



Supplementary Materials

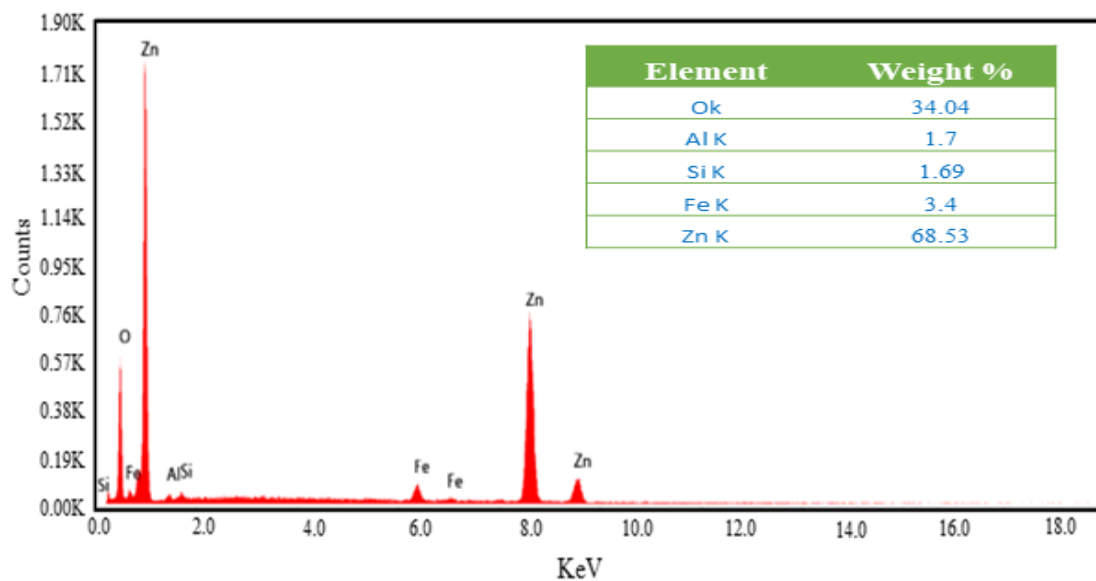


Fig. S1. EDX spectrum of MIL-53(Fe)/ZnO

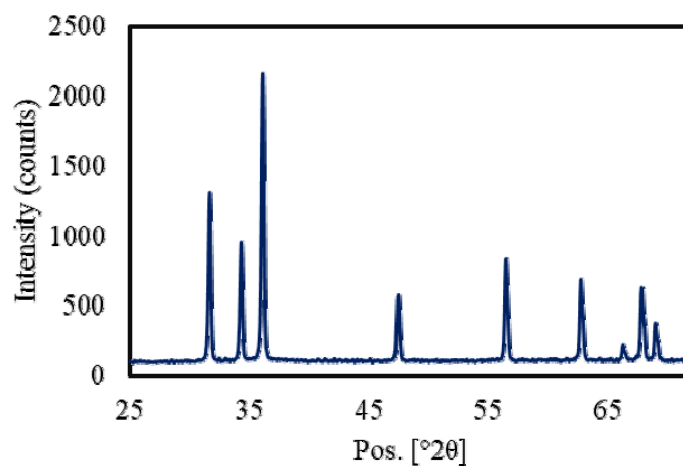


Fig. S2. XRD pattern of ZnO

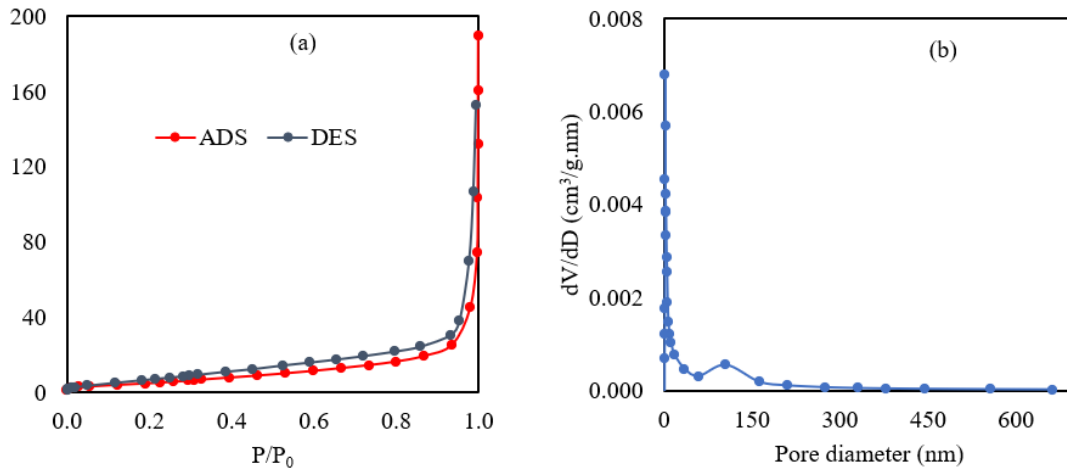


Fig. S3. (a) N₂ adsorption-desorption isotherms; (b) pore size distribution of MIL-53(Fe)/ZnO.

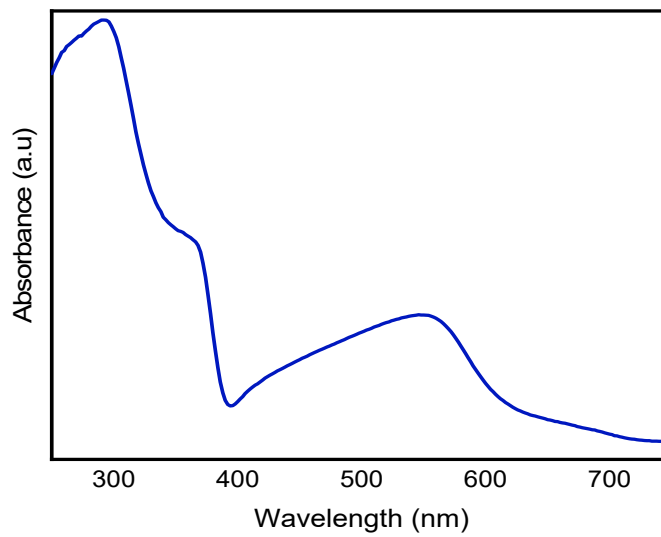


Fig. S4. UV-vis DRS spectra of MIL-53(Fe)/ZnO.

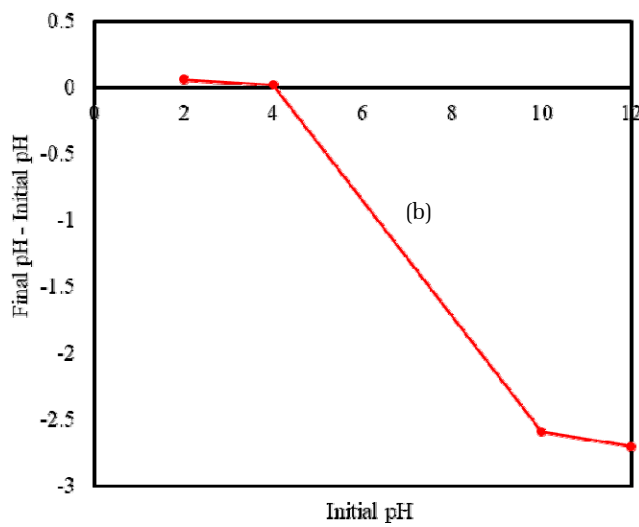


Fig. S5. Determination of point of zero charge MIL-53(Fe)/ZnO.

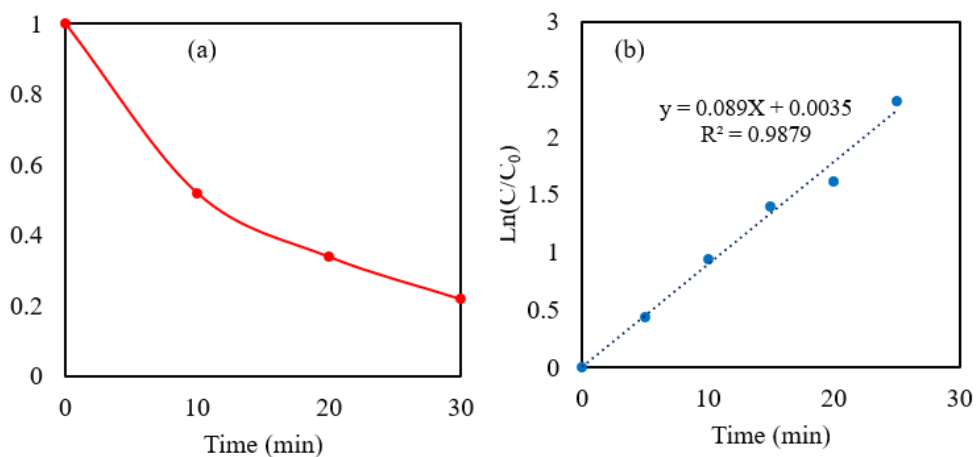


Fig. S6. (a) TOC removal of SMZ, (b) kinetic fitted curve; under the optimum conditions.

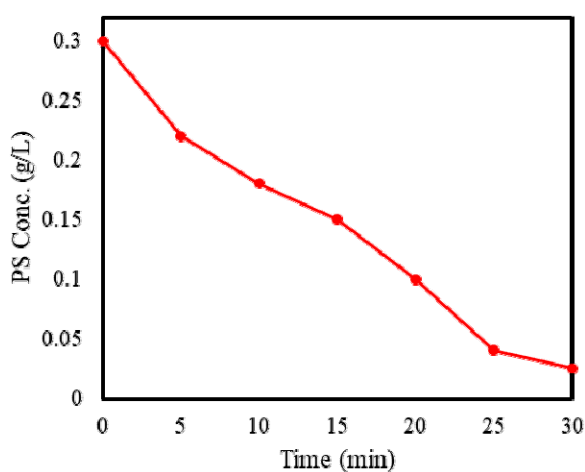


Fig. S7. The residual concentration of PS ions during the reaction under the optimum conditions.

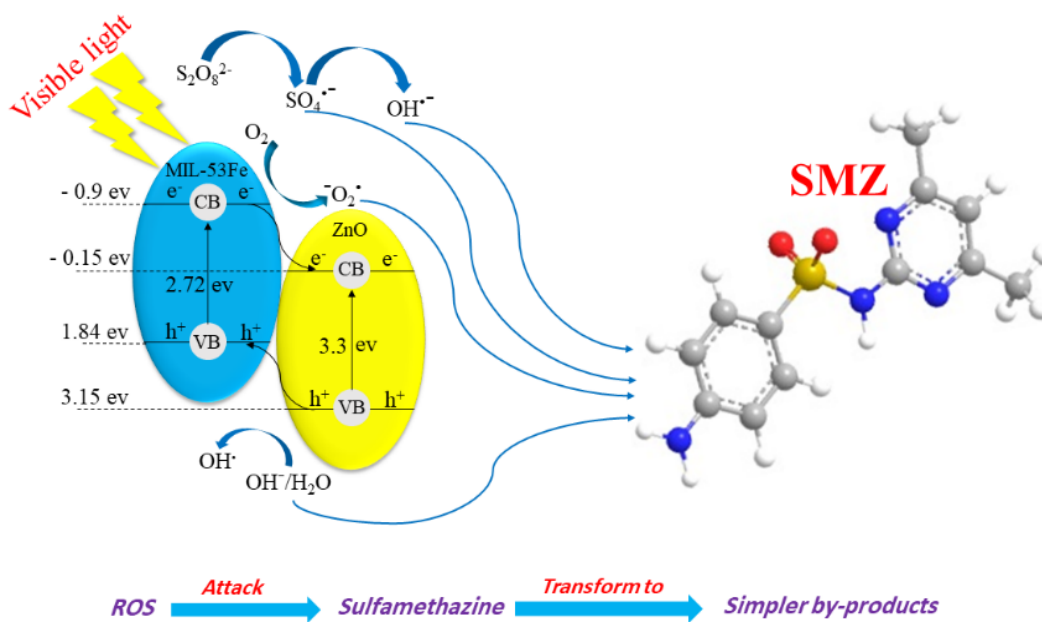


Fig. S8. A possible mechanism for the SMZ degradation by MIL-53(Fe)/ZnO system.

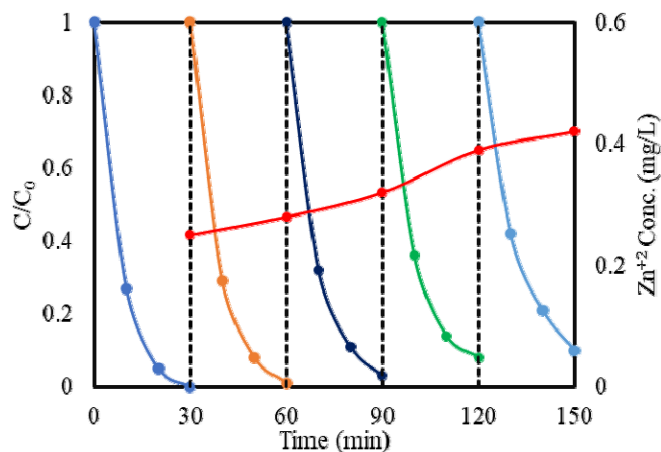


Fig. S9. Recycling experiment for the synthesized MIL-53(Fe)/ZnO during the photocatalytic process and the Zn²⁺ concentrations released to the solution after each run under the optimum conditions.

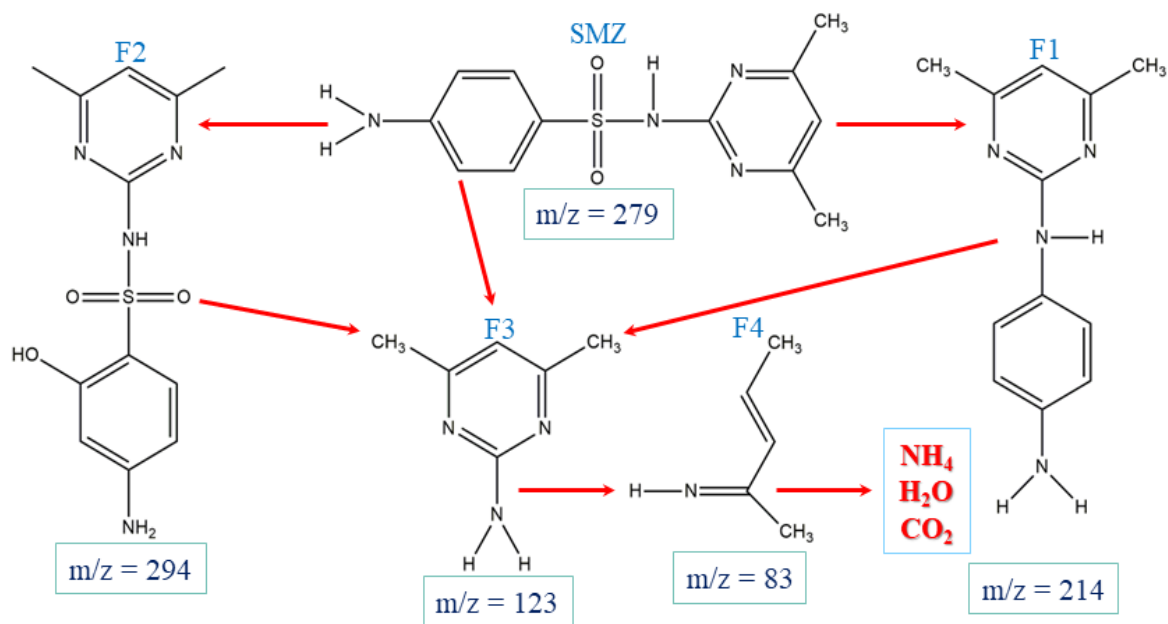


Fig. S10. The suggested degradation pathway of SMZ.

Table S1 BBD experimental levels and ranges of independent variables for SMZ degradation.

Independent variables	Units		Levels	
			-1	1
pH (X ₁)	-		3	11
Catalyst dose (X ₂)	g/L		0.2	1.0
Persulfate loading (X ₃)	g/L		0.1	0.5

Table S2 Characteristics of specific surface area and pore structure of MOFs and ZnO related samples prepared using different MOFs as reactive templates.

Samples	BET (m ² /g)	D(nm)	V (cc/g)
MIL-53(Fe)/ZnO	20.081	18.8	0.0944
MIL-53(Al)/ZnO	27.45	42.61	0.2925
MIL-53Fe	38.17	3.85	0.20
MIL-53Al	776.8	16.4	0.966

Table S3. The operating parameters of all experiments and the SMZ removal (%) from the response model and experimental work

Run	pH	Catalyst dose	P.S dose	% SMZ removal (Actual)	% SMZ removal (Predicted)
1	(-1)3	(-1)0.2	(0)0.3	100	98.35
2	(1)11	(-1)0.2	(0)0.3	44.47	43.98
3	(-1)3	(1)1	(0)0.3	75.85	75.29
4	(1)11	(1)1	(0)0.3	63.07	63.68
5	(-1)3	(0)0.6	(-1)0.1	47.11	47.19
6	(1)11	(0)0.6	(-1)0.1	19.48	18.40
7	(-1)3	(0)0.6	(1)0.5	60.42	62.55
8	(1)11	(0)0.6	(1)0.5	24.39	25.35
9	(0)7	(-1)0.2	(-1)0.1	6.88	7.93
10	(0)7	(1)1	(-1)0.1	13.38	13.33
11	(0)7	(-1)0.2	(1)0.5	25.07	26.16
12	(0)7	(0)0.6	(1)0.5	6.1	1.92
13	(0)7	(0)0.6	(0)0.3	7.24	8.42
14	(0)7	(0)0.6	(0)0.3	7.94	8.42
15	(0)7	(0)0.6	(0)0.3	8	8.42

Table S4. The ANOVA test for the efficiency of SMZ degradation.

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Model	9	12293.3	1365.92	214.19	0
Linear	3	2421.7	807.23	126.58	0
pH	1	2177	2177.01	341.38	0
Catalyst dose	1	4	3.96	0.62	0.466
PS dose	1	208	207.99	32.62	0.002
Square	3	9481.9	3160.65	495.63	0
pH*pH	1	6118.7	6118.66	959.48	0
Catalyst dose*Catalyst dose	1	1185	1184.96	185.82	0
PS dose*PS dose	1	484.5	484.53	75.98	0
2-Way Interaction	3	501.7	167.23	26.22	0.002
pH*Catalyst dose	1	456.9	456.89	71.65	0
pH*PS dose	1	17.6	17.64	2.77	0.157
Catalyst dose*PS dose	1	27.2	27.16	4.26	0.094
Error	5	31.9	6.38		
Lack-of-Fit	3	31.5	10.51	58.87	0.017
Pure Error	2	0.4	0.18		
Total	14	12325.2			

Text S1: Cost calculations

The dimensions of a cylindrical full-scale photocatalytic reactor are a diameter = 2.0 m, height = 2.0 m, wall thickness = 0.25 m, and floor thickness = 0.3 m. Accordingly, the total volume of reinforced concrete is 5.0 m³. The cost of total reinforced concrete was estimated based on the use of 350 kg/m³ of cement and 120 kg/m³ of steel including the cost of required equipment and labor to be 1500 \$. The cost of the mixer was 1000 \$ and the cost of the required connections for operation was assumed to be 500 \$. Therefore, the cost of the reactor construction and permanent facilities (C_{po}) was roughly calculated to be 3000 \$.

The cost of operation of one kg of the catalyst was determined to be 2.5 \$ including the cost of the precursors and chemicals. The dose of the catalyst was determined to be 0.2 kg/m³. The cost of one kg of sodium persulfate is about 1 \$. A sodium persulfate dose of 0.39 kg/m³ was considered for calculation. For the pH adjustment, the costs of HCl and NaOH were determined to be 0.04 \$/L and 0.03 \$/L, respectively. The number of lamps needed in large scale reactor to attain the same illumination intensity in lab-scale reactor is considered to be 10 lamps. The cost of lamps needed to illuminate one cubic meter of wastewater was assumed, as displayed in **Table S5**.

Table S5. Summary of cost estimation of the MIL-53(Fe)/ZnO/PS/Vis and MIL-53(Fe)/ZnO/UV.

Costs (\$/m ³)	AC	Cch	Clamp	Ec	OC	TC
MIL-53(Fe)/ZnO/PS/Vis	0.10	0.94	0.25	0.21	1.40	1.50
MIL-53(Fe)/ZnO/UV	0.10	0.55	1.5	0.30	2.35	2.45