Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Graphene encapsulated Fe_xCo_y nanocages derived from metal–organic frameworks as efficient activators for peroxymonosulfate

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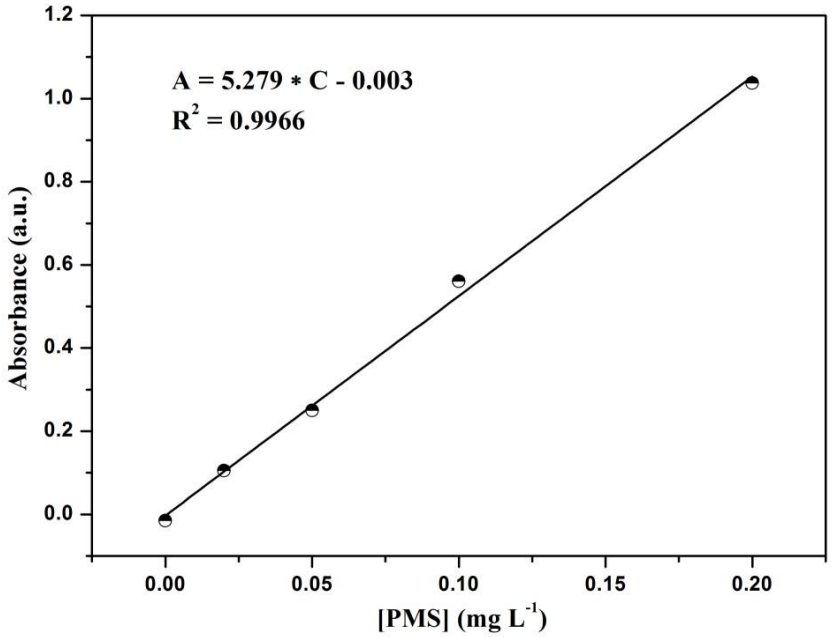


Fig. S1. The calibration curve of PMS concentration determined using iodometric method.

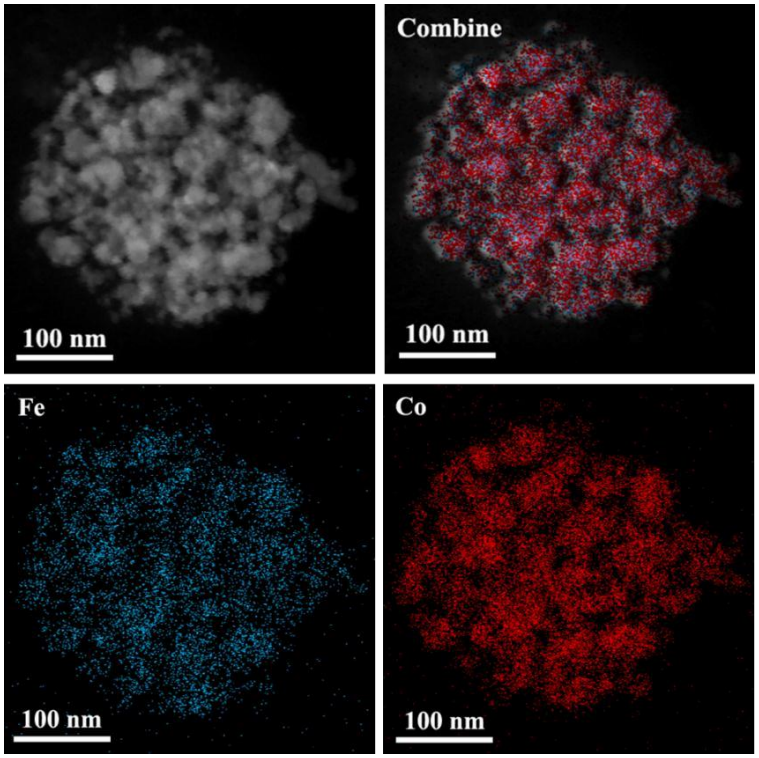


Fig. S2. EDS mapping of Fe_3Co_7@C-650 nanocages**.**

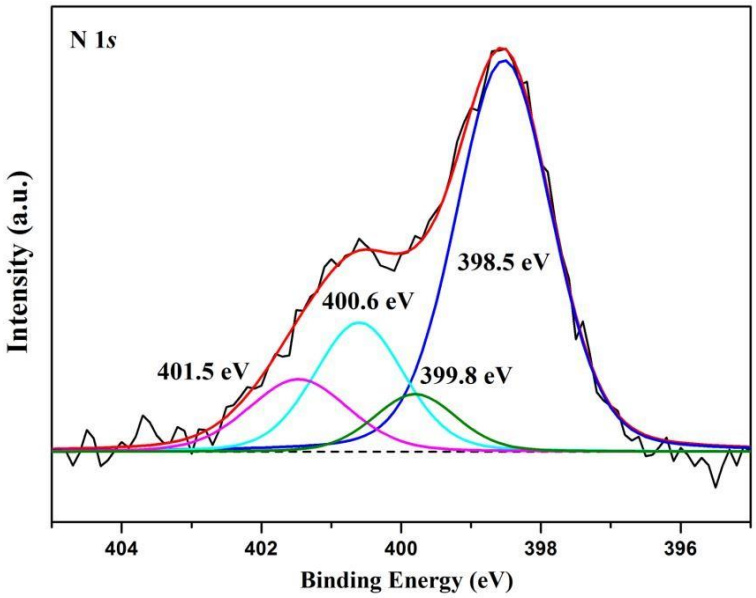


Fig. S3. High resolution XPS spectrum of N 1*s* for Fe_3Co_7@C-650 nanocages.

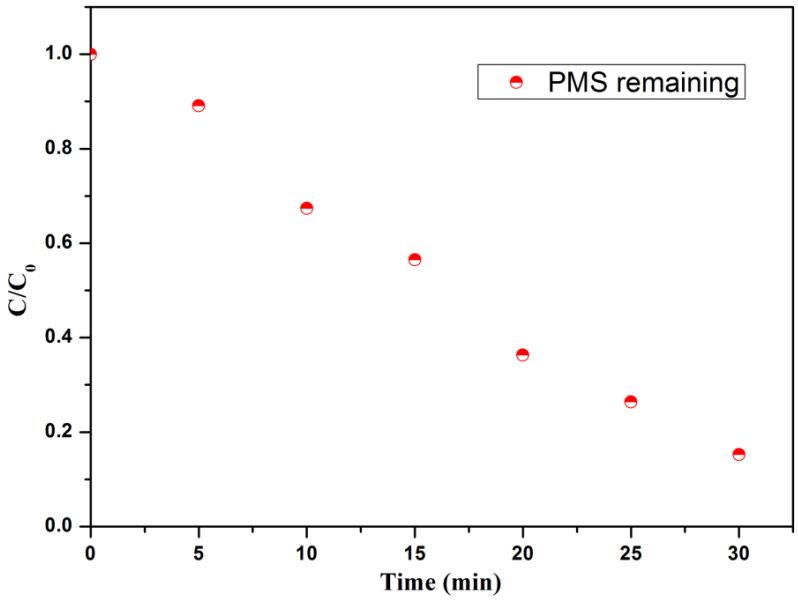


Fig. S4. The time courses of PMS remaining during the reaction**.** Reaction conditions: [BPA] = 20 mg L^{-1}, [PMS] = 0.2 g L^{-1}, catalyst = 0.1 g L^{-1}, initial solution pH = 6.0.

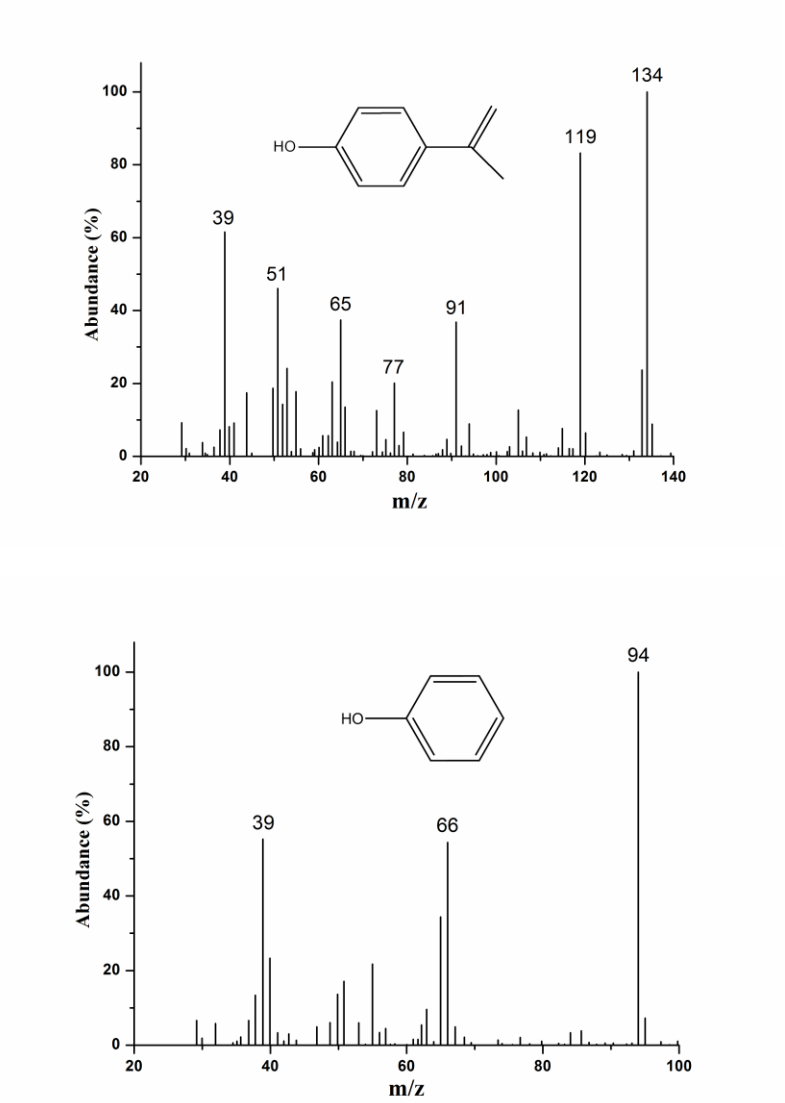


Fig. S5. GC-MS spectra of the intermediates.

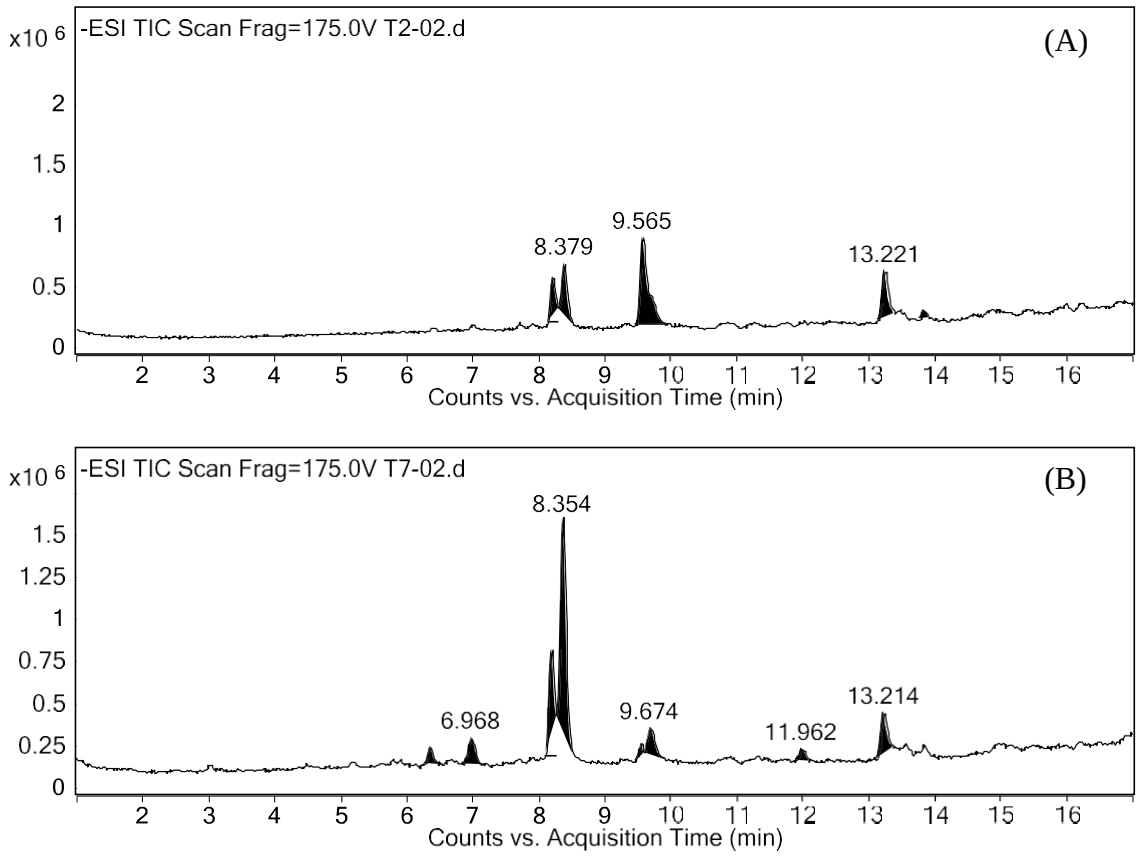
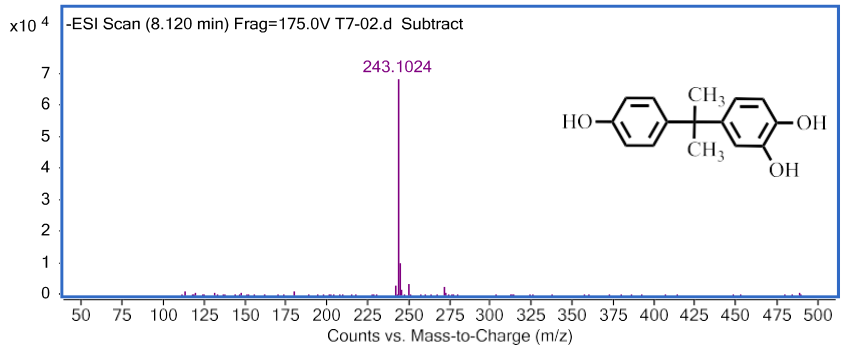
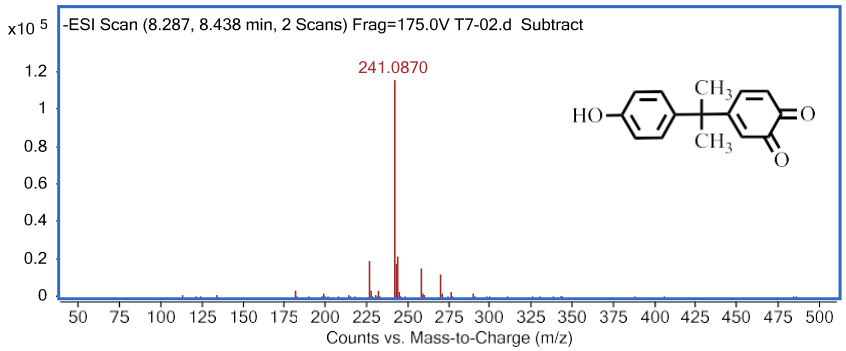
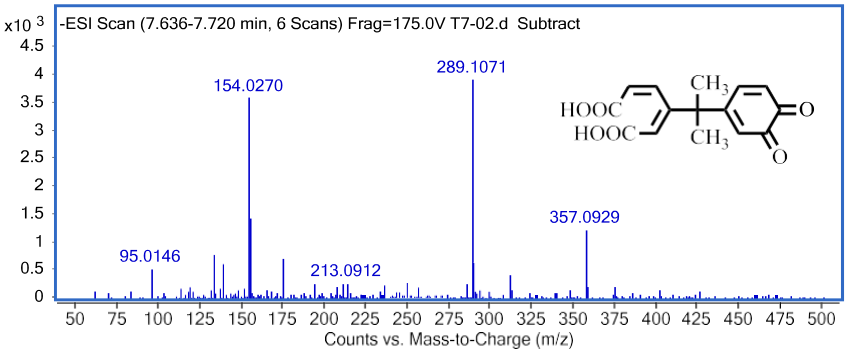
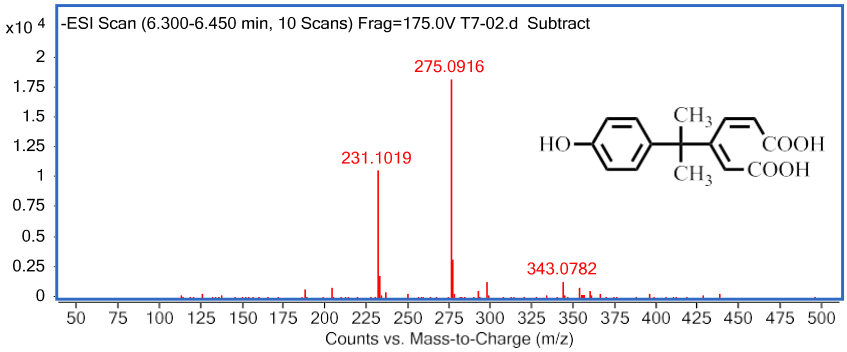


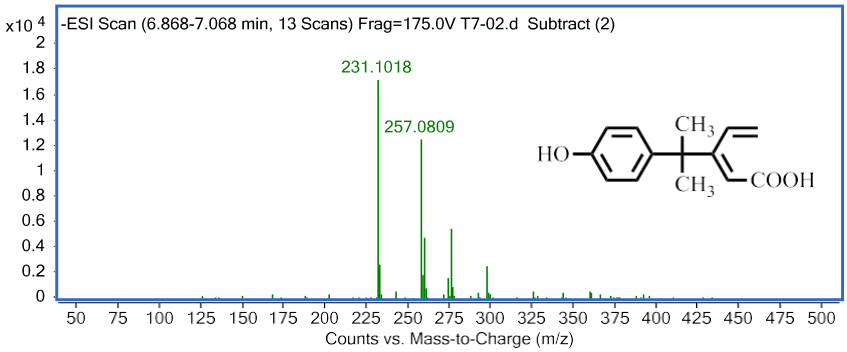
Fig. S6. LC-MS diagram for BPA degradation reaction by activation of PMS on Fe_3Co_7@C-650 nanocages after (A) 10 min and (B) 30 min. Reaction conditions: [BPA] = 20 mg L^{-1}, [PMS] = 0.2 g L^{-1}, catalyst = 0.1 g L^{-1}, initial solution pH = 6.0.


x10 4
-ESI Scan (8.120 min) Frag=175.0V T7-02.d Subtract
243.1024
HO
CH3
CH3
OH
OH
Counts vs. Mass-to-Charge (m/z)


x10 5
-ESI Scan (8.287, 8.438 min, 2 Scans) Frag=175.0V T7-02.d Subtract
241.0870
HO
CH3
CH3
O
O
Counts vs. Mass-to-Charge (m/z)


x10 3
-ESI Scan (7.636-7.720 min, 6 Scans) Frag=175.0V T7-02.d Subtract
154.0270
289.1071
357.0929
95.0146
213.0912
HOOC
HOOC
CH3
CH3
O
O
Counts vs. Mass-to-Charge (m/z)


x10 4
-ESI Scan (6.300-6.450 min, 10 Scans) Frag=175.0V T7-02.d Subtract
275.0916
231.1019
343.0782
HO
CH3
CH3
COOH
COOH
Counts vs. Mass-to-Charge (m/z)


x10 4
-ESI Scan (6.868-7.068 min, 13 Scans) Frag=175.0V T7-02.d Subtract (2)
231.1018
257.0809
HO
CH3
CH3
COOH
Counts vs. Mass-to-Charge (m/z)

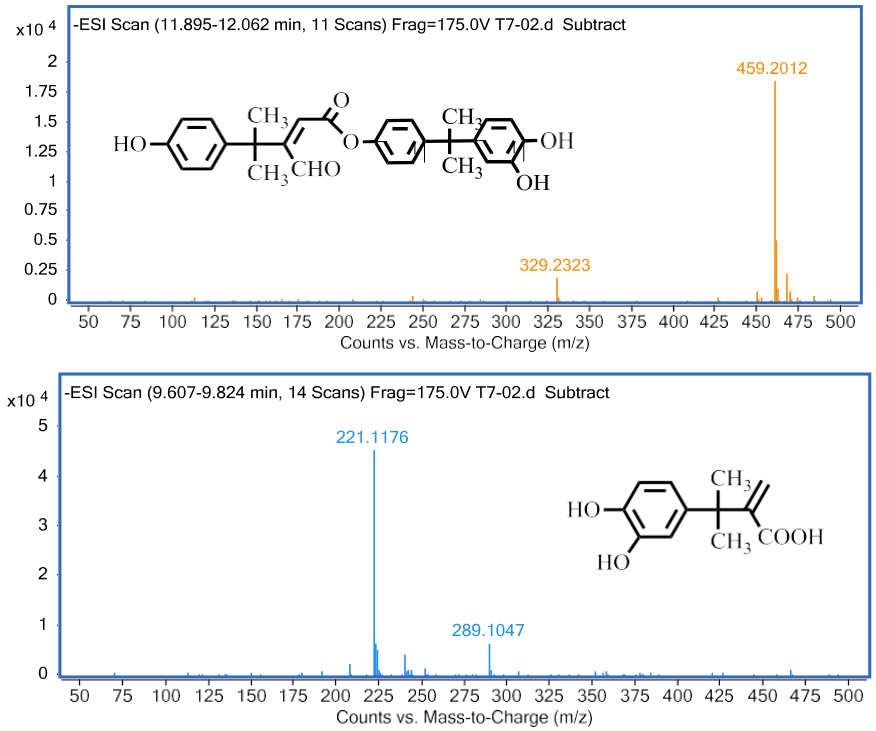


Fig. S7. LC-MS spectra of the intermediates.

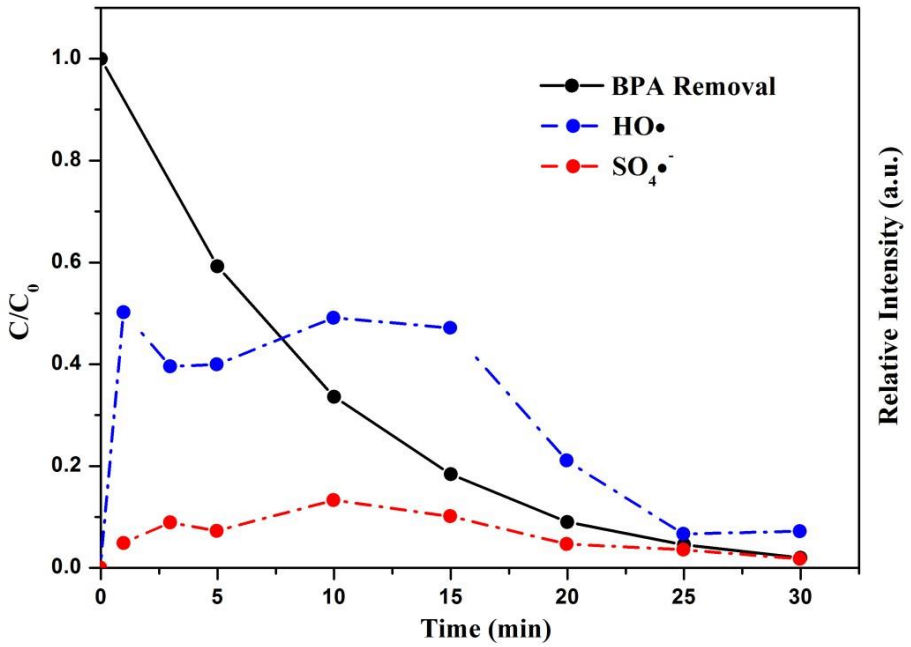


Fig. S8. BPA removal profile and relative intensity variations of DMPO-•OH and DMPO-SO_4•$^-$ during reaction. Reaction conditions: [BPA] = 20 mg L^{-1}, [PMS] = 0.2 g L^{-1}, catalyst = 0.1 g L^{-1}, T = 298 K, initial solution pH = 6.0.

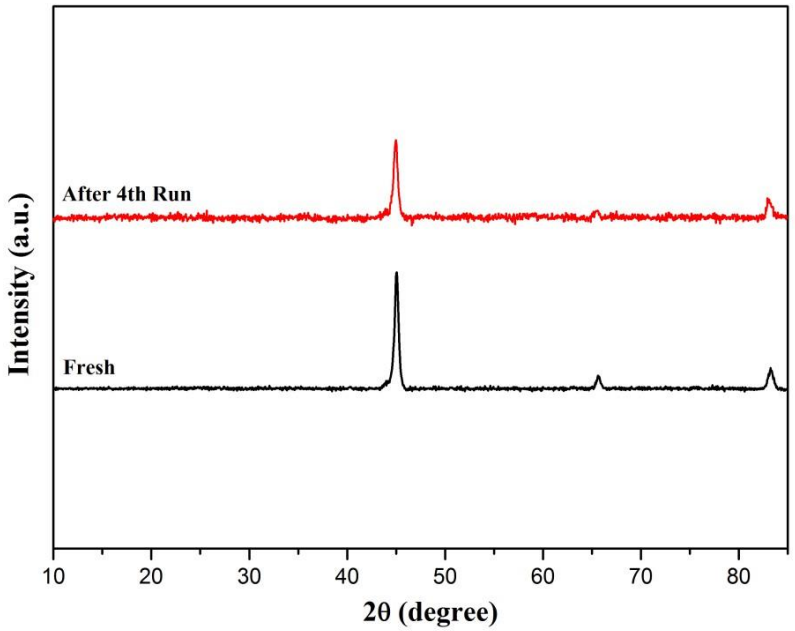


Fig. S9. The XRD patterns of Fe_3Co_7@C-650 before and after 4-cycle run. Reaction conditions: [BPA] = 20 mg L^{-1}, [PMS] = 0.2 g L^{-1}, catalyst = 0.1 g L^{-1}, initial solution pH = 6.0.

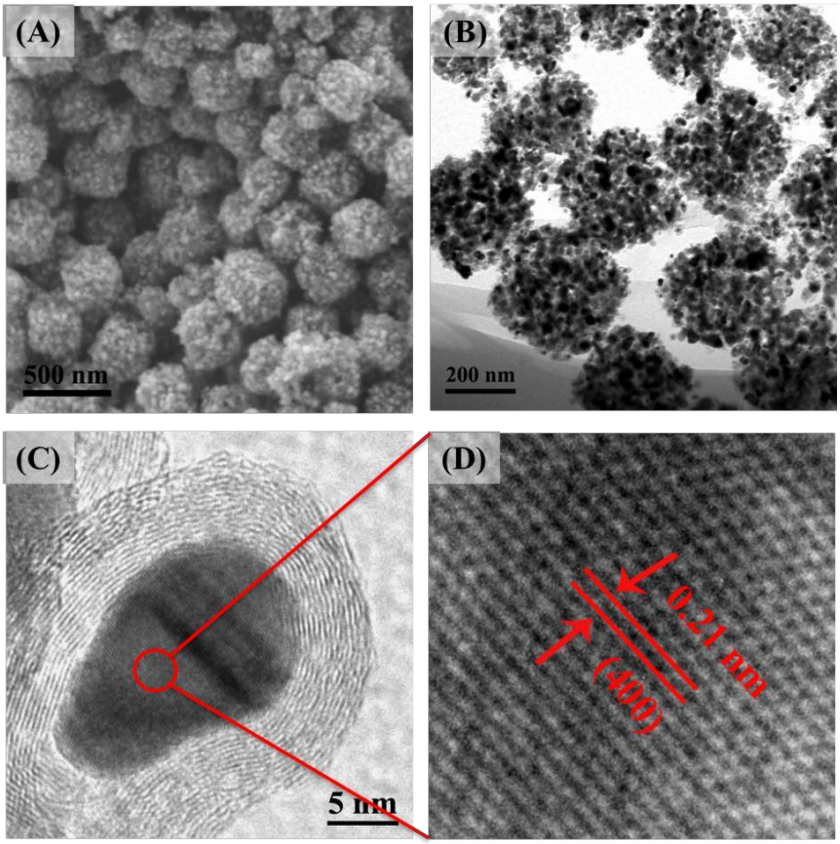


Fig. S10. (A) SEM image (B) TEM image, and (C, D) HR-TEM images of Fe_3Co_7@C-650 after 4-cycle run.

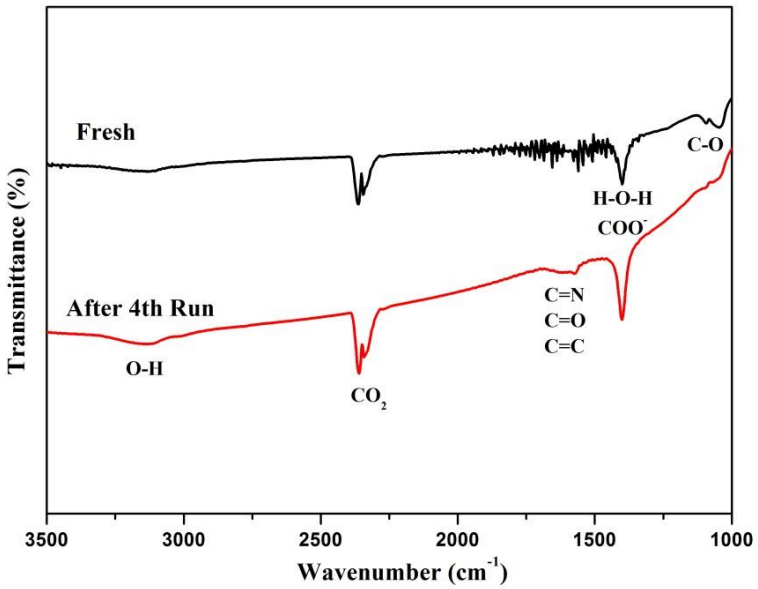


Fig. S11. FT-IR spectra of Fe_3Co_7@C-650 before and after 4-cycle run.

Table S1. The chemical compositions and average crystallite sizes of Fe_xCo_y@C nanicages

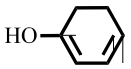
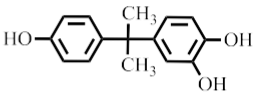
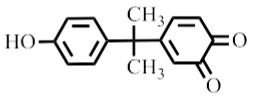
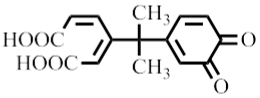
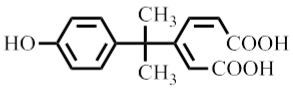
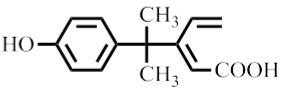
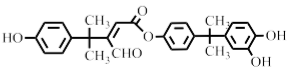
Nanocages	Metal content (%)				Average crystallite size
	Fe	Co	N	O	(nm)
Fe_3Co_7@C-500	17.66	52.14	16.93	13.27	17.6
Fe_3Co_7@C-650	24.84	71.01	1.01	3.14	23.9
Fe_3Co_7@C-800	24.68	69.85	1.81	3.66	30.7
Fe_2Co_8@C-500	18.16	68.67	8.17	5.00	15.9

Table S2. Room temperature ^{57}Fe Mössbauer parameters of Fe_xCo_y@C nanocages.

samples	Assignment	IS (mm s^{-1})	QS (mm s^{-1})	B_{hf} (T)	Γ (mm s^{-1})	Area (%)
Fe_2Co_8@C-500	Fe^0	0.00	0.02	32.4	0.32	32.4
	Fe^0	0.00	0.02	33.8	0.31	36.9
	Fe_2O_3	0.31	1.12	-	0.99	30.7
Fe_3Co_7@C-500	Fe^0	0.00	0.03	32.7	0.32	36.1
	Fe^0	0.00	0.00	34.1	0.34	40.6
	Fe_2O_3	0.34	1.14	-	1.00	23.3
Fe_3Co_7@C-650	Fe^0	0.00	0.03	32.9	0.32	39.9
	Fe^0	0.00	-0.01	34.2	0.34	60.1
Fe_3Co_7@C-800	Fe^0	0.00	0.01	33.2	0.31	60.2
	Fe^0	0.00	-0.01	34.4	0.28	39.8

Experimental errors are ± 0.02 mm s^{-1} for isomer shift (IS), ± 0.03 mm s^{-1} for quadrupole splitting (QS) and 1% for relative area. IS is relative to α-iron foil.

Table S3. Reaction intermediates identified by GC-MS and LC-MS

Compounds	Retention time (min)	Molecular weight (m/z)	Molecular structure
Product A	5.58 (GC-MS)	94	
Product B	10.84 (GC-MS)	134	
Product C	8.12 (LC-MS)	244	
Product D	8.44 (LC-MS)	242	
Product E	7.64 (LC-MS)	290	
Product F	6.30 (LC-MS)	276	
Product G	6.87 (LC-MS)	232	
Product H	11.90 (LC-MS)	460	
Product I	9.60 (LC-MS)	222