Supporting Information

Jinqi Li [1], Xueqi Wang [1], Huidong Tang [1], Jiachen Li [1], Jiacheng Bao [2], Yixing Ma [1,*], Kai Li [1], Xin Sun [1,*]

[1] Faculty of Environment Science and Engineering, Kunming University of Science and Technology, Kunming 650500, China.

[2] School of Resource & Environment and Safety Engineering, University of South China, Hengyang, 421001, China.

Corresponding Author:

Yixing Ma, E-mail address: mayixing99@kust.edu.cn

Xin Sun, E-mail address: sunxin_kmust@163.com

Text S1 Materials and Chemicals

H_2O_2 (30 wt%), calcium oxide (H_3BTC, ≥ 98.0%), $FeCl_3 \cdot 6H_2O$ (99.0%, AR), $FeCl_2 \cdot 4H_2O$ (99.0%, AR), $FeSO_4 \cdot 7H_2O$ (5% in H_2O), Reduced iron powder (AR), ethanol (EtOH, 99.7 %), NaOH(99.0%, AR) were purchased from Aladdin (Shanghai, China).All the solutions were prepared with ultrapure water.

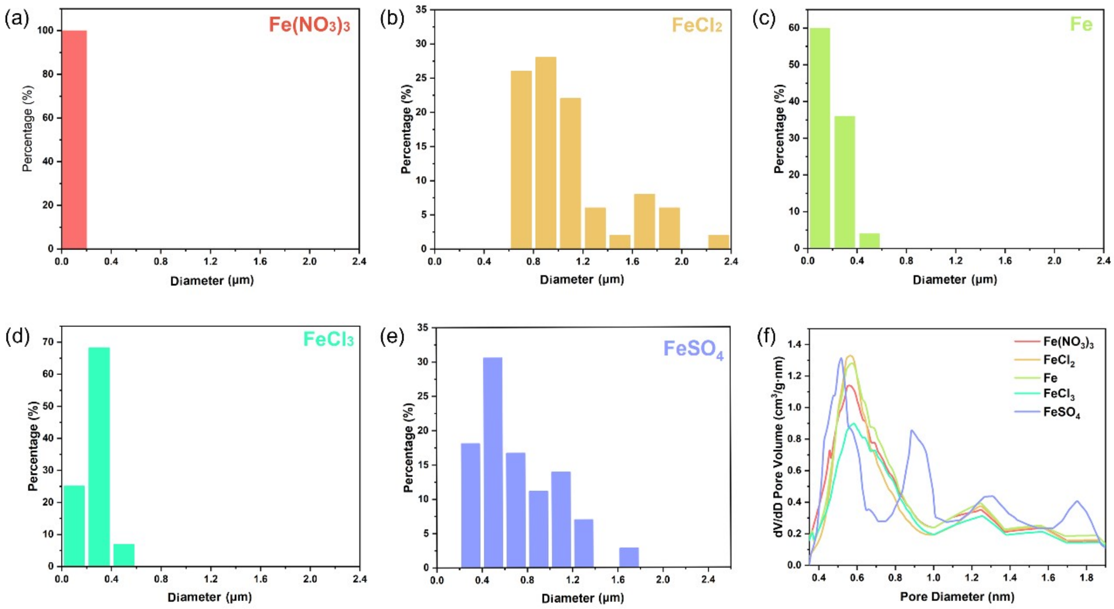

Fig. S1. Particle size distribution of MIL-100(Fe) prepared with different iron sources (a) $Fe(NO_3)_3$, (b) $FeCl_2$, (c) Fe, (d) $FeCl_3$, (e) $FeSO_4$, (f) Pore Size Distribution of MIL-100(Fe) prepared with different Iron sources.

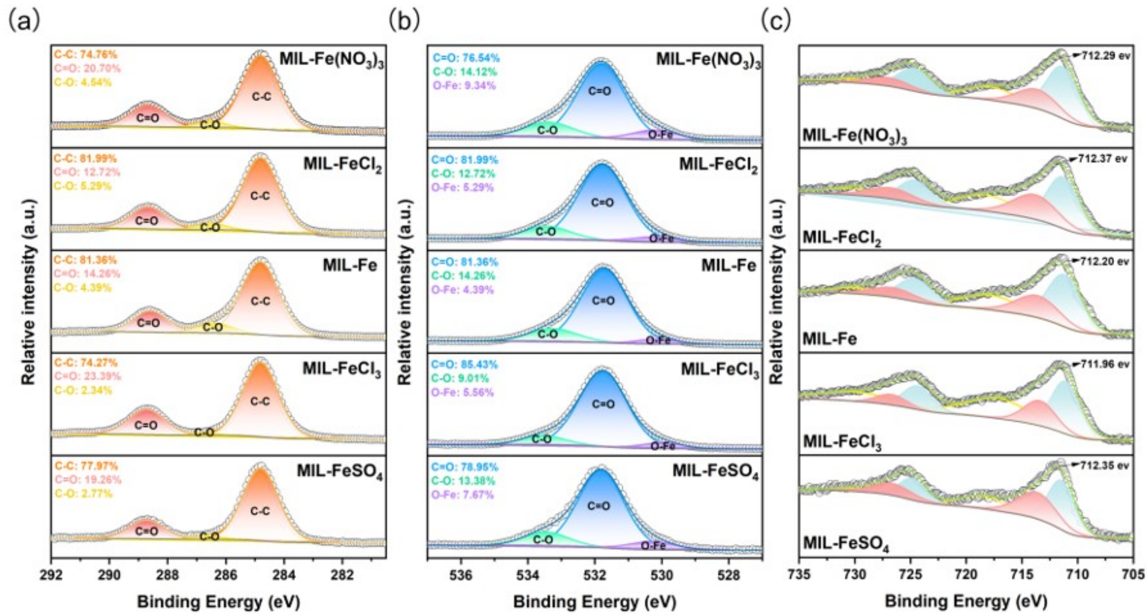

Fig. S2. XPS fine spectrum of MIL-100(Fe) prepared with different iron sources (a) C 1s, (b) O 1s, (c) Fe 2p.

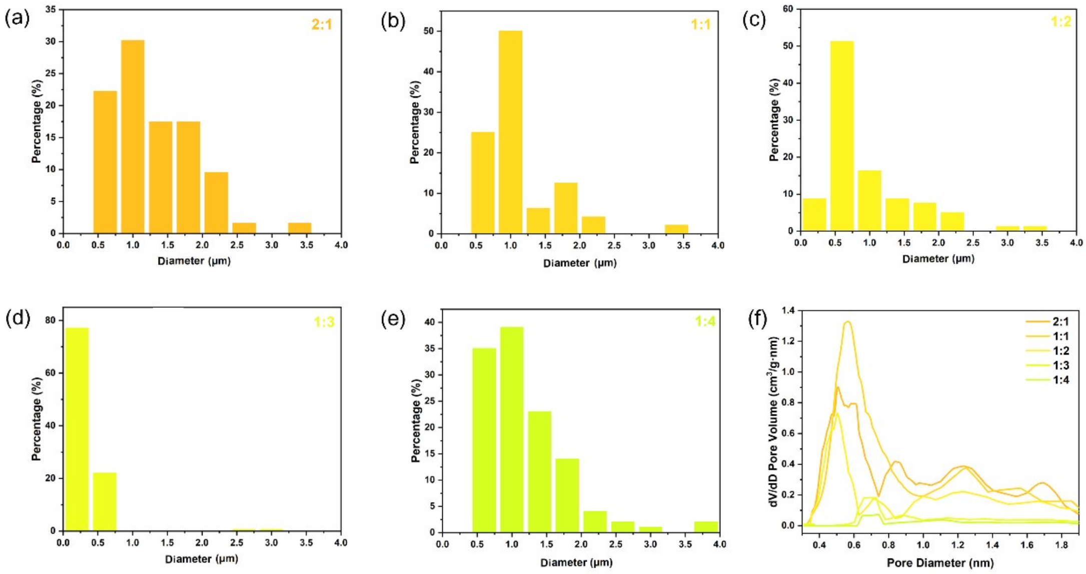

Fig. S3. Particle size distribution of MIL-100(Fe) prepared with different precursor ratios (a) 2:1, (b) 1:1, (c) 1:2,(d) 1:3, (e) 1:4, (f) Pore size distribution of MIL-100(Fe) prepared with different $FeCl_2/H_3BTC$ ratios.

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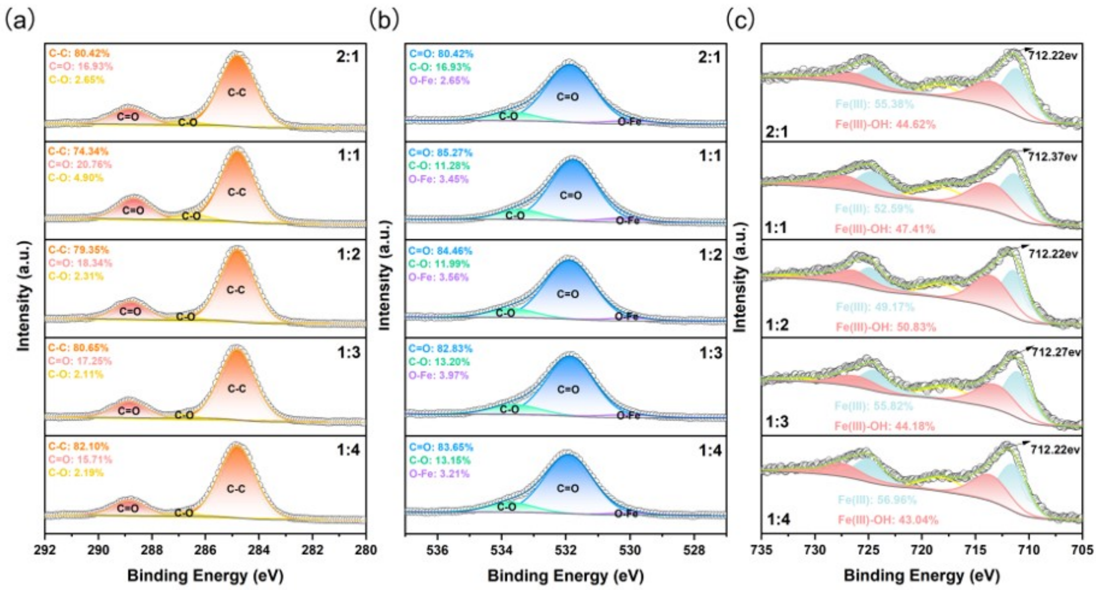

Fig. S4. XPS fine spectrum of MIL-100(Fe) prepared with different $FeCl_2/H_3BTC$ ratios (a) C 1s, (b) O 1s, (c) Fe 2p.

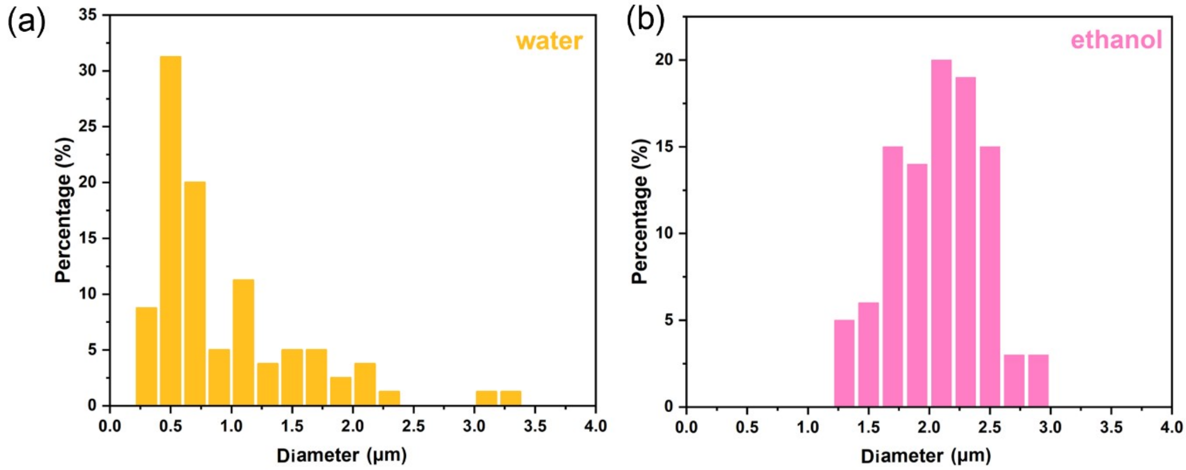

Fig. S5. Particle size distribution of MIL-100(Fe) prepared with different synthesis solvents (a) water, (b) ethanol.

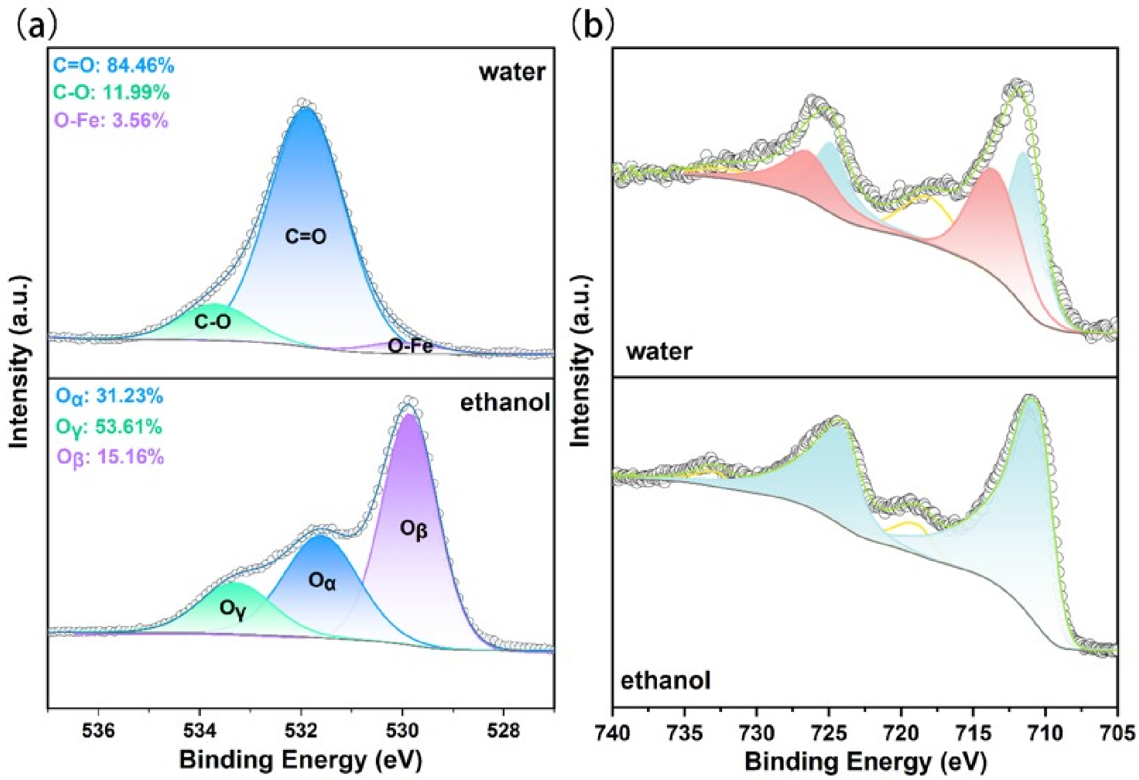

Fig. S6. XPS fine spectrum of MIL-100(Fe) prepared with different synthesis solvents (a) O1s, (b) Fe 2p.

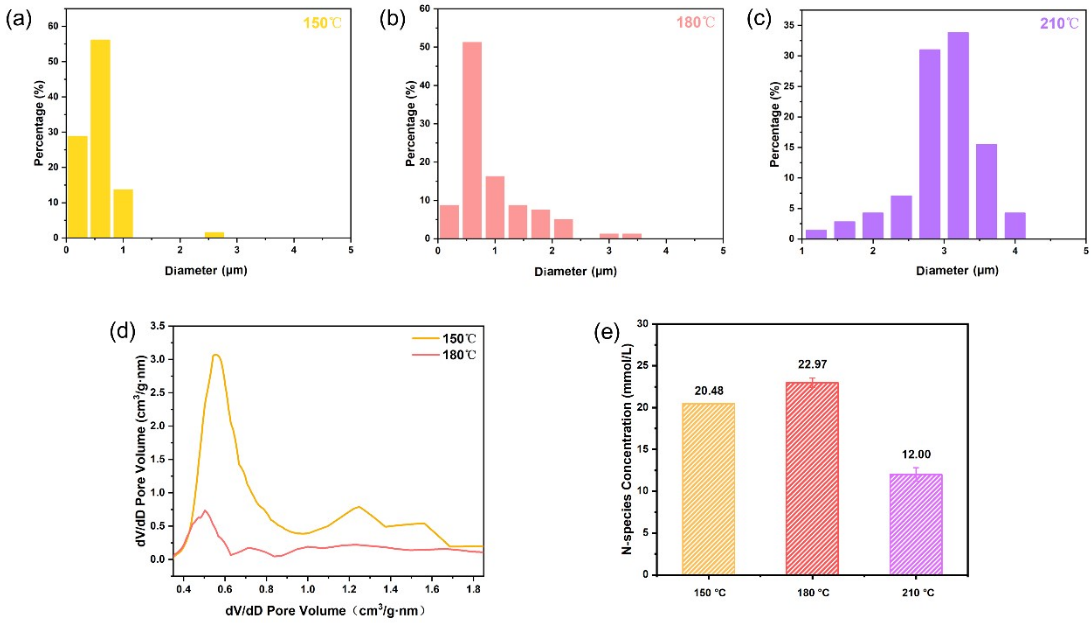

Fig. S7. Particle Size Distribution of MIL-100(Fe) prepared with different hydrothermal reaction temperatures (a) 150℃; (b) 180℃; (c) 210℃. (d)The Pore Size Distribution of MIL-100(Fe) prepared with different hydrothermal reaction temperatures, and (e) the absorption capacity of N species with denitrification efficiency ≥80%.

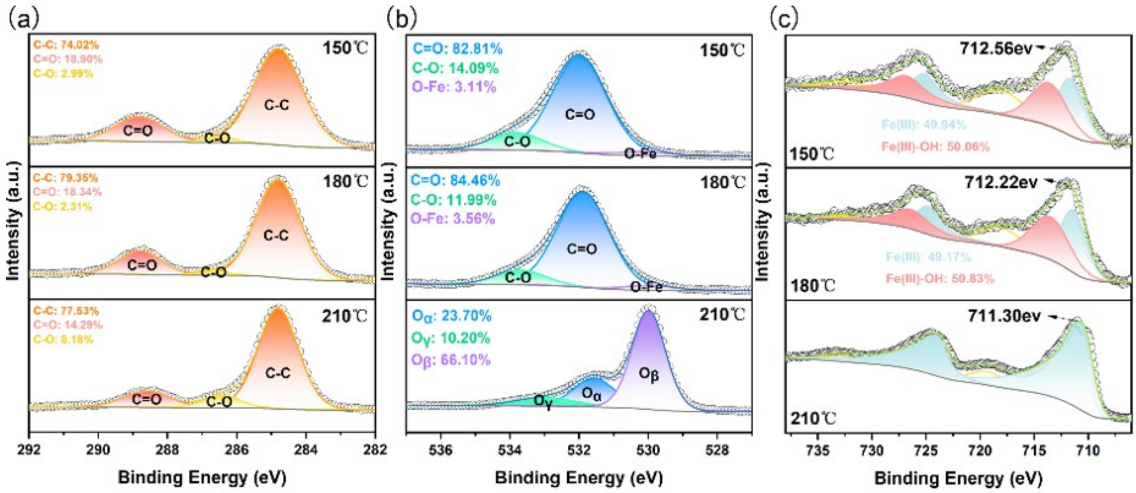

Fig. S8. XPS fine spectrum of MIL-100(Fe) prepared with different hydrothermal reaction temperatures (a) C 1s; (b) O1s; (c) Fe 2p.

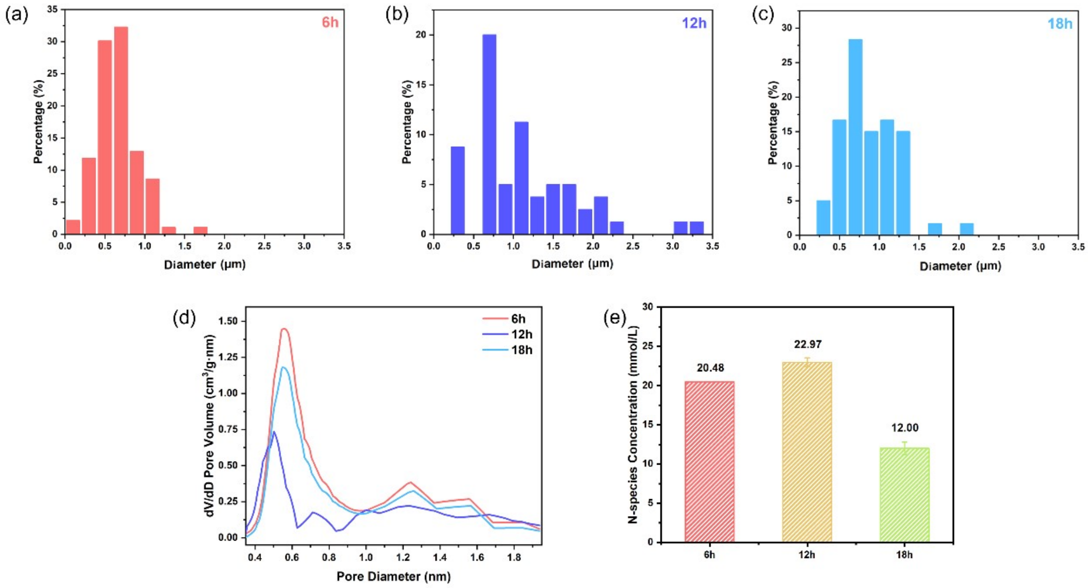

Fig. S9. Particle Size Distribution of MIL-100(Fe) prepared with different hydrothermal reaction times (a) 6 h; (b) 12 h; (c) 18 h (d)The Pore Size Distribution of MIL-100(Fe) prepared with different hydrothermal reaction times, and (e) the absorption capacity of N species with denitrification efficiency ≥80%.

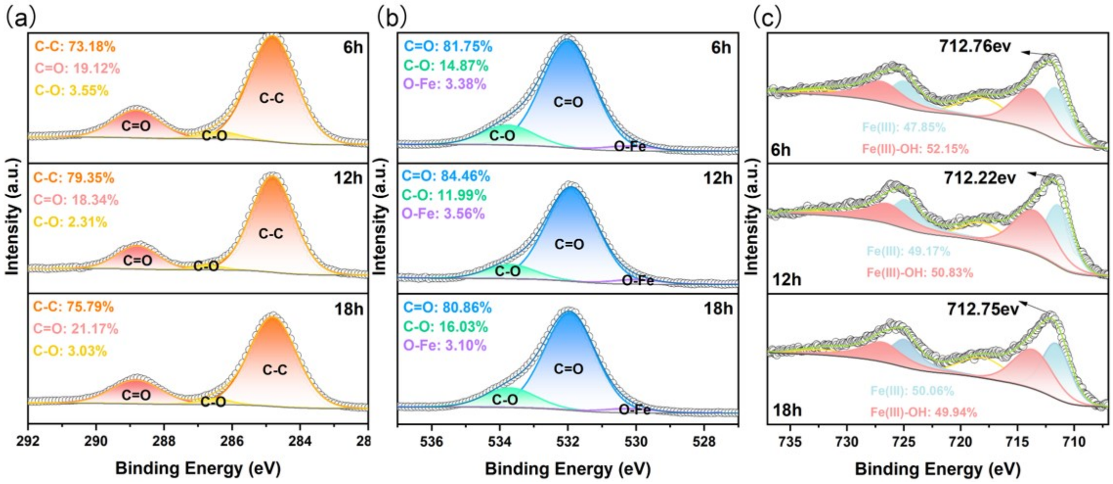

Fig. S10. XPS Fine Spectrum of MIL-100(Fe) prepared with different hydrothermal reaction times

(a) C 1s; (b) O 1s; (c) Fe 2p.

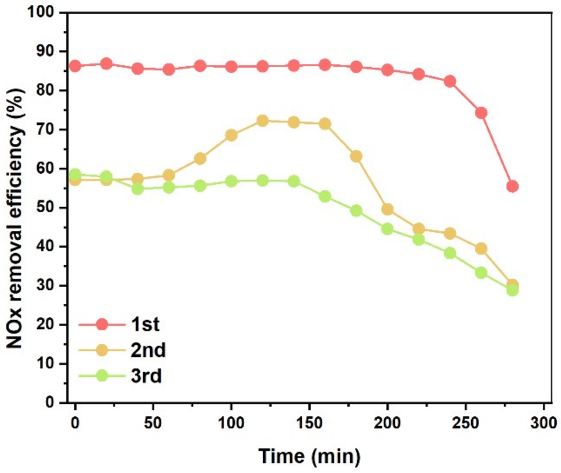

Fig. S11. Reusability of MIL-100(Fe).

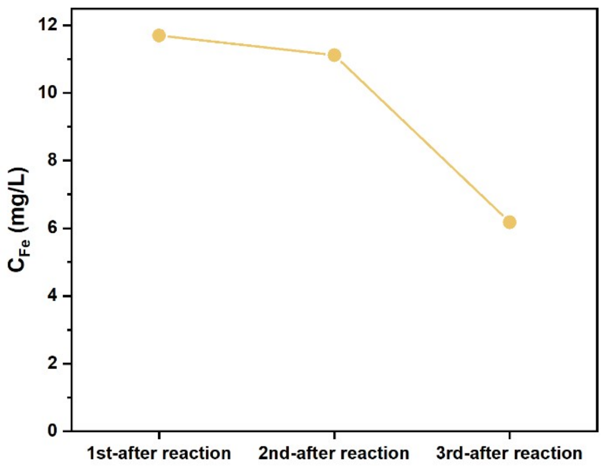

Fig. S12. Iron ion concentration as a function of reaction cycles.

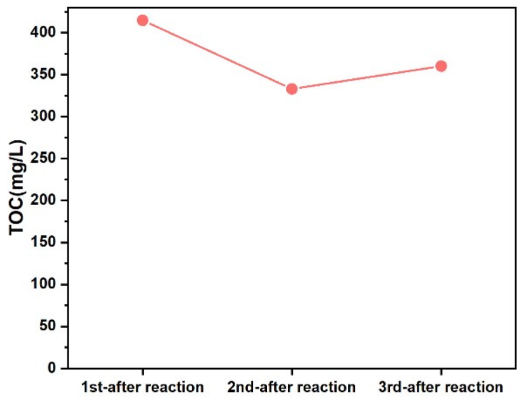

Fig. S13. Total organic carbon (TOC) concentration as a Function of Reaction Cycles.

Conditions		S_{BET} (m^2g^{-1})	V_p (cm^3g^{-1})	Average pore Diameter (nm)
Iron precursor	$Fe(NO_3)_3$	1519.55	0.90	2.37
	$FeCl_2$	1426.56	0.68	1.89
	Fe	1621.72	0.78	1.92
	$FeCl_3$	1303.80	1.04	2.64
	$FeSO_4$	1884.67	0.76	1.61

Table. S1. BET specific surface area data of MIL-100(Fe) prepared with different iron sources.

Samples	Surface atomic ratio	Bulk atomic ratio
$Fe(NO_3)_3$	16.19	23.52
$FeCl_2$	16.16	20.15
Fe	14.89	20.07
$FeCl_3$	18.25	15.13
$FeSO_4$	17.89	22.29

Table S2. Proportion of surface and bulk iron elements in MIL-100(Fe) prepared with different iron sources.

Conditions		$S_{BET}(m^2g^{-1})$	$V_p(cm^3g^{-1})$	Average pore diameter
	2:1	1439.82	0.65	1.81
	1:1	1426.56	0.68	1.89
Fe/BTC ratio	1:2	823.91	0.53	2.57
	1:3	195.60	0.20	4.09
	1:4	95.57	0.10	4.37

Table S3. BET specific surface area data of MIL-100(Fe) prepared with different $FeCl_2$/H_3BTC ratios.

Samples	Surface atomic ratio	Bulk atomic ratio
2：1	14.87	19.43
1：1	16.16	20.15
1：2	16.01	18.56
1：3	17.17	15.33
1：4	13.88	19.72

Table S4. Proportion of surface and bulk Fe elements in MIL-100(Fe) prepared with different $FeCl_2$/H_3BTC.

Conditions		$S_{BET}(m^2g^{-1})$	$V_p(cm^3g^{-1})$	Average pore Diameter
hydrothermal reaction temperatures	150 ℃	2870.95	1.43	1.99
	180 ℃	823.91	0.53	2.57

Table S5. BET specific surface area data of MIL-100(Fe) prepared with different hydrothermal reaction temperatures.

Samples	Surface atomic ratio	Bulk atomic ratio
150 ℃	13.14	18.14
180 ℃	16.01	18.56

Table S6. Proportions of surface and bulk Fe elements in MIL-100(Fe) prepared at different hydrothermal temperatures.

Conditions		$S_{BET}(m^2g^{-1})$	$V_p(cm^3g^{-1})$	Average pore Diameter
hydrothermal	6 h	1377.94	0.71	2.06
reaction	12 h	823.91	0.53	2.57
times	18 h	1145.76	0.66	2.50

Table S7. BET specific surface area data of MIL-100(Fe) prepared with different hydrothermal reaction time.

Samples	Surface atomic ratio	Bulk atomic ratio
6 h	13.27	18.60
12 h	16.01	18.56
18 h	12.39	16.90

Table S8. Proportions of surface and bulk Fe elements in MIL-100(Fe) synthesized at different hydrothermal durations.