

## Supporting Information

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Figure S10. Adsorption selectivity of CO<sub>2</sub> over CH<sub>4</sub> and N<sub>2</sub> for PHCTF-2b calculated from Henry's law initial slope method at 273 K.

### Experimental section:

Calculation methods for  $Q_{st}$ ,  $Q_0$ ,  $A_0$ ,  $K_H$  values:

The isosteric enthalpies ( $Q_{st}$ ) of CO<sub>2</sub> in PHCTFs were calculated from the adsorption isotherms measured at different temperatures in term of Clausius-Clapeyron equation:

$$\ln P = \frac{Q_{st}}{RT} + C \quad (1)$$

where  $R$ ,  $C$ ,  $P$  and  $T$  are the gas constant, equation constant, the pressure and temperature at the equilibrium state, respectively. The first virial coefficients ( $A_0$ ) are obtained from the slopes of the virial plots. From their intercepts,  $A_0$  values relating to gas-material interaction were calculated. Henry's law constants ( $K_H$ ) are calculated from the equation  $K_H = \exp(A_0)$ . Then, the limiting enthalpy of adsorption at zero surface CO<sub>2</sub> coverage ( $Q_0$ ) can be obtained in term of Vant Hoff equation:

$$\frac{d [\ln K_H]}{dT} = \frac{Q_0}{RT^2} \quad (2)$$

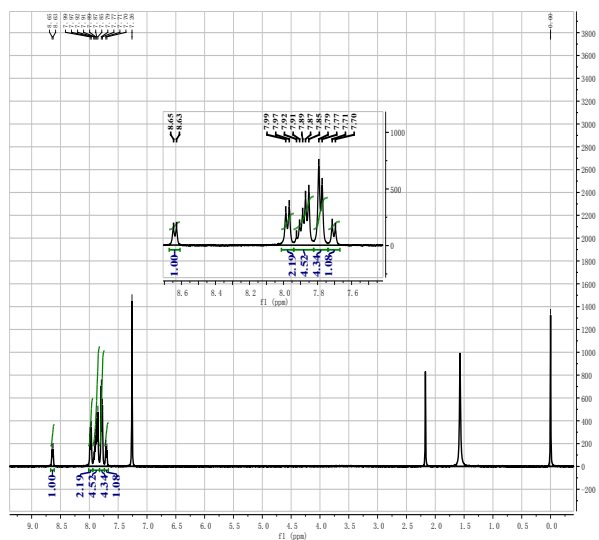


Figure S1.  $^1\text{H-NMR}$  spectrum of PHPZ-DN.

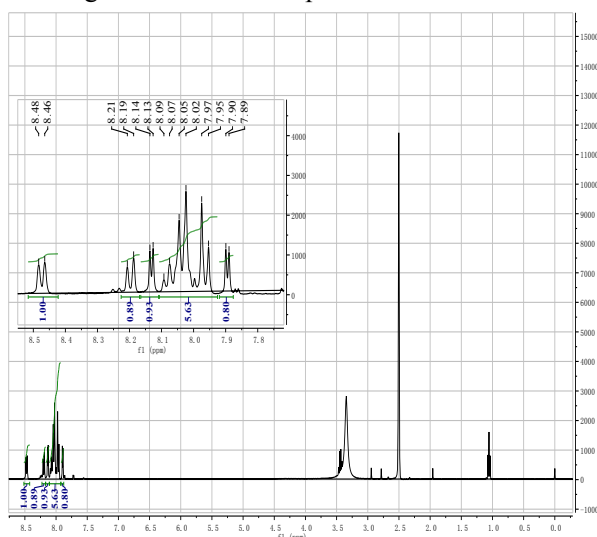


Figure S2.  $^1\text{H-NMR}$  spectrum of THPZ-DN.

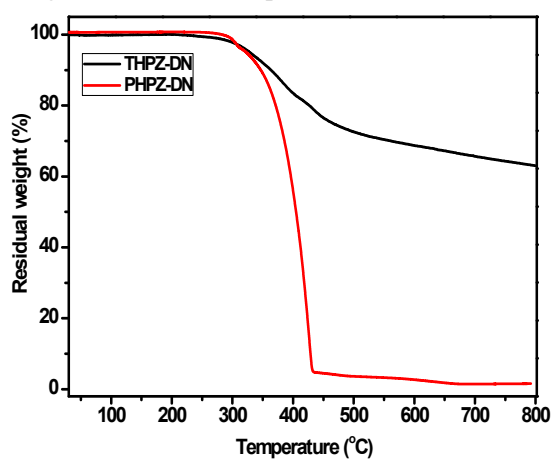


Figure S3. TGA thermograms of PHPZ-DN and THPZ-DN under nitrogen atmosphere.

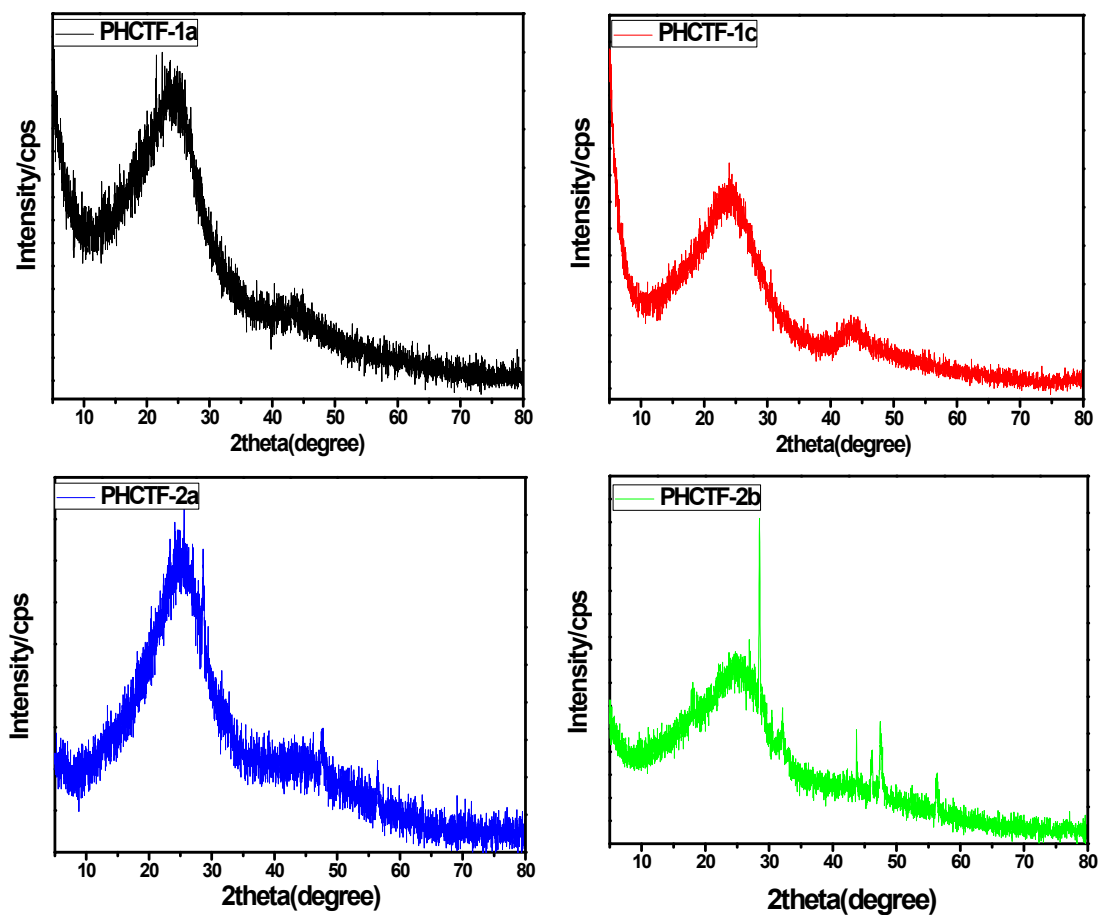


Figure S4. PXRD patterns of PHCTF-1a, PHCTF-1c, PHCTF-2a and PHCTF-2b.

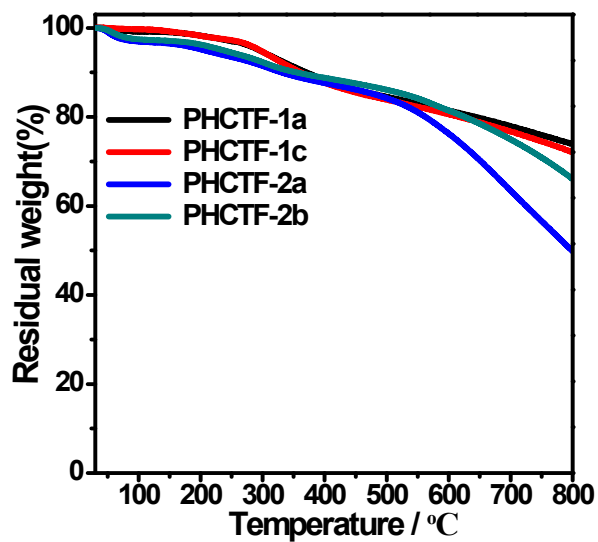


Figure S5. TGA curves of PHCTF-1a, PHCTF-1c, PHCTF-2a and PHCTF-2b in nitrogen atmosphere.

Table S1. Elemental analysis data of PHCTFs.

	Calculated(%)						Found(%)					
	C	H	N	S	C/N	C/H	C	H	N	S	C/N	C/H
PHCTF-1a	75.9	3.5	16.1	--	4.7	21.9	74.6	3.2	7.8	--	9.5	23.2
PHCTF-1b	75.9	3.5	16.1	--	4.7	21.9	74.3	3.0	7.4	--	10.0	24.8
PHCTF-1c	75.9	3.5	16.1	--	4.7	21.9	76.9	2.8	5.6	--	13.7	27.5
PHCTF-2a	67.8	2.8	15.8	9.1	4.3	24.2	56.9	2.5	13.8	3.0	4.1	22.8
PHCTF-2b	67.8	2.8	15.8	9.1	4.3	24.2	56.1	2.3	13.3	3.1	4.2	24.4

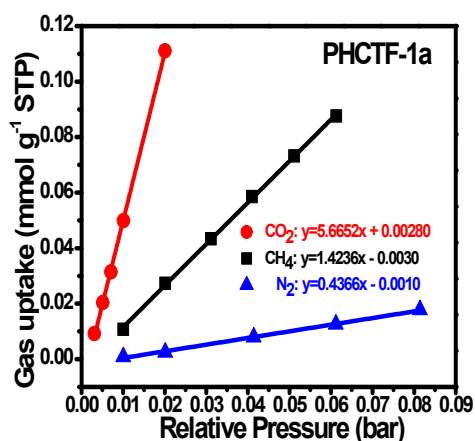


Figure S6. Adsorption selectivity of CO<sub>2</sub> over CH<sub>4</sub> and N<sub>2</sub> for PHCTF-1a calculated from Henry's law initial slope method at 273 K.

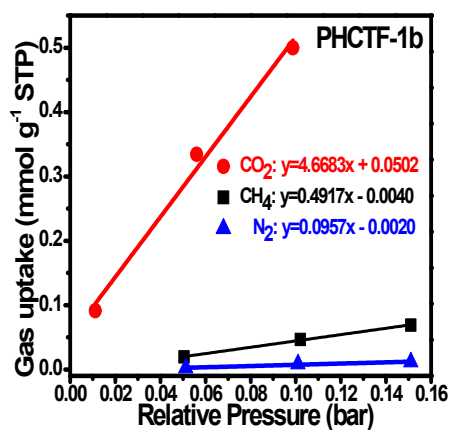


Figure S7. Adsorption selectivity of CO<sub>2</sub> over CH<sub>4</sub> and N<sub>2</sub> for PHCTF-1b calculated from Henry's law initial slope method at 273 K.

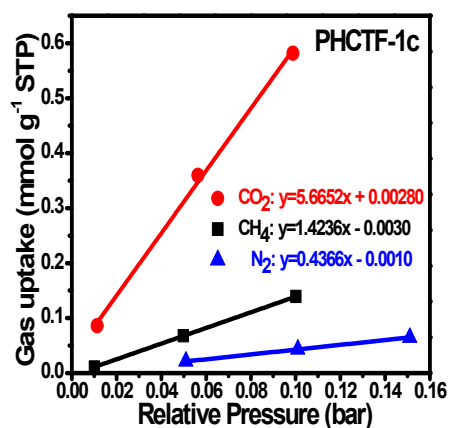


Figure S8. Adsorption selectivity of CO<sub>2</sub> over CH<sub>4</sub> and N<sub>2</sub> for PHCTF-1c calculated from Henry's law initial slope method at 273 K.

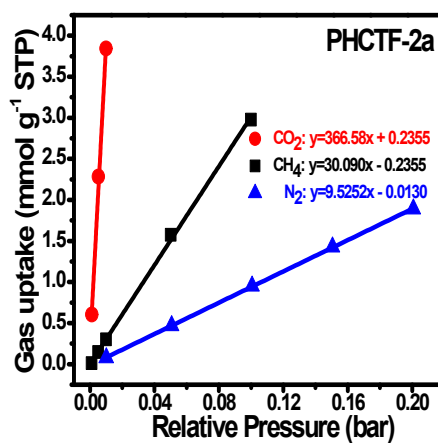


Figure S9. Adsorption selectivity of CO<sub>2</sub> over CH<sub>4</sub> and N<sub>2</sub> for PHCTF-2a calculated from Henry's law initial slope method at 273 K.

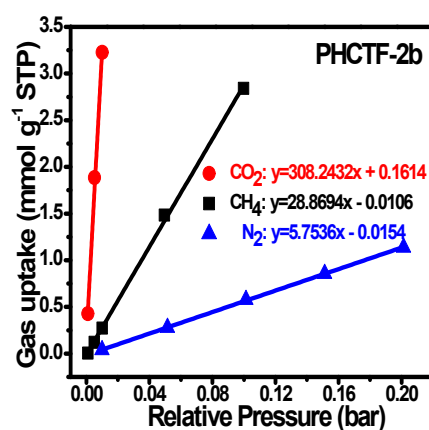


Figure S10. Adsorption selectivity of CO<sub>2</sub> over CH<sub>4</sub> and N<sub>2</sub> for PHCTF-2b calculated from Henry's law initial slope method at 273 K.