Supporting Information

Synthesis of "all-in-one" hypercross-linked organic polymers: Experimental and kinetic models for CO_2 chemical fixation and iodine adsorption

Experimental

All raw materials such as 1,4-bis (bromomethyl) benzene, N,N-dimethylethylenediamine, 1,2-dichloroethane, cyclohexane, methanol, phenol, butanophenol, octylphenol, dodecylphenol, pentadecylphenol were purchased from Aladdin Company. All epoxides used were purchased from Energy Chemical Reagents Co. Ltd. Chemicals are analytical grade and used directly without purification. The purity of CO_2 is 99.9% and was provided from Handan Anke Factory.

Characterizations

The FT-IR spectra were recorded on a Nicolet IS10 spectrometer ranging from 400 to 4000 cm^{-1}. The ^{13}C CP MAS NMR spectrum was checked on a JNM-ECZ600R spectrometer. XPS spectra were collected by Thermo Fisher Scientific K-Alpha spectrometer using an Al K Alpha source, and calibrated with C1s peak at 284.8 eV with energy of 150.0 eV. SEM was recorded on a Hitachi SU-8020 microscope with an acceleration voltage of 3.0 kV. Nitrogen adsorption isotherm was obtained from a Micromeritics ASAP 2460 at 77 K, and the sample was degassed at 100ºC for 6 h before

adsorption measurement. The basic sites of the samples were determined by temperature-programmed desorption (CO_2-TPD) on a Micromeritics Autochem II 2920 instrument. The programmed temperature range was 30–350°C, and the heating rate was 10 °C min^{-1}. CO_2 sorption isotherms were measured on a Micromeritics ASAP 2020 analyzer. The conversions of cyclic carbonates were detected on ^{1}H NMR spectra with a Bruker 400 spectrometer. The crude products were resolved in $CDCl_3$ in the presence of TMS as internal standard and the conversion was calculated on the proton peak area ration of ECH and product at 2.6 and 5.1 ppm. The products were determined by gas chromatography (FULI GC9720) using a flame ionization detector (FID) and a capillary column (30 m×0.32 mm×0.50 μm), the internal standard was ethyl acetate. Electronic (UV-Visible) spectra were recorded on a UV-3600 spectrophotometer, and measure the absorbance of the solution at 505 nm.
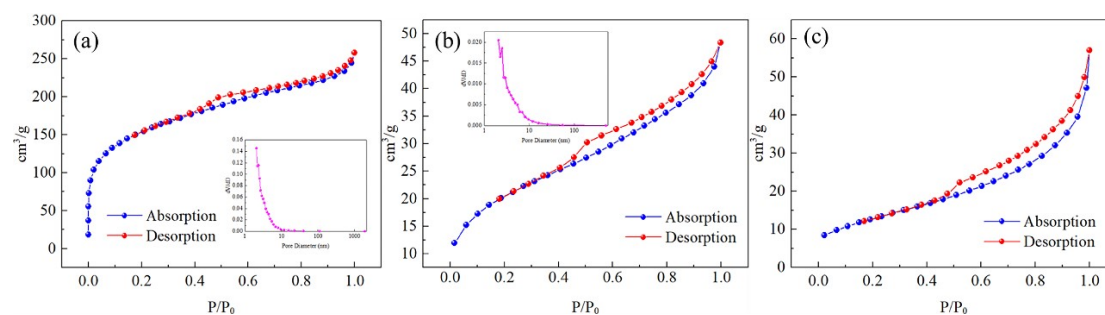

Fig. S1. N_2 adsorption and desorption isotherms and the pore size distribution of (a) HCP_{OH}-C_4 (b) HCP_{OH}-C_8 and (c) HCP_{OH}-C_{15}.

Table S1 The yield (%) of HCP_{OH}-C_{12} catalyzed CO_2 cycloaddition reaction under different pressures [a].

	8 h	**12 h**	20 h
0.1 MPa	51	67	86
0.6 MPa	68	76	92
1.0 MPa	74	83	97

[a] Reaction conditions: ECH (15 mmol), catalysts (70 mg), 90°C.
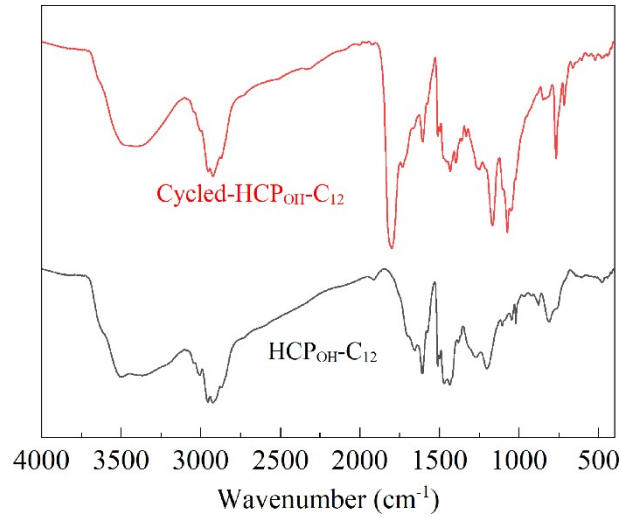
Fig. S2. FT-IR images of HCP_{OH}-C_{12} and Cycled-HCP_{OH}-C_{12}.

y=0.00616x+0.05079
R²=0.993

y=0.01524x+0.00645
R²=0.99

y=0.03454x-0.0297
R²=0.984

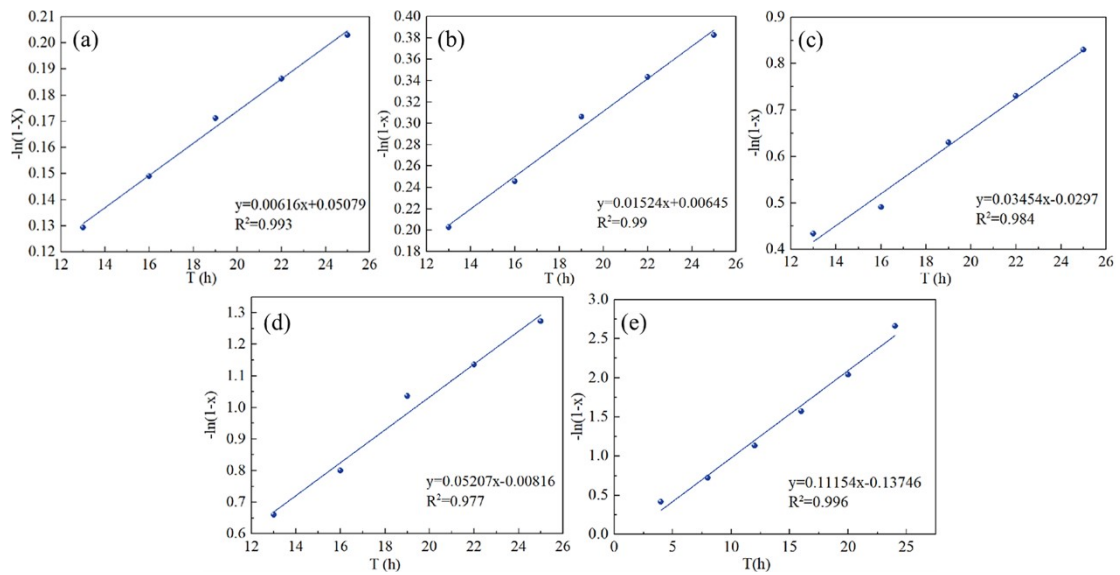y=0.05207x-0.00816
R²=0.977

y=0.11154x-0.13746
R²=0.996

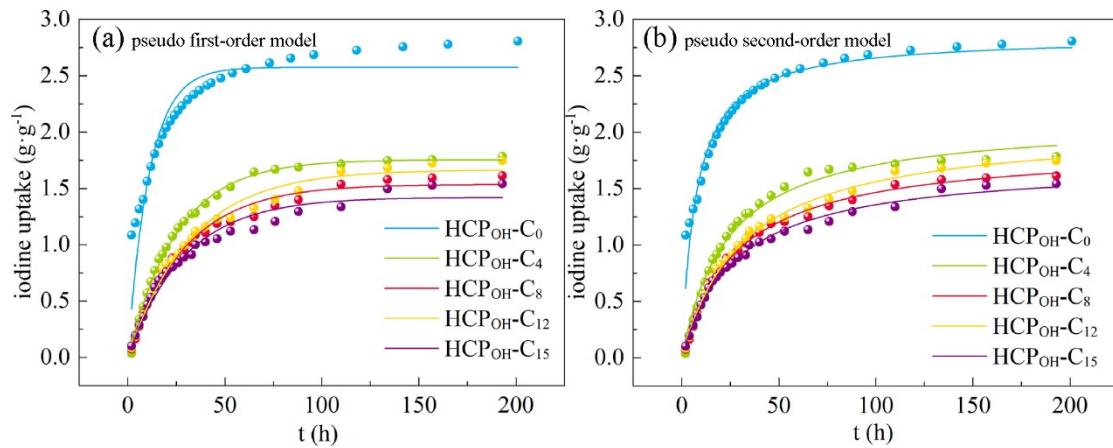**Fig. S3.** Plot -ln(1-x) -T(h) at different temperatures. (a) 50℃ (b) 60℃ (c) 70℃ (d) 80℃ (e) 90℃.

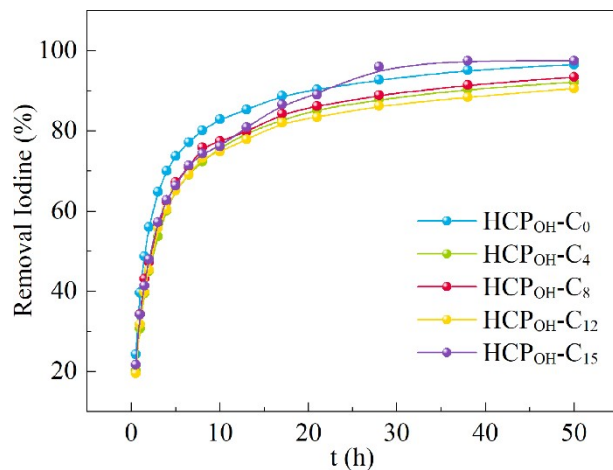**Fig. S4**. Adsorption kinetics of iodine vapor on HCP_{OH}-C_n.

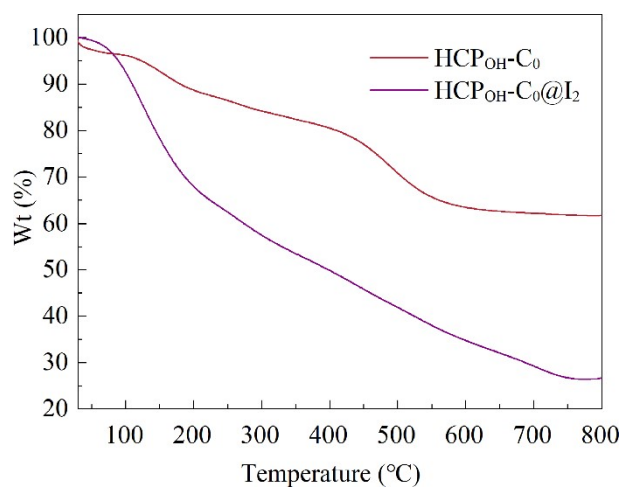**Fig. S5.** Release of iodine upon heating $HCP_{OH}-C_n@I_2$ at 120°C.

Fig. S6. TGA analysis of $HCP_{OH}-C_0$ before and after iodine vapor adsorption.

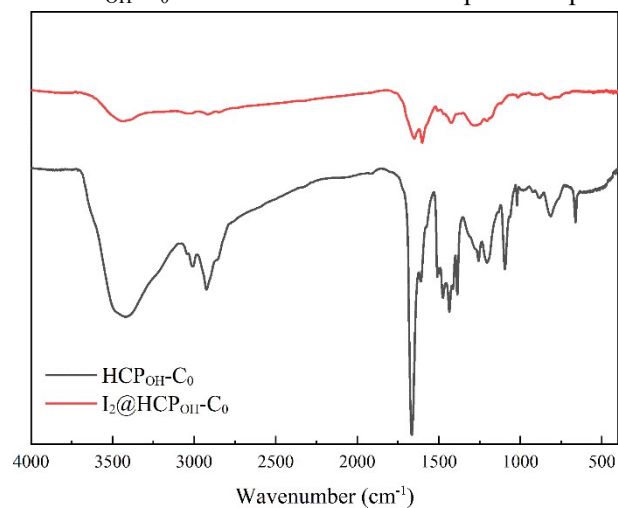**Fig. S7.** FT-IR spectra of $HCP_{OH}-C_0$ before and after adsorption of iodine vapor.
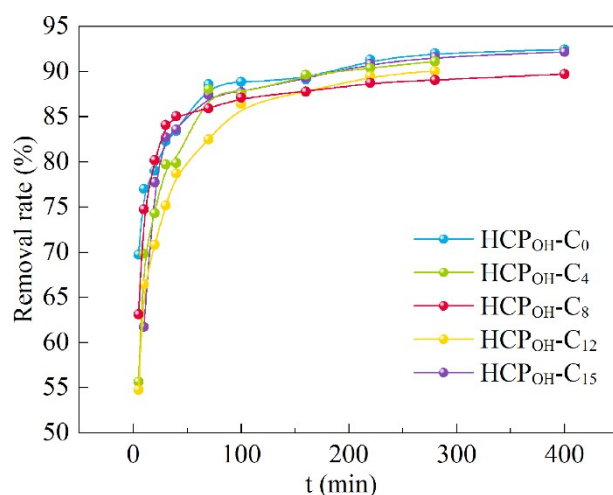
Fig. S8. The removal rate of iodine solution by HCP_{OH}-C_n.

Table S2 Pseudo-first-order and pseudo-second-order kinetic parameters of iodine solution in HCP_{OH}-C_0

Absorbent	Q_e (mg·g^{-1})	Pseudo first order kinetics			Pseudo second order kinetics		
		K_1 (min^{-1})	Q_e (mg·g^{-1})	R^2	K_2 (mg·g^{-1}·min^{-1})	Q_e (mg·g^{-1})	R^2
HCP_{OH}-C_0	177	0.26	169.9	0.73	0.002	178	0.97

Table S3 Langmuir and Freundlich parameters for iodine adsorption in cyclohexane solution.

	Langmuir model			Freundlich model		
	Q_{max}(mg·g^{-1})	K_L(L·mg^{-1})	R^2	K_F	1/n	R^2
298K	247.56	0.03133	0.99	28.612	0.4032	0.96
308K	252.81	0.03938	0.99	32.059	0.4001	0.97

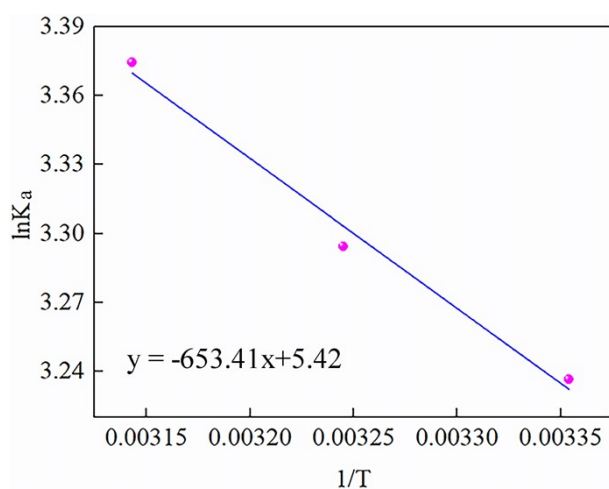

$y = -653.41x + 5.42$

Fig. S9. Thermodynamic parameter diagram of HCP_{OH}-C_0 adsorption in iodine solution.
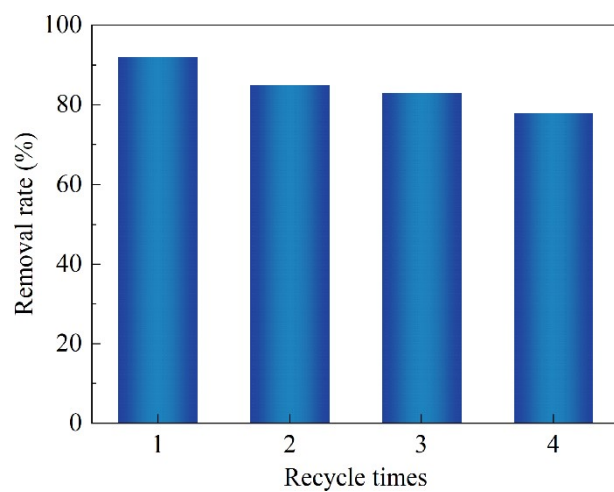
Fig. S10. Recyclability of HCP_{OH}-C_0 for iodine solution after four regeneration cycles