Highly efficient PMS activation by nZVI@MoS_2 via Mo-Fe interfaces synergistic interaction for rapid degradation of ofloxacin

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Text S1 Materials

Ferric sulfate heptahydrate ($FeSO_4·7H_2O$), Molybdenum (MoS_2, 99.5%), Ofloxacin (OFL, 98%), PMS ($2KHSO_5·KHSO_4·K_2SO_4$), sodium thiosulfate ($Na_2S_2O_3·5H_2O$), Sulfadiazine (SDZ), 2,4-dichlorophenol (2,4-DCP), Ciprofloxacin (CIP), methanol (MeOH), tert-butanol (TBA), p-Benzoquinone (p-BQ), L-Histidine (L-His), formic acid (HCOOH, HPLC≥99%), potassium dihydrogen phosphate (KH_2PO_4), sodium sulfate (Na_2SO_4), sodium nitrate ($NaNO_3$), sodium bicarbonate ($NaHCO_3$), sodium chloride (NaCl) and humic acid (HA) were purchased from Shanghai Maclin Biochemical Technology Co., Ltd. Sodium borohydride ($NaBH_4$) was obtained from Damao Chemical Reagent Factory (Tianjin, China). 5,5-dimethy-1-pyroflax-oxide (DMPO), 2,2,6,6-tetramethylpiperidine (TEMP) were bought from Aladdin Reagent Co., Ltd. (China).

Text S2 Characterization and analytical methods

The microstructure and elemental distribution of the nZVI@MoS_2 composite were examined by scanning and transmission electron microscopy (SEM, GeminiSEM 500, ZEISS, Germany; TEM, HT7700, Hitachi, Japan), together with high-resolution TEM (JEM-2100, JEOL, Japan). Crystalline phases and surface functional groups were identified using X-ray diffraction (XRD, MXPAHF, Japan) and Fourier transform infrared spectroscopy (FTIR-1500, USA), while the specific surface area and pore structure were determined by the Brunauer–Emmett–Teller (BET) method (Autosorb-iQ, Quantachrome, USA). Surface elemental composition and chemical states before and after reaction were analyzed by X-ray photoelectron spectroscopy (XPS, ESCALAB QXi, Thermo Scientific, USA). Transformation products of ofloxacin (OFL) were identified by liquid chromatography–mass spectrometry (LC–MS, 1290 II–6460, Agilent, USA), and mineralization efficiency was assessed by total organic carbon (TOC) analysis (Multi N/C

3100, Jena, Germany).

Reactive oxygen species generated in the nZVI@MoS_2/PMS system were detected using electron paramagnetic resonance (EPR, A300 EMX PLUS, Bruker, Germany). The experimental parameters were set as follows: magnetic field center at 3500 G; microwave frequency of 9.8 GHz; microwave power of 2.0 mW; modulation frequency of 4.0 G; modulation amplitude of 4.0 G; sweep width of 200 G; receiver gain of 3.54×10^4; time constant of 41.0 ms; sweep time of 15 s; and 15 scans were accumulated. DMPO was used as the spin-trapping agent for detecting •OH, $SO_4^{\bullet-}$ in aqueous solution, as well as $O_2^{\bullet-}$ in methanol. TEMP was employed as the spin trap to detect $^1O_2$ in aqueous solution (Chen et al., 2024; Qi et al., 2025; Su et al., 2025).

The concentration of OFL was quantified by ultra-performance liquid chromatography (UPLC, 1260 Infinity II Prime, Agilent, USA) equipped with a C18 column and UV detection at 294 nm. The mobile phase consisted of 0.1% (v/v) formic acid in water and methanol (7:3), with a flow rate of 1.0 mL min^{-1} at 30 °C. Real water matrices, including domestic well water and three Chaohu Lake samples (Anhui Province, China) with different pollution levels, were used to evaluate practical applicability.

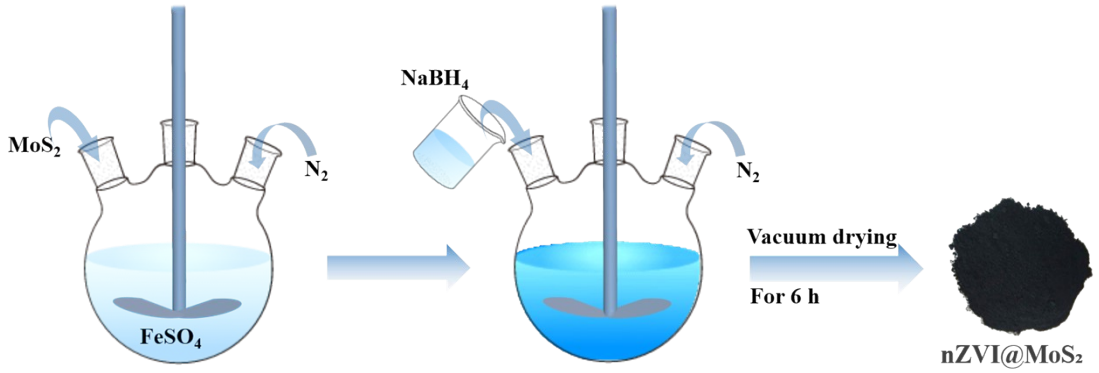


Fig. S1 Schematic for preparation of nZVI@MoS_2.

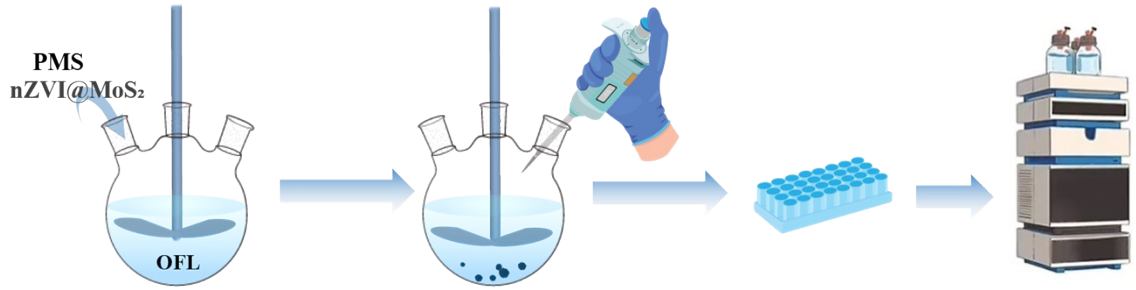


Fig. S2 Schematic diagram of the experimental process.

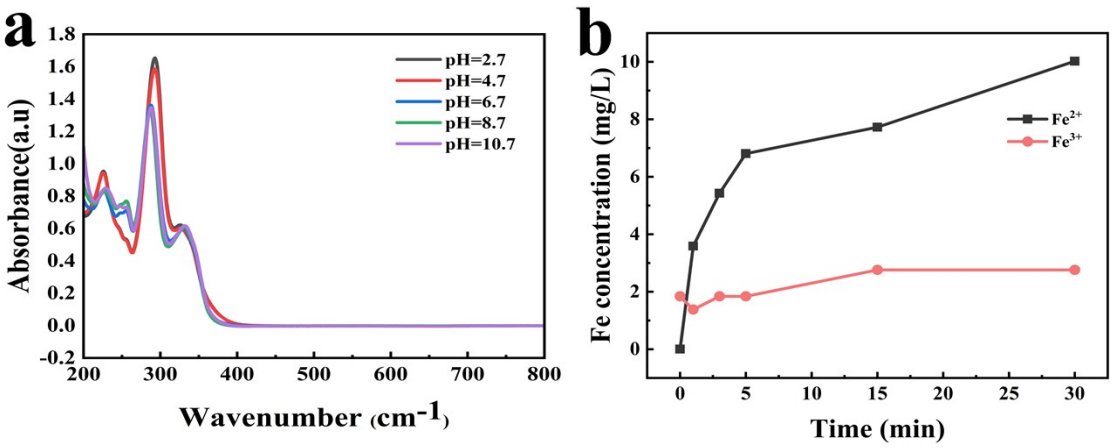


Fig. S3 (a) UV-Vis spectra of OFL under different pH conditions (2.7-10.7); (b) Concentrations of Fe^{3+} and Fe^{2+} in nZVI@MoS_2/PMS system for degradation of OFL.

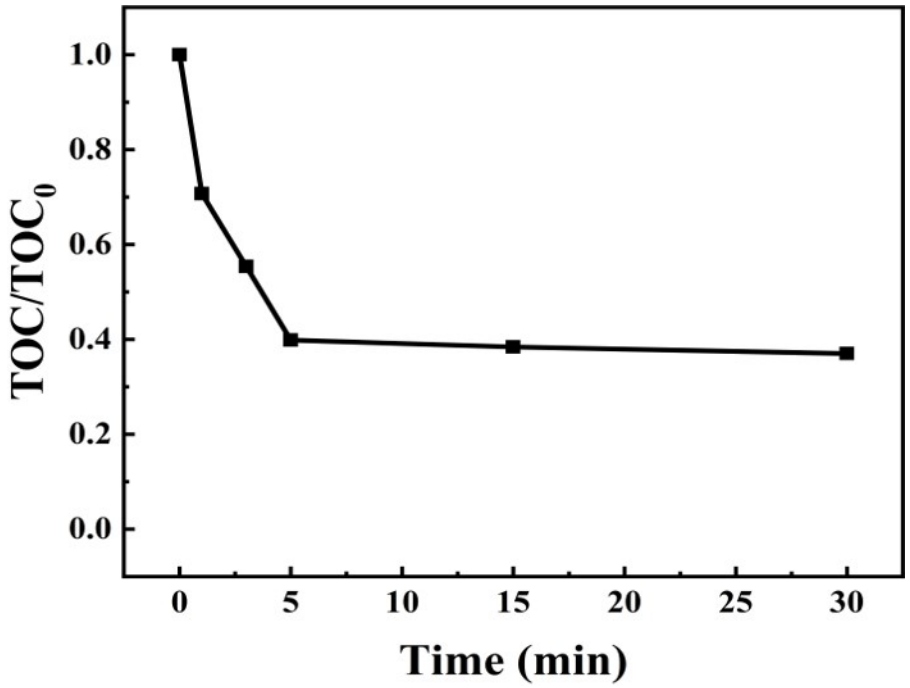
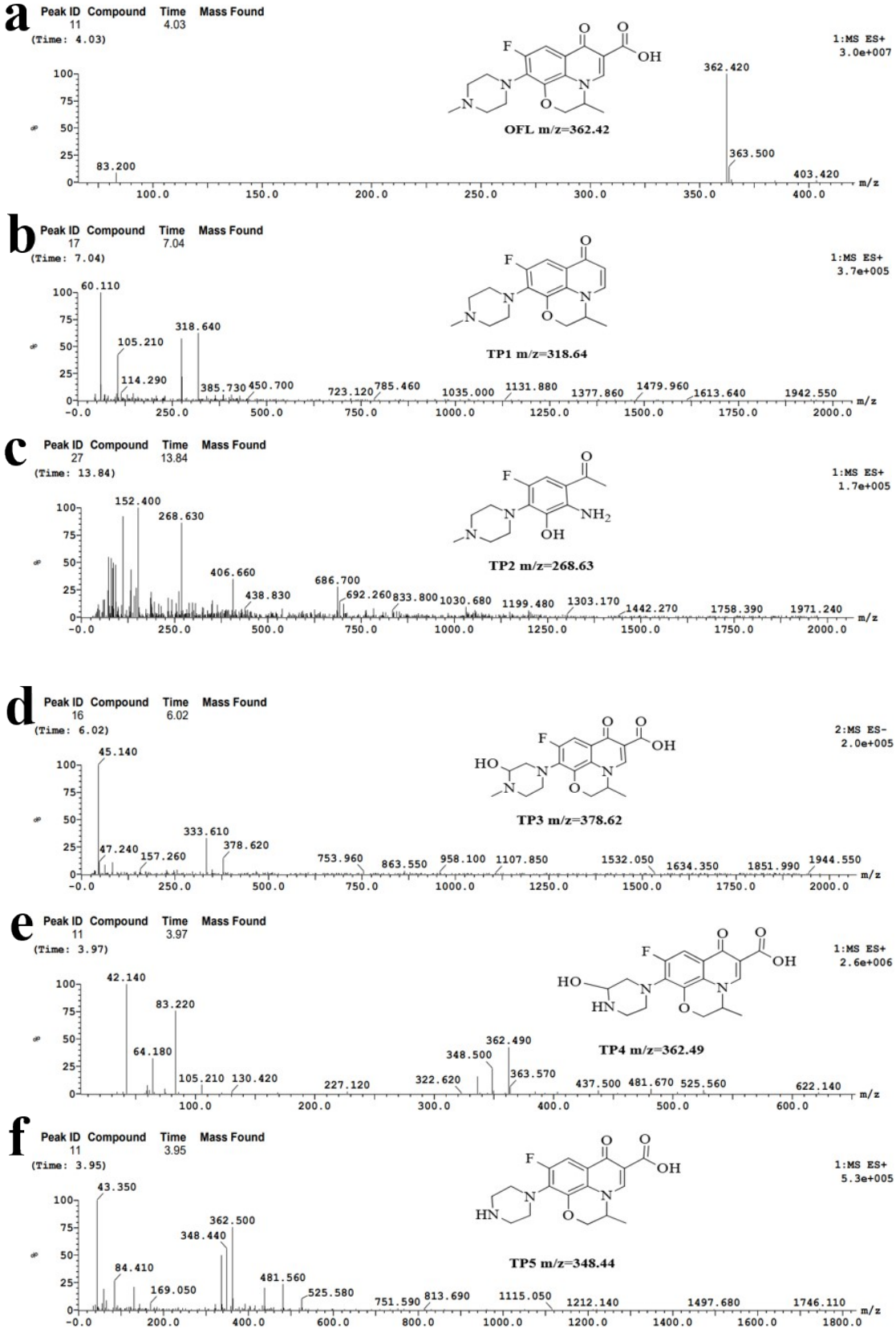


Fig. S4 Variation of TOC removal with reaction time for OFL in nZVI@MoS_2/PMS system. Reaction conditions: [nZVI@MoS_2] = 0.1 g/L, [PMS] = 0.2 mM, Mo/Fe (20 wt% Mo), initial pH = 6.7, [OFL] = 30 mg/L, t = 25 °C.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Peak ID Compound Time Mass Found
11 4.03
(Time: 4.03)
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3.0e+007
362.420
363.500
403.420
83.200
OFL m/z=362.42
b
Peak ID Compound Time Mass Found
17 7.04
(Time: 7.04)
1:MS ES+
3.7e+005
60.110
318.640
105.210
114.290
385.730
450.700
723.120
785.460
1035.000
1131.880
1377.860
1479.960
1613.640
1942.550
TP1 m/z=318.64
c
Peak ID Compound Time Mass Found
27 13.84
(Time: 13.84)
1:MS ES+
1.7e+005
152.400
268.630
406.660
438.830
686.700
692.260
833.800
1030.680
1199.480
1303.170
1442.270
1758.390
1971.240
TP2 m/z=268.63
d
Peak ID Compound Time Mass Found
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(Time: 6.02)
2:MS ES-
2.0e+005
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47.240
157.260
333.610
378.620
753.960
863.550
958.100
1107.850
1532.050
1634.350
1851.990
1944.550
TP3 m/z=378.62
e
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83.220
64.180
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363.570
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525.560
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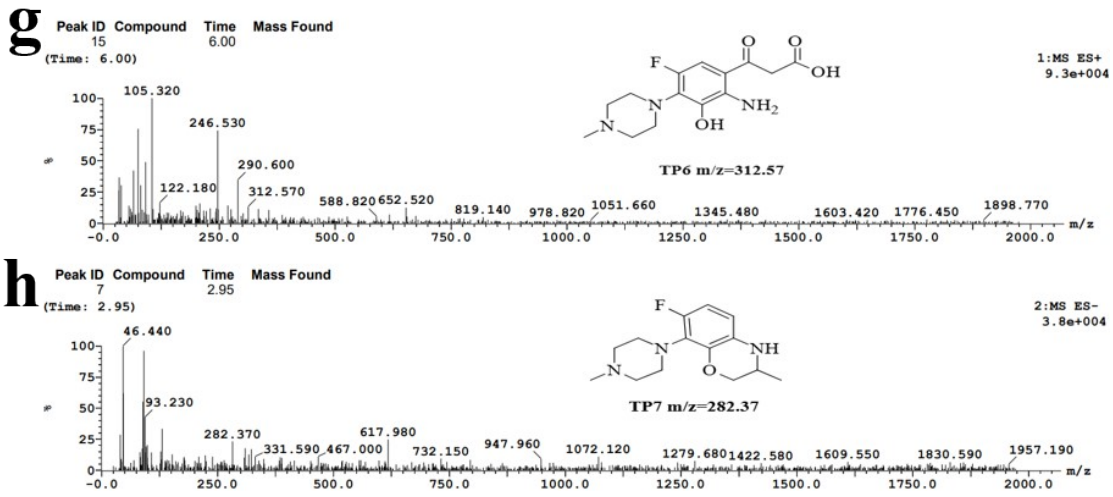

Fig. S5 LC-MS fragment patterns of OFL degradation intermediates by nZVI@MoS_2/PMS system.

Table S1

Surface area, pore size, and pore volume of the catalyst.

Catalyst	S_{BET} (m^2/g)	Pore size (nm)	Pore volume (cm^3/g)
nZVI	14.72	1.54	0.06
MoS_2	5.56	1.66	0.03
nZVI@MoS_2	20.98	2.01	0.08

Table S2

Comparisons of OFL degradation in different systems.

Catalyst	Catalyst Dosage	PMS Concentration	OFL Concentration	Time (min)	Removal Efficiency (%)	References
$LaFeO_3$@ZIF-67	0.4 g/L	1 mM	20 mg/L	15	92.48%	(41)
$CuFe_2O_4$-Mt	0.4 g/L	2 mM	40 mg/L	60	85.2%	(40)
$CoFe_2O_4$/C	0.04 g/L	0.8 mM	20 mg/L	12	96.8%	(39)
nZVI@MoS_2	0.1 g/L	0.2 mM	30 mg/L	30	97.4%	this study

Table S3

Index parameters of the lake water and domestic well water.

Water	Cl^- (mg/L)	SO_4^{2-} (mg/L)	NO_3^- (mg/L)	PO_4^{3-} (mg/L)
Lake water (Slight)	233.67	221.60	1.66	0.05
Lake water (Moderate)	249.54	265.46	1.54	0.04
Lake water (Severe)	277.25	253.16	3.98	0.21
Groundwater (Domestic well)	885.34	130.52	118.52	0.01

Table S4

ECOSAR toxicity analysis of OFL and intermediates.

Compound	Acute toxicity Logarithmic-transformed toxicity value			Chronic toxicity Logarithmic-transformed toxicity value		
	Fish (96hr LC50)	Daphnid (48hr LC50)	Green Algae (96hr EC50)	Fish	Daphnid	Green Algae
OFL	7.702	7.267	6.358	6.469	5.731	5.356
TP1	4.174	3.850	3.397	3.071	2.620	2.641
TP2	3.193	2.909	2.624	2.138	1.792	1.957
TP3	8.777	8.295	7.191	7.488	6.627	6.084
TP4	8.950	8.460	7.321	7.652	6.768	6.195
TP5	7.549	7.120	6.237	6.323	5.601	5.248
TP6	7.803	7.361	6.421	6.561	5.804	5.403
TP7	1.726	0.800	0.720	0.495	-0.286	0.240

Very toxic Toxic Harmful Not harmful

References

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