Electronic Supplementary Information

Resorcinol-Formaldehyde Based Nanostructured Carbons for CO_2 Adsorption: Kinetics, Isotherm and Thermodynamic Studies

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Calculations of energy duty for desorption

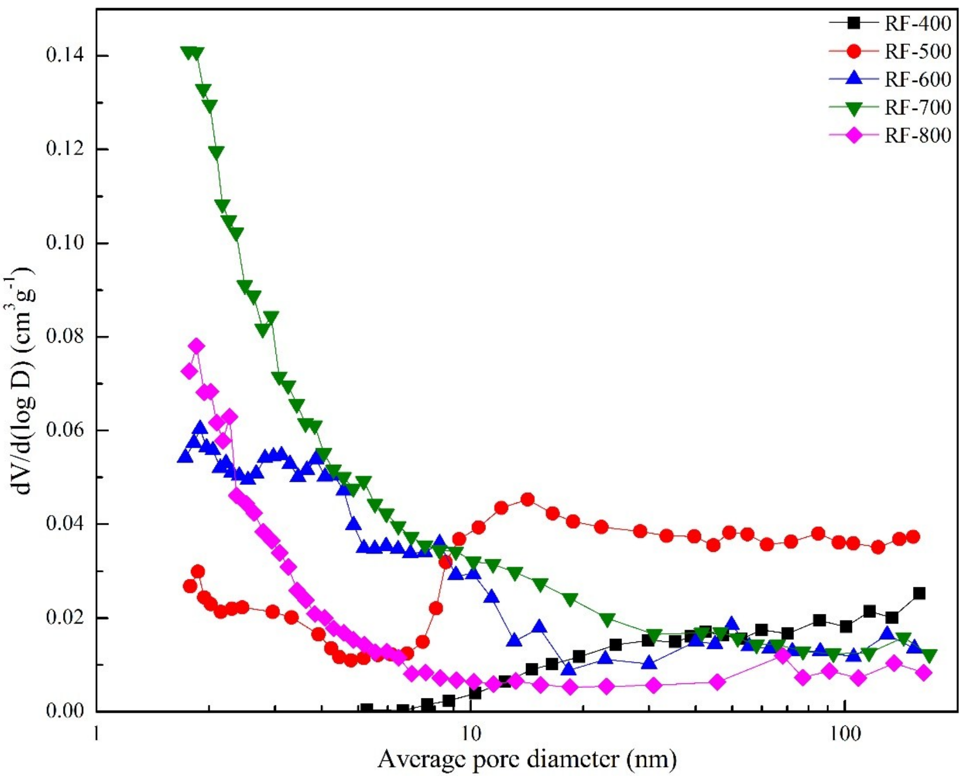

Fig. S1 Pore size distribution of nanostructured carbons.

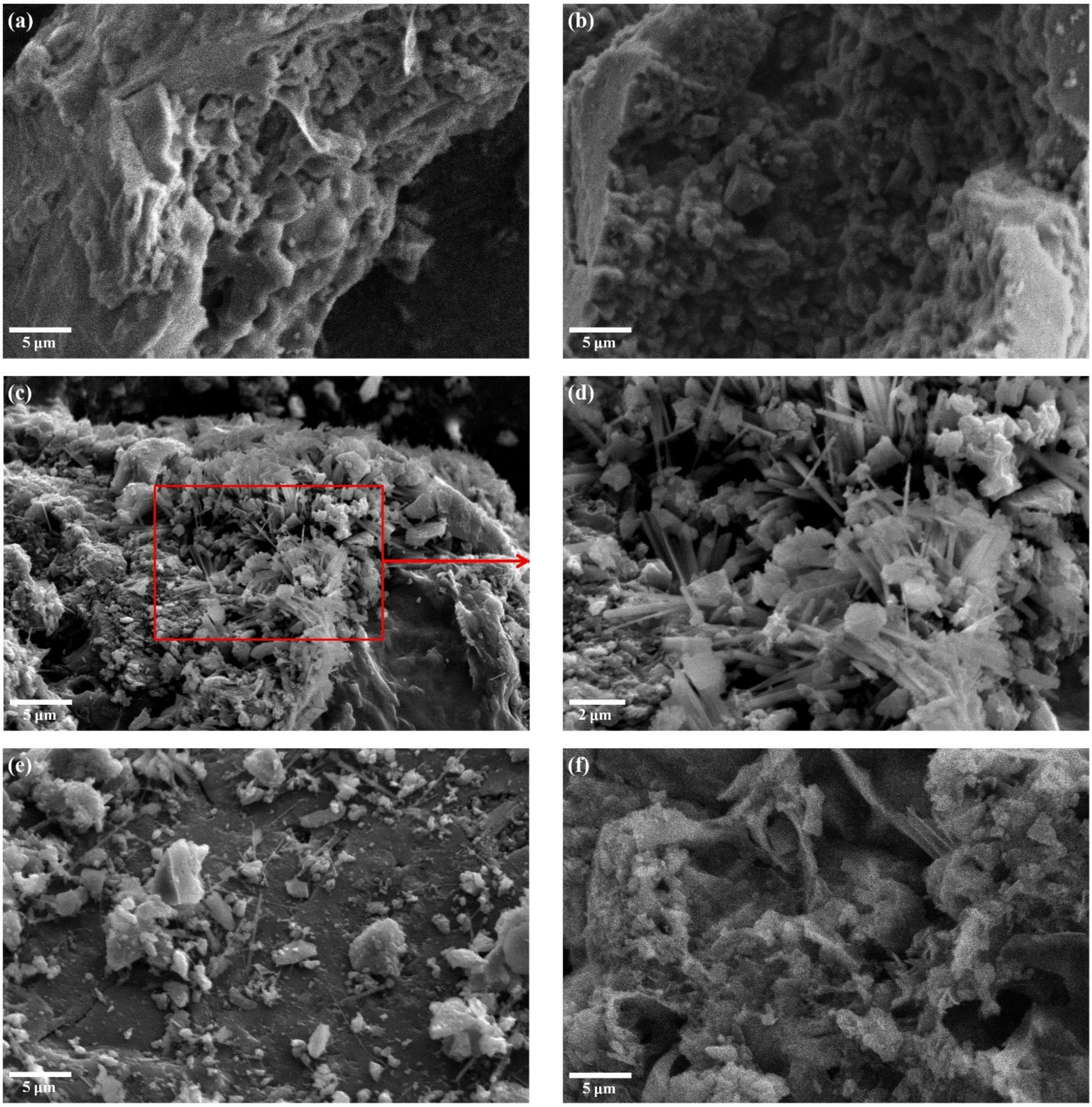

Fig. S2 SEM image of **(a)** RF-500, **(b)** RF-600 **(c, d)** RF-700, (**e)** RF-800, and **(f)** RF-C.

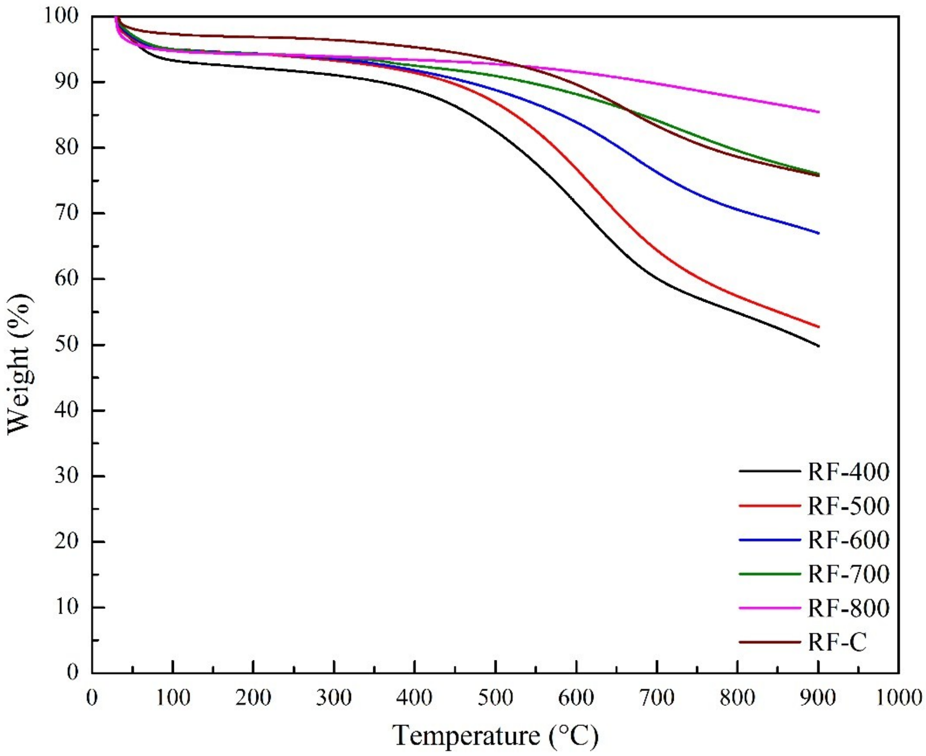

Fig. S3 Thermogravimetric profiles of the prepared carbons.

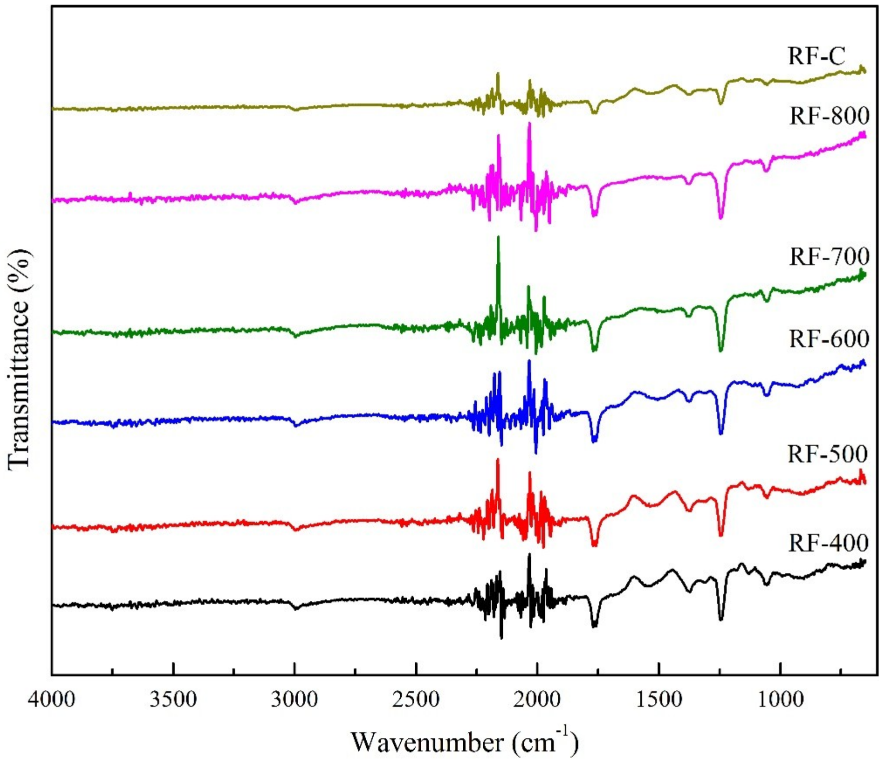

Fig. S4 FTIR spectra of porous carbons obtained from RF resin.

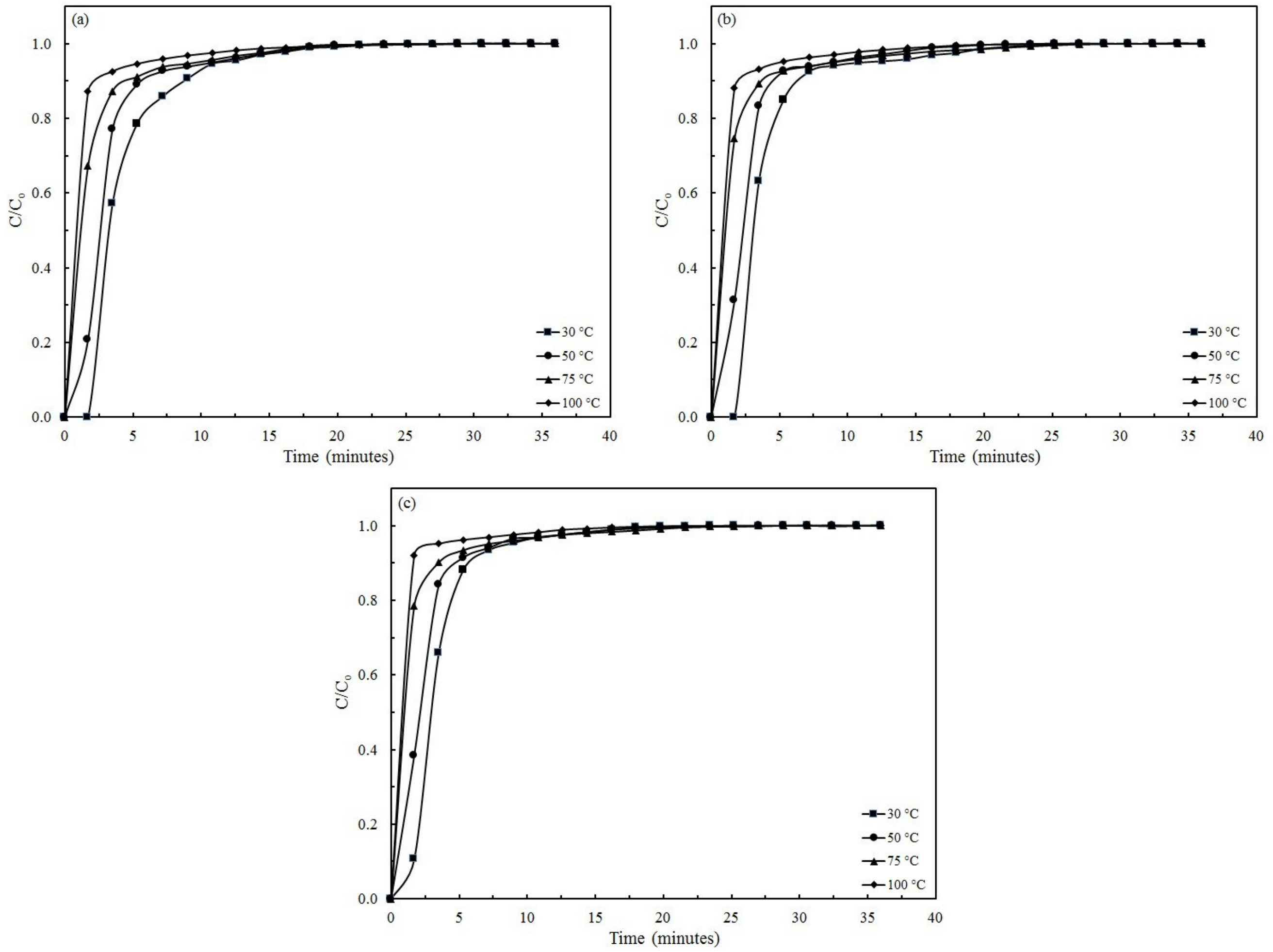

Fig. S5 Breakthrough profiles for RF-700 at **(a)** 7.5%, **(b)** 10%, and **(c)** 12.5% feed CO_2 concentration at different adsorption temperatures.

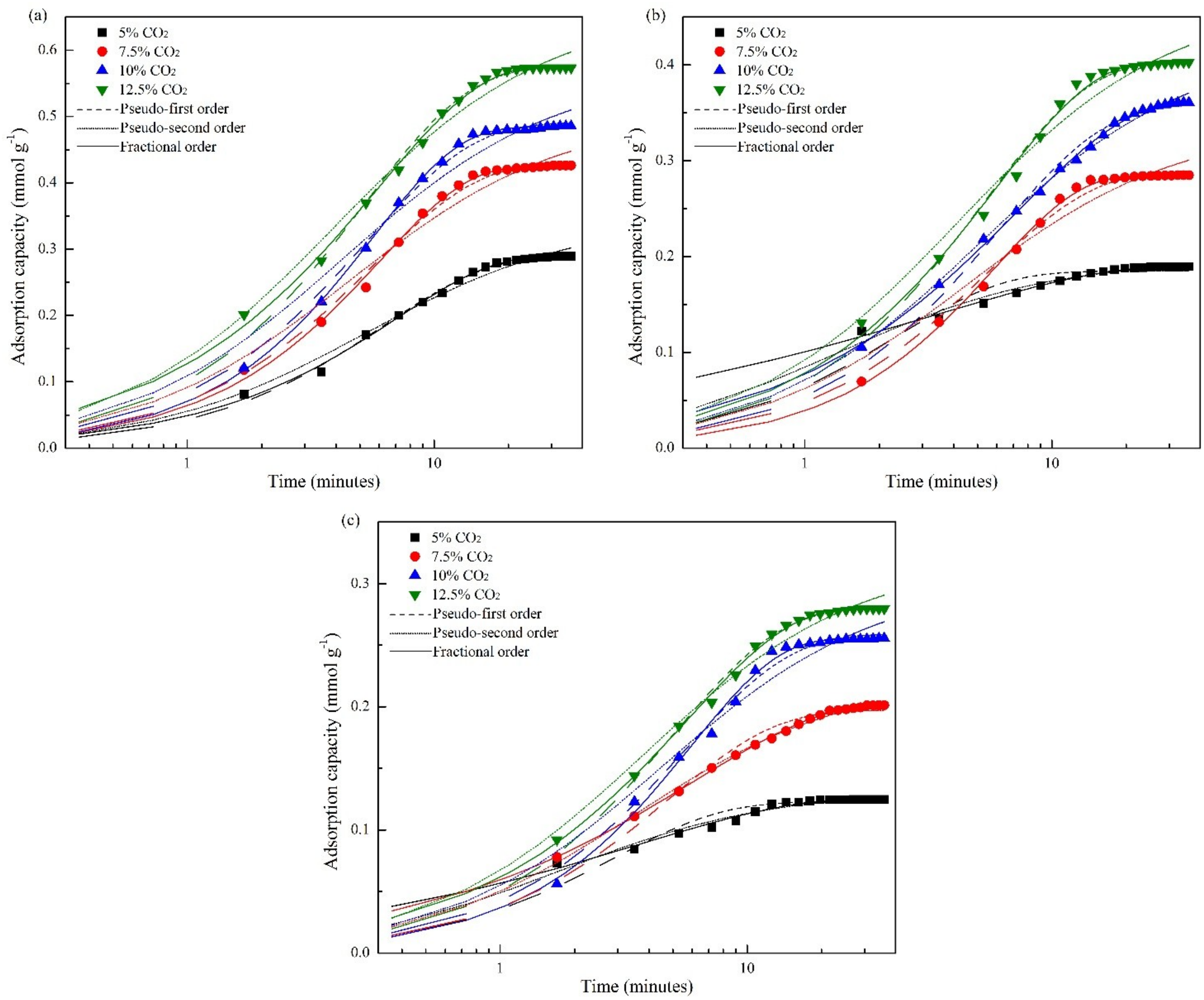

Fig. S6 Comparison of kinetic models for CO_2 uptake on RF-700 at (a) 50 °C, (b) 75 °C, and (c) 100 °C as a function of feed concentration

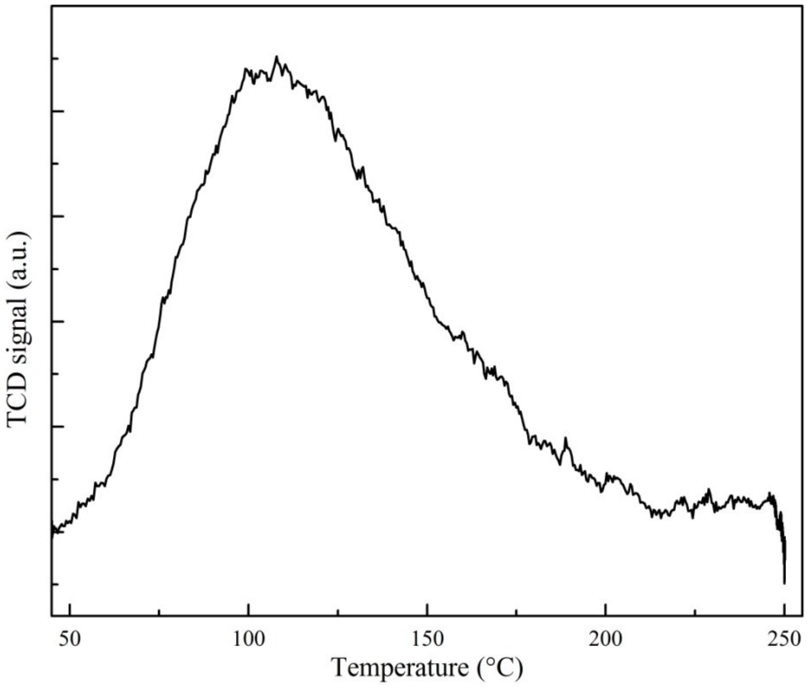

Fig. S7 Temperature programmed desorption profile of CO_2 of RF-700.

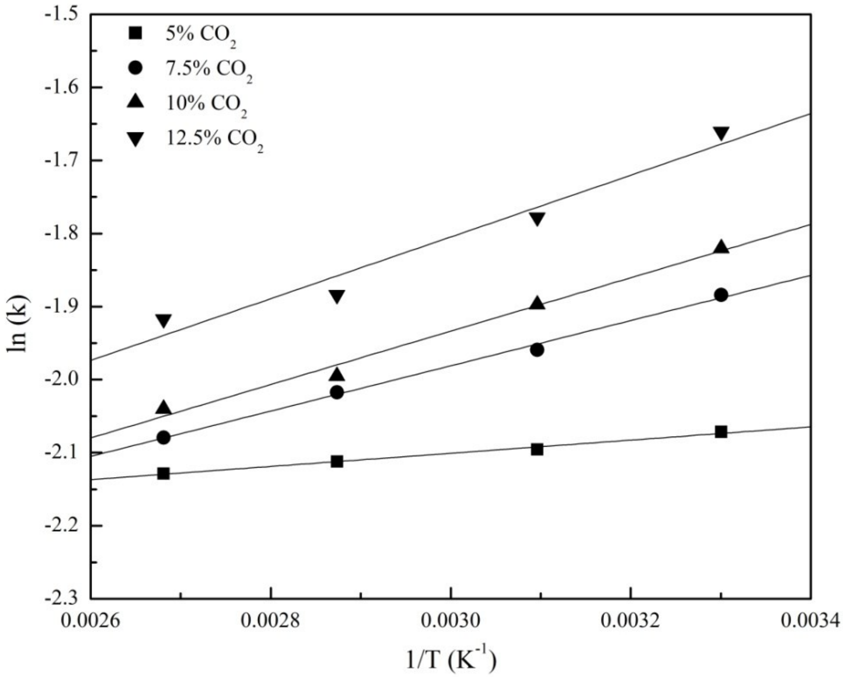

Fig. S8 Arrhenius plot for kinetic rate constants obtained from fractional order kinetic model.

Table S1 Deconvolution of C1s photoelectron envelope of RF-derived carbons

Sample		C1	C2	C3	C4	C5
RF-400	BE	284.10	285.50	286.42	288.40	-
	FWHM	1.99	1.27	1.68	2.53	-
	A %	60.08	25.22	13.83	0.88	0.00
RF-500	BE	284.55	285.27	286.30	288.70	-
	FWHM	1.29	1.09	1.45	2.11	-
	A %	35.72	40.87	19.24	4.17	0.00
RF-600	BE	284.32	285.21	286.24	288.36	-
	FWHM	1.85	1.45	1.65	2.23	-
	A %	54.69	22.32	15.44	7.55	0.00
RF-700	BE	284.25	285.14	-	288.56	-
	FWHM	1.18	1.96	-	4.3	-
	A %	58.02	24.44	0.00	17.54	0.00
RF-800	BE	284.45	285.41	-	288.18	283.44
	FWHM	1.47	2.24	-	2.24	1.29
	A %	17.71	14.67	0.00	8.35	59.27
RF-C	BE	284.42	285.13	286.43	288.31	-
	FWHM	0.86	0.94	1.48	1.90	-
	A%	54.43	23.17	15.27	7.13	0.00

$^{\alpha}$*BE*: Binding energy (eV); *FWHM*: Full width at half maximum (eV); *A%*: relative area percentage

Table S2 Deconvolution of O1s photoelectron envelope of RF-derived carbons

Sample		O1	O2	O3
RF-400	BE	531.81	532.80	533.46
	FWHM	1.73	1.38	1.69
	A %	31.25	40.68	28.07
RF-500	BE	531.21	532.23	533.24
	FWHM	2.36	1.34	1.41
	A %	57.06	26.02	16.92
RF-600	BE	531.67	532.38	533.21
	FWHM	1.57	1.33	1.43
	A %	34.34	39.15	26.51
RF-700	BE	531.35	532.16	533.11
	FWHM	1.80	1.35	1.84
	A %	26.58	36.10	37.32
RF-800	BE	531.22	532.11	-
	FWHM	1.54	1.10	-
	A %	80.55	19.45	0.00
RF-C	BE	531.67	532.29	533.60
	FWHM	1.45	1.54	1.66
	A%	39.93	33.29	26.79

$^{\alpha}$*BE*: Binding energy (eV); *FWHM*: Full width at half maximum (eV); *A%*: relative area percentage

Table S3 Kinetic model parameters for CO_2 adsorption on RF-700 at different adsorption temperatures and CO_2 concentrations

Adsorption temperature (ºC)	CO_2 concentration (volume%)	Pseudo-first order model				Pseudo-second order model				Fractional order model					
		k_1 (min^{-1})	q_e (mmol g^{-1})	R^2	Error %	k_2 (g $mmol^{-1}$ min^{-1})	q_e (mmol g^{-1})	R^2	Error %	k_n ($mmol^{1-m}$ g^{m-1} min^{-n})	q_e (mmol g^{-1})	n	m	R^2	Error %
30	5	0.160	0.410	0.993	4.458	0.378	0.489	0.974	9.014	0.126	0.402	0.898	1.020	0.997	4.207
	7.5	0.147	0.574	0.998	1.991	0.242	0.690	0.993	5.569	0.152	0.578	1.009	1.036	0.999	1.682
	10	0.190	0.712	0.996	2.854	0.289	0.826	0.974	8.303	0.162	0.703	1.106	1.048	0.999	2.200
	12.5	0.192	0.764	0.993	5.435	0.269	0.887	0.973	11.128	0.190	0.763	1.326	1.353	0.996	3.710
50	5	0.160	0.292	0.997	3.960	0.549	0.346	0.987	5.430	0.123	0.289	0.754	0.871	0.998	3.140
	7.5	0.179	0.432	0.995	3.649	0.437	0.504	0.975	7.082	0.141	0.426	0.838	1.020	0.997	3.268
	10	0.189	0.491	0.996	3.435	0.411	0.570	0.973	9.654	0.150	0.484	0.863	1.076	0.999	0.951
	12.5	0.195	0.577	0.995	4.585	0.389	0.662	0.987	3.835	0.169	0.576	0.862	1.097	0.998	2.272
75	5	0.424	0.185	0.955	6.551	3.761	0.198	0.992	2.923	0.121	0.190	0.590	0.370	0.998	1.450
	7.5	0.183	0.290	0.994	3.694	0.665	0.338	0.969	9.741	0.133	0.285	0.762	0.693	0.998	1.931

	10	0.164	0.359	0.994	4.719	0.478	0.422	0.997	1.620	0.136	0.363	0.770	0.739	0.999	1.297
	12.5	0.188	0.406	0.994	4.132	0.519	0.468	0.981	4.654	0.152	0.403	0.793	0.875	0.996	3.013
100	5	0.342	0.123	0.960	6.981	4.377	0.133	0.989	3.350	0.119	0.125	0.655	0.467	0.995	2.124
	7.5	0.208	0.197	0.984	6.393	1.277	0.224	0.995	1.752	0.125	0.202	0.703	0.607	0.999	0.546
	10	0.180	0.259	0.993	5.583	0.729	0.303	0.971	11.862	0.130	0.255	0.748	1.052	0.996	3.107
	12.5	0.200	0.280	0.997	3.222	0.822	0.321	0.989	3.773	0.147	0.280	0.775	1.114	0.999	1.262

Calculations of energy duty for desorption

1. Sensible heat

Adsorption conditions:

Adsorption temperature: 30 °C

Feed gas concentration: 12.5% CO_2 in N_2

Pressure: 1 atm

Desorption conditions:

Desorption temperature: 200 °C

Purge gas: 100% N_2

Temperature difference, $\Delta T = (200 - 30)\ ℃ = 170\ ℃ = 170\ K$

Specific heat capacity of the prepared carbon (RF-700), C_p = 1.215 J g^{-1} K^{-1}

CO_2 adsorption capacity of RF-700 $= 0.76\ mmol\ CO_2\ per\ g\ adsorbent$

$= 0.76 \times 10^{-3} mol\ CO_2\ per\ g\ adsorbent$

$$Sensible\ heat = \frac{C_p \Delta T}{adsorption\ capacity}$$

$$= \frac{1.215 \times 170}{0.76 \times 10^{-3}}\ J\ per\ mole\ CO_2$$

$$= 271{,}776.3\ J\ per\ mole\ CO_2$$

$Sensible\ heat = 271.8\ kJ\ per\ mole\ CO_2$

Assuming that 75% of the sensible heat required for heating the adsorbent material can be recovered using indirect or direct in a heat exchange,

Net sensible heat required in the process $= (25\%\ of\ 271.8)\ kJ\ per\ mole\ CO_2$

$Sensible\ heat = 67.9\ kJ\ per\ mole\ CO_2$

2. Isosteric heat of adsorption

Isosteric heat of adsorption was obtained from CO_2 adsorption isotherms by using Clausius-Clapeyron equation.

$Isosteric\ heat\ of\ adsorption,\ Q_{st} = 15.74\ kJ\ per\ mole\ CO_2$

3. Thermal energy input

$$Thermal\ energy\ input\ =\ Desorption\ heat\ +\ Sensible\ heat$$

$$= (15.74 + 67.9)\ kJ\ per\ mole\ CO_2$$

$$Thermal\ energy\ input = 83.64\ kJ\ per\ mole\ CO_2$$

$$= \frac{83.64}{44}\ kJ\ per\ g\ CO_2$$

$$= 1.9\ kJ\ per\ g\ CO_2 = 1.9\ MJ\ per\ kg\ CO_2$$

Hence desorption of 1 kg CO_2 requires energy equal to 1.9 MJ which is obtained from the burning of fossil fuels.

4. CO_2 generated

Assuming fuel used for energy production is Bituminous coal.

CO_2 generated from burning of Bituminous coal = 205.3 lbs per Million Btu

$$CO_2\ generated\ = \frac{205.3\ \times 0.454}{1.055\ \times\ 10^9}\ kg\ CO_2 per\ J$$

$$= 8.84 \times 10^{-8}\ kg\ CO_2 per\ J$$

$$= 0.0884\ kg\ CO_2 per\ MJ$$

i.e. to generate 1 MJ of energy from burning of bituminous coal 0.0884 kg of CO_2 is generated.

$$CO_2 adsorption\ capacity\ = 0.76\ mmol\ CO_2\ per\ g\ adsorbent$$

$$= 0.76\ mol\ CO_2\ per\ kg\ adsorbent$$

$$= (0.76 \times 44)\ g\ CO_2\ per\ kg\ adsorbent$$

$$= 33.44\ g\ CO_2\ per\ kg\ adsorbent$$

$$= 0.03344\ kg\ CO_2\ per\ kg\ adsorbent$$

Basis: 1 kg adsorbent

$$CO_2 adsorbed\ = 0.03344\ kg\ CO_2\ per\ kg\ adsorbent$$

Energy required to desorb 0.03344 kg CO_2 = $(1.9 \times 0.03344) MJ = 0.064\ MJ$

Hence CO_2 generated from combustion of fossil fuel = $(0.0884\ \times 0.064) kg\ CO_2$

$$CO_2\ generated = 0.0056\ kg\ CO_2$$

Therefore, energy required for desorption of 0.03344 kg CO_2 per kg adsorbent is equivalent to the generation of 0.0056 kg of CO_2 per kg adsorbent.