

Text S1 Chemicals:

The following chemicals were obtained from Aladdin Chemistry Co., Ltd, China: Sulfamethoxazole, humic acid (HA), 5,5-dimethyl-1-pyrroline-N-oxide (DMPO, C₆H₁₁NO), 2,2,6,6-tetramethylpiperidine (TEMP, C₉H₁₉N), furfuryl alcohol (FFA, C₅H₆O₂), P-benzoquinone (BQ, C₆H₄O₂) and methanol (chromatographic grade, CH₃OH). The following chemicals were purchased from Guangzhou Chemical Reagent Factory (China): sodium hydroxide (NaOH), sulfuric acid (H₂SO₄), hydrochloric acid (HCl) and sodium sulphate (Na₂SO₄). Persulfate, iron nitrate nonahydrate (FeCl₂·4H₂O) and 2-methylimidazole (2-MeIM, C₄H₆N₂) were purchased from Macklin. Zinc nitrate hexahydrate (Zn (NO₃)₂·6H₂O) was provided by Alfa Aesar Chemical Co., Ltd. Methanol (CH₃OH), ethanol (C₂H₅OH), potassium iodide (KI) and Tert-butyl alcohol (TBA) were obtained from Tianjin Chemical Co., Ltdj. Nafion solution was purchased from Shanghai Hesun Electric Co., Ltd (China). Acetic acid (chromatographic grade, CH₃COOH) was provided by Tianjin Kermel Chemical Reagent Co., Ltd (China). Except special notes, all reagents used in this work were analytical reagents (A.R.) and used without any further purification. Deionized water was purified by millipore reverse osmosis (RO) system and used throughout the whole experiment.

Text S2 Synthesis of FeMIL:

FeCl₂·4H₂O (5 mmol, 0.99 g), 2-aminoterephthalic acid (2-BDC) (5 mmol, 0.83 g) were added to N,N-dimethylformamide (DMF) (25 mL) and stirred for 30 min at first. The mixture was then poured into a 100 mL Teflon-lined steel autoclave, placed in a fan oven preheated to 150 °C and maintained for 12 h, and then the autoclave was cooled to room temperature in air. The product was obtained by centrifugation and successively washed by DMF, methanol and water. The resulting solid was dried in a vacuum oven at 60 °C for 12 h to remove H₂O molecules. The resulting powder

was stored at room temperature in a covered glass container until needed.

Text S3 Characterization

X-ray diffraction (XRD, Bruker D8-Advance) was analyzed over arrange of $2\theta=5-80^\circ$ using Cu $K\alpha_1$ radiation to detect the crystal structure. Transmission electron microscopy and high angle annular dark field scanning TEM (HAADF-STEM) were performed at FEI Tecnai G2 f20 s-twin, 200kV. X-ray photoelectron spectroscopy (XPS) data were obtained by Thermo K-Alpha⁺ equipped with monochrome Al $K\alpha$ X-ray source using powder compression method. The C1s peak binding energy at 284.7eV was used as the calibration reference. The surface area was determined by the Brunauer-Emmett-Teller (BET) method using a surface area analyzer (ASAP 2460 Version 2.00, Micromeritics), and the pore size distribution was analyzed by the Barrett-Joyner-Halenda(BJH). Before the physical adsorption measurement of nitrogen, the sample degassed for 5 hours at 150 °C vacuum. The aberration-corrected high-angle annular dark field scanning transmission electron microscopy (AC HAADF-STEM) images were investigated by Themis Z (FEI, USA) equipped with energy-dispersive X-ray spectroscopy (EDS) mapping at an accelerating voltage of 200 kV.

Text S4 Analytical Methods

Electro chemical measurements were performed in a conventional three-electrode system with the Fe(MIL)-N-C catalyst as the working electrode. The electrolyte for i-t curve was $\text{Na}_2\text{SO}_4(0.1 \text{ M})$, $\text{Na}_2\text{SO}_4(0.1 \text{ M}) +$ and $\text{Na}_2\text{SO}_4(0.1 \text{ M}) + \text{PMS} (0.4\text{g/L}) + \text{BPA} (20\text{mg/L})$ respectively. Radicals were detected by electron paramagnetic resonance (EPR) (Japan, JESFA200) with DMPO and TEMPO as the spinning-trap agent. The EPR test was carried out when the reaction time were 0 min, 5 min and 10 min.

Text S5

In this study, kinetic model pseudo-first-order were used to describe the kinetic parameters of the catalytic process of SMX degradation, which is expressed as:

$$-\ln\left(\frac{C_t}{C}\right) = kt \quad (\text{S1})$$

Where C ($\text{mg}\cdot\text{L}^{-1}$) is the SMX concentration after adsorption equilibrium, C_t ($\text{mg}\cdot\text{L}^{-1}$) is the SMX quantity at the time of $t = t$, t (min) represents the reaction time, and k (min^{-1}) refers to the pseudo-first order degradation rate constant (min^{-1}), The values of $-\ln(C_t/C_0)$ are linearly correlated with t , and k values are determined from the slope of the linear plot.

Text S6

All calculations were simulated with the software of Materials Studio. The lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO) were calculated by Doml3 package. During the structure optimization process, generalized gradient approximation (GGA) with function of Perdew-Burke-Ernzerhof (PBE) was utilized to describe the electron interaction energy of exchange correlation.

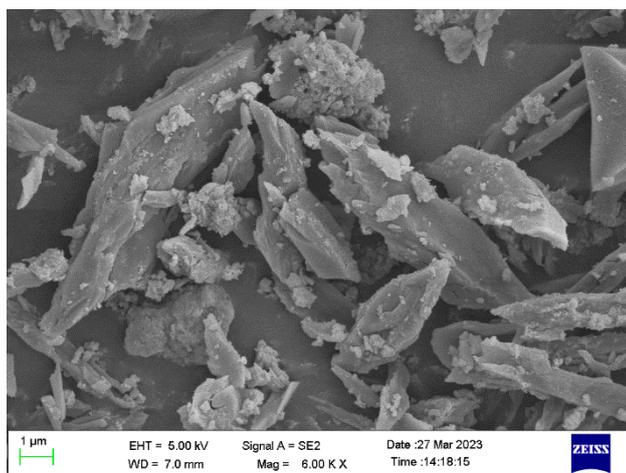


Figure S1. SEM of P-FeMIL.

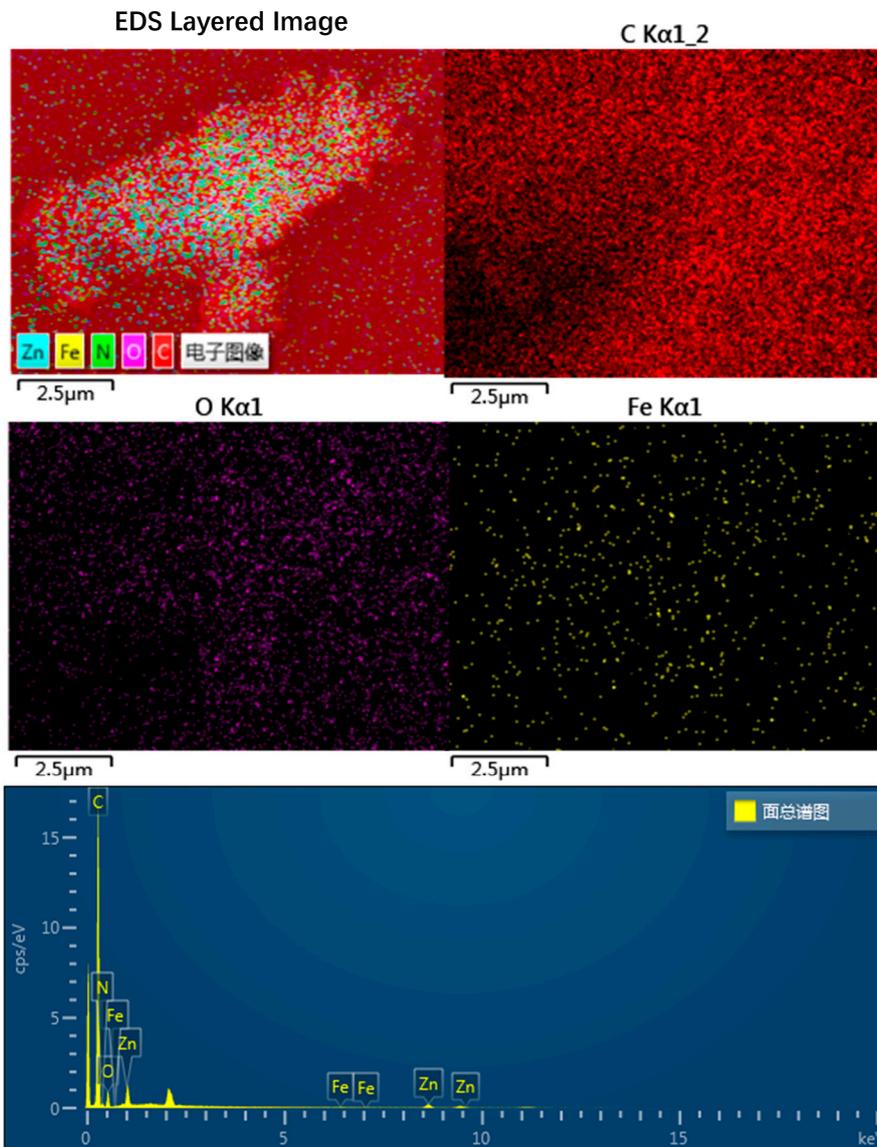
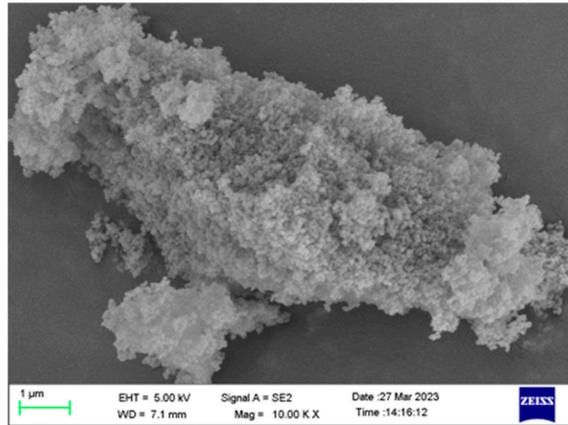


Figure S2. SEM of FeMIL-ZIF and EDX of FeMIL-ZIF.

Table S1. Elemental content.

element	wt%	Atom %
C	76.78	82.99
N	7.49	6.94
O	11.33	9.19
Fe	0.11	0.03
Zn	4.29	0.85
Total	100.00	100.00

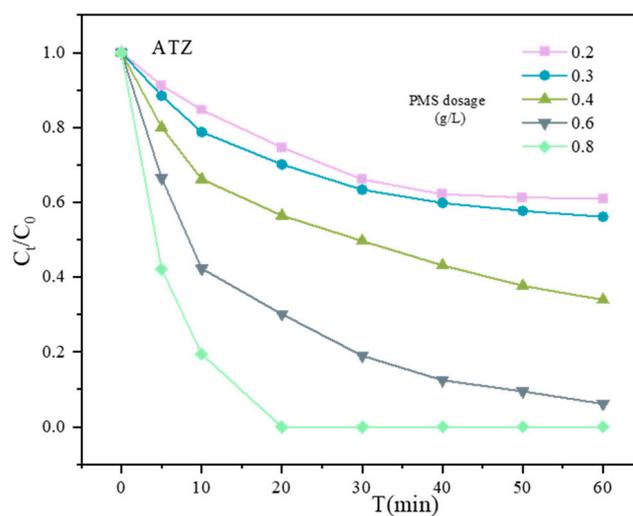


Figure S3. Effect of PMS dosage on ATZ degradation.

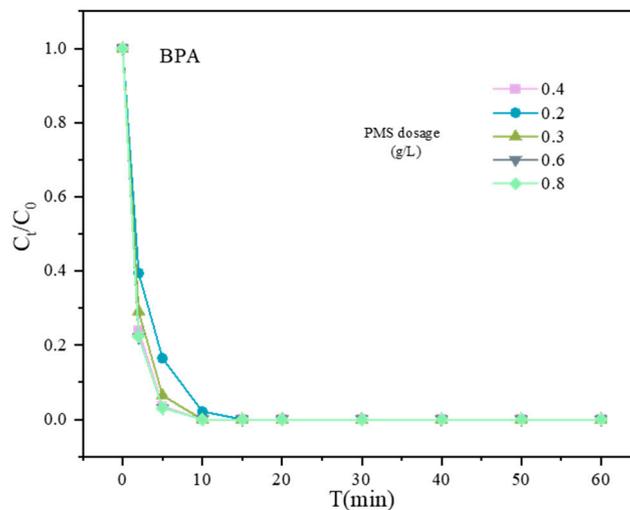


Figure S4. Effect of PMS dosage on BPA degradation.