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Electronic Supplementary Information for

Chemical fixation of carbon dioxide catalyzed via covalent triazine frameworks as metal free heterogeneous catalysts without cocatalyst

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Table S 1 Overview of the detailed synthesis parameters used for the CTFs discussed in this work

Materials	2,5-DCP /g	$ZnCl_2$ /g	Mass ratio of $ZnCl_2$/monomer	Reaction conditions
2,5-DCP-CTF-0	1	10	1:10	400 ℃/40 h
2,5-DCP-CTF-1	1	10	1:10	600 ℃/40 h
2,5-DCP-CTF-2	1	12	1:12	400 ℃/20 h and 600 ℃/20 h
2,5-DCP-CTF-3	1	10	1:10	400 ℃/20 h and 600 ℃/20 h
2,5-DCP-CTF-4	1	12	1:12	400 ℃/20 h and 600 ℃/60 h

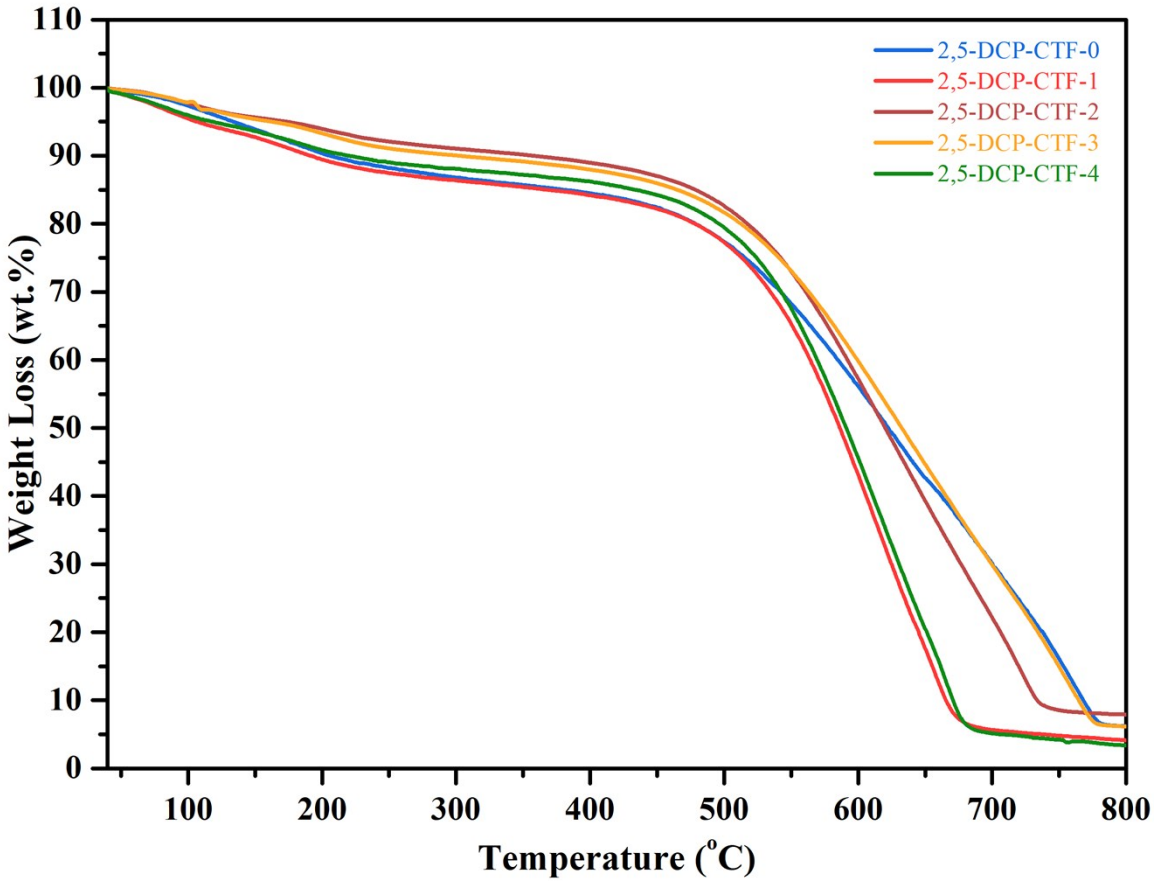


Fig. S1 TGA curves of 2,5-DCP-CTF under air.

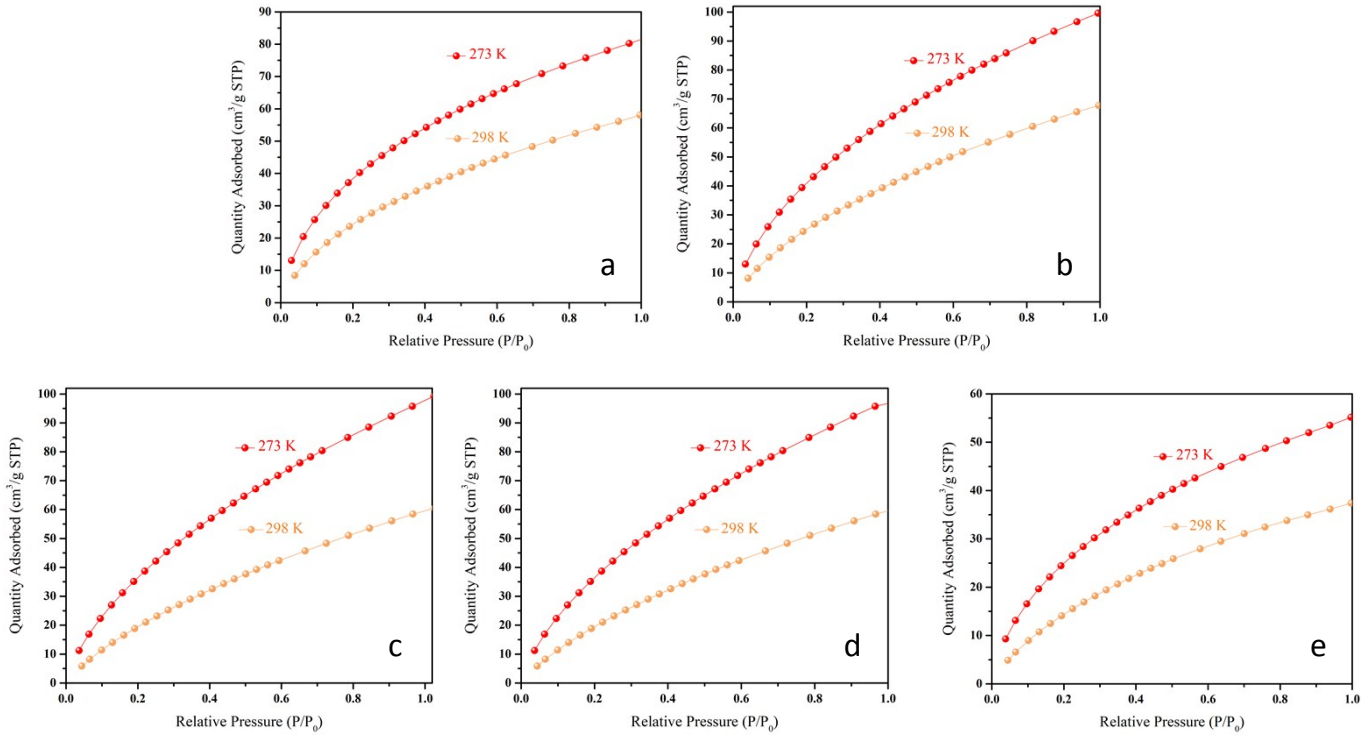


Fig. S2 CO_2 adsorption isotherms and the dual-site Langmuir to fit the CO2 adsorption isotherms of 2,5-DCP-CTF-0, 2,5-DCP-CTF-1, 2,5-DCP-CTF-2, 2,5-DCP-CTF-3, 2,5-DCP-CTF-4 measured at 273 K and 298K (symbol : CO_2 adsorption isotherms, line: the dual-site Langmuir to fit the CO2 adsorption isotherms).

Dual-site Langmuir parameter for adsorption of CO2 in 2,5-DCP-CTF. These parameters were determined by fitting adsorption isotherms for temperatures ranging from 278 K to 473 K.

2,5-DCP-CTF-0: $$q = q_A + q_B = \frac{q_{sat,A} b_A p}{1 + b_A p} + \frac{q_{sat,B} b_B p}{1 + b_B p}$$

$q_{sat,A}$ = 213.60 cm³/g

$q_{sat,B}$ = 34.03 cm³/g

$$b_A = b_{A0} \exp\left(\frac{E_A}{RT}\right);$$

b_{A0} = 2.38x10^{-7} KPa^{-1}

E_A =17.12 kJ mol^{-1}

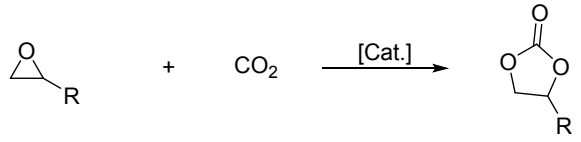
$$b_B = b_{B0} \exp\left(\frac{E_B}{RT}\right)$$

b_{B0} =7.94x10^{-7} kPa^{-1}

E_B =32.55 kJ mol^{-1}

Table S2. Overview of the detailed parameters determined by fitting adsorption isotherms for temperatures ranging from 273 K to 298 K.

entry	$q_{sat,A}$	$q_{sat,B}$	b_{A0}	E_A	b_{B0}	E_B	Q_{st}
	cm^3/g	cm^3/g	KPa^{-1}	$kJ\ mol^{-1}$	KPa^{-1}	$kJ\ mol^{-1}$	$kJ\ mol^{-1}$
2,5-DCP-CTF-0	213.60	34.03	$2.38x10^{-7}$	172.12	$7.94x10^{-7}$	32.55	32.55
2,5-DCP-CTF-1	192.97	32.32	$1.42x10^{-6}$	19.26	$1.03x10^{-6}$	27.66	27.66
2,5-DCP-CTF-2	239.99	20.94	$3.36x10^{-7}$	21.69	$1.07x10^{-7}$	31.88	31.88
2,5-DCP-CTF-3	240.12	19.06	$3.32x10^{-7}$	18.59	$1.08x10^{-7}$	30.06	30.06
2,5-DCP-CTF-4	86.78	15.51	$8.80x10^{-10}$	21.45	$1.77x10^{-10}$	32.03	32.03



Scheme S1 Cycloaddition of CO_2 to different starting epoxides.

Table S3 Synthesis of cyclic carbonates from epoxides and CO_2 catalyzed by 2,5-DCP-CTF-0.

Entry	Epoxide	Conversion/%[b]	Selectivity /%[b]	Yeild /%
1[a]	epbromohydrin	97.5	85.6	83
2[a]	propyleneoxide	98.4	41.5	41
3[a]	styreneoxide	51.9	95.0	49

[a] Reaction conditions: 18 mmol epichlorohydrin, 100 mg catalyst, 130 ℃, 10 bar CO_2, 4 h, without solvent.

[b] Determined by GC-MS using toluene as internal standard.

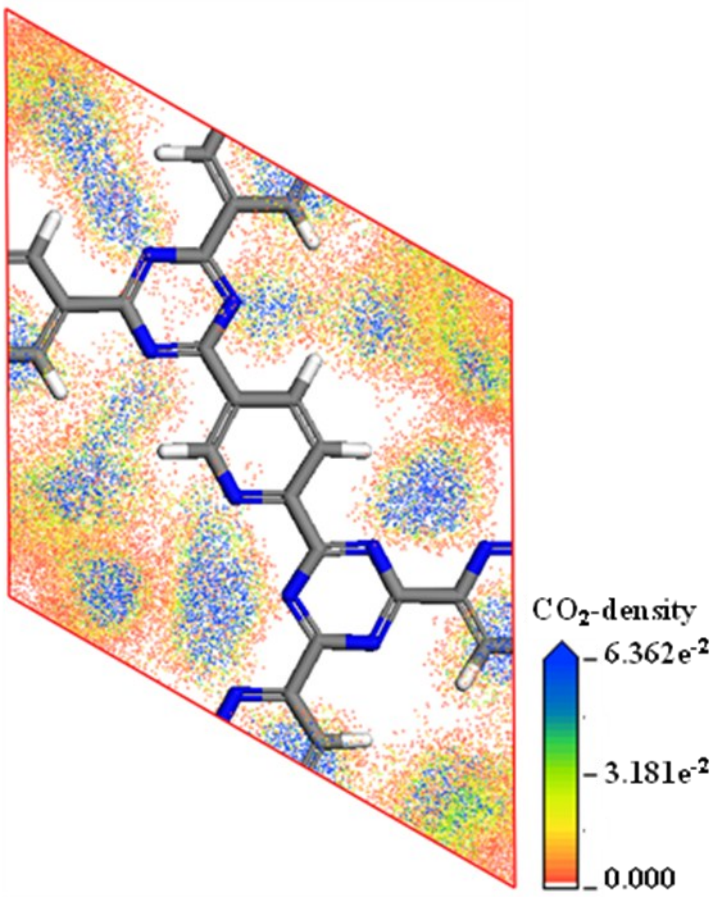


Fig. S3 Density field for CO_2 in 2,5-DCP-CTF at 273 K and 30 bar (blue: N; gray: C; white: H) computed by Sorption.