

Supplementary

CuFeS₂/MXene-Modified Polyvinylidene Fluoride Membrane for Antibiotics Removal through Peroxymonosulfate Activation

Dongyang Zhang ¹, Kunfu Li ¹, Lei Fang ^{1,2,*} and Huishan Chen ¹

¹ Key Laboratory of Drinking Water Safety and Distribution Technology of Zhejiang Province, College of Civil Engineering and Architecture, Zhejiang University, Hangzhou 310058, China

² Future Water Laboratory, Innovation Center of Yangtze River Delta, Zhejiang University, Jiaxing 314000, China

* Correspondence: fanglei1999@zju.edu.cn

Note S1. Synthesis of CuFeS₂/MXene.

Ti₃AlC₂ was added to the etching solution of LiF and HCl, maintaining 45 °C for 24 hours. After the reaction, the obtained product was repeatedly rinsed with water, and separated by centrifugation until the pH of the supernatant reached 5. After drying, MXene was obtained.

Adding 0.46 g MXene, 0.01 mol CuCl, 0.01 mol FeCl₃·6H₂O and 0.02 mol (NH₂)₂CS sequentially, CuFeS₂/MXene was prepared by hydrothermal synthesis (200 °C, 10 h). The precipitate was centrifuged three times with water and anhydrous ethanol respectively, and dried in vacuum. Besides, CuFeS₂ was synthesized by the similar procedure without the addition of MXene.

Table S1. The mass loss of modified materials.

r/min	control	PEG	PEG + GA
500	52.1%	15.4%	9.6%
1000	59.7%	22.6%	12.7%
1500	67.7%	27.6%	19.9%

Table S2. Data related to the Fukui function.

Site	Atom	Charge (-1) (e/A)	Charge (0) (e/A)	Charge (+1) (e/A)	f ⁰	f ⁻
1	N	-0.1054	-0.0838	0.0523	0.079	0.136
2	C	0.0454	0.0677	0.1571	0.056	0.089
3	C	0.0162	0.0223	0.0408	0.012	0.018
4	C	0.0519	0.0586	0.0804	0.014	0.022
5	C	0.0592	0.0830	0.1808	0.061	0.098
6	C	0.0099	0.0830	0.0359	0.013	-0.047
7	C	0.0153	0.0192	0.0338	0.009	0.015
8	C	0.0540	0.0581	0.0790	0.012	0.021
9	N	-0.0936	-0.0908	-0.0672	0.013	0.024
10	C	0.1750	0.1951	0.2045	0.015	0.009
11	O	-0.4069	-0.3751	-0.3586	0.024	0.017
12	O	-0.1623	-0.1255	-0.1085	0.027	0.017
13	C	0.0208	0.0655	0.1069	0.043	0.041
14	C	0.0106	0.0516	0.0838	0.037	0.032
15	C	0.0224	0.0577	0.1232	0.050	0.065
16	C	0.0357	0.0558	0.0773	0.021	0.021
17	C	-0.0549	-0.0327	0.0232	0.039	0.056
18	C	-0.0913	0.0045	0.0598	0.076	0.055
19	N	-0.0582	-0.0137	-0.0050	0.027	0.009
20	C	-0.0040	0.1437	0.1728	0.088	0.029
21	C	-0.0958	-0.0592	-0.0389	0.028	0.020
22	C	0.0268	0.1157	0.1353	0.054	0.020
23	O	-0.1552	-0.1449	-0.1220	0.017	0.023
24	C	0.0621	0.0840	0.0894	0.014	0.005
25	C	0.0155	0.0460	0.0604	0.022	0.014
26	C	0.0110	0.0399	0.0523	0.021	0.012
27	O	-0.3963	-0.3085	-0.2764	0.060	0.032
28	C	0.1092	0.1420	0.1900	0.040	0.048
29	F	-0.1172	-0.0918	-0.0624	0.027	0.029

Table S3. Single model and its correlation coefficient.

model	expression	PVDF membrane	catalytic membrane + PMS
complete blocking (n=2)	$\ln J_0 - \ln J = At$	R ² =0.9276	R ² =0.9586
standard blocking (n=1.5)	$\frac{1}{J^{0.5}} - \frac{1}{J_0^{0.5}} = Bt$	R ² =0.9510	R ² =0.9673
intermediate blocking (n=1)	$\frac{1}{J} - \frac{1}{J_0} = Ct$	R ² =0.9710	R ² =0.9755
cake filtration (n=0)	$\frac{1}{J^2} - \frac{1}{J_0^2} = Dt$	R ² =0.9944	R ² =0.9885