

Electron Trap Engineering in g-C₃N₄ with Molecular Mo₃S₄ Clusters for Visible-Light-Driven Photocatalysis

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SUPPORTING INFORMATION

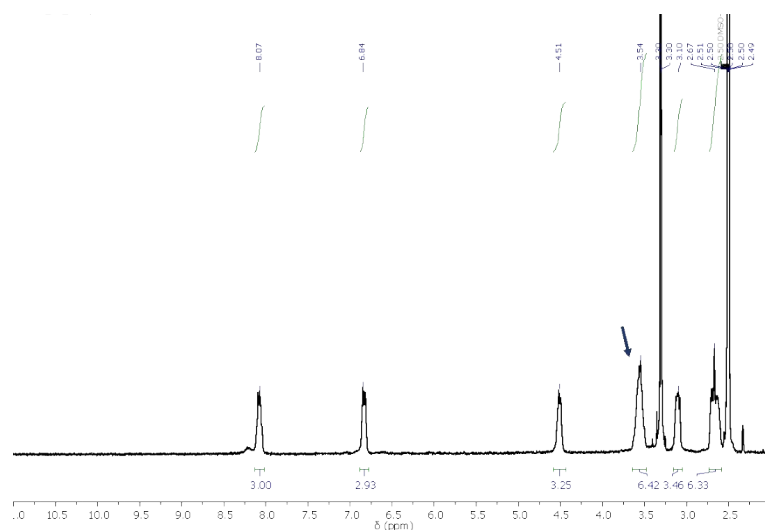


Figure S1. ¹H-NMR spectrum of the [Mo₃S₄Cl₃(en)₃]Cl complex in DMSO-*d*₆.

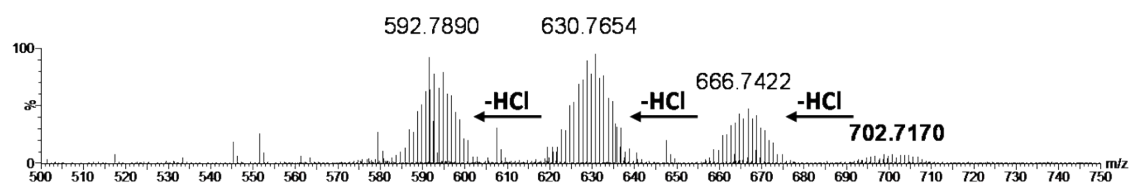


Figure S2. HRMS (ESI-TOF) spectrum of the $[\text{Mo}_3\text{S}_4\text{Cl}_3(\text{en})_3]\text{Cl}$ complex registered at 20 V in CH_3CN .

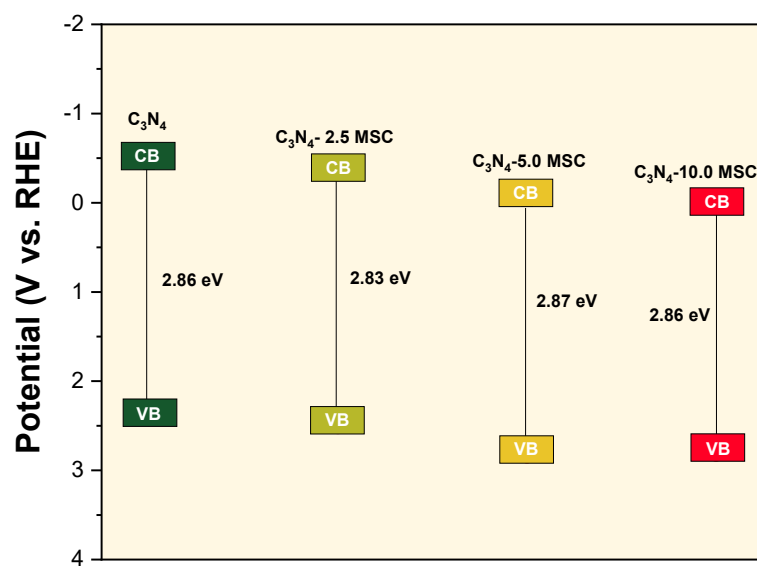


Figure S3. Valence and conduction band positions estimated from Mott-Schottky plots.

Table S1. Summary of the flat band potentials, carrier donor density and charge transfer resistance for pristine g-C₃N₄ and MSC-modified g-C₃N₄ materials.

Material	Flat band potential (V vs Ag/AgCl)	Flat band potential (V vs RHE)	Carrier Donor Density ($\times 10^{21} \text{ cm}^{-3}$)	R_s (Ω)	R_{ct} ($\text{k}\Omega$)
C₃N₄	-1.14	-0.43	0.56	76.74	8938
C₃N₄-2.5MSC	-1.02	-0.31	2.29	34.58	7877
C₃N₄-5.0MSC	-0.73	-0.02	2.39	49.5	4436
C₃N₄-10.0MSC	-0.64	0.07	3.42	34.54	1677

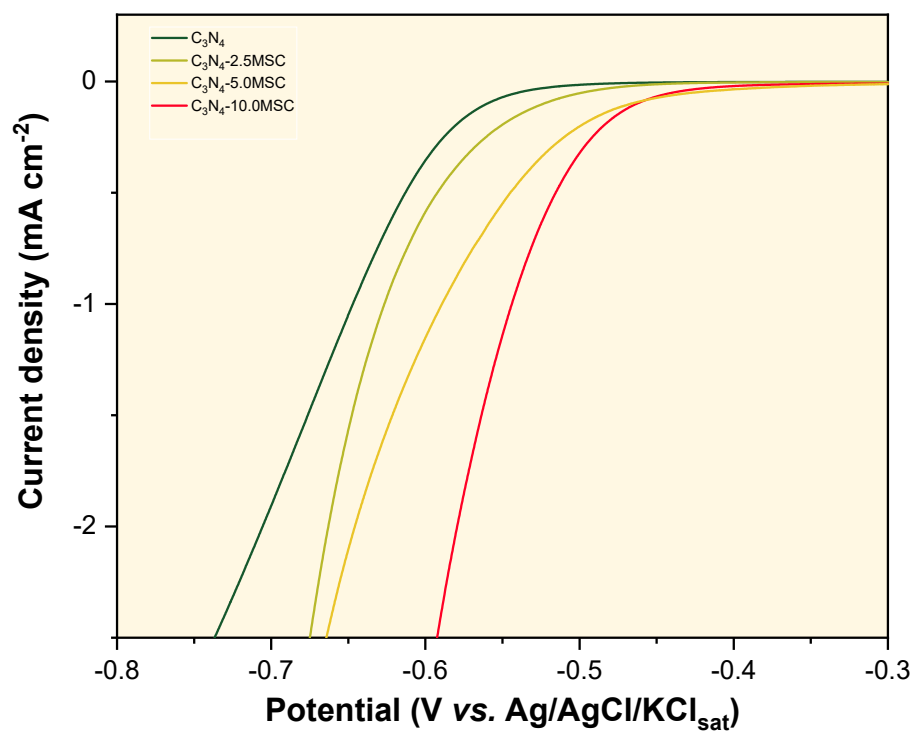


Figure S4. Polarization curves for HER registered in 0.5 M Na_2SO_4 .

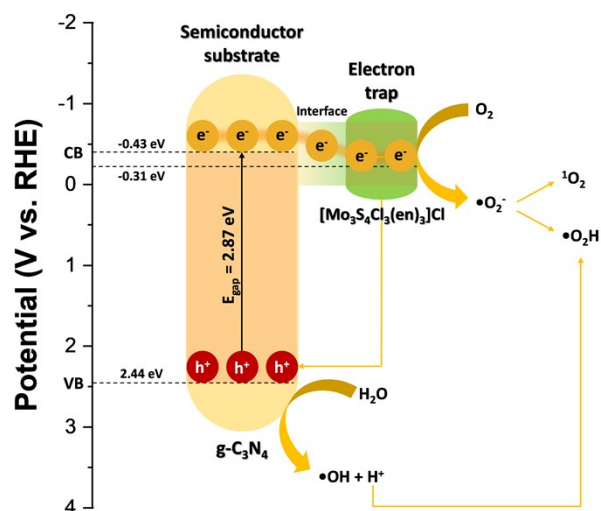


Figure S5. A schematic representation of the electron transfer pathway in $g\text{-C}_3\text{N}_4/[\text{Mo}_3\text{S}_4\text{Cl}_3(\text{en})_3]\text{Cl}$.

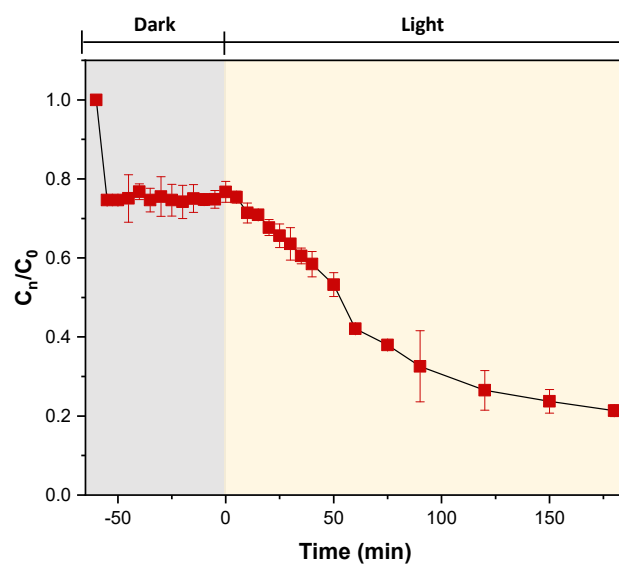


Figure S6. Photocatalytic degradation profile of CIP using the sample with 1.25 wt% of $[\text{Mo}_3\text{S}_4\text{Cl}_3(\text{en})_3]\text{Cl}$ cluster.

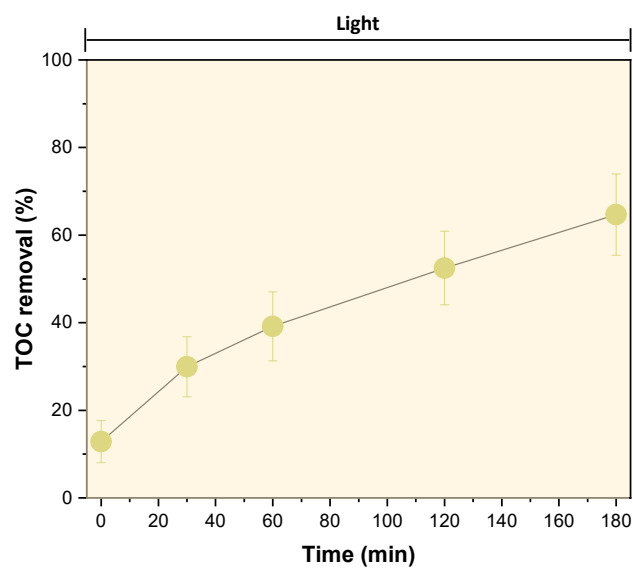


Figure S7. TOC removal evolution using the sample with 2.5 wt% of $[\text{Mo}_3\text{S}_4\text{Cl}_3(\text{en})_3]\text{Cl}$ cluster.

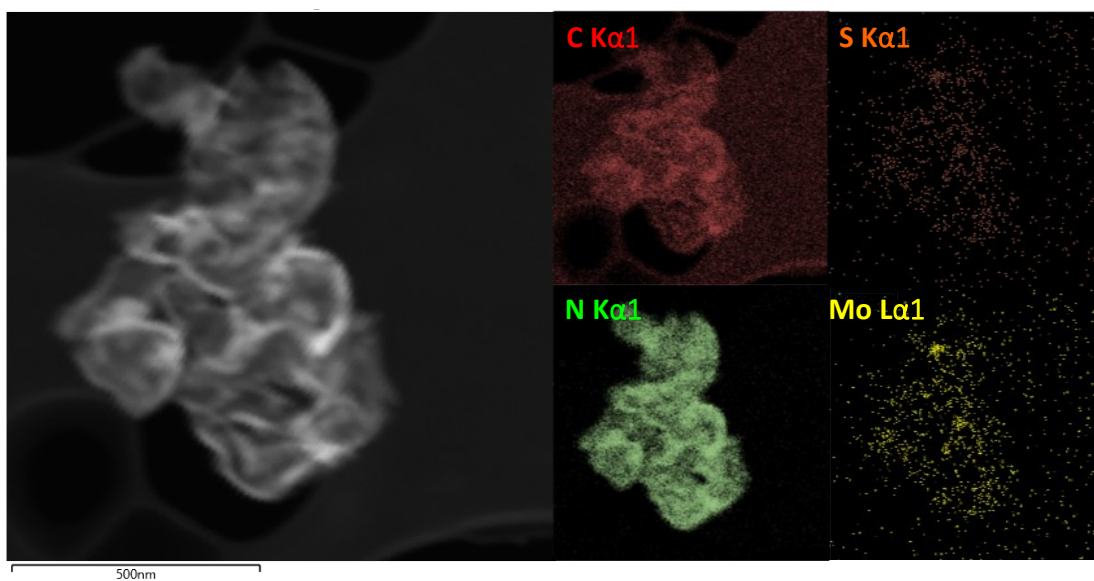


Figure S8. Characterization of the sample with 2.5 wt% of $[\text{Mo}_3\text{S}_4\text{Cl}_3(\text{en})_3]\text{Cl}$ cluster after the photocatalytic recycle.

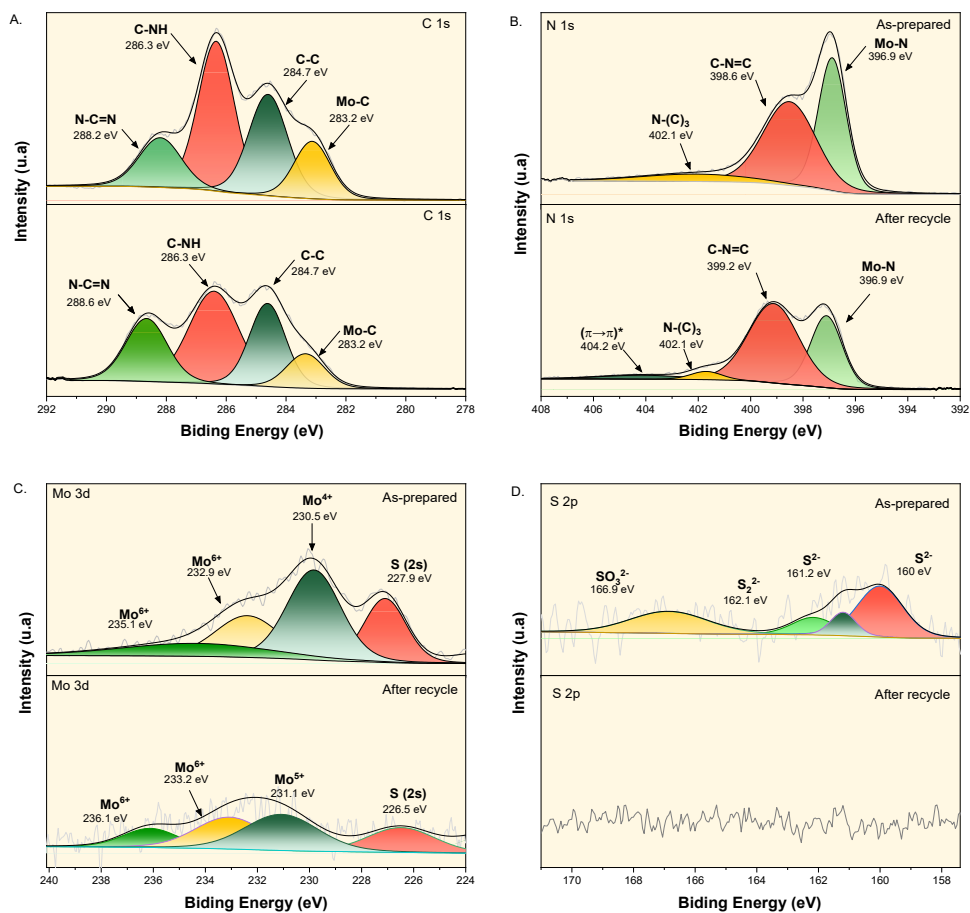


Figure S9. High Resolution XPS spectra of the C_3N_4 -2.5MSC before and after reaction: (A) C 1s, (B) N 1s, (C) Mo 3d, and (D) S 2p.

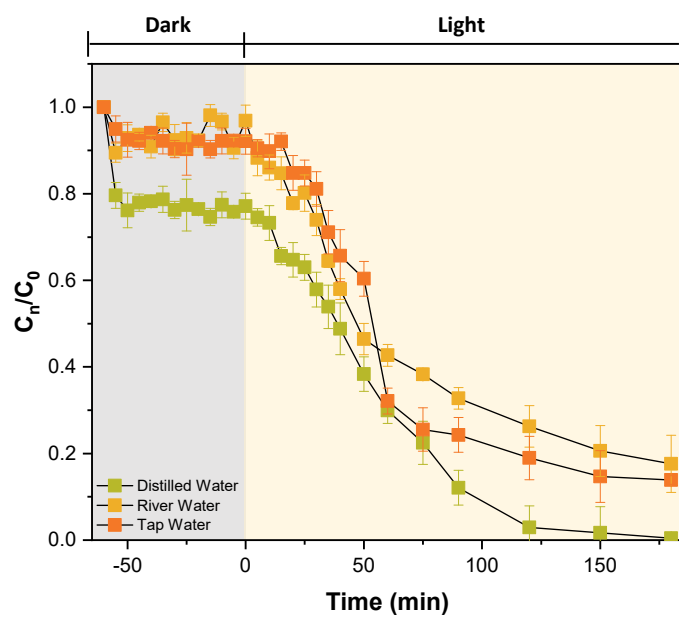


Figure S10. Photocatalytic performance using untreated tap and river water at pH 8.3.

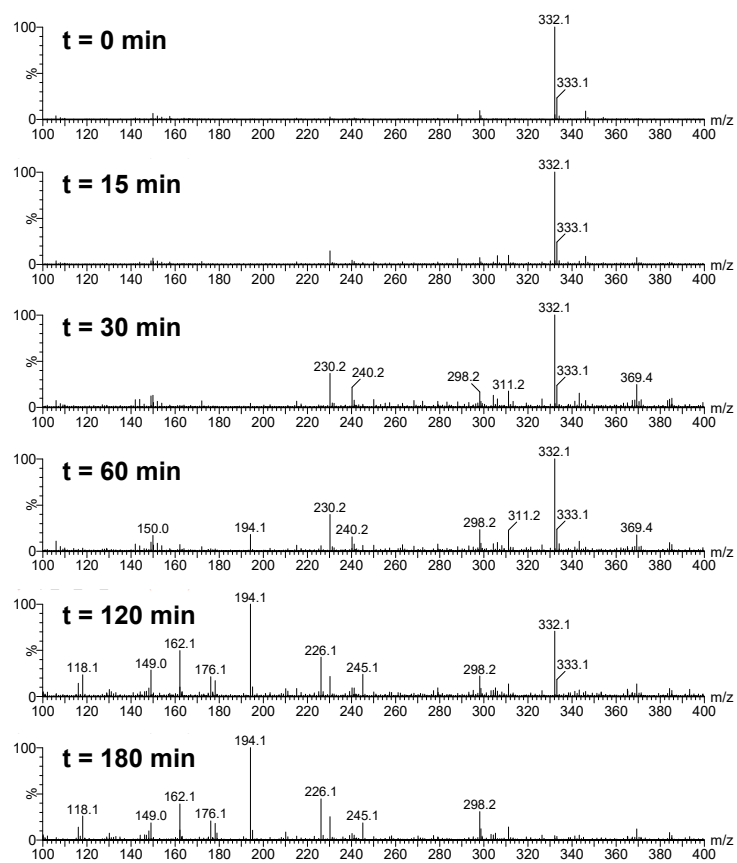


Figure S11. HRMS spectra of the CIP photodegradation at different times.