Synergistic Mechanism of FeS₂/ACFs Self-standing Membrane in Highly Efficient Electro-Fenton Degradation: Carbon Nanodefects and Free Radicals Analysis

Huiying Zhang^a, Shuyan Yu^{a,*}, Shunzheng Zhao^a, Congju Li ^{a,b *}

^aSchool of Energy and Environmental Engineering, University of Science and Technology Beijing, Beijing

100083, China;

^bCollege of Textiles, Donghua University, Shanghai, 201620, China.

*Corresponding author: Professor. Congju Li, <u>congjuli@126.com</u>

Dr. Shuyan Yu, yushuyan@ustb.edu.cn



Figure S1 Schematic diagram of an electro-Fenton reaction device



Figure S2 TC standard curve



Figure S3 Schematic representation of the effect of different pH on TC degradation



Figure S4 UV-Vis spectra before and after a single passage of 50 mg/l OTC+TC mixed solution through $FeS_2/ACFs$ membrane



Figure S5 Possible TC degradation intermediates



Fig. S6 Schematic diagram of TC structure and atomic number

Table S 1 Elemental content in FeS ₂ /ACFs								
electrode	C/%	Fe/%	S/%					
FeS ₂ /C/ACFs	79.70	7.53	12.77					

Cathode Anode Degradation H_2O_2 catalyst time Refere concentration loading and efficiency nce (mmol/l)/air (mmol/l) pumping speed NAC-1000/GF Pt 1.765 0.5 83.07% in 120 min [1] CNT Fe 0.887 97.21% in 25 min [2] -Ti/RuO₂-IrO₂ CF 1 l/min 0.1 >95% in 60 min [3] MnFe-LDH@BC 0.5 l/min 94.2% in 500 min Pt [4] Fe-GAC (particles) 5.5 0.693 92.6% in 60 min [5] 100% in 20 min ZIF-8/ACFs Pt 0.6 l/min 0.6 [6] Ti Ru-Ir Ti 82.7% in 60 min [7] 0.15 l/min 1.79 FeS₂/ACFs Ti 20 100% single pass This work

Table S 2 Comparison table between FeS₂/ACFs and other jobs

 Table S 3 Fukui function calculation of TC											
	Atom	f	\mathbf{f}^+	\mathbf{f}^0		Atom	f	\mathbf{f}^+	f^0		
1	С	0.007	0.016	0.011	33	Н	0.024	0.056	0.04		
2	С	0.01	0.04	0.025	34	Н	0.017	0.05	0.034		
3	С	-0.003	0.001	-0.001	35	Η	0.025	0.061	0.043		
4	С	0	0.038	0.019	36	Η	0.021	0.025	0.023		
5	С	0.002	0.007	0.005	37	Н	0.032	0.007	0.019		
6	С	0.009	0.051	0.03	38	Н	0.002	0.023	0.012		
7	С	-0.002	-0.011	-0.007	39	Н	0.026	0.027	0.026		
8	С	-0.01	-0.006	-0.008	40	Н	0.03	0.014	0.022		
9	С	0.025	0	0.013	41	Н	0.024	0.025	0.025		
10	С	0.01	0.088	0.049	42	Η	-0.003	0.03	0.014		
11	С	-0.02	0.073	0.026	43	Η	0.001	-0.002	-0.001		
12	С	-0.004	-0.01	-0.007	44	Η	0.012	0.017	0.014		
13	С	-0.006	-0.005	-0.005	45	Η	0.014	0.029	0.021		
14	С	-0.009	-0.013	-0.011	46	Н	0.011	0.021	0.016		
15	С	-0.007	-0.006	-0.006	47	Η	0.02	0.011	0.016		
16	С	0.043	0.01	0.026	48	Н	0.022	0.012	0.017		
17	С	0.01	0.004	0.007	49	Н	0.048	0.017	0.033		
18	С	0.022	0.001	0.011	50	Н	0.038	0.007	0.023		
19	С	0.026	0.003	0.014	51	Н	0.015	-0.004	0.006		
20	С	-0.005	-0.008	-0.007	52	Н	0.032	0.022	0.027		
21	0	0.003	0.015	0.009	53	Н	-0.005	0.005	0		
22	Ο	0.005	0.022	0.014	54	Н	0.016	-0.007	0.004		
23	Ο	0.034	0.089	0.062	55	Н	0.016	0.01	0.013		
24	0	0.008	0.069	0.038	56	Н	0.028	0.021	0.024		
25	Ο	0.064	0.024	0.044							
26	0	0.151	0.008	0.08							
27	0	0.135	0.011	0.073							
28	0	0.03	0.017	0.024							
29	Ν	0.039	0.007	0.023							
30	Ν	0	0.003	0.001							
31	С	-0.014	-0.008	-0.011							
32	С	-0.016	-0.008	-0.012							

Table S 3 Fukui function calculation of TC

Reference:

[1]Han S, Wang Z, Pi X, et al. Promotion of tetracycline degradation by electro-Fenton: controlling the reaction zone by N-doped modified activated carbon cathode[J]. Journal of Cleaner Production, 2022, 370: 133524.

[2] Dai C, Shi S, Chen D, et al. Study on the mechanism of tetracycline removal in electrocoagulation coupled with electro-fenton reaction system with Fe anode and carbon nanotube cathode[J]. Chemical Engineering Journal, 2022, 428: 131045.

[3] Chen S, Tang L, Feng H, et al. Carbon felt cathodes for electro-Fenton process to remove tetracycline via synergistic adsorption and degradation[J]. Science of the total environment, 2019, 670: 921-931.

[4] Xu M, Wei J, Chen X, et al. Satisfactory degradation of tetracycline by a pH-universal MnFe-LDH@ BC cathode in electric fenton process: Performances, mechanisms and toxicity assessments[J]. Journal of Environmental Chemical Engineering, 2022, 10(5): 108409.

[5] He Z, Xu X, Wang B, et al. Evaluation of iron-loaded granular activated carbon used as heterogeneous fenton catalyst for degradation of tetracycline[J]. Journal of Environmental Management, 2022, 322: 116077.

[6] Yu F, Wang L, Ma H, et al. Zeolitic imidazolate framework-8 modified active carbon fiber as an efficient cathode in electro-Fenton for tetracycline degradation[J]. Separation and Purification Technology, 2020, 237: 116342.

[7] Xu Z, Teng R, Xu L, et al. Assembly of Amorphizing Porous Bimetallic Metal-Organic Frameworks Spheres with Zn–O–Fe Cluster and Coordination Deficiency via Ligand Competition for Efficient Electro-Fenton Catalysis[J]. Advanced Functional Materials, 2024: 2401248.