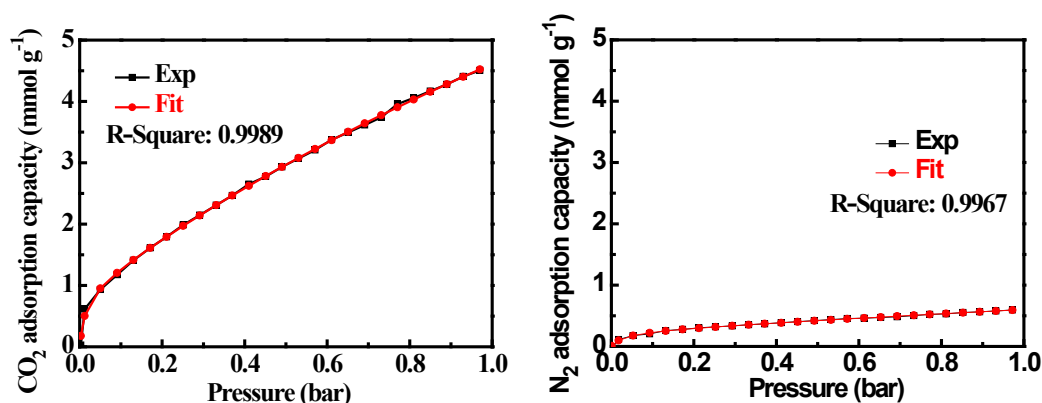


Fig. S2. CO₂ and N₂ gas adsorption isotherms for SA-2N-P at 298 K (black). The red lines correspond to dual-site Langmuir equation fit.

2. The adsorption selectivity, S_{ads} , for binary mixtures of **1** and **2**, is defined as follows:

$$S_{ads} = \frac{q_1 / q_2}{p_1 / p_2} \quad (2)$$

where q_i is the amount of i adsorbed and p_i is the partial pressure of i in the mixture

for CO₂ over N₂ in flue-gas streams (typically 15% CO₂ and 85% N₂) was estimated from the experimental single-component isotherms. The SA-2N-P exhibits high adsorption selectivity of 29 for CO₂ over N₂ at 295 K and 1 bar.

References:

- S1. Z. W Liu, F. Peng, H. J. Wang, H. Yu, W. X. Zheng and J. Yang, *Angew. Chem. Int. Ed.*, 2011, **123**, 3315.
- S2. D. S. Yang, D. Bhattacharjya, S. Inamdar, J. Park and J. S. Yu, *J. Am. Chem. Soc.* 2012, **134**, 16127.
- S3. C. H. Choi, S. H. Park and S. I. Woo, *J. Mater. Chem.*, 2012, **22**, 12107
- S4. W. G. Lu, J. P. Sculley, D. Q. Yuan, R. Krishna, Z. W. Wei, and H. C. Zhou, *Angew. Chem., Int. Ed.*, 2012, **51**, 7480.
- S5. W. G. Lu, D. Q. Yuan, J. Sculley, D. Zhao, R. Krishna and H. C. Zhou, *J. Am. Chem. Soc.*, 2011, **133**, 18126.
- S6. Y. F. Zhao, L. Zhao, K. X. Yao, Y. Yang, Q. Zhang and Y. Han, *J. Mater. Chem.*, 2012, **22**, 19726.
- S7. Y. F. Zhao, X. Liu, K. X. Yao, L. Zhao and Y. Han, *Chem. Mater.*, 2012, **24**, 4725.