Supporting Information

Simultaneous Catalysis of Sulfite Oxidation and Uptake of Heavy Metals by Bifunctional Activated Carbon Fiber in Magnesia Desulfurization

Figure S1 XPS spectrum of 40% Co-ACFs

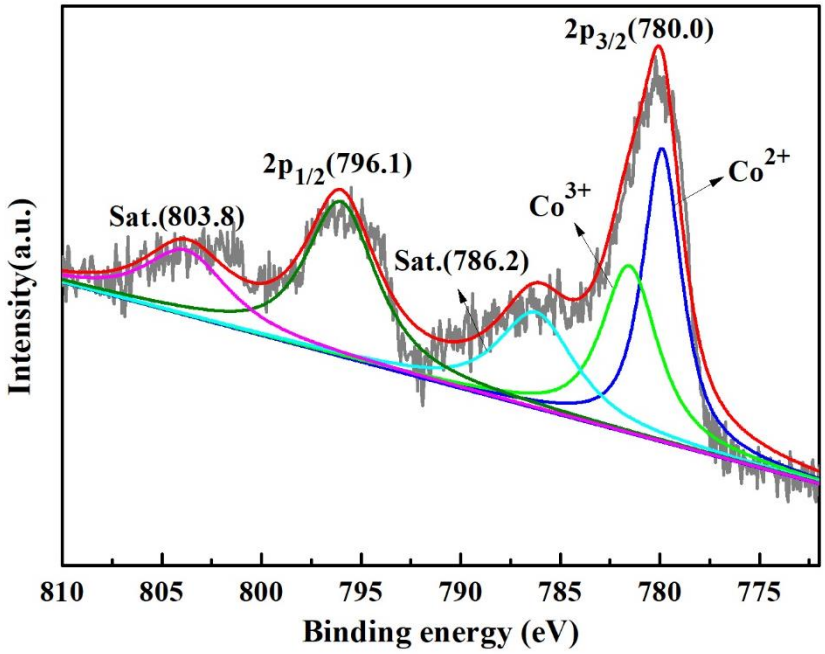

Figure S2 Catalysis performance of Co-ACFs after four cycles

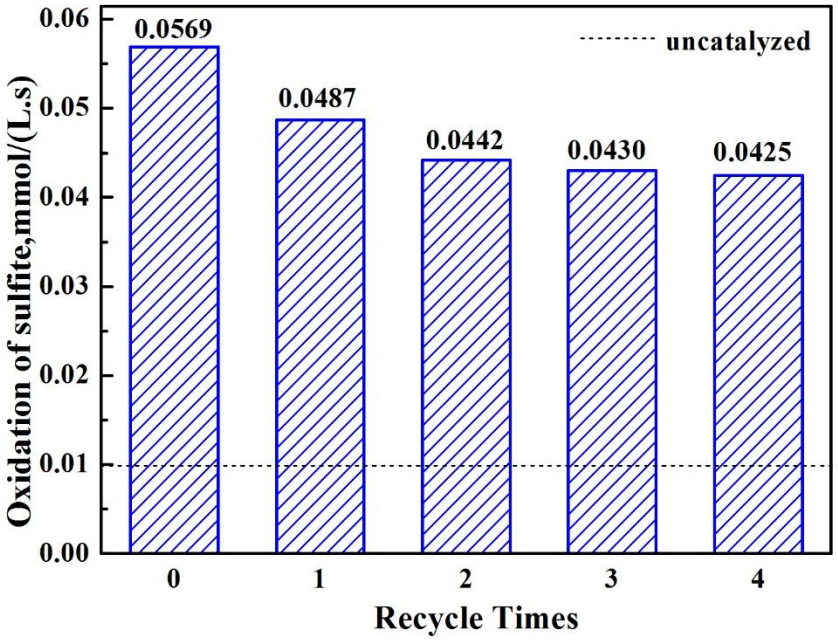

Figure S2 demonstrated that the catalytic performance of Co-ACFs declined substantially after the first and second cycles, and then remained basically the same. Although the oxidation rate decreased by about 25% from 0.0569 to 0.0425 mmol/(L·s) after four recycles, the catalytic reaction rate was still promoted by over 4.2 times compared with the uncatalyzed counterpart, which can accelerate the oxidation of magnesium sulfite. These results indicated that the developed Co-ACFs catalyst-adsorbent is stable, enabling the feasibility for application in a real desulfurization process. The calcined Co-ACFs will be squeezed into spherical particles by the binder, so that the shedding of the cobalt active component can be further prohibited.

Figure S3 Comparison of the catalysis activity of Co-based catalysts on magnesium sulfite oxidation at a concentration of 0.5 g/L

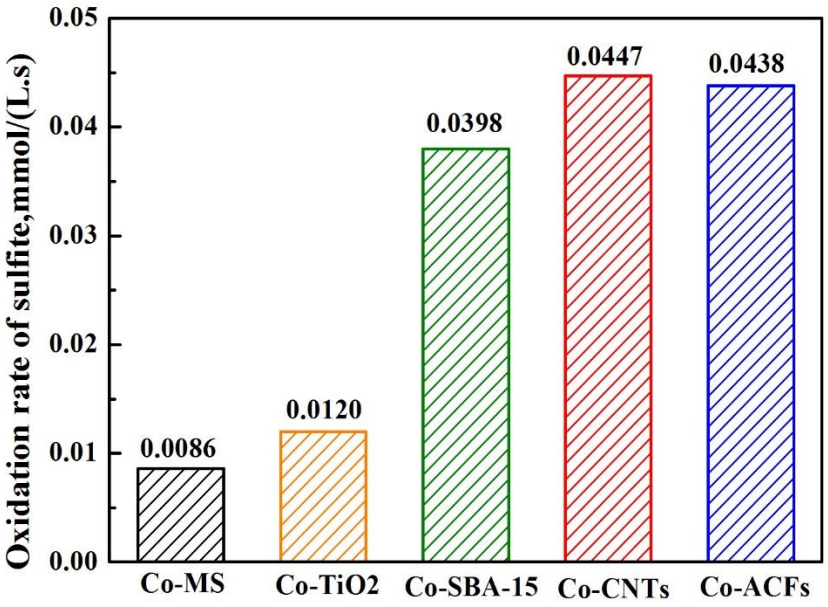

Table S1 Comparison of adsorption capacities for heavy metals onto different absorbents.

adsorbent	ion	Fitting models	kinetic parameters		Qm(mg/g)	Ref.
			k_2	q_e		
Co-CNTs	Hg	Langmuir	0.29	4.9	166.7	[1]
SBA-15-SH	Hg	Freundlich	0.011	189.87	195.6	[2]
Fe3O4 NPs@AC@SO3H	Cd	Langmuir	0.01	35.4	119.04	[3]
HS-mSi@MOF-5	Cd	Langmuir	0.001	91.996	98.0366	[4]
ZrO(OH)2/VMT	Ni	Langmuir	0.03	80.25	90.21	[5]
HWSAC	Ni	Langmuir	0.0056	31.75	61.92	[6]
ACF	Hg	Langmuir	\	\	198.8	[7]
ACF	Cd	Langmuir	\	\	2.33	[8]
ACC	Ni	Langmuir			2.296	[9]
MO-ACF	Cd	Langmuir	0.9562	\	14.88	[8]
ACF-Ox	Ni	Langmuir	\	\	21.12	[10]
ACF modification via by sulphuric acid	Hg	Langmuir	0.019	\	300.3	[7]
Co-ACF	Hg	Langmuir	0.46	4	333.3	This work
	Cd	Langmuir	0.07	5.32	500	
	Ni	Langmuir	0.09	9.34	52.6	

1. Wang, L.; Qi, T.; Hu, M.; Zhang, S.; Xu, P.; Qi, D.; Wu, S.; Xiao, H., Inhibiting Mercury Re-emission and Enhancing Magnesia Recovery by Cobalt-Loaded Carbon Nanotubes in a Novel Magnesia Desulfurization Process. *Environ. Sci. Technol.* **2017,** *51*, (19), 11346-11353.

2. Shen, Y.; Jiang, N.; Liu, S.; Zheng, C.; Wang, X.; Huang, T.; Guo, Y.; Bai, R., Thiol functionalization of short channel SBA-15 through a safe, mild and facile method and application for the removal of mercury (II). *J. Environ. Chem. Eng.* **2018,**

6, (4), 5420-5433.

3. Nejadshafiee, V.; Islami, M. R., Adsorption capacity of heavy metal ions using sultone-modified magnetic activated carbon as a bio-adsorbent. *Mater. Sci. Eng., C* **2019,** *101*, 42-52.

4. Zhang, J.; Xiong, Z.; Li, C.; Wu, C., Exploring a thiol-functionalized MOF for elimination of lead and cadmium from aqueous solution. *J. Mol. Liq.* **2016,** *221*, 43-50.

5. Liu, D.; Deng, S.; Vakili, M.; Du, R.; Tao, L.; Sun, J.; Wang, B.; Huang, J.; Wang, Y.; Yu, G., Fast and high adsorption of Ni(II) on vermiculite-based nanoscale hydrated zirconium oxides. *Chem. Eng. J.* **2019,** *360*, 1150-1157.

6. Kong, J.; Gu, R.; Yuan, J.; Liu, W.; Wu, J.; Fei, Z.; Yue, Q., Adsorption behavior of Ni(II) onto activated carbons from hide waste and high-pressure steaming hide waste. *Ecotoxicol. Environ. Saf.* **2018,** *156*, 294-300.

7. Nabais, J.; Carrott, P.; Ribeiro Carrott, M. M.; Silvestre, S.; Durán-Valle, C., Adsorption of Aqueous Mercury(II) Species by Commercial Activated Carbon Fibres with and without Surface Modification. *Adsorpt. Sci. Technol.* **2007,** *25*, 199-215.

8. Chen, Y.; Peng, L.; Zeng, Q.; Yang, Y.; Lei, M.; Song, H.; Chai, L.; Gu, J., Removal of trace Cd(II) from water with the manganese oxides/ACF composite electrode. *Clean Technol Environ Policy* **2014,** *17*, (1), 49-57.

9. Duman, O.; Ayranci, E., Attachment of benzo-crown ethers onto activated carbon cloth to enhance the removal of chromium, cobalt and nickel ions from aqueous solutions by adsorption. *J. Hazard. Mater.* **2010,** *176*, (1-3), 231-8.

10. Berber-Mendoza, M. S.; Mart ńez-Costa, J. I.; Leyva-Ramos, R.; Amezquita Garcia, H. J.; Medell ń Castillo, N. A., Competitive Adsorption of Heavy Metals from Aqueous Solution onto Oxidized Activated Carbon Fiber. *Water Air Soil Pollut.* **2018,** *229*, (8).