

Photocatalytic activity of 2D-MoS₂ in the reductive degradation of bromophenol blue.

SUPPLEMENTARY

Table S1. Qualitative and quantitative analysis of 2D-MoS₂

	BE (eV)	At. Conc. (%)	Assignments
S 2p _{3/2}	162.6	2.08	MoS ₂
S 2p _{1/2}	164.0	1.04	
S 2p _{3/2}	169.2	5.37	SO ₄ ²⁻
S 2p _{1/2}	170.4	2.69	
Mo 3d _{5/2}	229.6	0.92	MoS ₂
Mo 3d _{3/2}	232.7	0.61	
Mo 3d _{5/2}	233.7	2.21	Mainly Mo(SO ₄) ₃ ; MoO ₃ (residual); Mo(CO ₃) ₃ (residual)
Mo 3d _{3/2}	236.8	1.47	
C 1s	284.7	21.53	sp ² (and sp ³ at 285 eV)
	286.2	10.06	C-N and C-O-C (or C-O)
	288.6	2.43	CO ₃ ²⁻
	291.1	1.57	π-π*
O 1s	528.8	0.71	MoO ₃
	532.1	34.11	SO ₄ ²⁻ (and O=C, residual)
	533.9	5.71	O-C
	537.5	1.69	H ₂ O
Na 1s	1071.8	2.65	Na ⁺
S 2s	226.7	—	MoS ₂
	233.2	—	SO ₄ ²⁻
N 1s (overlapping Mo 3p _{5/2})	401.9	3.15	N from hydrazine chloride (no chlorine is detected)
Atomic ratios			<i>Observations</i>
S(SO ₄ ²⁻)/S(S ²⁻)		2.58	S(sulfate)/S(sulfide) for S 2p
S(S ²⁻)/Mo _(3d, 229.6; 232.8)		2.03	As expected
[S(SO ₄ ²⁻) + C(CO ₃ ²⁻) + O(O ²⁻)] /Mo _(3d, 233.8; 236.8)		3.05	Compatible with Mo(SO ₄) ₃ , Mo(CO ₃) ₃ and MoO ₃
Oxidized species / O		1.02	
O _{532.1} /S(SO ₄ ²⁻)		4.08	As expected (subtracting O=C contribution)

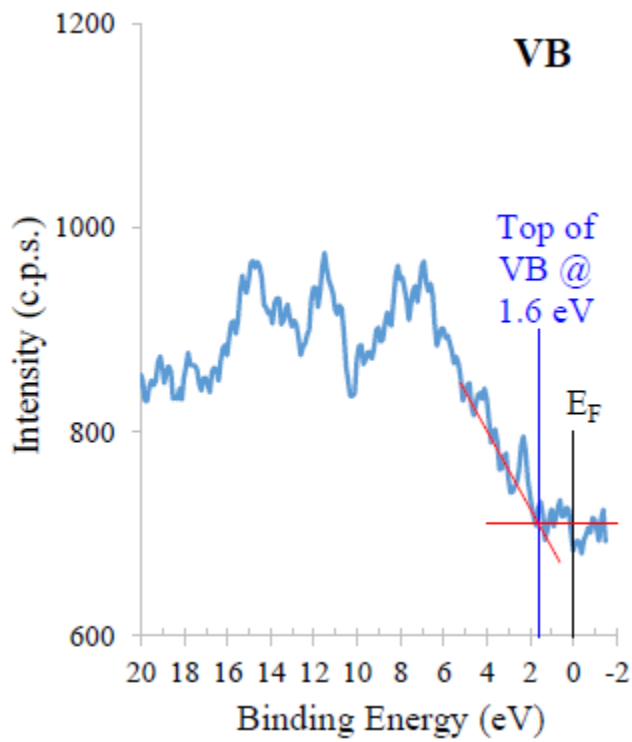
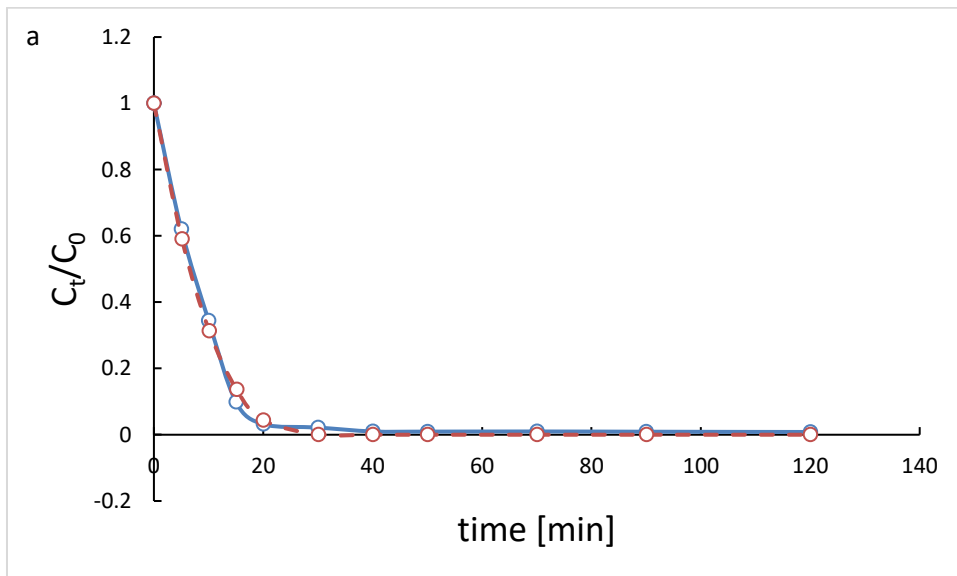


Figure S1. XPS Valence Band. The spectrum was smoothed (with a linear Savitzky-Golay function with Kernel width of 3), corrected from the charge shift, and the source satellites were subtracted.



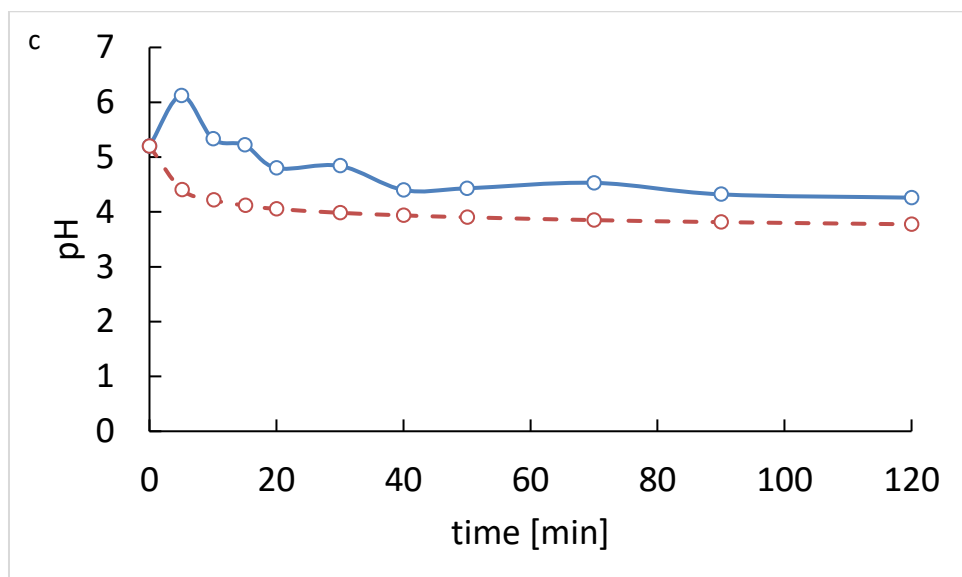
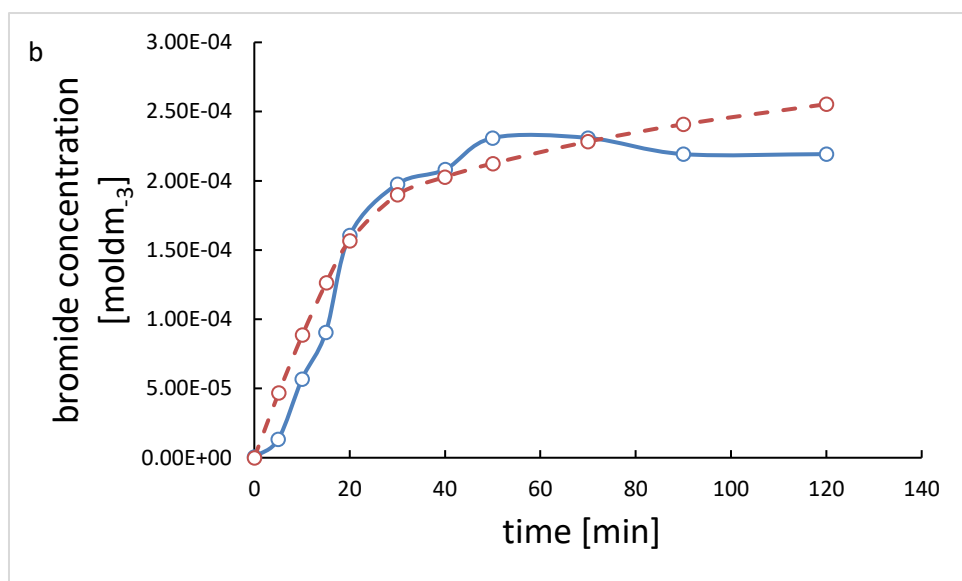


Figure S2. Comparison of the obtained and simulated results (actual results - blue, simulated results - red) of BPB decay (a), bromide production (b), pH changes of the reaction mixture (c) over time. The simulation was performed based on the proposed mechanism.

Table S2. The rate constants of reactions considered for the kinetic simulation of PFOA decomposition under ionizing radiation in N₂O-saturated aqueous solutions [1,2].

No.	Reaction	Rate constant [dm ³ mol ⁻¹ s ⁻¹]
1.	$2 e_{\text{aq}}^- \rightarrow \text{H}_2 + 2 \text{OH}^-$	1.1×10^{10}
2.	$e_{\text{aq}}^- + \text{H}^\bullet \rightarrow \text{H}_2 + \text{OH}^-$	2.5×10^{10}
3.	$e_{\text{aq}}^- + \text{}^\bullet\text{OH} \rightarrow \text{OH}^-$	3.0×10^{10}
4.	$e_{\text{aq}}^- + \text{H}^+ \rightarrow \text{H}^\bullet$	2.3×10^{10}
5.	$2 \text{H}^\bullet \rightarrow \text{H}_2$	1.55×10^{10}
6.	$\text{}^\bullet\text{OH} + \text{tert-Butanol} \rightarrow \text{H}_2\text{O}$	6×10^8
7.	$\text{H}^\bullet + \text{tert-Butanol} \rightarrow \text{H}_2\text{O}$	1×10^5
8.	$\text{H}^\bullet + \text{}^\bullet\text{OH} \rightarrow \text{H}_2\text{O}$	7.0×10^9
9.	$\text{H}^\bullet + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{}^\bullet\text{OH}$	10
10.	$\text{H}^\bullet + \text{OH}^- \rightarrow e_{\text{aq}}^- + \text{H}_2\text{O}$	2.2×10^7
11.	$e_{\text{aq}}^- + \text{BPB} \rightarrow \text{products} + \text{Br}^-$	1.1×10^{10}
12.	$\text{H}^\bullet + \text{BPB} \rightarrow \text{products} + \text{Br}^-$	2.9×10^9

References

[1] G.V. Buxton, C.L. Greenstock, W.P. Helman, A.B. Ross. 1988 *J. Phys. Chem. Ref. Data*, **17** 513-886.

[2] A.J. Elliot, A. 1989 *Radiat. Phys. Chem.* **34** 753-758.