

Electronic Supplementary Information

Leveraging the Machine Learning for Predicting the Photocatalysis Performance of g-C₃N₄/CdS/MoS₂-based Heterostructure Nanocomposite

Preeti Kumari^{1,2}, Chandni Devi^{1,2,*}, Mukesh Kumar^{1,2}, Surender Kumar Sharma³, Ravi Pratap Singh³, Kamlesh Yadav⁴, Gaurav Kumar Yogesh^{1,†}

¹Department of Physics and Astrophysics, School of Basic Sciences, Central University of Haryana, Mahendergarh, 123031, India

²Department of Applied Science and Humanities, School of Engineering and Technology, Central University of Haryana, Mahendergarh, 123031, India

³Department of Physics, Central University of Punjab, Bathinda-151401, Punjab, India

⁴Department of Physics, University of Allahabad, Prayagraj-211002, Uttar Pradesh, India

^{*,†}Corresponding Author Email: chandni@cuh.ac.in, yogeshgaurav26@gmail.com

Results and Discussion

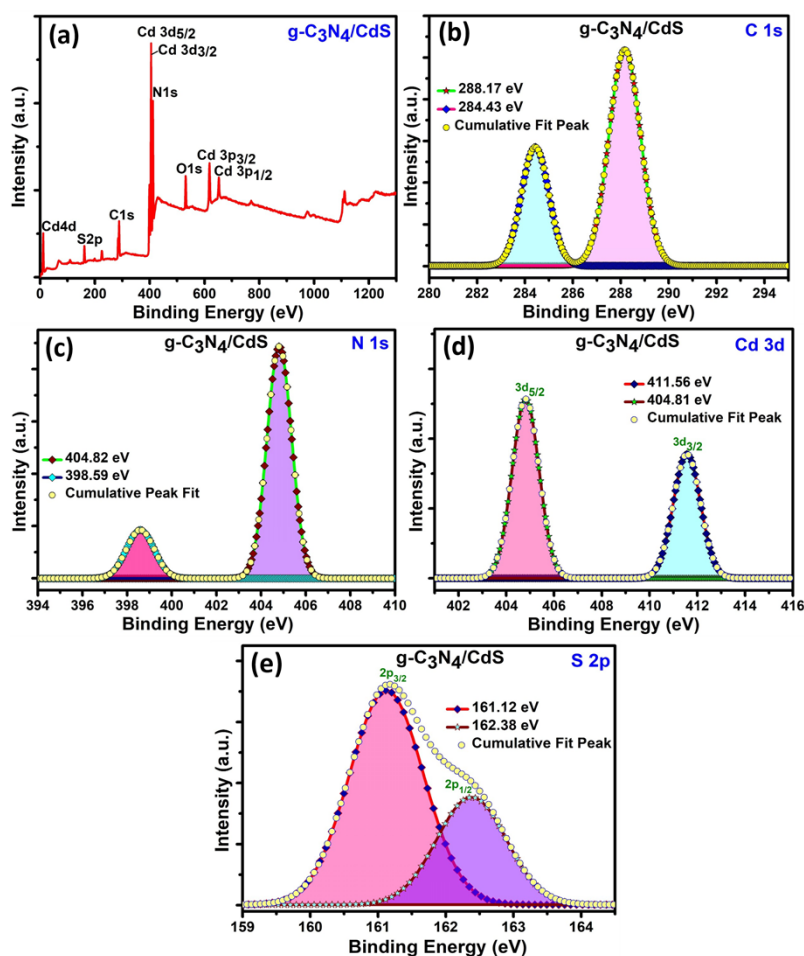


Fig. S1. XPS spectra (a) high-resolution scan, (b) C 1s peak, (c) N 1s peak, (d) Cd 3d, and (e) S 2p peaks of g-C₃N₄/CdS.

Table S1. Fitting parameter of XPS spectra of g-C₃N₄, g-C₃N₄/CdS

Sample	Peak	Position (eV)	Remark
g-C ₃ N ₄	C 1s (C=C bonding)	284.46	
	C 1s (N=C-N)	287.98	
	N 1s (C=N-C)	398.43	
	N 1s ((C)3-N)	400.06	
	N 1s (II- excitation)	404.08	
	O 1s	532.13	
g-C ₃ N ₄ /CdS	C 1s (N=C-N)	288.17	$\Delta BE_{N=C-N} = 0.19 \text{ eV}$ $\Delta BE_{N=C-N} = 0.16 \text{ eV}$ $\Delta BE_{\text{II-excitation}} = 0.73 \text{ eV}$
	N 1s (C=N-C)	398.59	
	N 1s (II- excitation)	404.82	
	O 1s	531.30	
	Cd 3d5/2	404.81	
	Cd 3d3/2	411.56	
	S 2p3/2	161.12	
	S 2p1/2	162.38	

Table S2. Data set used for training of ML models

S.N o.	Nanocatalyst	Source	Dye	Power (W)	Dose (mg)	Solution (ml)	Concentration (ppm)	Time (min.)	Efficiency (%)	Ref.
1	g-C ₃ N ₄ /WS ₂	Sunlight	MB		50	50	50	120	95	¹
2	CdS/CQDs/g-C ₃ N ₄	Xenon	MB	300	100	100	10	120	98	²
3	g-C ₃ N ₄ /CdS	CDMR	MB	70	200	200	20	100	95	³
4	CdS @Cu/g-C₃N₄	Xenon	MB	350	7	35	10	20	85	⁴
5	MoS ₂ /g-C ₃ N ₄	UV	RhB	100	50	80	30	360	90	⁵
6	g-C₃N₄ @ ZnO-MoS₂	LED	MB	10	5	50	0.71	180	95	⁶
7	g-C ₃ N ₄ /CdS	LED	RhB	20	25	100	10	90	95	⁷
8	g-C ₃ N ₄ /MoS ₂	Xenon	RhB	500	50	50	10	120	99.6	⁸
9	MnS/g-C ₃ N ₄	Xenon	MB	300	10	30		140	95.5	⁹
10	g-C ₃ N ₄ /CdS	Sunlight	TC		50	100	20	40	96.2	¹⁰
11	g-C ₃ N ₄ /CdS	Sunlight	CIP		50	100	20	40	80	¹⁰
12	g-C ₃ N ₄ /CdS	Metalhalide	RhB	400	5	25	0.71	40	99	¹¹
13	g-C ₃ N ₄ -CdS	Xenon	MB	500	80	200	25	180	90.45	
14	CdS/ g-C ₃ N ₄ /NiFe ₂ O ₄	Xenon	RBBR	500	30	30	20	180	96	¹²
15	2D g-C ₃ N ₄ /CdS	Xenon	Cr	300	50	100	100	50	99	¹³
16	CdS/g-C ₃ N ₄	LED	MO	200	50	100	10	210	99.7	¹⁴
17	F-BiVO ₄ /g-C ₃ N ₄ /CdS	Xenon	Cr	500	50	50	20	5	98	¹⁵
18	F-BiVO ₄ /g-C ₃ N ₄ /CdS	Xenon	CIP	500	50	50	20	30	90	¹⁵
19	g-C ₃ N ₄ /CdS/BiVO ₄	Halogen	MB	500	10	30	20	120	94.5	¹⁶
20	g-C ₃ N ₄ /CdS	Xenon	Ery	35	25	50	50	60	81.02	¹⁷
21	g-C ₃ N ₄ /BiOBr/CdS	Tungsten	TC	150	500	100	20	70	99.4	¹⁸

22	2D g-C ₃ N ₄ /CdS	Sunlight	Nitrophenol		50	100	30	50	99	19
23	2D g-C ₃ N ₄ /CdS	Sunlight	Nitrophenol		50	100	30	50	79	19
24	PAN/g-C ₃ N ₄ /CdS	Tungsten	RhB	250	20	100	10	15	92	20
25	CdS/TiO ₂ /g-C ₃ N ₄	LED	RhB	50	10	50	25	180	99	21
26	g-C ₃ N ₄ /Cu @ CdS	Sunlight	MB		50	80	20	120	95	22
27	g-C ₃ N ₄ /Cu @ CdS	Sunlight	CIP		30	80	25	90	76	22
28	P/N-type NdCoO ₃ /g-C ₃ N ₄	Sunlight	EBT	400	75	50	5	120	95.8	23
29	g-C ₃ N ₄ /MoS ₂ -PANI	Sunlight	BPA				20	60	92.66	19
30	g-C ₃ N ₄ /MoS ₂	Sunlight	BPA				20	60	69.8	19
31	g-C ₃ N ₄ /MoS ₂ -PANI	Sunlight	BPA				30	60	88.59	19
32	g-C ₃ N ₄ /MoS ₂ -PANI	Sunlight	BPA				40	60	85.76	19
33	g-C ₃ N ₄ /MoS ₂ -PANI	Sunlight	BPA				50	60	82.79	24
34	g-C ₃ N ₄ /MoS ₂ -PANI	Sunlight	BPA				60	60	78.68	24
35	g-C ₃ N ₄ /MoS ₂	Xenon	AB1	300	25	50	0.5	60	97.5	20
36	g-C ₃ N ₄ /MoS ₂	Xenon	AB1	300	25	50	4	60	63.3	25
37	g-C ₃ N ₄ /MoS ₂	Xenon	RhB	300	25	50	10	90	85	25
38	GO/g-C ₃ N ₄ /MoS ₂	Xenon	MB	500	20	50	20	60	99	26
39	Ag ₃ PO ₄ /g-C ₃ N ₄ @MoS ₂	Xenon	AMA	300	30	50	20	90	99.9	27
40	g-C ₃ N ₄ /MoS ₂	UV	Hypophosphite	35	5	50	50	90	93.45	28
41	g-C ₃ N ₄ /MoS ₂	Xenon	MB	500	50	100	20	120	94	29
42	g-C ₃ N ₄ /MoS ₂	Xenon	RhB	300	50	50	10	60	87.4	30
43	g-C ₃ N ₄ /MoS ₂ QDs	Xenon	RhB	500	30	50	20	120	62	31
44	GO/g-C ₃ N ₄ /MoS ₂	Xenon	RhB	500	20	50	20	60	77.2	21
45	GO/g-C ₃ N ₄ /MoS ₂	Xenon	CV	500	20	50	20	60	70.3	26
46	GO/g-C ₃ N ₄ /MoS ₂	Xenon	Cr	500	20	50	10	120	80	26
47	MoS ₂ -coupled g-C ₃ N ₄	Sunlight	MB		20	100	20	105	98	32
48	MoS ₂ -ZrO ₂ /g-C ₃ N ₄	Xenon	RhB	300	100	100	30	40	99.8	33
49	g-C ₃ N ₄ /MoS ₂ /MnO OH	Xenon	MB	130	15	25		70	94	34
50	MoS ₂ -g-C ₃ N ₄	Sunlight	RhB		25	100	5	360	78	35
51	g-C ₃ N ₄ /MoS ₂	Xenon	RhB	500	50	100		120	100	36
52	g-C ₃ N ₄ /MoS ₂	Xenon	MO	500	50	100		120	79	36
53	g-C ₃ N ₄ /MoS ₂	Xenon	Cr	300	10	100	20	120	91.6	37
54	MoS ₂ /g-C ₃ N ₄	LED	RhB	100	5	100	10	180	99.7	38
55	g-C ₃ N ₄ :MoS ₂ : ZnO-Ag hybrid nanocomposite	Halogen	MB	500	60	100		100	95.29	39
56	MoS ₂ /g-C ₃ N ₄ -P	Sunlight	MB		20	100	5	80	95	40

57	MoS ₂ /g-C ₃ N ₄ -M	Sunlight	MB		20	100	5	80	82	40
58	g-C ₃ N ₄ /MoS ₂ /GO	Tungsten	RhB	150	100	100	5	60	99	41
59	g-C ₃ N ₄ /MoS ₂ /GO	Tungsten	Chlorophen ol	150	100	100	5	60	89	41
60	g-C ₃ N ₄ /MoS ₂ /GO	Tungsten	RhB	150	20	50	5	60	78	41
61	MoS ₂ /g-C ₃ N ₄ /Bi ₂₄ O ₃₁ C ₁₁₀	Xenon	TC	300	10	50	20	50	97.5	42
62	g-C ₃ N ₄ /MoS ₂	Tungsten	MB	150	15	50	3.5	120	98	43
63	g-C ₃ N ₄ /MoS ₂	Xenon	MB		15	100	20	60	98	44
64	g-C ₃ N ₄ /MoS ₂	Ultrasoni c	Levofloxaci n		60	60	10	140	75.81	45
65	g-C ₃ N ₄ /MoS ₂	Ultrasoni c	MB		60	60	10	14	98.43	45
66	g-C ₃ N ₄ /MoS ₂	Xenon	RhB	500	30	150	0.71	120	94	46
67	g-C ₃ N ₄ /MoS ₂ with hollow structure	Xenon	Tetracycline	300	10	50	10	90	98.49	42
68	g-C ₃ N ₄ /MoS ₂ with hollow structure	Xenon	Cu	300	10	50	5	90	99.9	42
69	g-C ₃ N ₄ /MoS ₂	Xenon	Sulfasalazin e		20	100	20	90	97	43
70	g-C ₃ N ₄ /MoS ₂	Xenon	RhB	350	20	50	10	90	99.4	44
71	g-C ₃ N ₄ /MoS ₂	Sunlight	MB		30	100	10	180	81	

References

1. Nawaz A, Goudarzi S, Saravanan P, Zarrin H. Z-scheme induced g-C₃N₄/WS₂ heterojunction photocatalyst with improved electron mobility for enhanced solar photocatalysis. *Sol Energy*. 2021;228(February):53-67. doi:10.1016/j.solener.2021.09.040
2. Feng S, Chen T, Liu Z, Shi J, Yue X, Li Y. Z-scheme CdS/CQDs/g-C₃N₄ composites with visible-near-infrared light response for efficient photocatalytic organic pollutant degradation. *Sci Total Environ*. 2020;704. doi:10.1016/j.scitotenv.2019.135404
3. Shenoy S, Tarafder K, Sridharan K. Graphitic C₃N₄/CdS composite photocatalyst: Synthesis, characterization and photodegradation of methylene blue under visible light. *Phys B Condens Matter*. 2020;595(June):412367. doi:10.1016/j.physb.2020.412367
4. Li C, Zhai Q, Liu W, Yang Q, Li Q, Zhang X. Facile fabrication of CdS/Cu-doped g-C₃N₄ heterojunction for enhanced photocatalytic degradation of methylene blue. *J Mater Sci Mater Electron*. 2023;34(23):1-15. doi:10.1007/s10854-023-11055-9
5. Tran Huu H, Thi MDN, Nguyen VP, et al. One-pot synthesis of S-scheme MoS₂/g-C₃N₄ heterojunction as effective visible light photocatalyst. *Sci Rep*. 2021;11(1):1-12. doi:10.1038/s41598-021-94129-0
6. Sahu D, Panda NR. Synthesis of novel nanocomposite of g-C₃N₄ coated ZnO–MoS₂ for energy storage and photocatalytic applications. *Chemosphere*. 2024;350(December 2023):141014. doi:10.1016/j.chemosphere.2023.141014
7. Fang J, Xie K, Kang Q, Gou Y. Facile fabrication of g-C₃N₄/CdS heterojunctions with enhanced visible-light photocatalytic degradation performances. *J Sci Adv Mater Devices*. 2022;7(1). doi:10.1016/j.jsamd.2021.100409
8. Fan Y, Yang Y ning, Ding C. Preparation of g-C₃N₄/MoS₂ Composite Material and Its Visible Light Catalytic Performance. *J Inorg Organomet Polym Mater*. 2021;31(12):4722-4730. doi:10.1007/s10904-021-

9. Muhammad Tahir Farid H, Altuijri R, Abu El Maati L, Hussain Jawhari A. One pot development of MnS/g-C₃N₄ nanocomposite via hydrothermal synthesis for photodegradation of methylene blue. *Inorg Chem Commun.* 2023;155(July):111003. doi:10.1016/j.inoche.2023.111003
10. Siddhardhan E V., Steephen A, Jose M, Arumanayagam T. Efficient removal of TC and CIP antibiotics by surface modified g-C₃N₄/CdS nanocomposite under sunlight irradiation. *Dye Pigment.* 2024;225(February):112052. doi:10.1016/j.dyepig.2024.112052
11. Wang M, Wang M, Peng F, Sun X, Han J. Fabrication of g-C₃N₄ Nanosheets Anchored With Controllable CdS Nanoparticles for Enhanced Visible-Light Photocatalytic Performance. *Front Chem.* 2021;9(October):1-10. doi:10.3389/fchem.2021.746031
12. El-Sabban HA, Mady AH, Diab MA, Attia SY, Mohamed SG. Construction of novel dual Z-scheme heterojunction of ternary CdS/g-C₃N₄/NiFe₂O₄ magnetically retrievable nanocomposite for boosted photocatalytic and energy storage applications. *Surfaces and Interfaces.* 2024;44(October 2023):103798. doi:10.1016/j.surfin.2023.103798
13. Ren Y, Gong T. Fabrication of 2D g-C₃N₄/CdS core-shell heterojunction with effective photocatalytic activity for dye degradation and reduction of Cr(VI) under visible light. *J Mater Sci Mater Electron.* 2021;32(12):16845-16853. doi:10.1007/s10854-021-06245-2
14. Lin C, Zhang Y, Zhang SY, et al. Facile Fabrication of a Novel g-C₃N₄/CdS Composites Catalysts with Enhanced Photocatalytic Performances. *ES Energy Environ.* 2023;20:1-13. doi:10.30919/esee8c860
15. Yang Z, Yang J, Li L, et al. A novel F-BiVO₄/g-C₃N₄/CdS dual S-scheme heterojunction for high efficient photocatalytic removal of multiple pollutants. *Appl Surf Sci.* 2024;672(June):160738. doi:10.1016/j.apsusc.2024.160738
16. Saad M, Bahadur A, Iqbal S, et al. Development of stable S-scheme 2D-2D g-C₃N₄/CdS nanoheterojunction arrays for enhanced visible light photomineralisation of nitrophenol priority water pollutants. *Sci Rep.* 2024;14(1):1-11. doi:10.1038/s41598-024-52950-3
17. Afzal MI, Shahid S, Mansoor S, Javed M, Iqbal S. Fabrication of a Ternary Nanocomposite g-C₃N₄/Cu@CdS with Superior Charge Separation for Removal of Organic Pollutants and Bacterial Disinfection from Wastewater under Sunlight Illumination. *Toxics.* 2022;657(10):1-13.
18. Kianipour S, Razavi FS, Hajizadeh-Oghaz M, et al. The synthesis of the P/N-type NdCoO₃/g-C₃N₄ nano-heterojunction as a high-performance photocatalyst for the enhanced photocatalytic degradation of pollutants under visible-light irradiation. *Arab J Chem.* 2022;15(6):103840. doi:10.1016/j.arabjc.2022.103840
19. Ahamad T, Naushad M, Alzahrani Y, Alshehri SM. Photocatalytic degradation of bisphenol-A with g-C₃N₄/MoS₂-PANI nanocomposite: Kinetics, main active species, intermediates and pathways. *J Mol Liq.* 2020;311:113339. doi:10.1016/j.molliq.2020.113339
20. Song R, Yao L, Sun C, et al. Electrospun Membranes Anchored with g-C₃N₄/MoS₂ for Highly Efficient Photocatalytic Degradation of Aflatoxin B1 under Visible Light. *Toxins (Basel).* 2023;15(2). doi:10.3390/toxins15020133
21. Wu M hong, Li L, Xue Y cheng, et al. Fabrication of ternary GO/g-C₃N₄/MoS₂ flower-like heterojunctions with enhanced photocatalytic activity for water remediation. *Appl Catal B Environ.* 2018;228(2010):103-112. doi:10.1016/j.apcatb.2018.01.063
22. Liu H, Chen H, Ding N. Visible Light-Based Ag₃ PO₄/g-C₃ N₄ @MoS₂ for Highly Efficient Degradation of 2-Amino-4-acetylaminoanisole (AMA) from Printing and Dyeing Wastewater. *Int J Environ Res Public Health.* 2022;19(5). doi:10.3390/ijerph19052934
23. Guan W, He K, Du J, et al. Improvement of Photocatalytic Performance for the g-C₃N₄/MoS₂ Composite

Used for Hypophosphite Oxidation. *J Nanomater.* 2020;2020. doi:10.1155/2020/8461543

24. Zhong Z, Xu R, He H, Zhuang Q, Huang L. Construction of 2D g-C₃N₄/MoS₂ heterojunction photocatalyst for enhanced degradation of pollution under visible light. *Desalin Water Treat.* 2019;137:234-242. doi:10.5004/dwt.2019.23160
25. Fan Y, Yang Y ning, Ding C, Wang H jun. Degradation of rhodamine B by g-C₃N₄/MoS₂ composite photocatalyst. *Ferroelectrics.* 2022;595(1):146-155. doi:10.1080/00150193.2022.2079465
26. Azhar A, Basit MA, Mehmood W, et al. Synchronized wet-chemical development of 2-dimensional MoS₂ and g-C₃N₄/MoS₂ QDs nanocomposite as efficient photocatalysts for detoxification of aqueous dye solutions. *Colloids Surfaces A Physicochem Eng Asp.* 2023;657. doi:10.1016/j.colsurfa.2022.130581
27. Krishnasamy M, Rajendran R, Vignesh S, et al. Facile synthesis of efficient MoS₂-coupled graphitic carbon nitride Z-scheme heterojunction nanocomposites: photocatalytic removal of methylene blue dye under solar light irradiation. *Environ Sci Pollut Res.* 2023;31(34):46513-46525. doi:10.1007/s11356-023-26418-2
28. Xu L, Lv J, Zhao Z, Sun G. A Novel Photocatalyst MoS₂-ZrO₂/g-C₃N₄ and Its Photocatalytic Properties. *Russ J Phys Chem A.* 2023;97(6):1302-1312. doi:10.1134/S003602442306016X
29. Sekar M, Saravanan K, Prasath M, Bharathi Bernadsha S. An investigation on the synthesis and characterization of MoS₂ nanoflowers draped g-C₃N₄ nano sheet (g-C₃N₄ / MoS₂ / MnOOH) ternary composite for the efficient photocatalytic applications. *Chem Phys Impact.* 2024;9(May):100665. doi:10.1016/j.chphi.2024.100665
30. Ansari SA, Cho MH. Simple and Large Scale Construction of MoS₂-g-C₃N₄ Heterostructures Using Mechanochemistry for High Performance Electrochemical Supercapacitor and Visible Light Photocatalytic Applications. *Sci Rep.* 2017;7(February):1-11. doi:10.1038/srep43055
31. Zheng J, Zhang B, Wang Z. Electron-assisted synthesis of g-C₃N₄/MoS₂ composite with dual defects for enhanced visible-light-driven photocatalysis. *RSC Adv.* 2020;11(1):78-86. doi:10.1039/d0ra10148f
32. Tian C, Yu H, Zhai R, et al. Visible Light Photoactivity of g-C₃N₄/MoS₂ Nanocomposites for Water Remediation of Hexavalent Chromium. *Molecules.* 2024;29(3). doi:10.3390/molecules29030637
33. Moghimifar Z, Yazdani F, Tabar-Heydar K, Sadeghi M. Photocatalytic Hydrogen Evolution Under Visible Light Using MoS₂/g-C₃N₄ Nano-Photocatalysts. *Catal Letters.* 2024;154(3):1255-1269. doi:10.1007/s10562-023-04389-w
34. Elavarasan N, Vignesh S, Srinivasan M, et al. Integrating gC₃N₄ nanosheet with MoS₂ and ZnO-Ag: Remarkably enhanced photocatalytic performance under visible-light irradiation. *Colloids Interface Sci Commun.* 2021;44(June):100474. doi:10.1016/j.colcom.2021.100474
35. Hassan HM ul, Tawab SA, Khan MI, et al. Reduce the recombination rate by facile synthesis of MoS₂/g-C₃N₄ heterostructures as a solar light responsive catalyst for organic dye degradation. *Diam Relat Mater.* 2023;140(PA):110420. doi:10.1016/j.diamond.2023.110420
36. Kumaresan N, Karuppasamy P, Pandian MS, Ramasamy P. Formation of face-contact interaction in 2D/2D/2D heterostructure ternary nanocomposites of g-C₃N₄/MoS₂/GO for effective photocatalytic activity against the organic pollutants under the visible light irradiation. *J Mater Sci Mater Electron.* 2022;33(15):11970-11988. doi:10.1007/s10854-022-08159-z
37. Kang J, Jin C, Li Z, Wang M, Chen Z, Wang Y. Dual Z-scheme MoS₂/g-C₃N₄/Bi₂₄O₃₁Cl₁₀ ternary heterojunction photocatalysts for enhanced visible-light photodegradation of antibiotic. *J Alloys Compd.* 2020;825:153975. doi:10.1016/j.jallcom.2020.153975
38. Senthilnathan S, Ganesh Kumar K, Sugunraj S, et al. MoS₂ modified g-C₃N₄ composite: A potential candidate for photocatalytic applications. *J Saudi Chem Soc.* 2023;27(5):101717. doi:10.1016/j.jscs.2023.101717
39. Lyu H, Zhu W, Chen K, Gao J, Xie Z. 3D flower-shaped g-C₃N₄/MoS₂ composite with structure defect for

- synergistic degradation of dyes. *J Water Process Eng.* 2024;57(October 2023):104656. doi:10.1016/j.jwpe.2023.104656
40. He Y, Ma Z, Junior LB. Distinctive binary g-C₃N₄/MoS₂ heterojunctions with highly efficient ultrasonic catalytic degradation for levofloxacin and methylene blue. *Ceram Int.* 2020;46(8):12364-12372. doi:10.1016/j.ceramint.2020.01.287
 41. Qi YR, Liang QH, Lv RT, Shen WC, Kang FY, Huang ZH. Subject Category : Subject Areas : Synthesis and photocatalytic activity of mesoporous g-C₃N₄ / MoS₂ hybrid catalysts. *R Soc.* Published online 2018:2-10.
 42. Liu J, Dong Y, Zhang Y, Liu W, Xu J, Lin H. Enhanced synergistic performance of g-C₃N₄/MoS₂ with hollow structure for tetracycline photocatalytic degradation in complex environments: Performance and mechanism. *J Clean Prod.* 2024;451(April):141983. doi:10.1016/j.jclepro.2024.141983
 43. Sharma G, Naushad M, ALOthman ZA, Iqbal J, Bathula C. High interfacial charge separation in visible-light active Z- scheme g-C₃N₄/MoS₂ heterojunction: Mechanism and degradation of sulfasalazine. *Chemosphere.* 2022;308(P1):136162. doi:10.1016/j.chemosphere.2022.136162
 44. Cui Z, Wu H, Bai K, et al. Fabrication of a g-C₃N₄/MoS₂ photocatalyst for enhanced RhB degradation. *Phys E Low-Dimensional Syst Nanostructures.* 2022;144(July). doi:10.1016/j.physe.2022.115361