Electronic Supplementary Information for

Benzimidazole functionalized Covalent Triazine Frameworks for CO_2 capture

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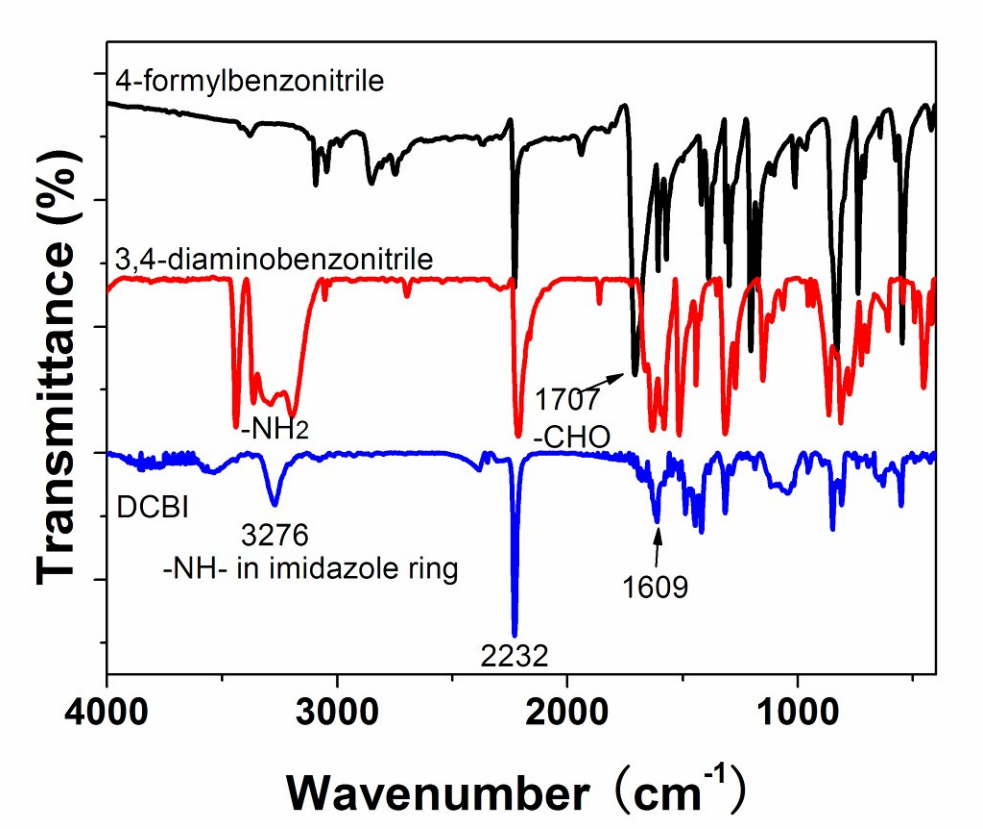

Fig. S1 FT-IR spectra of DCBI and corresponding reactants (KBr pellets)

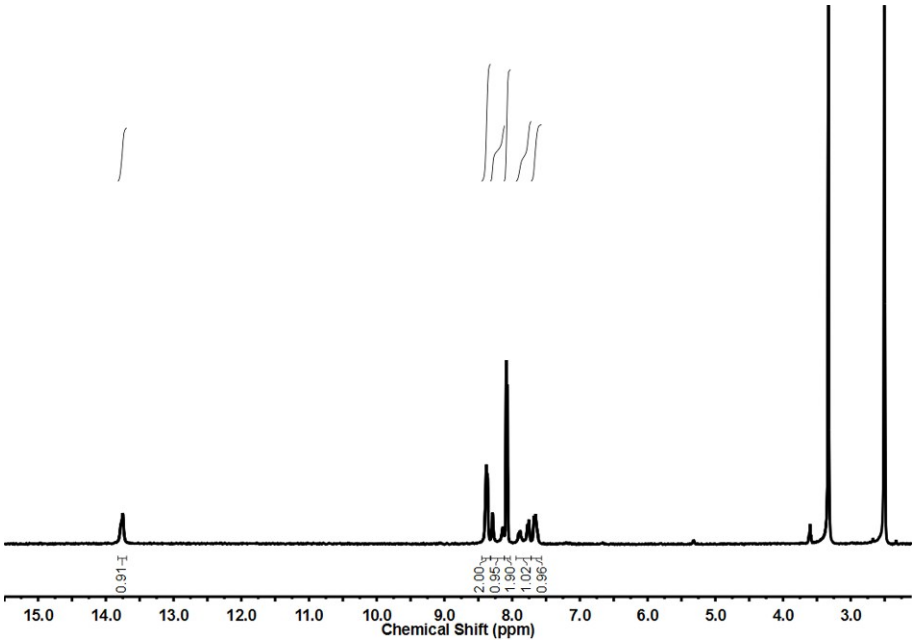

Fig. S2 ^{1}H NMR spectrum of DCBI (DMSO-d_6, 400 MHz)

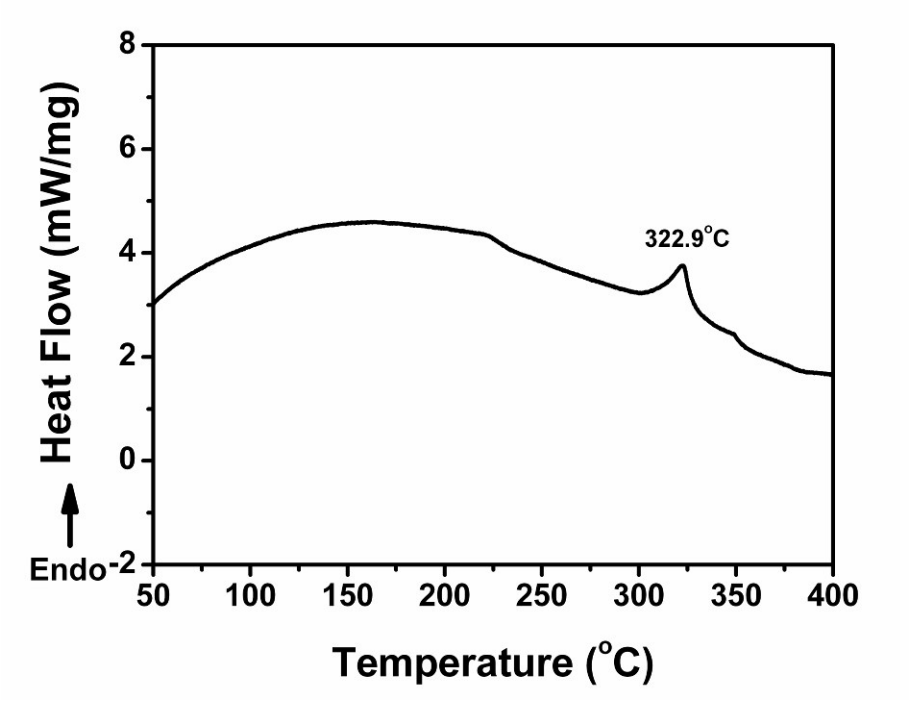

Fig. S3 DSC curve of DCBI (N_2, 10 °C /min)

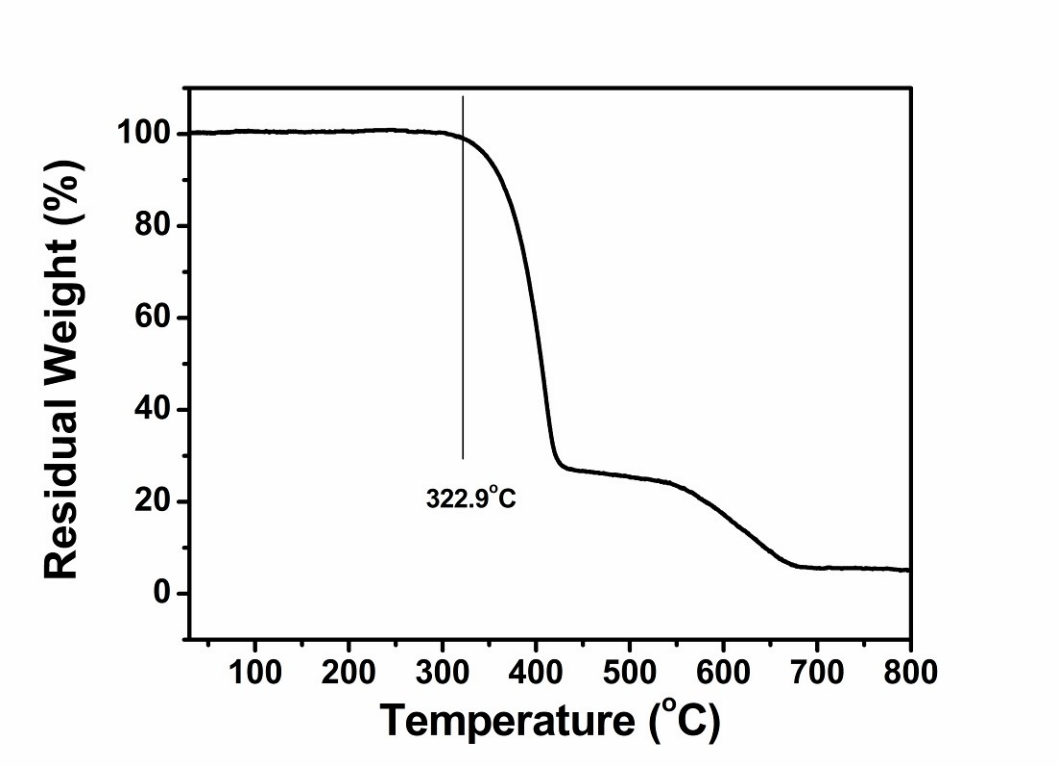

Fig. S4 TGA curve of DCBI (N_2, 10 °C /min)

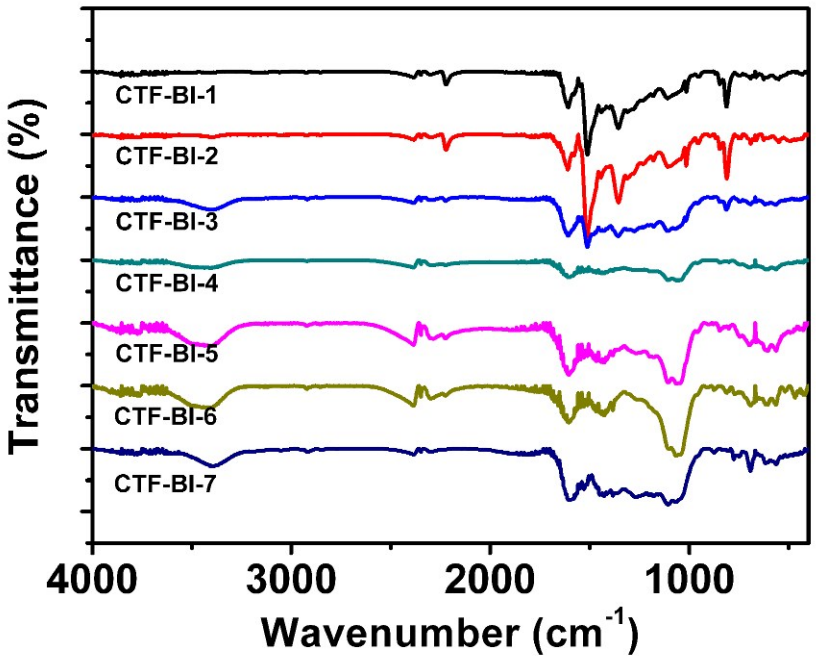

Fig. S5 FT-IR spectra of the CTF-BIs obtained from different ratios of $ZnCl_2$ to DCBI (KBr pellets)

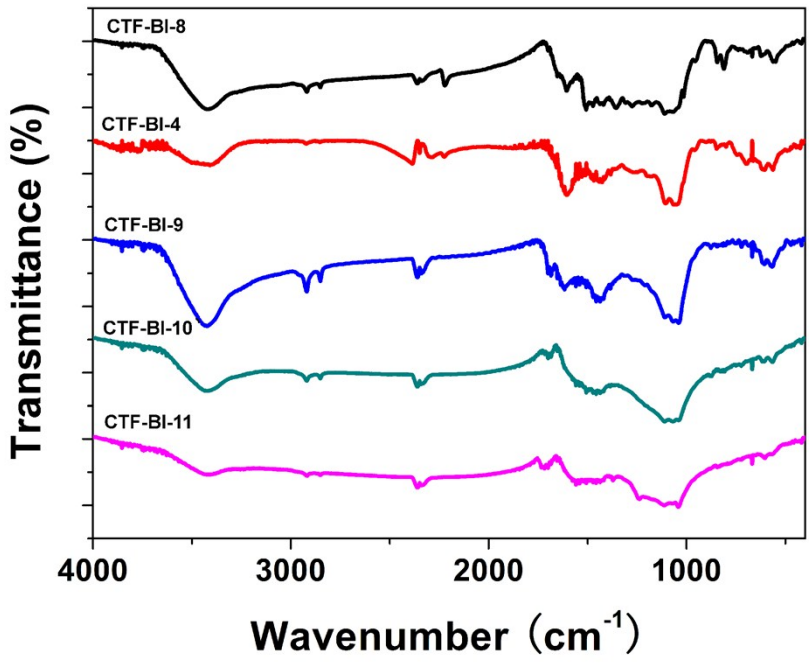

Fig S6 FT-IR spectra of the CTF-BIs obtained from different reaction temperatures.

(KBr pellets)

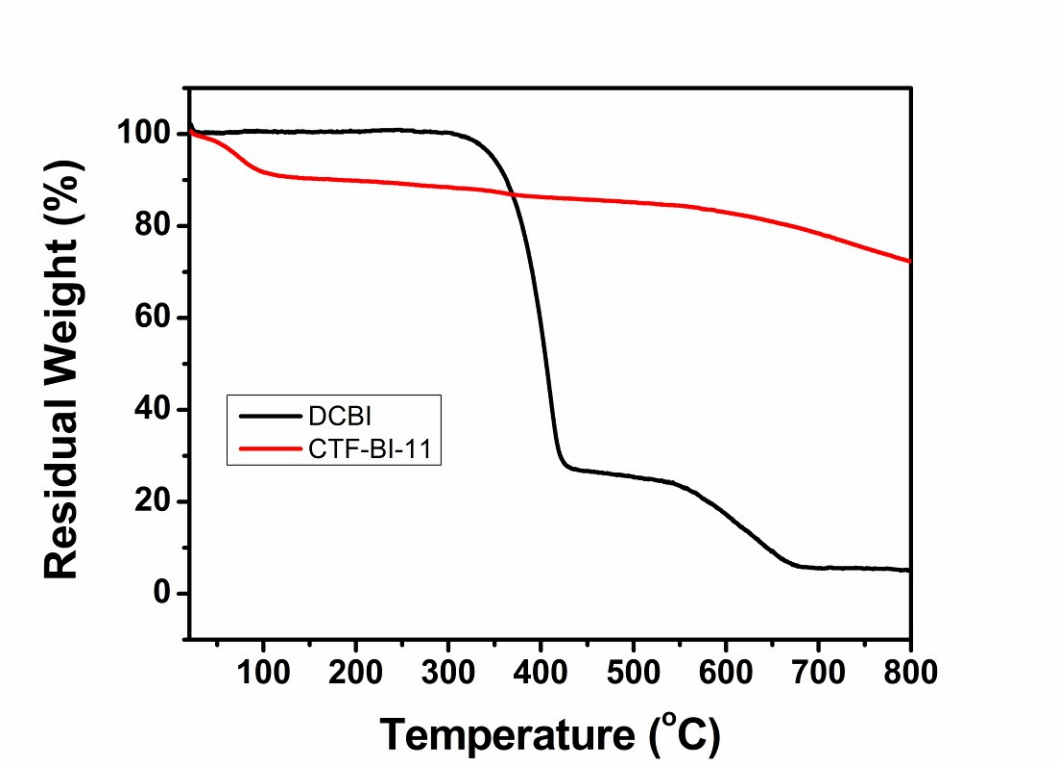

Fig. S7 TGA curve of DCBI and CTF-BI-11 (N_2, 10 °C /min)

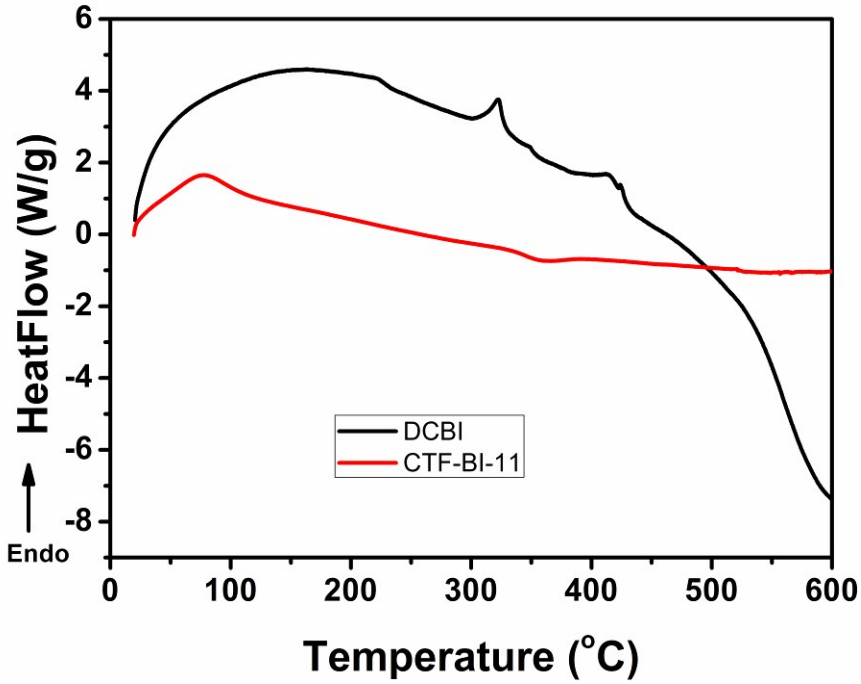

Fig. S8 DSC curves of DCBI and CTF-BI-11 (10 °C/min, N_2)

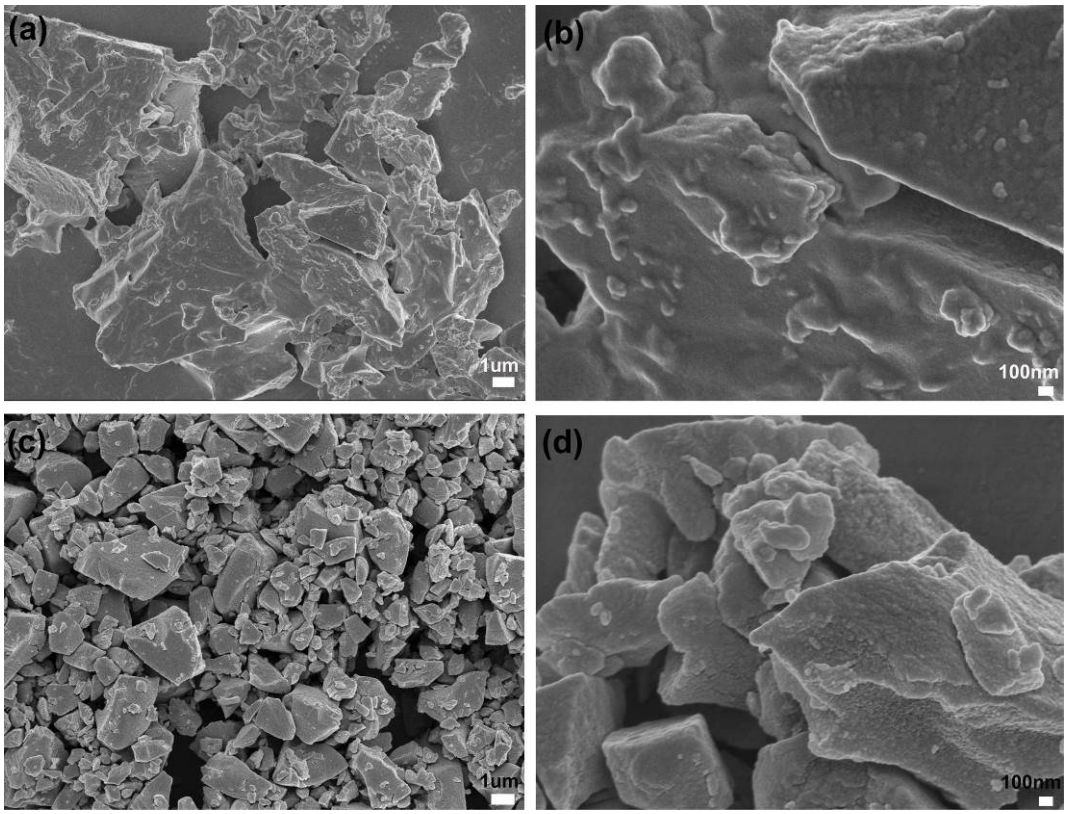

Fig. S9 FESEM images of CTF-BI-4 (a) and (b) and CTF-BI-11 (c) and (d)

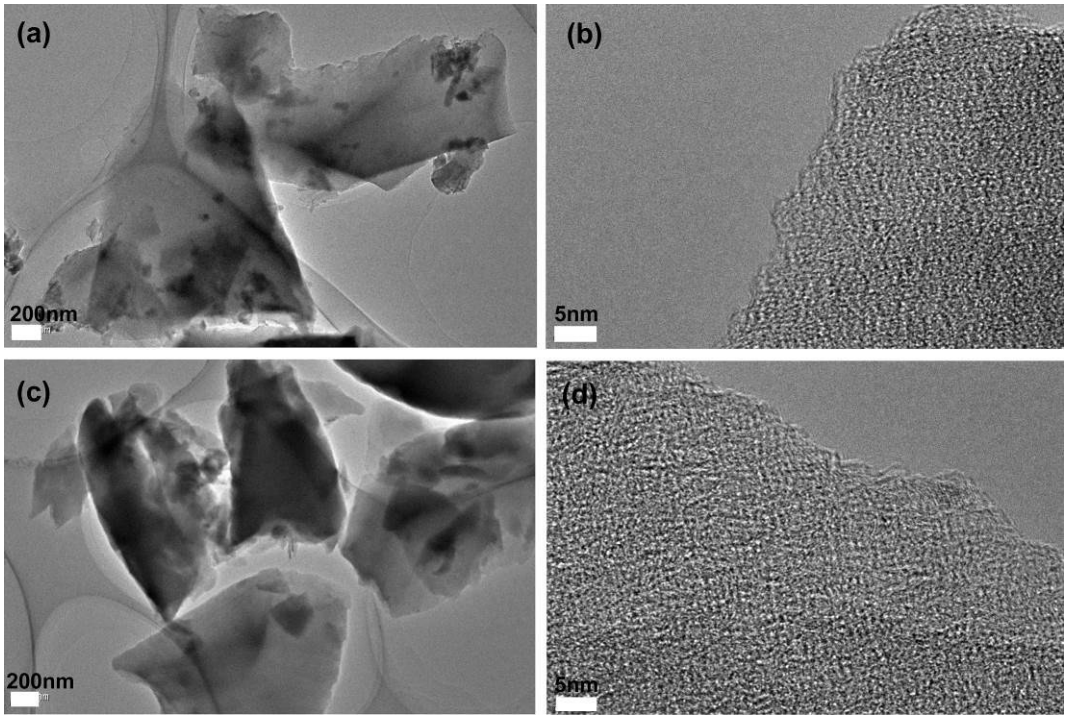

Fig. S10 TEM images of CTF-BI-4 (a) and (b) and CTF-BI-11 (c) and (d)

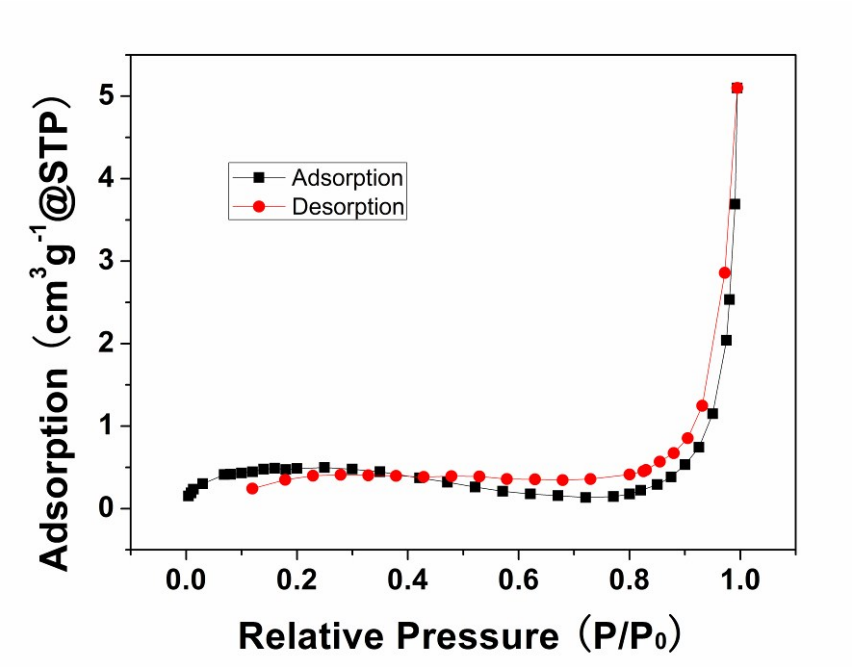

Fig. S11 Nitrogen adsorption and desorption isotherms at 77.3 K for CTF-BI-S

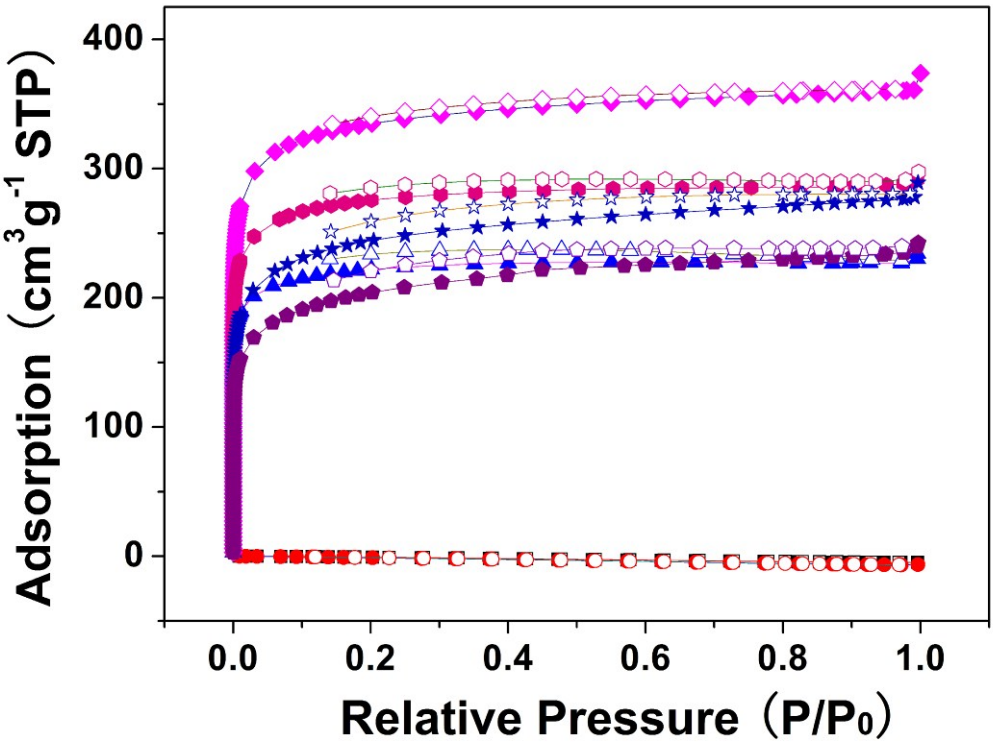

Fig. S12 Nitrogen adsorption and desorption isotherms at 77.3 K for all CTF-BIs derived from different ratios of $ZnCl_2$ to DCBI.

(Filled symbols for adsorption and Unfilled symbols for desorption. Square: CTF-BI-1; Circle: CTF-BI-2; Triangle: CTF-BI-3; Diamond: CTF-BI-4; Hexagon: CTF-BI-5; Star: CTF-BI-6; Pentagon: CTF-BI-7)

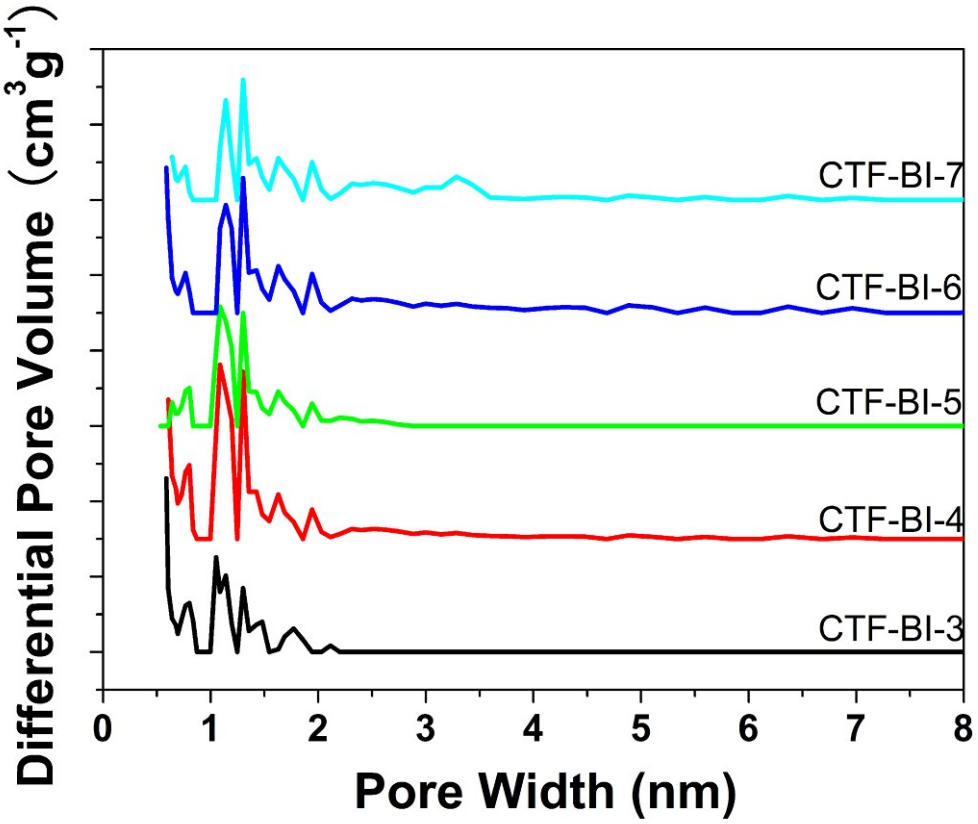

Fig. S13 Pore size distributions (PSD) calculated by the NLDFT method for all CTF-BIs derived from different ratios of $ZnCl_2$ to DCBI

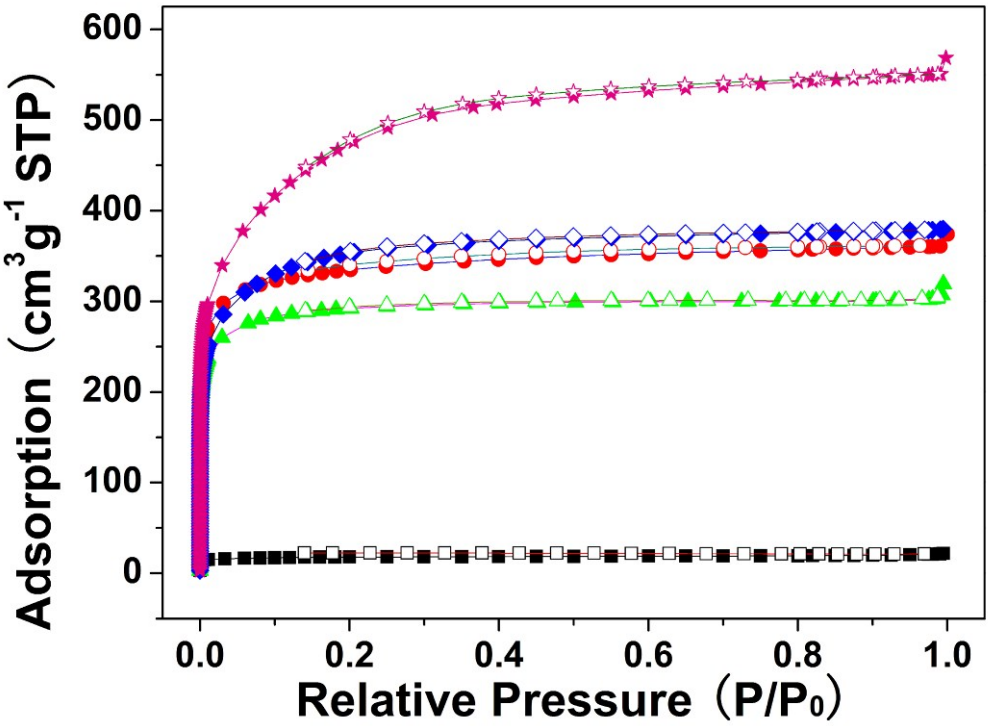

Fig. S14 Nitrogen adsorption and desorption isotherms at 77.3 K for all CTF-BIs obtained from different reaction temperatures

(Filled symbols for adsorption and Unfilled symbols for desorption. Square: CTF-BI-8; Circle: CTF-BI-4; Triangle: CTF-BI-9; Diamond: CTF-BI-10; Star: CTF-BI-11)

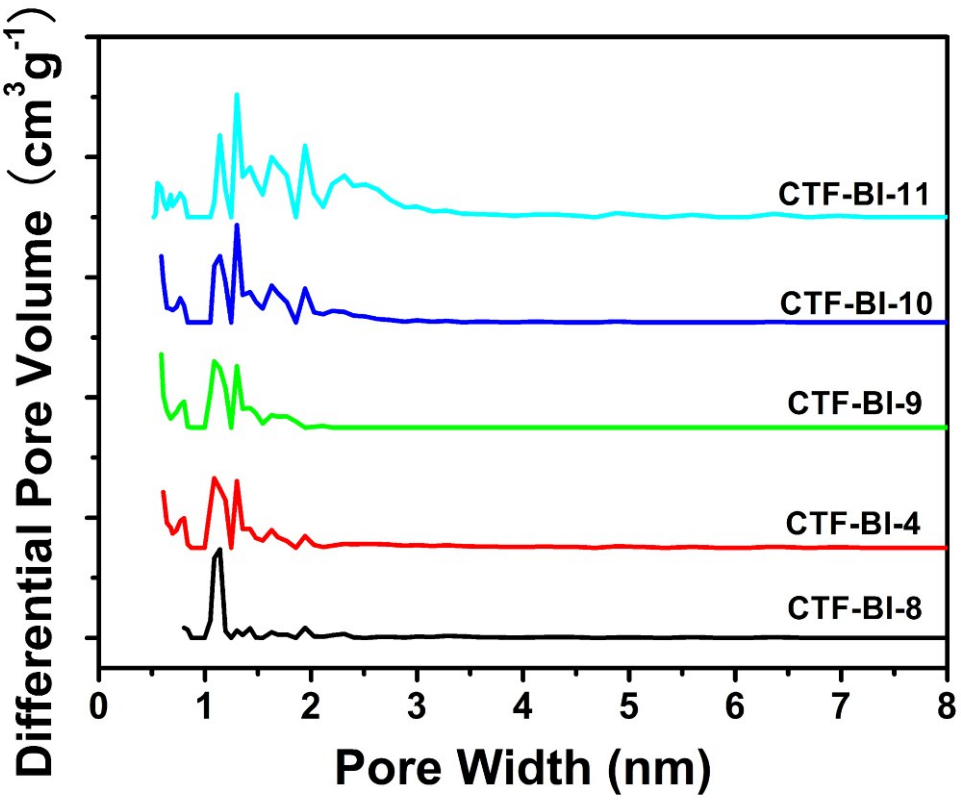

Fig. S15 Pore size distributions (PSD) calculated by the NLDFT method for all CTF-BIs obtained from different reaction temperatures

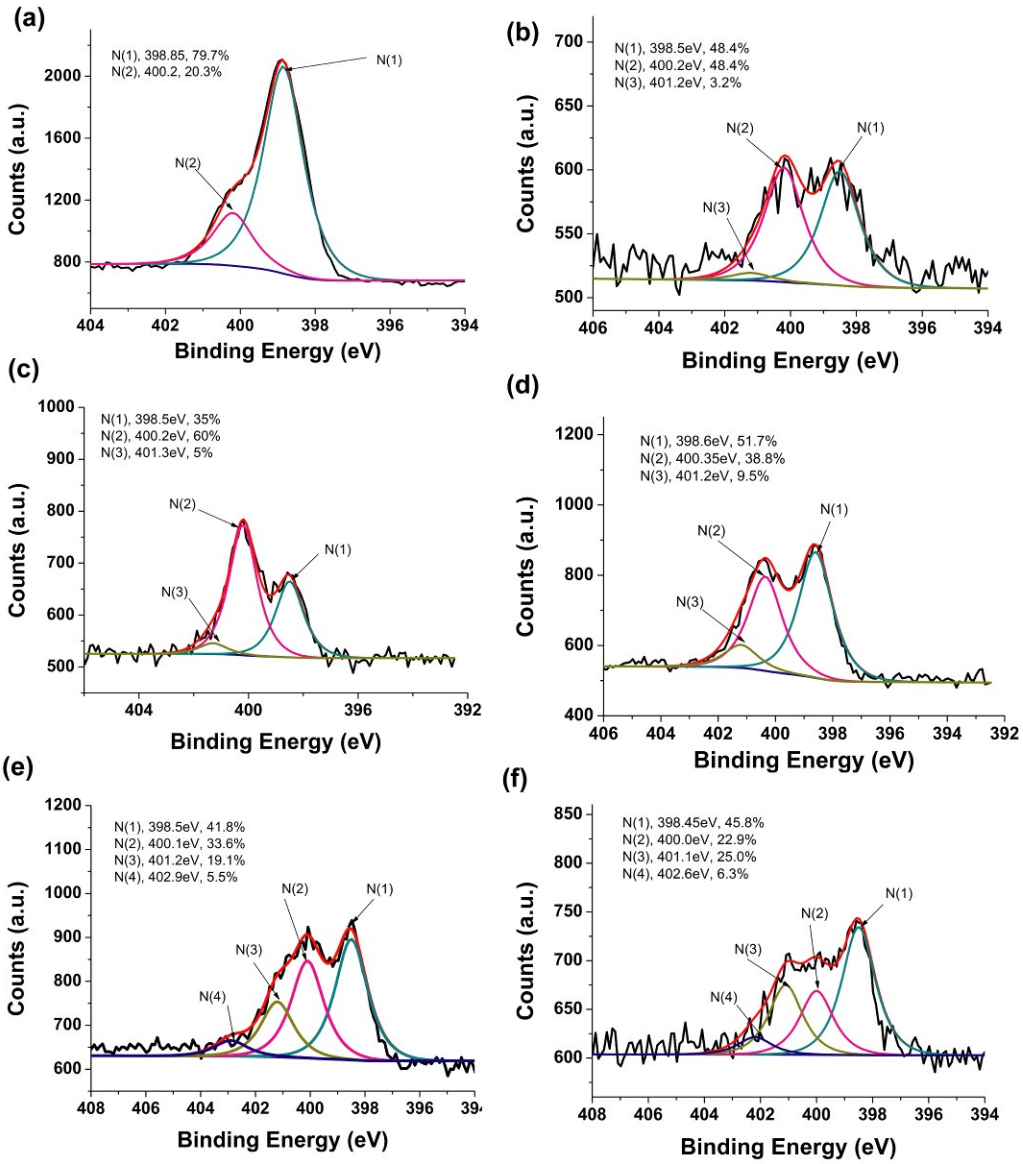

Fig. S16 High resolution N1s XPS spectra of (a) DCBI, (b) CTF-BI-8 (350 °C), (c) CTF-BI-4 (400 °C), (d) CTF-BI-9 (450 °C), (e) CTF-BI-10 (500 °C), and (f) CTF-BI-11 (550 °C)

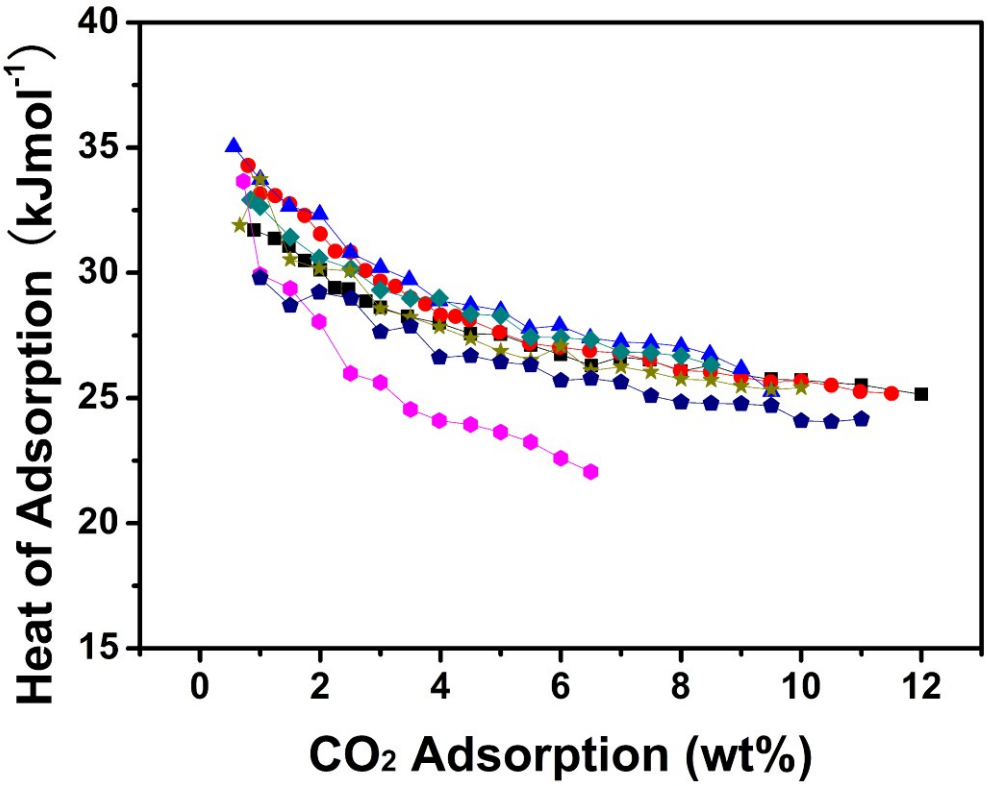

Fig. S17 Heats of Adsorption for the CTF-BIs

(Square: CTF-BI-4; Circle: CTF-BI-11; Triangle: CTF-BI-3; Diamond: CTF-BI-6; Hexagon: CTF-BI-7; Star: CTF-BI-9; Pentagon: CTF-BI-10)

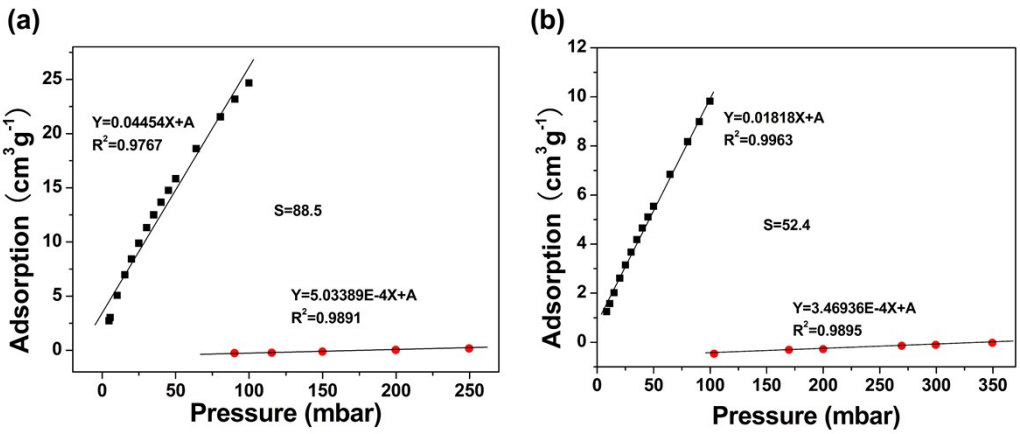

Fig. S18 CO_2/N_2 selectivity for CTF-BI-3 at (a) 273 K and (b) 303 K, calculated using the Henry's Law constants in the linear low pressure range (0~100 mbar for CO_2 and 100~400 mbar for N_2)

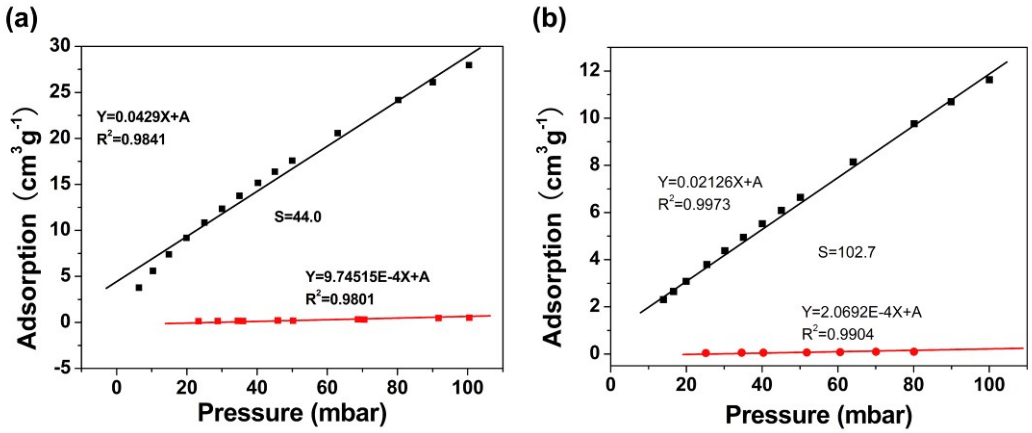

Fig. S19 CO_2/N_2 selectivity for CTF-BI-4 at (a) 273 K and (b) 303 K, calculated using the Henry's Law constants in the linear low pressure range (0~100 mbar)

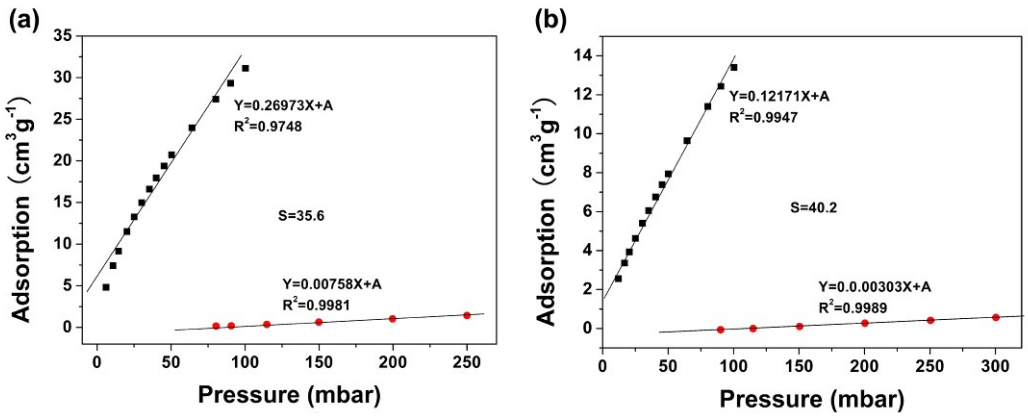

Fig. S20 CO_2/N_2 selectivity for CTF-BI-5 at (a) 273 K and (b) 303 K, calculated using the Henry's Law constants in the linear low pressure range (0~100 mbar for CO_2 and 50~300 mbar for N_2)

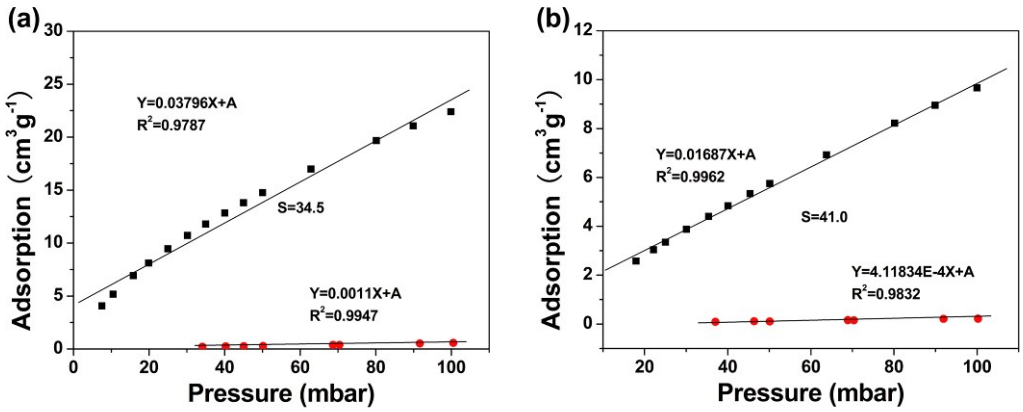

Fig. S21 CO_2/N_2 selectivity for CTF-BI-6 at (a) 273 K and (b) 303 K, calculated using the Henry's Law constants in the linear low pressure range (0~100 mbar)

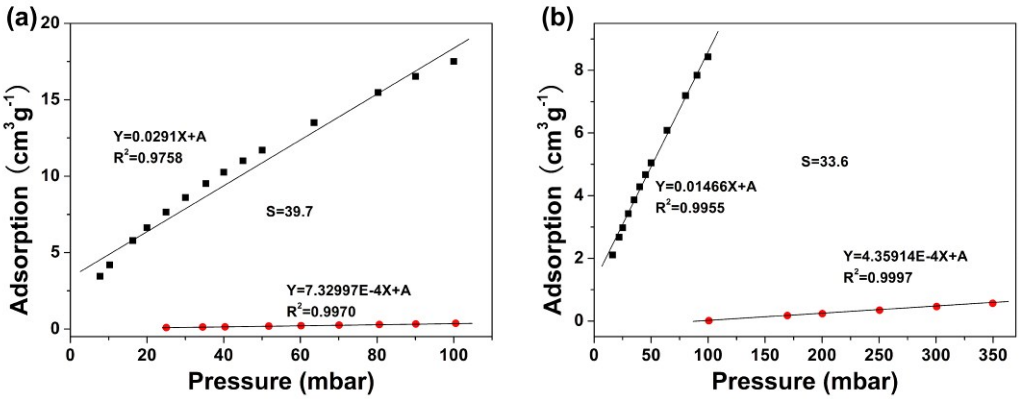

Fig. S22 CO_2/N_2 selectivity for CTF-BI-7 at (a) 273 K and (b) 303 K, calculated using the Henry's Law constants in the linear low pressure range (0~100 mbar for CO_2 and 100~350 mbar for N_2 at 303 K)

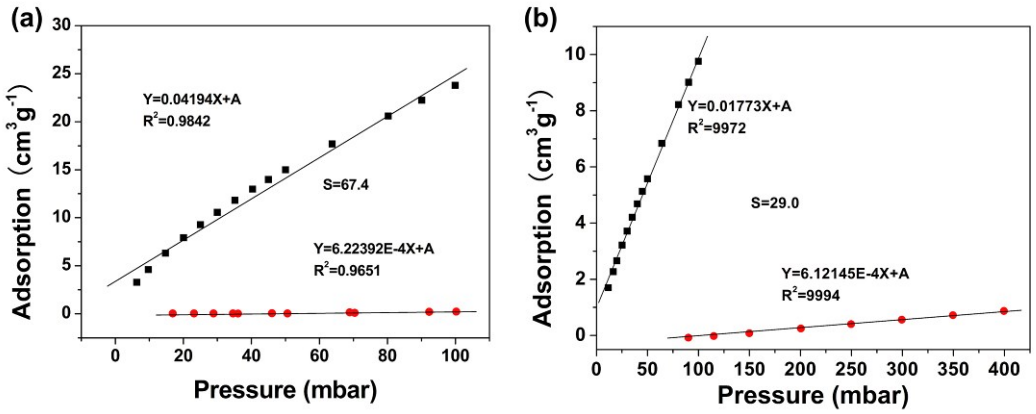

Fig. S23 CO_2/N_2 selectivity for CTF-BI-9 at (a) 273 K and (b) 303 K, calculated using the Henry's Law constants in the linear low pressure range (0~100 mbar for CO_2 and 100~400 mbar for N_2 at 303 K)

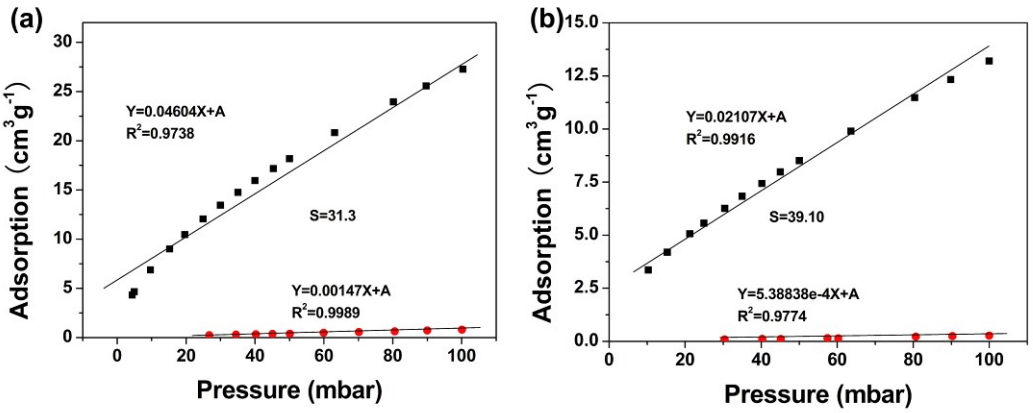

Fig. S24 CO_2/N_2 selectivity for CTF-BI-10 at (a) 273 K and (b) 303 K, calculated using the Henry's Law constants in the linear low pressure range (0~100 mbar)

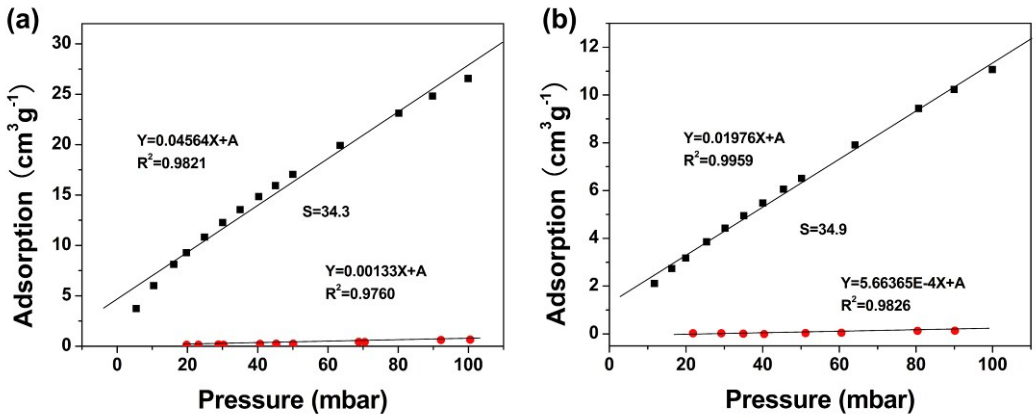

Fig. S25 CO_2/N_2 selectivity for CTF-BI-11 at (a) 273 K and (b) 303 K, calculated using the Henry's Law constants in the linear low pressure range (0~100 mbar)

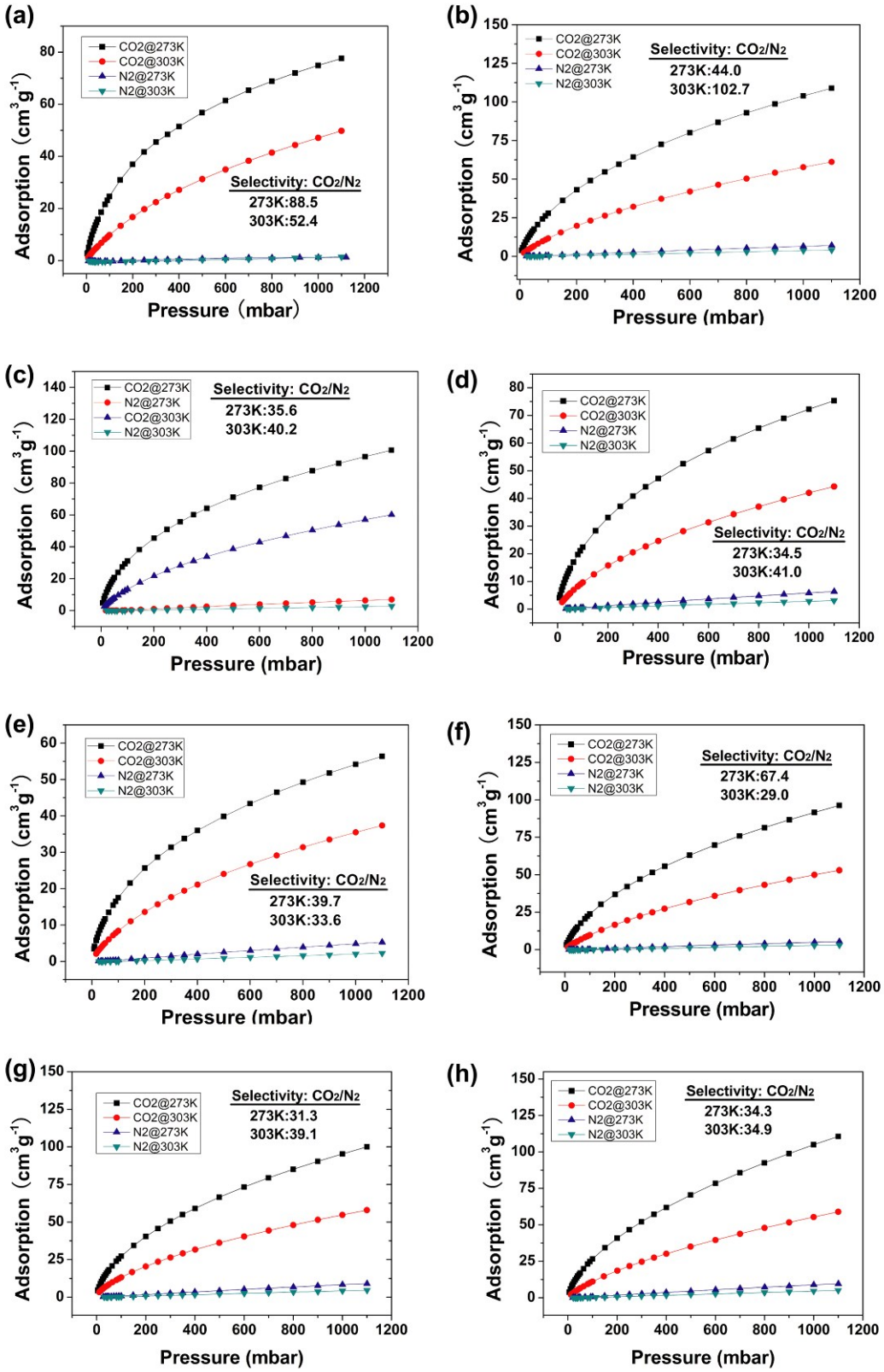

Fig. S26 CO_2/N_2 selectivities for (a) CTF-BI-3, (b) CTF-BI-4, (c) CTF-BI-5, (d) CTF-BI-6, (e) CTF-BI-7, (f) CTF-BI-9, (g) CTF-BI-10, and (h) CTF-BI-11, calculated using the Henry's Law constants in the linear low pressure range.

Table S1 Elemental Analysis of the CTF-BIs

Code	N (%)	C (%)	H (%)
Calculated	22.94	73.76	3.30
CTF-BI-8	16.18	63.03	3.419
CTF-BI-4	14.72	65.94	3.884
CTF-BI-9	12.11	55.83	3.376
CTF-BI-10	11.63	68.71	2.385
CTF-BI-11	10.95	58.87	2.779