ChemistryOPEN

Supporting Information

High Gas Uptake and Selectivity in Hyper-Crosslinked Porous Polymers Knitted by Various Nitrogen-Containing Linkers

Ziyan Jia,[a, b] Jiannan Pan,[b] and Daqiang Yuan*[a]

open_201700073_sm_miscellaneous_information.pdf

Ideal adsorbed solution theory (IAST) selectivity studies:

In order to estimate the CO_2/N_2 separation efficiency for the HCPs, a single-site Langmuir-Freundlich model was used to get selectivity parameters according to the ideal adsorbed solution theory (IAST) of Myers and Prausnitz.[1] The IAST calculations were carried out for binary mixture containing 15 % CO_2 (y1) and 85 % N_2 (y2), which is typical of flue gases. The pure component isotherms of CO_2 and N_2 measured at 273 K and 295 K were fitted with the single-site Langmuir-Freundlich model:

$$\boldsymbol{N = \mathrm{A}\frac{bP^c}{1 + bP^c}}$$

N: molar loading of species i, mmol/g

A: saturation capacity of species i, mmol/g

P: pressure, kPa

b: constant, kPa^{-1}

c: constant

The adsorption selectivities, S_{ads}, for binary mixtures of CO_2/N_2, defined by $S_{\mathrm{ads}} = \frac{x_1/x_2}{y_1/y_2}$

S_{ads}: adsorption selectivity

x_i: the mole fractions of component i in the adsorbed phases

y_i: the mole fractions of component i in the bulk phases

[1] Myers, A. L.; Prausnitz, J. M. AICHE J. 1965, 11, 121.

Figure S1. Color of the HCP-1-4 (from left to right). .

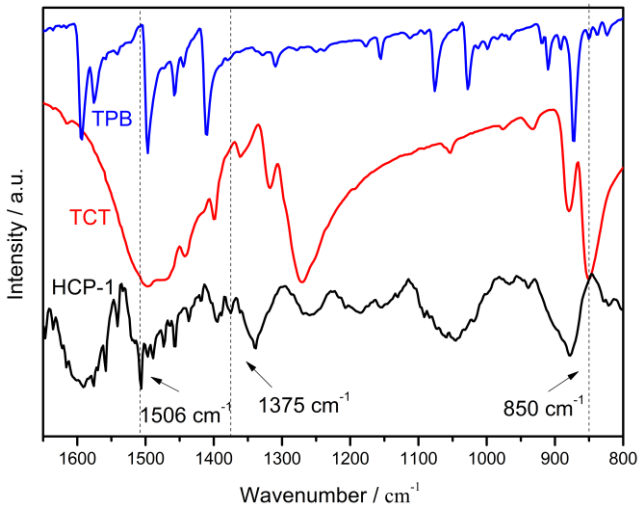

Figure S2. FT-IR spectra of HCP-1 and related starting materials.

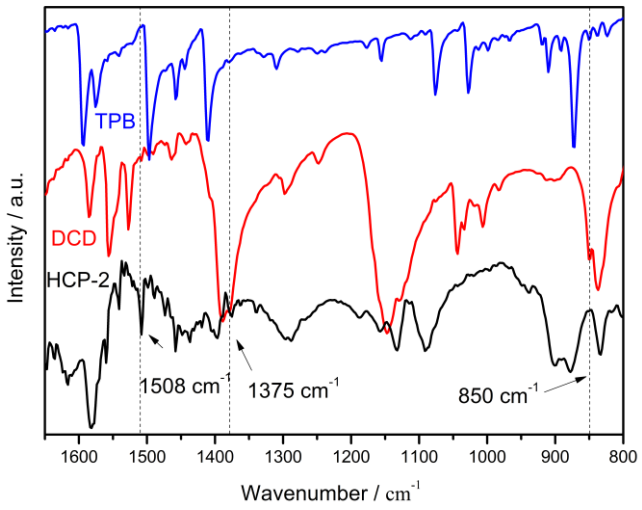

Figure S3. FT-IR spectra of HCP-2 and related starting materials.

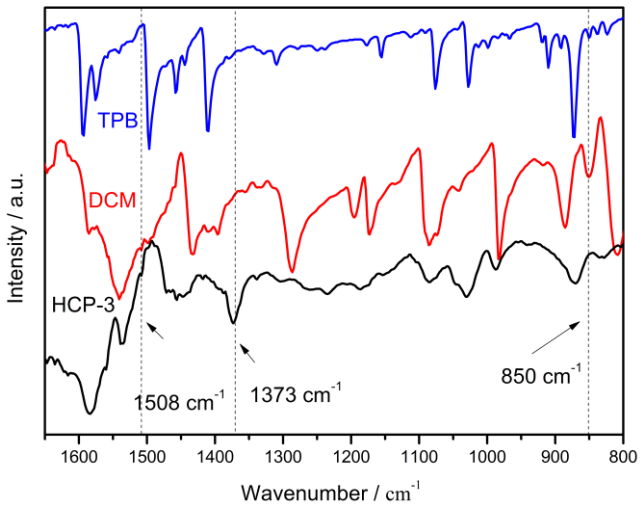

Figure S4. FT-IR spectra of HCP-3 and related starting materials.

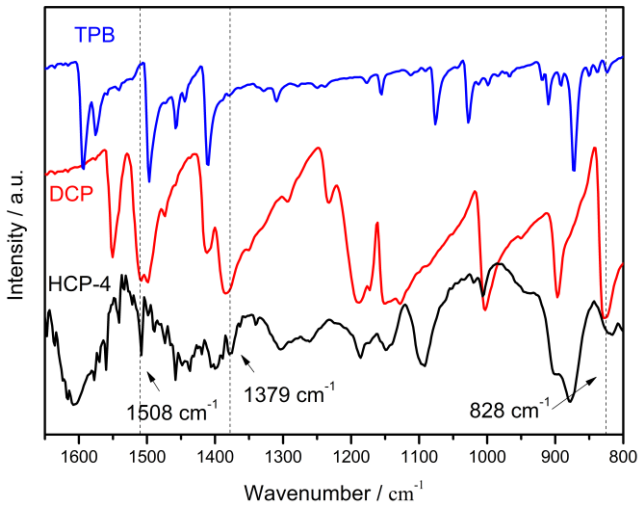

Figure S5. FT-IR spectra of HCP-4 and related starting materials.

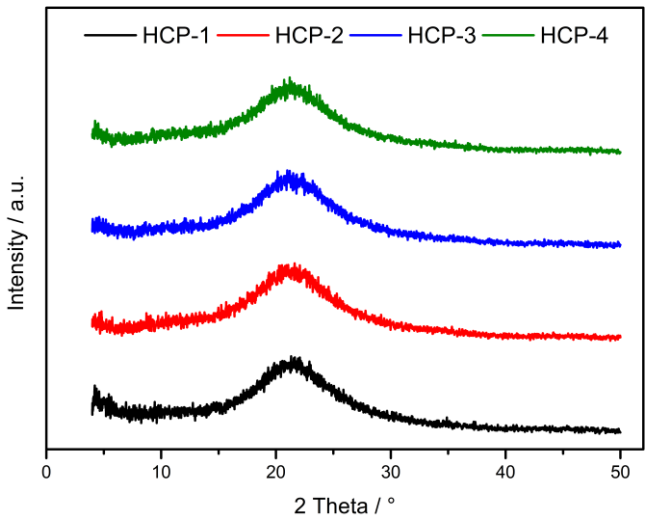

Figure S6. X-ray diffraction patterns of HCP-1-4.

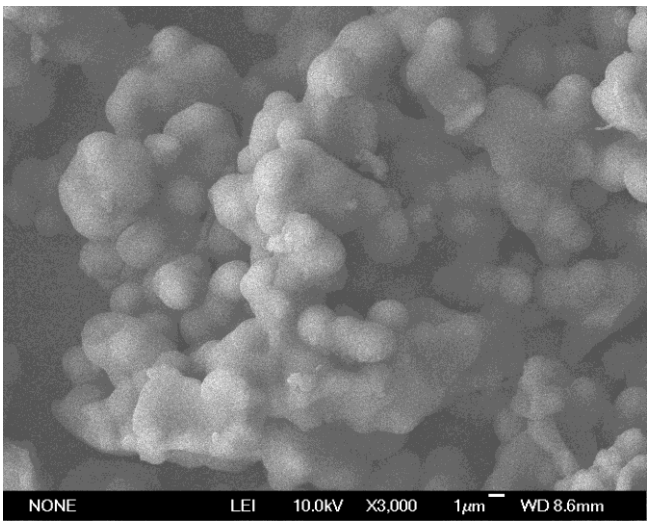

Figure S7. SEM image of HCP-1.

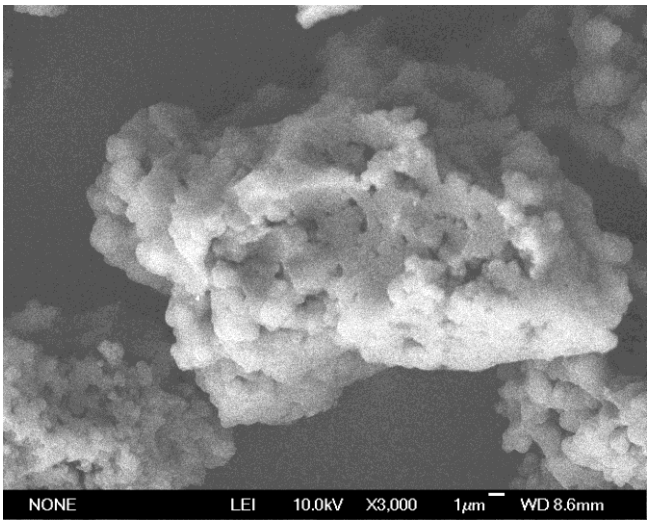

Figure S8. SEM image of HCP-2.

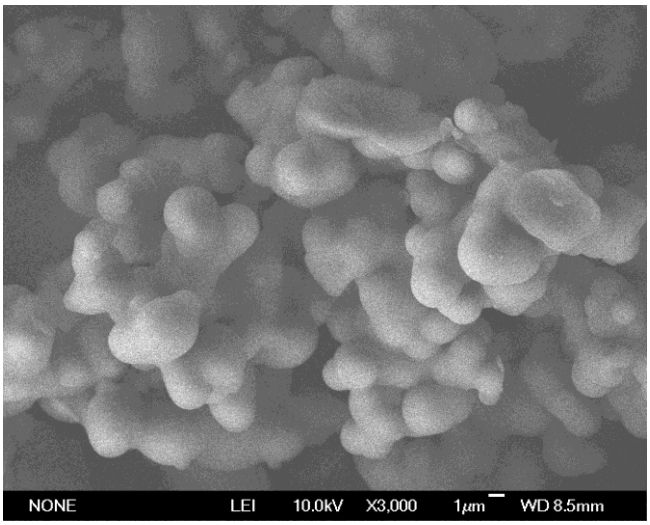

Figure S9. SEM image of HCP-3.

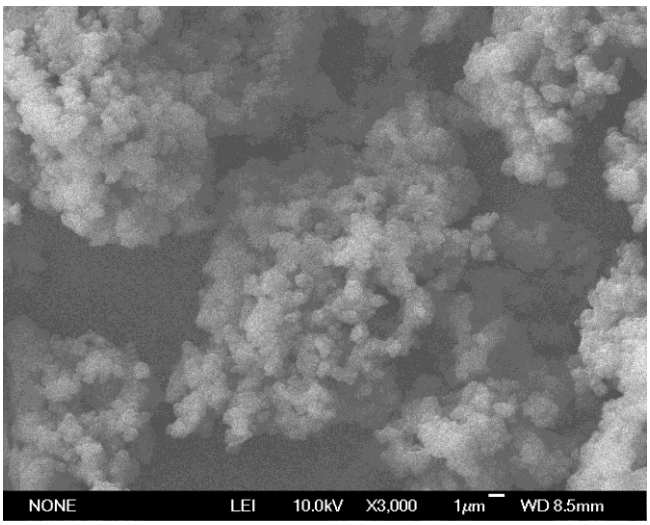

Figure S10. SEM image of HCP-4.

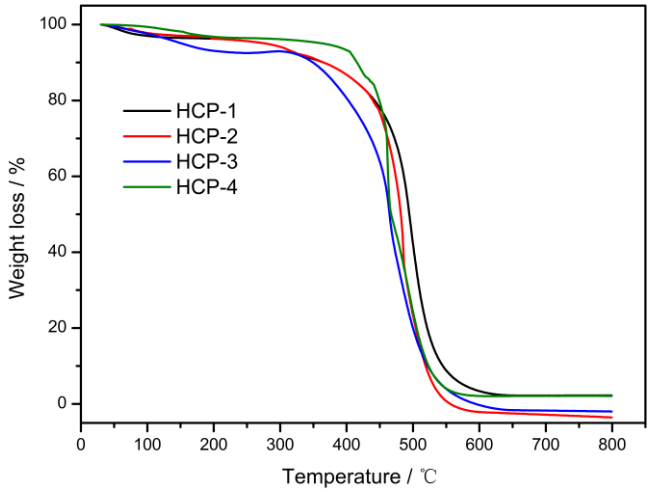

Figure S11. Thermogravimetric analysis of HCP-1-4 under air atmosphere.

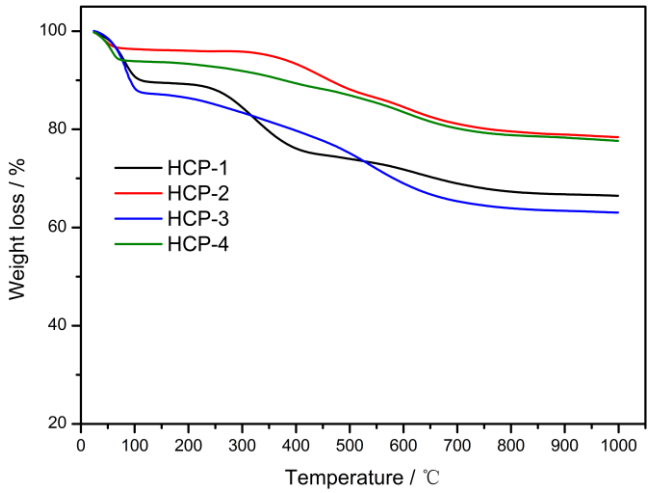

Figure S12. Thermogravimetric analysis of HCP-1-4 under nitrogen atmosphere.

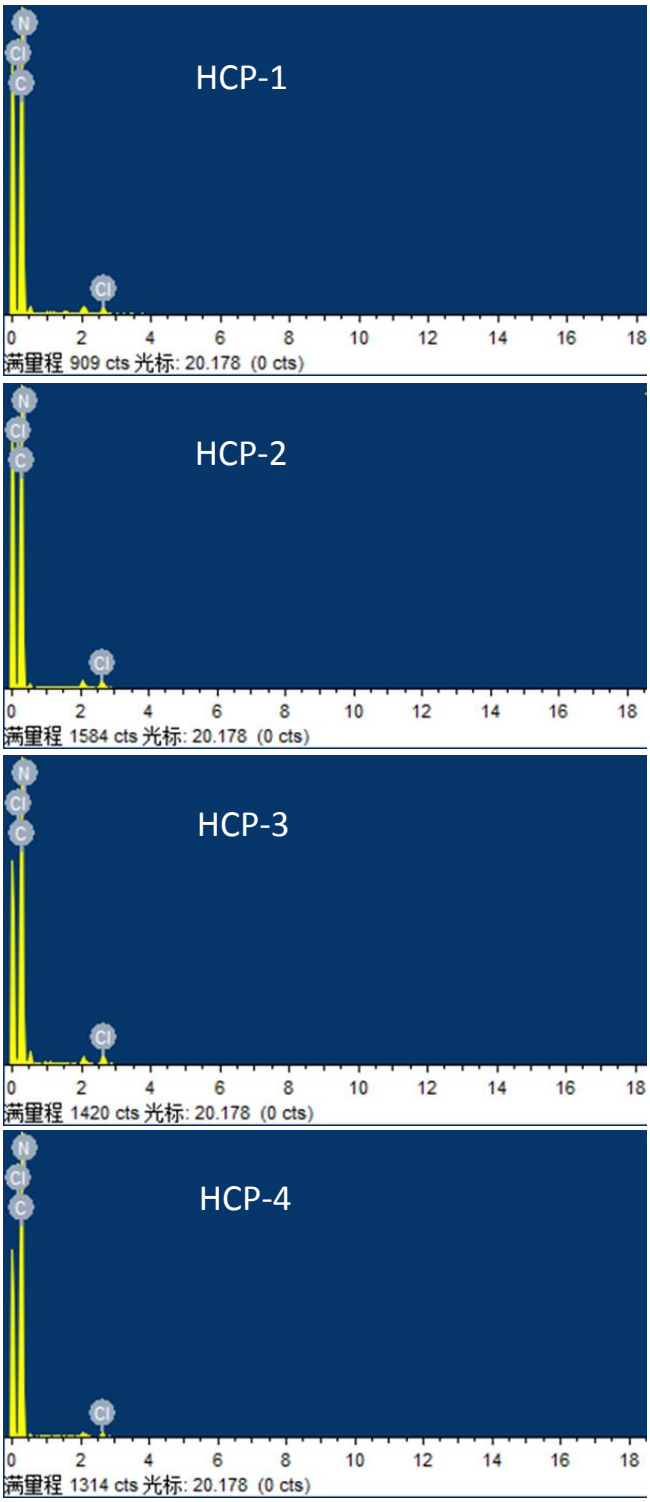

Figure S13. EDS analysis of HCP-1-4.

Table S1 The weight percentages of different elements in HCPs.

Polymers	C (%)	H (%)	N (%)	Cl (%)	Al (%)
HCP-1	70.45	5.70	5.95	1.05	0.29
HCP-2	81.85	4.61	1.82	1.26	0.40
HCP-3	71.46	5.72	4.52	1.92	0.34
HCP-4	85.21	4.85	1.08	1.34	0.25