Electronic Supplementary Information

Synthesis of polybenzoxazine based nitrogen-rich porous carbons for carbon dioxide capture

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Contents

Table S1 Elemental and XPS analysis of all samples.

Sample	Elemental analysis (wt. %)				XPS analysis (at. %)		
	C	H	N	O	C	N	O
NPC-c	78.31	2.33	5.67	13.69	87.90	4.51	7.59
NPC-0	78.28	2.25	5.32	14.15	87.75	4.36	7.89
NPC-1	77.96	2.27	5.27	14.50	87.10	4.26	8.64
NPC-2	77.63	2.22	5.25	14.90	87.05	4.24	8.87
NPC-3	77.60	2.20	5.24	14.96	86.75	4.23	9.02
NPC-4	77.54	2.15	5.21	15.10	86.59	4.18	9.23

Table S2 XPS peak positions and relative content of N species in the NPCs.

Sample	N-6	N-5	N-Q	N-X
	398.5 eV	400.2 eV	401 eV	403 eV
NPC-c	32.51	51.18	11.18	5.14
NPC-0	33.72	44.17	13.43	8.68
NPC-1	30.98	51.43	12.19	5.39
NPC-2	29.08	54.54	12.86	3.51
NPC-3	25.37	56.26	13.75	4.62
NPC-4	21.47	59.27	14.19	5.07

Table S3 Elemental and XPS analysis of NPC-2 and NPC-2-HCl.

Sample	Elemental analysis (wt. %)				XPS analysis (at. %)			
	C	H	N	O	C	N	O	Cl
NPC-2	77.63	2.22	5.25	14.90	87.05	4.24	8.87	-
NPC-2-HCl	76.55	2.84	5.22	15.38	83.14	4.05	9.75	3.06

Table S4 The textural properties and CO_2 uptakes of NPC-2 and NPC-2-HCl.

Sample	S_{BET} (m^2 g^{-1})	S_{micro} (m^2 g^{-1})	V_{total} (cm^3 g^{-1})	CO_2 uptake (mmol g^{-1})		CO_2 uptake/S_{BET} (μmol m^{-2})	
				0 °C	25 °C	0 °C	25 °C
NPC-2	1255.9	1108.4	0.63	6.35	4.02	5.06	3.20
NPC-2-HCl	1171.3	1056.5	0.60	4.79	3.09	4.09	2.64

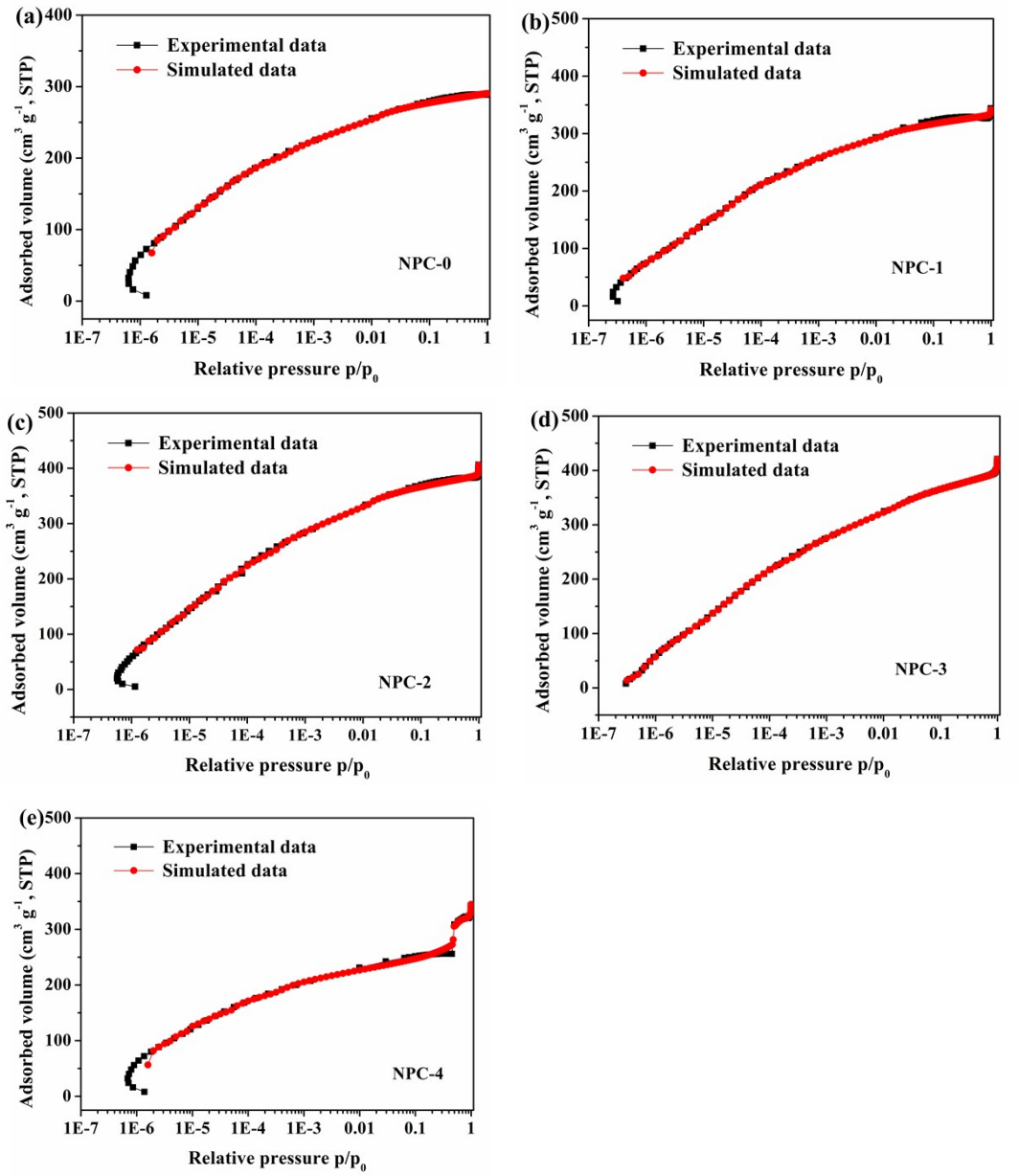

Fig. S1 DFT fit between the carbon slit adsorption branch kernel (red circle) and the experimental data (nitrogen adsorption, black square) for (a) NPC-0, (b) NPC-1, (c) NPC-2, (d) NPC-3, and (e) NPC-4.

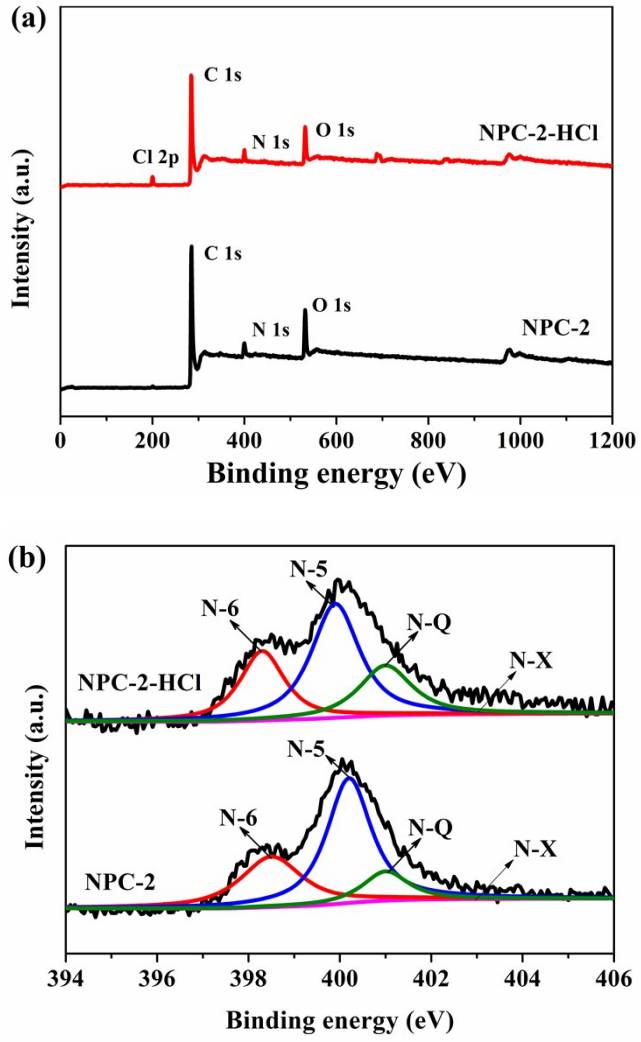

Fig. S2 XPS spectrum of NPC-0 and NPC-2-HCl (a) survey spectra, and (b) N 1s spectra.

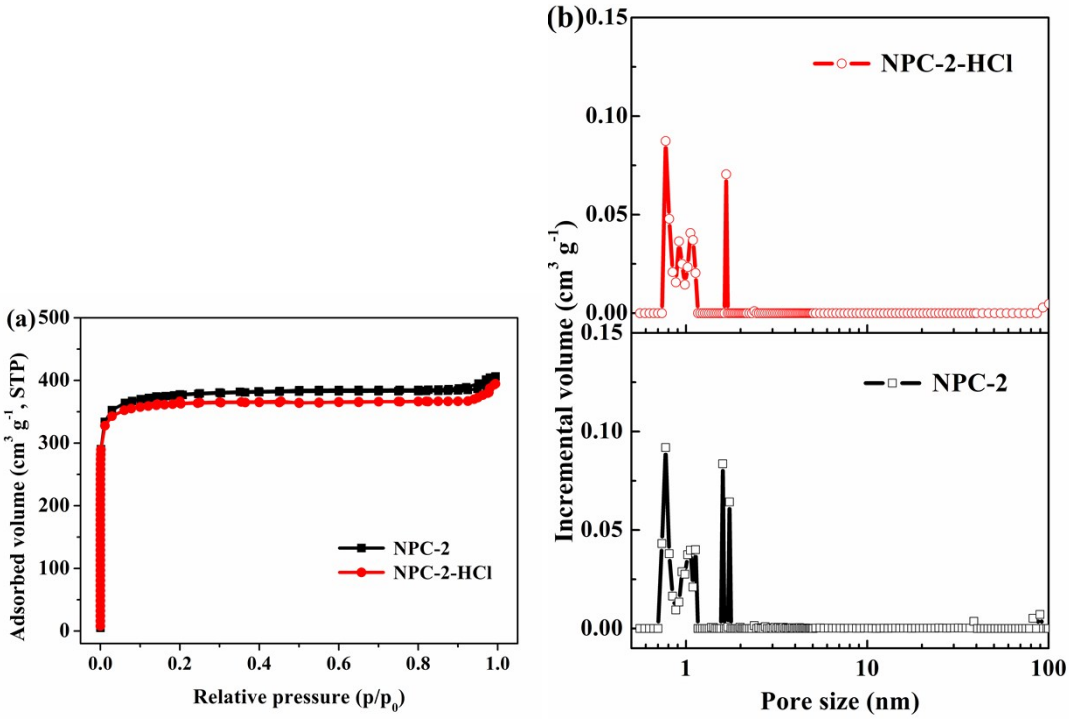

Fig. S3 (a) N_2 sorption isotherms and (b) DFT pore size distributions for the NPC-2 and NPC-2-HCl.

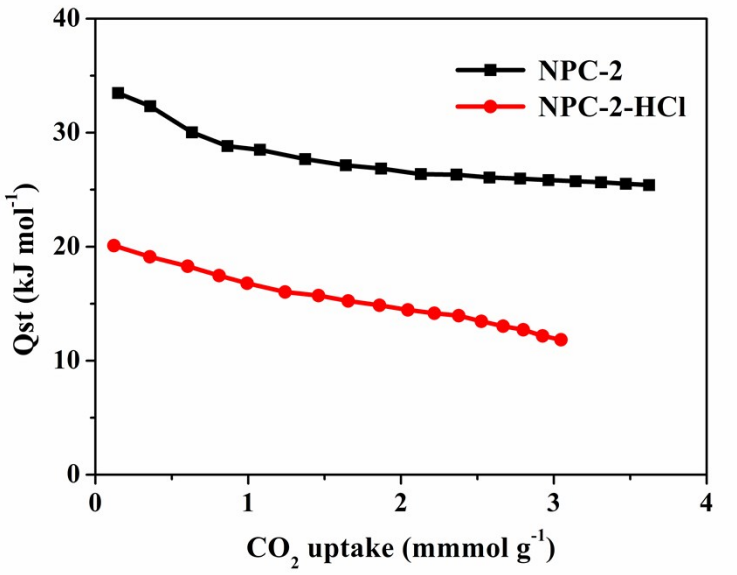

Fig. S4 Isosteric heat of CO_2 adsorption for NPC-2 and NPC-2-HCl.

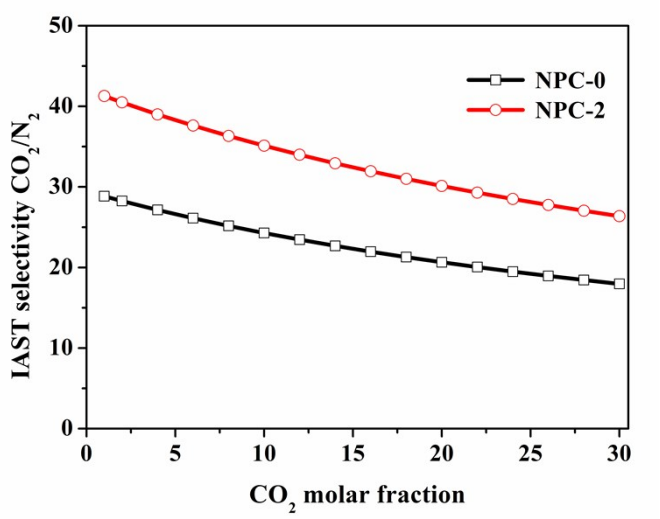

Fig. S5 CO_2/N_2 selectivity versus CO_2 molar fraction with the overall pressure of 1.0 bar. The calculations were based on the single-component gas adsorption data at 25 ^oC by the IAST method.

Firstly, the experimental single-component gas CO_2 adsorption isotherms of NPC-0 and NPC-2 can be modeled adequately using a single-site Langmuir model:[1,2]

$$q_i = q_{i,sat} \times \frac{b_i p_i}{1 + b_i p_i}$$

where b_i is the Langmuir constant, Pa^{-1}; p_i is the bulk gas phase pressure of species i, Pa; q_i is the molar loading of species i, mmol g^{-1}; $q_{i,sat}$ is the saturation capacity of species i, mmol g^{-1}.

The fitted parameters of the CO_2 adsorption isotherm data at 25 ^oC for NPC-0 and NPC-2 using a single-site Langmuir model are listed in the following table, which are aimed to enable application of IAST in simulating the property of each adsorbent under a mixed CO_2/N_2 gas.

The fitted parameters derived from the single-site Langmuir model.

Sample	$q_{i,sat}$ (mmol g^{-1})	$b_i \times 10^5$ (Pa^{-1})	R-square
NPC-0	4.4179	2.130	0.9920
NPC-2	5.7683	1.987	0.9928

Reference:

1 Y. F. Zhao, X. Liu, K. X. Yao, L. Zhao, Y. Han. *Chem. Mater.*, 2012, **24**, 4725-4734.

2 J. A. Mason, K. Sumida, Z. R. Herm, R. Krishna, J. R. Long. *Energy Environ. Sci.*, 2011, **4**, 3030-3040.