Support Materials

Sulfur Vacancy on MoS₂ Enhanced the Activation of Peroxymonosulfate through the Co-existence of Radical and Non-radical Pathways to Degrade Organic Pollutants in Wastewater

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Figure S1 Preparation step of MoS₂-300 catalyst.





Figure S2 Comparison of darkness and LED illumination on degradation of RhB. Reaction conditions: [RhB] = 10 mg/L, [PMS] = 1.0 mM, $[MoS_2-300] = 1.0 \text{ g/L}$, initial pH = 3.0.

Figure S3



Figure S3 Effect of the treated time on the degradation of RhB. Reaction conditions: $[RhB] = 10 \text{ mg/L}, [PMS] = 1.0 \text{ mM}, [MoS_2-300] = 1.0 \text{ g/L}, initial pH = 3.0, in the darkness.}$





Figure S4 Removal of RhB with different oxidation system. Reaction conditions: $[RhB] = 10 \text{ mg/L}, [Oxidants] = 1.0 \text{ mM}, [MoS_2-300] = 1.0 \text{ g/L}, initial pH = 3.0, in the darkness.}$





Figure S5 Removal of organic pollutants. Reaction conditions: [Pollutants] = 10 mg/L, [MoS₂-300] = 1.0 g/L, [PMS] = 1.0 mM, initial pH = 3.0, in the darkness.

Figure S6



Figure S6 Changes of solution pH before and after the reaction.

Figure S7



Figure S7 (a) Removal of RhB without or with regeneration; (b) XRD patterns of fresh and used MoS₂ catalysts; (c) SEM image of used MoS₂-300 catalyst. Reaction conditions: [RhB] = 10 mg/L, [PMS] = 0.5 mM, [MoS₂-300] = 1.0 g/L, initial pH = 3.0, in the darkness.



Figure S8 Decomposition of PMS. Reaction conditions: [RhB] = 10 mg/L, $[MoS_2-300] = 1.0 \text{ g/L}$, [PMS] = 1.0 mM, initial pH = 3.0, in the darkness.

Figure S8

Table S1 Changes of surface Mo(IV) concentration, ratios of Mo(IV) and Mo(VI), and 2H-MoS₂ and 1T-MoS₂ phases in catalysts with different temperatures by XPS characterization ^{*a*}.

Catalysts	Mo(IV)	Mo(IV)/Mo(VI)	2H-MoS ₂ /1T-MoS ₂ ^b	2H-MoS ₂ /1T-MoS ₂ ^c
MoS ₂	98.3%	57.8	0.48	0.50
MoS ₂ -300	85.1%	5.7	0.62	0.66
MoS ₂ -500	58.8%	1.4	0.28	no

^{*a*}: Based on the peak area of each component; ^{*b*}: Mo 3d; ^{*c*}: S 2p.

Catalysts	Mo (mg/L)	S (mg/L)
MoS ₂ -300	36.2	91.6

Table S2 The concentrations of detected elements in reaction solution after the fifthreaction by ICP-MS.