

S-doping Fe-Ce composites derived from PBA to accelerate Fe(III)/Fe(II) cycle in the Fenton-like process

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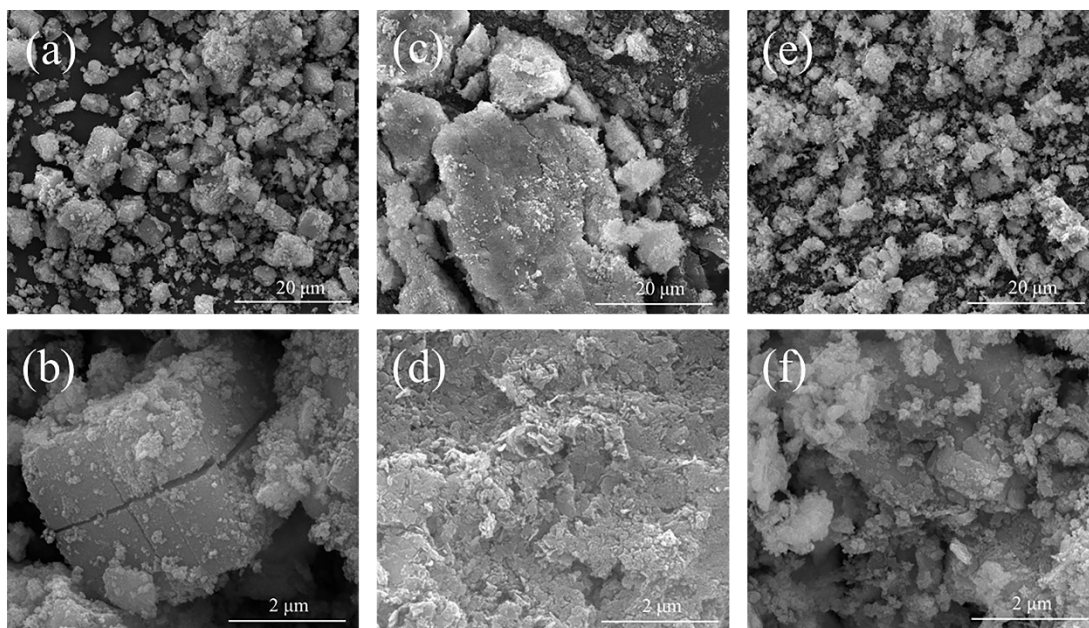


Fig. S1 SEM images of (a, b) Fe-Ce-S-H, (c, d) Fe-Ce-N and (e, f) Fe-Ce-S-N.

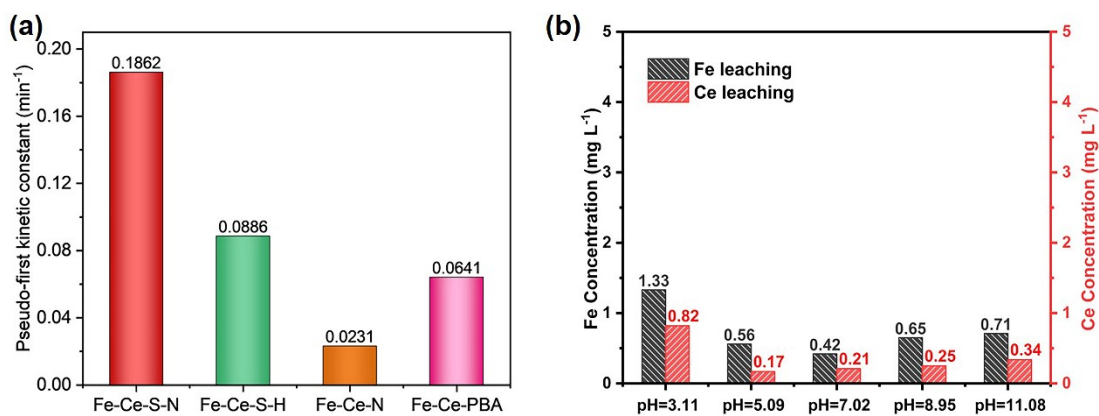


Fig. S2 (a) Reaction kinetic rate constants of SMZ under various reaction systems; (b) metal leaching concentration of Fe-Ce-S-N at different pH. Reaction conditions: $[\text{SMZ}] = 20 \text{ mg L}^{-1}$, $[\text{Catalyst}] = 0.2 \text{ g L}^{-1}$, $[\text{H}_2\text{O}_2] = 15 \text{ mM}$, $\text{pH} = 5.0$, $T = 25 \text{ }^\circ\text{C}$.

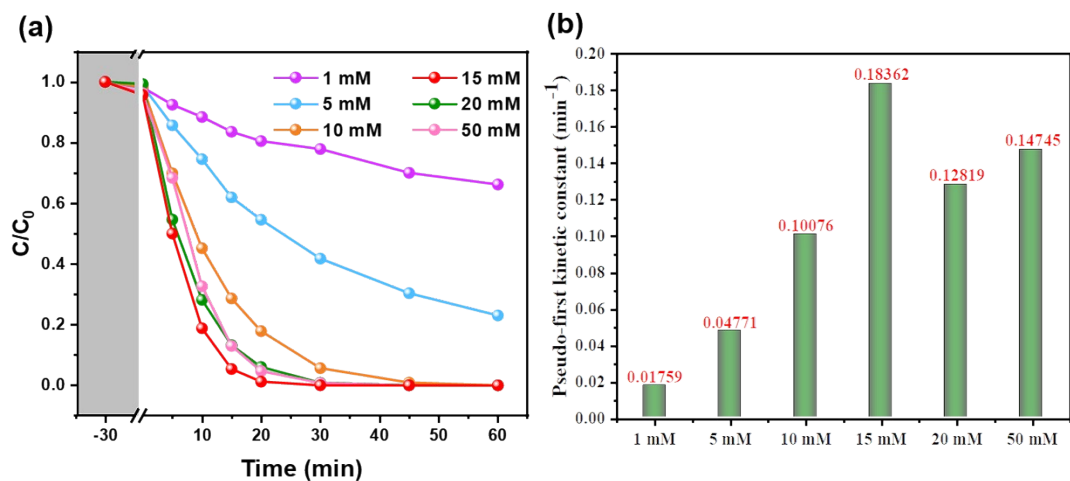


Fig. S3 Removal and reaction kinetic rate constants of SMZ under different H_2O_2 concentration.

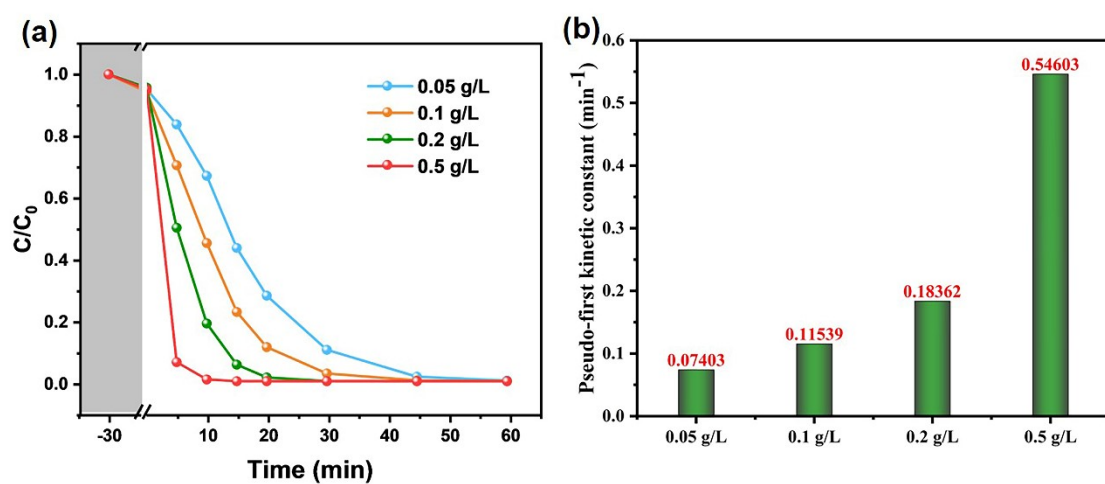


Fig. S4 Removal and reaction kinetic rate constants of SMZ under different catalyst dosage.

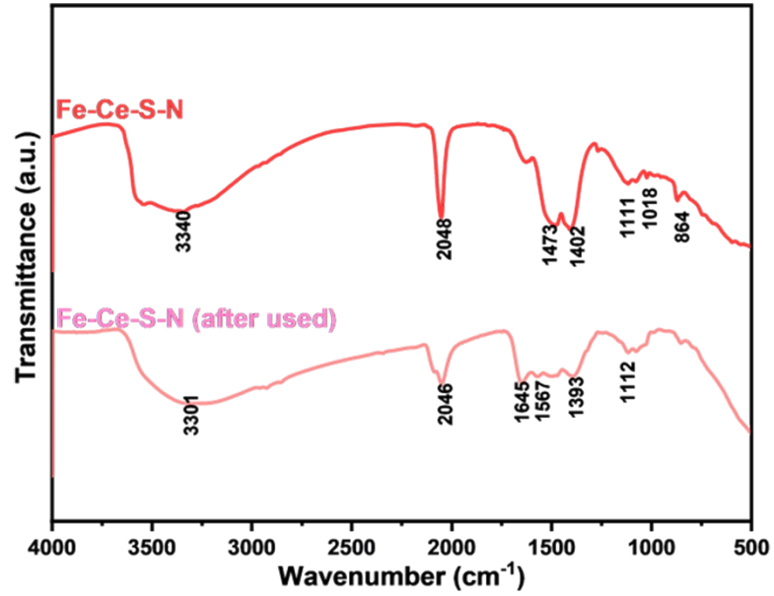


Fig. S5 FT-IR spectra of Fe-Ce-S-N catalyst before and after cycling reactions.

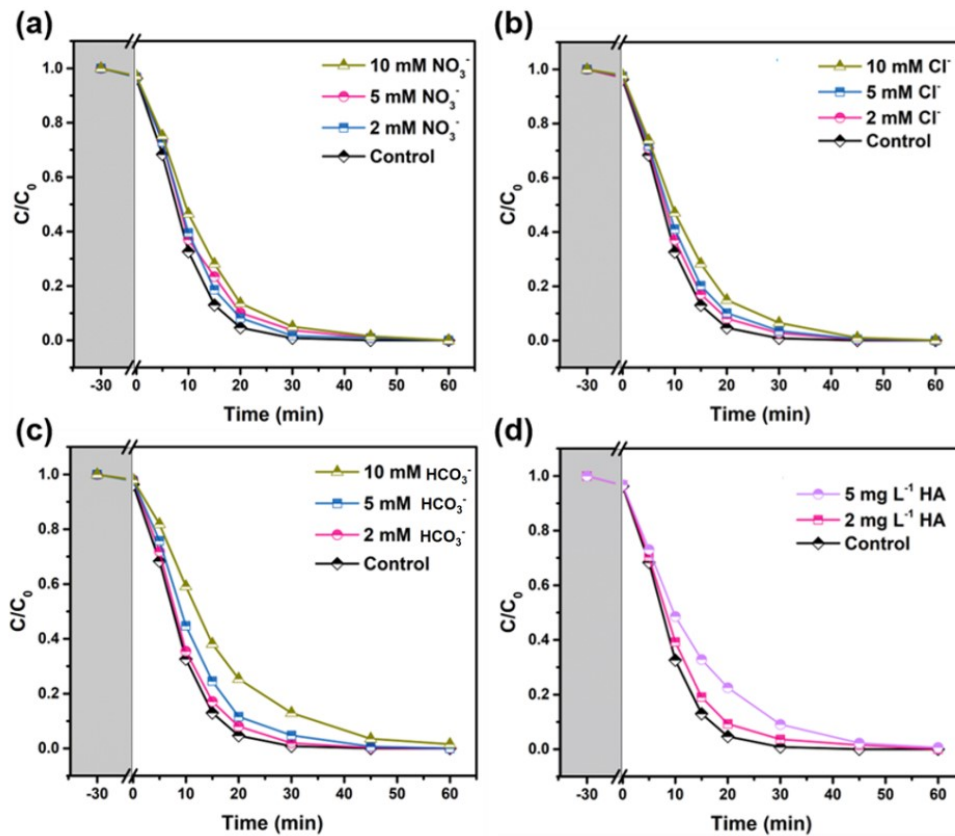


Fig. S6 Influence of inorganic anions and HA on SMZ degradation in the Fe-Ce-S-N/H₂O₂ system.

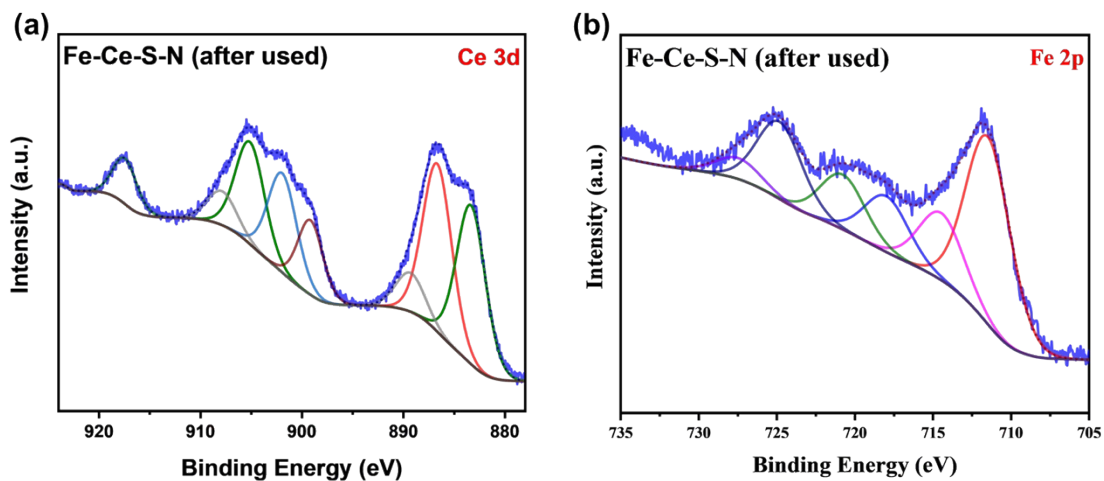


Fig. S7 High-resolution (a) Ce 3d and (b) Fe 2p XPS spectra of Fe-Ce-S-N after used.

Table S1 Metal leaching concentrations of catalysts obtained from different synthesized precursors

catalysts	Fe-Ce-PBA	Fe-Ce-S-N	Fe-Ce-S-H	Fe-Ce-N
Fe (mg L ⁻¹)	1.49	0.56	1.86	0.33
Ce (mg L ⁻¹)	0.54	0.17	0.73	0.09

Table S2. The corresponding Fe and Ce leaching concentration in different cycles.

Cycle	Fe (mg L ⁻¹)	Ce (mg L ⁻¹)
1 st	0.56	0.17
2 nd	0.44	0.14
3 rd	0.21	0.09
4 th	0.19	0.02

Table S3. Ratio of Fe(II)/Fe(III) and Ce(III)/Ce(IV) in Fe-Ce-S-N before and after used according to XPS characterization.

	Fe-Ce-S-N	Fe-Ce-S-N (used)
Fe ^{II} / Fe ^{II} +Fe ^{III}	0.282	0.373
Ce ^{III} / Ce ^{III} +Ce ^{IV}	0.726	0.530

Table S4. Toxicity classification according to the Globally Harmonized System.

Toxicity range (ppm)	Classification
LC ₅₀ /EC ₅₀ /ChV >100	Not harmful
10 < LC ₅₀ /EC ₅₀ /ChV ≤ 100	Harmful
1 < LC ₅₀ /EC ₅₀ /ChV ≤ 10	Toxic
LC ₅₀ /EC ₅₀ /ChV ≤ 1	Very toxic

Table S5. Predicted acute and chronic toxicity of SMZ and its products.

Compound	Acute toxicity (mg L ⁻¹)			Chronic toxicity (ChV) (mg L ⁻¹)		
	Fish (LC ₅₀)	Daphnid (LC ₅₀)	Green Algae (EC ₅₀)	Fish	Daphnid	Green Algae
SMZ	410.762	1.872	6.615	2.337	0.086	10.402
P1	5024.836	17859.785	91.284	1.899	186.877	29.324
P2	72773.367	553000	926.545	10.326	1948.60 2	148.545
P3	23716.477	136000	343.806	4.812	715.978	71.042
P4	76.877	91.187	2.335	0.12	4.597	2.049
P5	687.255	1603.323	15.206	0.447	30.668	7.182
P6	2152.689	5945	44.009	1.126	89.292	17.809
P7	8171.387	89.181	5959.974	2348.73 1	533.427	305.021
P8	443.424	0.735	3.637	3.637	0.051	5.375
P9	54.649	1.889	29.022	6.880	2.556	2.867
P10	1558.699	781.268	585.355	131.267	53.523	68.128
P11	4086.931	329.657	589.029	782.461	18.524	147.559
P12	266000	15422.803	53035	140000	628.185	10446.307
P13	20634.932	135000	281.289	3.534	588.522	51.538
P14	167.761	410.048	0.731	9.234	1.594	0.175
P15	306.332	483.427	8.139	0.33	16.189	5.499

Not harmful
 Harmful
 Toxic
 Very toxic