

## Supporting Information

### Tables

# **Synthesis, characterization and adsorption capacity of magnetic carbon composites activated by CO<sub>2</sub>: implication to the catalytic mechanisms of iron salts**

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**Table S1** Condition of mobile phase and wavelength of eight PPCPs in HPLC analysis

PPCP	Wavelength (nm)	Mobile Phase	Volume Ratio
sulfamethoxazole (SMX)	265		67:33
sulfapyridine (SPY)	265	TFA (0.1%) <sup>a</sup> : water	62:38
carbamazepine (CMZ)	285		80:20
sulfathiazole (STZ)	265		80:20
diclofenac sodium (DCF)	276	TFA (0.1%): methanol	10:90
quinindium (QND)	245		62:38
bisphenol A (BPA)	280	methanol: water	75:25
triclosan (TCS)	280		90:10

<sup>a</sup> TFA: trifluoroacetic acid.

**Table S2** Surface areas and porosities of MCs derived from different iron salt type (750°C of activation temperature and 2 h of hold time)

Sample	$S_{\text{BET}}^a$ (m <sup>2</sup> /g)	$S_{\text{mic}}^b$ (m <sup>2</sup> /g)	$S_{\text{mic}}/S_{\text{BET}}$ (%)	$V_{\text{mic}}^c$ (cm <sup>3</sup> /g)	$V_{\text{t}}^d$ (cm <sup>3</sup> /g)	$V_{\text{mic}}/V_{\text{t}}$ (%)
<i>MC-Cl-5</i>	703.0	509	72.4	0.225	0.408	55.1
<i>MC-Ox-5</i>	393.0	331	84.2	0.165	0.296	55.7
<i>MC-N-5</i>	345.0	315	91.3	0.158	0.216	73.1
<i>MC-S-5</i>	247.0	201	81.4	0.105	0.144	72.9
<i>MC-Ci-5</i>	60.0	46	76.7	0.023	0.053	43.4

<sup>a</sup> Brunauer-Emmett-Teller (BET) surface area measured using N<sub>2</sub> adsorption at  $P/P_0$  of 0.04-0.3.

<sup>b</sup> Micropore surface area calculated using the  $t$ -plot method.

<sup>c</sup> Micropore volume calculated using the  $t$ -plot method.

<sup>d</sup> Total pore volume determined at  $P/P_0 = 0.99$ .

**Table S3** Yields, ash, Fe contents, and elemental compositions for MCs derived from different iron salt types (750°C of activation temperature and 2 h of hold time)

Sample	Yield (%)	Ash (%)	Fe (%)	C (%)	N (%)	H (%)	Carbon Retention (%) <sup>b</sup>
<i>MC-Cl-5</i>	26.6	39.05	28.67	37.98	0.55	BDL <sup>a</sup>	15.76
<i>MC-Ox-5</i>	31.8	31.49	20.64	48.97	0.49	BDL	24.32
<i>MC-N-5</i>	34.1	29.84	24.32	44.48	0.64	BDL	23.68
<i>MC-S-5</i>	32.1	40.18	24.90	41.23	0.29	BDL	20.63
<i>MC-Ci-5</i>	24.1	95.79	51.78	4.17	0.04	BDL	1.57

<sup>a</sup> BDL: below detectable level.

$${}^b \text{Carbon retention (\%)} = \frac{M_{\text{sample}} \times C_{\text{sample}}}{M_{\text{hydrochar}} \times C_{\text{hydrochar}}}$$

where  $M_{\text{sample}}$  is the final mass (g) of sample;  $M_{\text{hydrochar}}$  is the mass (g) of hydrochar added;  $C_{\text{sample}}$  and  $C_{\text{hydrochar}}$  are carbon contents (%) of sample and hydrochar, respectively. ( $M_{\text{hydrochar}} = 3$  g;  $C_{\text{hydrochar}} = 64.07$  %)

**Table S4** Mössbauer parameters at room temperature of as-prepared MCs derived from different iron salt types (750°C of activation temperature and 2 h of hold time)

Sample	Component	HMF (KOe) <sup>a</sup>	IS (mm/s) <sup>b</sup>	QS (mm/s) <sup>c</sup>	$\Gamma/2$ (mm/s) <sup>d</sup>	Mole percentage (%)
<i>MC-Ox-5</i>	Fe <sub>3</sub> O <sub>4</sub>	459.63	0.54	0	0.27	43.1
		497.15	0.16	0.05	0.26	56.9
<i>MC-N-5</i>	Fe <sub>3</sub> O <sub>4</sub>	461.43	0.69	0	0.21	41.9
		497.79	0.29	0.03	0.22	58.1
<i>MC-S-5</i>	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub> (s) <sup>e</sup>	0	0.49	0.67	0.24	15.2
	Fe <sub>3</sub> O <sub>4</sub>	462.86	0.88	0	0.26	50.2
		489.22	0.39	0.10	0.16	34.6
<i>MC-Ci-5</i>	Fe <sub>3</sub> O <sub>4</sub>	458.64	0.51	0	0.31	59.6
		493.93	0.14	0.03	0.20	40.4

<sup>a</sup> HMF: hyperfine magnetic fields.

<sup>b</sup> IS: isomer shift.

<sup>c</sup> QS: quadrupole splitting.

<sup>d</sup>  $\Gamma/2$ : half line width.

<sup>e</sup> s: superparamagnetic.

**Table S5** Fe content analyses during acid leaching experiments at pH 2 for MCs activated at different iron salt types (750°C of activation temperature and 2 h of hold time)

Sample	Fe Leaching Concentration (mg/L)	Fe Leaching Percentage (%)
<i>MC-Cl-5</i>	4.13 ± 0.06	0.72 ± 0.01
<i>MC-Ox-5</i>	1.92 ± 0.03	0.47 ± 0.01
<i>MC-N-5</i>	2.97 ± 0.01	0.61 ± 0.01
<i>MC-S-5</i>	32.32 ± 0.38	6.49 ± 0.08
<i>MC-Ci-5</i>	2.82 ± 0.02	0.27 ± 0.01

**Table S6** Yields, ash, Fe contents, and elemental compositions for the MCs derived from different FeCl<sub>3</sub> loading content (750°C of activation temperature and 2 h of hold time)

Sample	Yield (%)	Ash (%)	Fe (%)	C (%)	N (%)	H (%)	Carbon Retention (%) <sup>b</sup>
<i>MC-CI-0</i>	36.9	10.13	-	71.43	1.04	BDL	41.09
<i>MC-CI-1</i>	17.0	21.64	8.14	53.66	0.86	BDL	14.24
<i>MC-CI-2</i>	25.2	22.39	11.43	54.04	0.73	BDL	21.21
<i>MC-CI-5</i>	25.7	51.23	29.12	35.54	0.53	BDL	14.23
<i>MC-CI-10</i>	31.6	80.61	45.51	19.07	0.32	BDL	9.41
<i>MC-CI-20</i>	35.6	93.43	59.70	0.15	BDL <sup>a</sup>	BDL	0.08

<sup>a</sup> BDL: below detectable level.

$$^b \text{ Carbon retention (\%)} = \frac{M_{\text{sample}} \times C_{\text{sample}}}{M_{\text{hydrochar}} \times C_{\text{hydrochar}}}$$

where  $M_{\text{sample}}$  is the final mass (g) of sample;  $M_{\text{hydrochar}}$  is the mass (g) of hydrochar added;  $C_{\text{sample}}$  and  $C_{\text{hydrochar}}$  are carbon contents (%) of sample and hydrochar, respectively. ( $M_{\text{hydrochar}} = 3$  g;  $C_{\text{hydrochar}} = 64.07$  %)

**Table S7** Surface areas and porosities of MCs derived from different FeCl<sub>3</sub> loading content (750°C of activation temperature and 2 h of hold time)

Sample	$S_{\text{BET}}^a$ (m <sup>2</sup> /g)	$S_{\text{mic}}^b$ (m <sup>2</sup> /g)	$S_{\text{mic}}/S_{\text{BET}}$ (%)	$V_{\text{mic}}^c$ (cm <sup>3</sup> /g)	$V_{\text{t}}^d$ (cm <sup>3</sup> /g)	$V_{\text{mic}}/V_{\text{t}}$ (%)
<i>MC-Cl-0</i>	539.9	502	93.0	0.224	0.253	88.5
<i>MC-Cl-1</i>	908.0	806	88.8	0.402	0.547	73.5
<i>MC-Cl-2</i>	648.0	560	86.4	0.281	0.408	68.9
<i>MC-Cl-5</i>	733.0	626	85.4	0.312	0.463	67.4
<i>MC-Cl-10</i>	385.0	280	72.7	0.137	0.286	47.9
<i>MC-Cl-20</i>	1.4	0	0.0	0.001	0.007	10.0

<sup>a</sup> Brunauer-Emmett-Teller (BET) surface area measured using N<sub>2</sub> adsorption at  $P/P_0$  of 0.04-0.3.

<sup>b</sup> Micropore surface area calculated using the  $t$ -plot method.

<sup>c</sup> Micropore volume calculated using the  $t$ -plot method.

<sup>d</sup> Total pore volume determined at  $P/P_0 = 0.99$ .



**Table S8** Mössbauer parameters at room temperature of as-prepared MCs derived from different FeCl<sub>3</sub> loadings (750°C of activation temperature and 2 h of hold time)

Sample	Component	HMF (KOe) <sup>a</sup>	IS (mm/s) <sup>b</sup>	QS (mm/s) <sup>c</sup>	Γ/2 (mm/s) <sup>d</sup>	Mole percentage (%)
<i>MC-Cl-1</i>	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub> (s) <sup>e</sup>	0	0.42	0.07	0.52	34.5
	Fe <sub>3</sub> O <sub>4</sub>	457.19	0.71	0.04	0.39	44.1
		491.18	0.27	0.02	0.18	21.4
<i>MC-Cl-2</i>	$\alpha$ -Fe <sub>2</sub> O <sub>3</sub> (s)	0	0.37	0.51	0.27	19.4
	Fe <sub>3</sub> O <sub>4</sub>	457.23	0.79	0.02	0.25	54.3
		488.38	0.41	0.05	0.14	26.3
<i>MC-Cl-5</i>	Fe <sub>3</sub> O <sub>4</sub>	458.14	0.68	0	0.28	70.2
		485.87	0.26	0.07	0.15	29.8
<i>MC-Cl-10</i>	Fe <sub>3</sub> O <sub>4</sub>	460.90	0.83	0	0.24	69.2
		485.55	0.39	0.07	0.13	30.8
<i>MC-Cl-20</i>	Fe <sub>3</sub> O <sub>4</sub>	465.36	0.60	0	0.19	56.9
		489.45	0.12	0.08	0.17	43.1

<sup>a</sup> HMF: hyperfine magnetic fields.

<sup>b</sup> IS: isomer shift.

<sup>c</sup> QS: quadrupole splitting.

<sup>d</sup> Γ/2: half line width.

<sup>e</sup> s: superparamagnetic.

**Table S9** Fe content analyses during acid leaching experiments at pH 2 for MCs activated at different FeCl<sub>3</sub> loadings (750°C of activation temperature and 2 h of hold time)

Sample	Fe Leaching Concentration (mg/L)	Fe Leaching Percentage (%)
<i>MC-CI-0</i>	-	-
<i>MC-CI-1</i>	3.96 ± 0.02	2.44 ± 0.01
<i>MC-CI-2</i>	3.85 ± 0.14	1.68 ± 0.06
<i>MC-CI-5</i>	4.34 ± 0.02	0.74 ± 0.01
<i>MC-CI-10</i>	3.84 ± 0.04	0.42 ± 0.01
<i>MC-CI-20</i>	3.92 ± 0.50	0.28 ± 0.04

**Table S10** Physicochemical properties of PPCPs and  $q_m$  values for PPCP adsorption onto the *MC-Cl-5* sample.

PPCP	$q_m$ (mmol/g) <sup>a</sup>	Log $K_{OW}$ <sup>b</sup>	Melting Points (°C)
sulfamethoxazole (SMX)	0.82	0.89	167
sulfapyridine (SPY)	0.91	0.35	191
carbamazepine (CMZ)	0.72	2.45	190
sulfathiazole (STZ)	0.91	0.05	202
diclofenac sodium (DCF)	0.57	3.91	288
quinindium (QND)	0.65	2.88	174
bisphenol A (BPA)	0.86	3.32	150
triclosan (TCS)	1.28	4.76	55

<sup>a</sup>  $q_m$ : the maximum adsorption capacity in Langmuir adsorption model.

<sup>b</sup>  $K_{OW}$ : octanol-water partition coefficient.