Supporting Information

Design and Synthesis of PANI/GO/MoS_2 Nanocomposites via Oxidative Polymerization for Efficient Photocatalytic Applications: Organic Pollutant Degradation and Hydrogen Generation

Pritam Hait[a], Rajeev Mehta[b], and Soumen Basu[a*]

[a] Department of Chemistry and Biochemistry, TIET-Virginia Tech Center of Excellence in Emerging Materials, Thapar Institute of Engineering & Technology, Patiala-147004, India.

[b] Department of Chemical Engineering, TIET-Virginia Tech Center of Excellence in Emerging Materials, Thapar Institute of Engineering & Technology, Patiala-147004, India.

*Corresponding author: E-mail: soumen.basu@thapar.edu (Dr. Soumen Basu)

S1. Chemicals used in the synthesis procedure:

The following chemicals were used for the synthesis of the materials: graphite fine powder (98%, LOBA CHEMIE), aniline (99%, LOBA CHEMIE), hydrochloric acid (36%, LOBA CHEMIE), ammonium persulfate (98%, SDFCL), thiourea (99.5%-100%, LOBA CHEMIE), Ammonium Molybdate (98%, LOBA CHEMIE), potassium permanganate (99%, LOBA CHEMIE), sodium nitrite (97%, LOBA CHEMIE), and hydrogen peroxide (30% solution, RANKEM). Methyl Orange was purchased from CDH Chemical.

S2. Instrument specifications:

The as-prepared nanocomposites were characterized by various characterization techniques. The ultraviolet-visible absorption spectra of the synthesized materials were measured utilizing a UV-vis spectrophotometer instrument (Shimadzu UV 2600). Photoluminescence spectra were recorded utilizing a spectrofluorometer instrument (Shimadzu RF-6000). The shape of the prepared composite was analyzed using field emission scanning electron microscopy (FESEM, JEOL). The functional groups present in the materials were identified using Fourier

transform infrared (FTIR) spectroscopy (Shimadzu IRTracer-100). The X-ray Photoelectron Microscopy (XPS) analysis was performed using a monochromatic aluminium source, specifically Al ka radiation, on an Omicron ESCA instrument with an energy of 1486.7 eV. Brunauere-Emmette-Teller (BET) method and Barrette-Joynere-Halenda (BJH) method were done by Belsorp Mini II instrument. The degraded products and possible Intermediate by-products of the degradation product were analysed by Gas Chromatography Mass Spectrometry (GCMS, Bruker SHS-40). The amount of hydrogen produced by photocatalytic water splitting was measured using GC-TCD (nucon 5765).

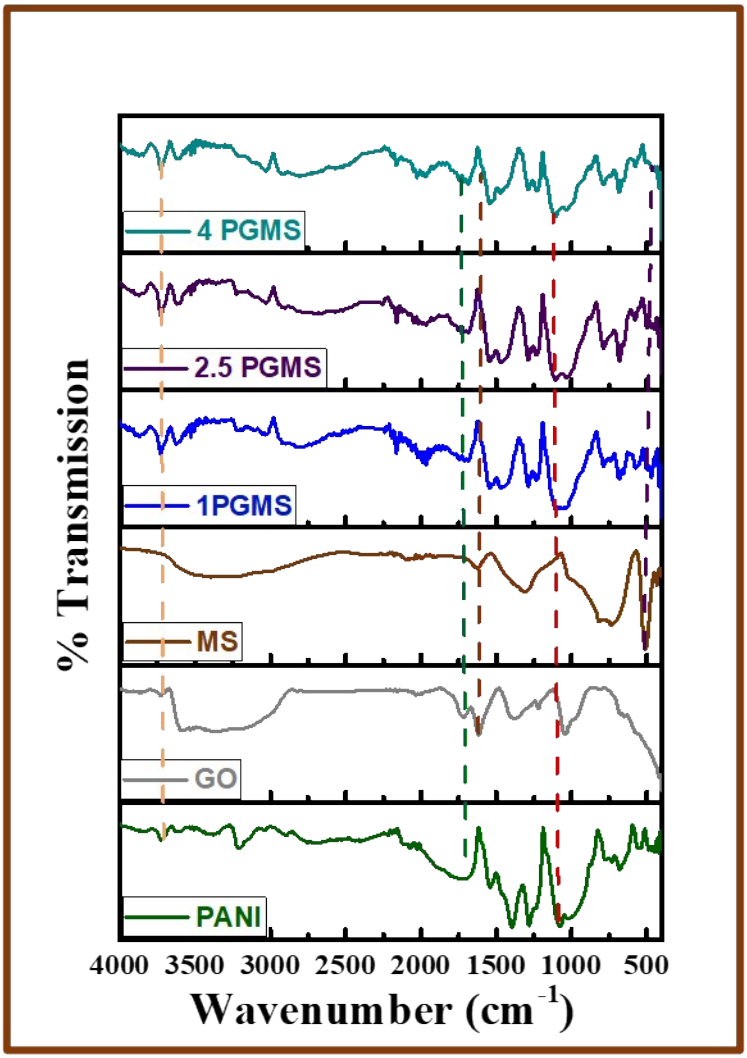


Fig. S1: FTIR of PANI, GO, MoS_2, 1PGMS, 2.5PGMS, and 4PGMS.

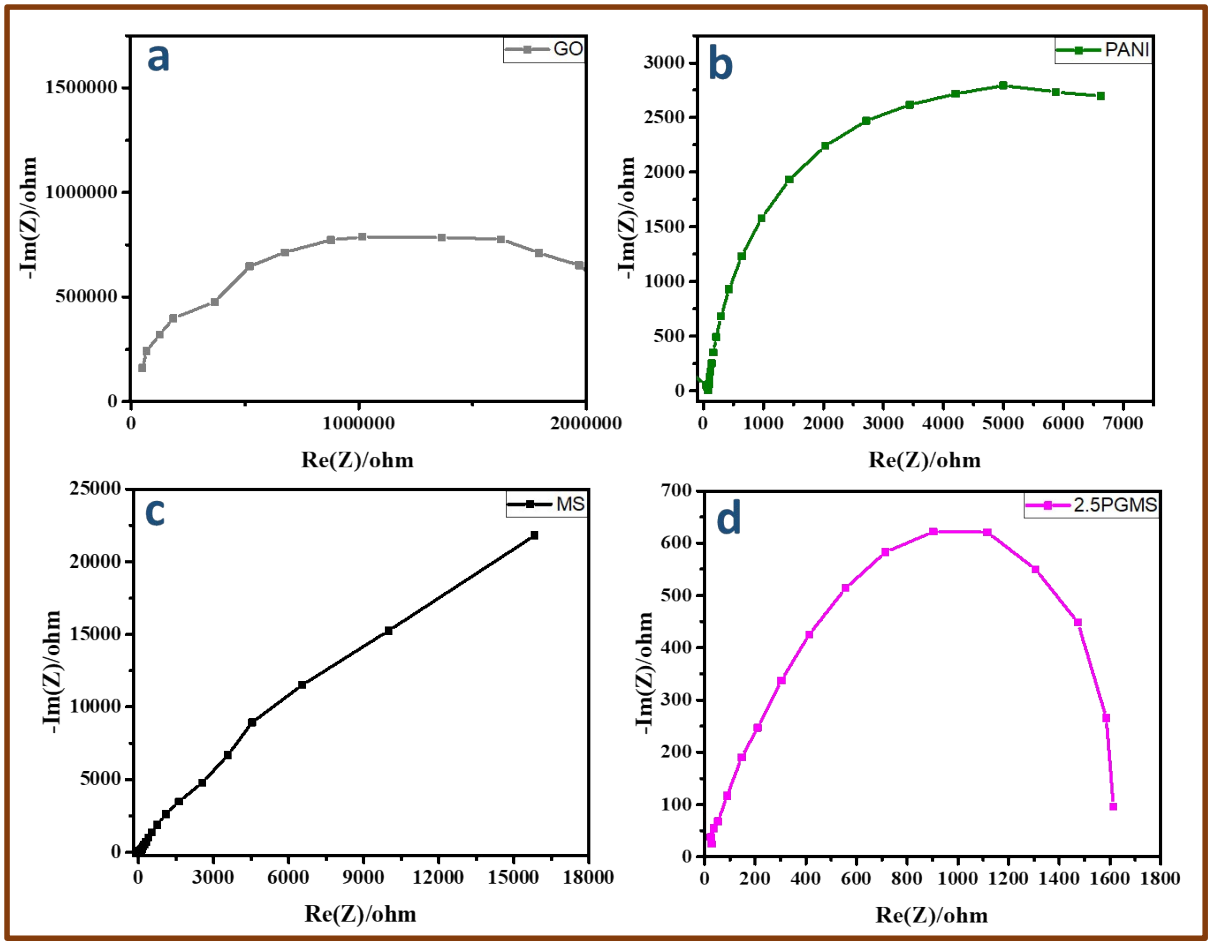


Fig. S2: EIS plot of (a) GO, (b) PANI, (c) MS, and (d) 2.5PGMS.

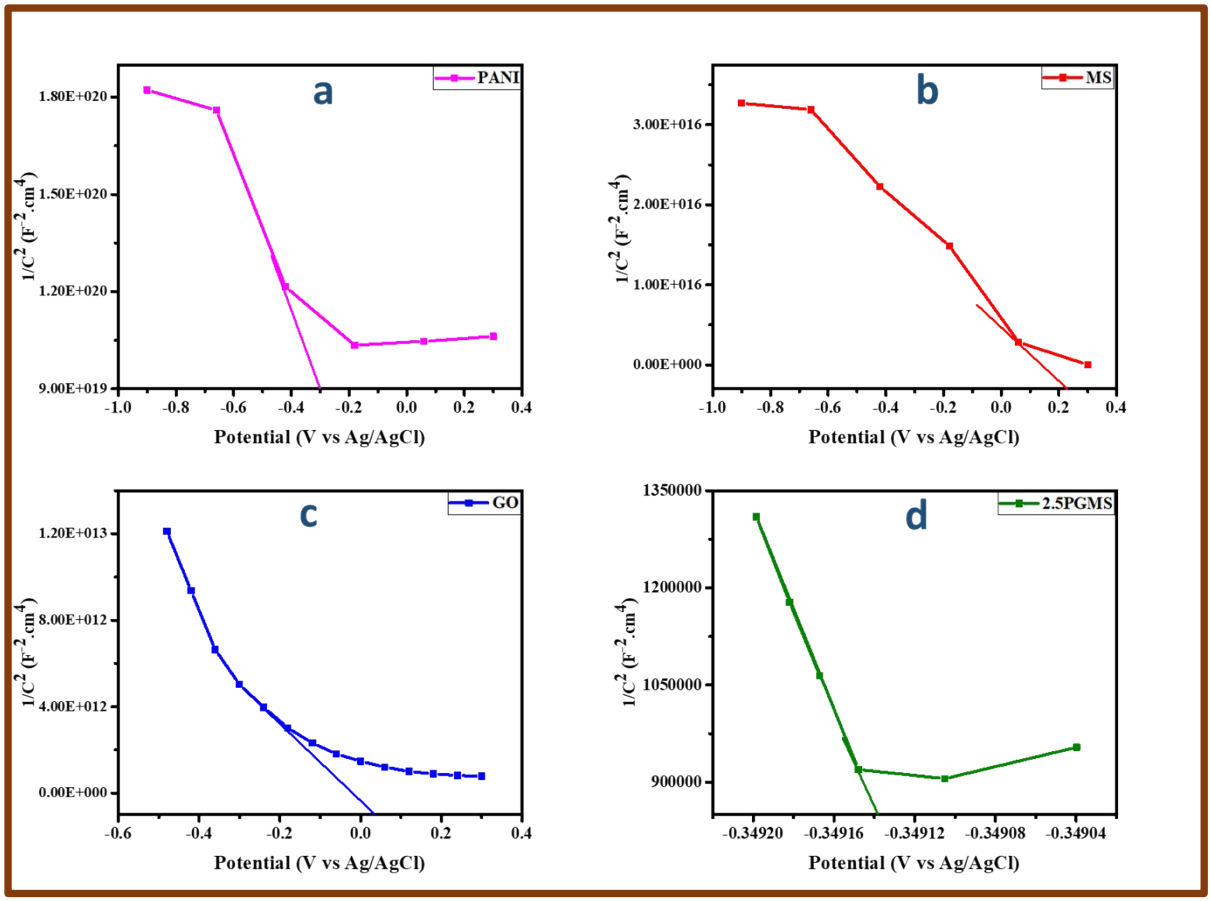


Fig S3: Mott-Schottky plot of (a) PANI (b) MS (c) GO (d) 2.5PGMS.

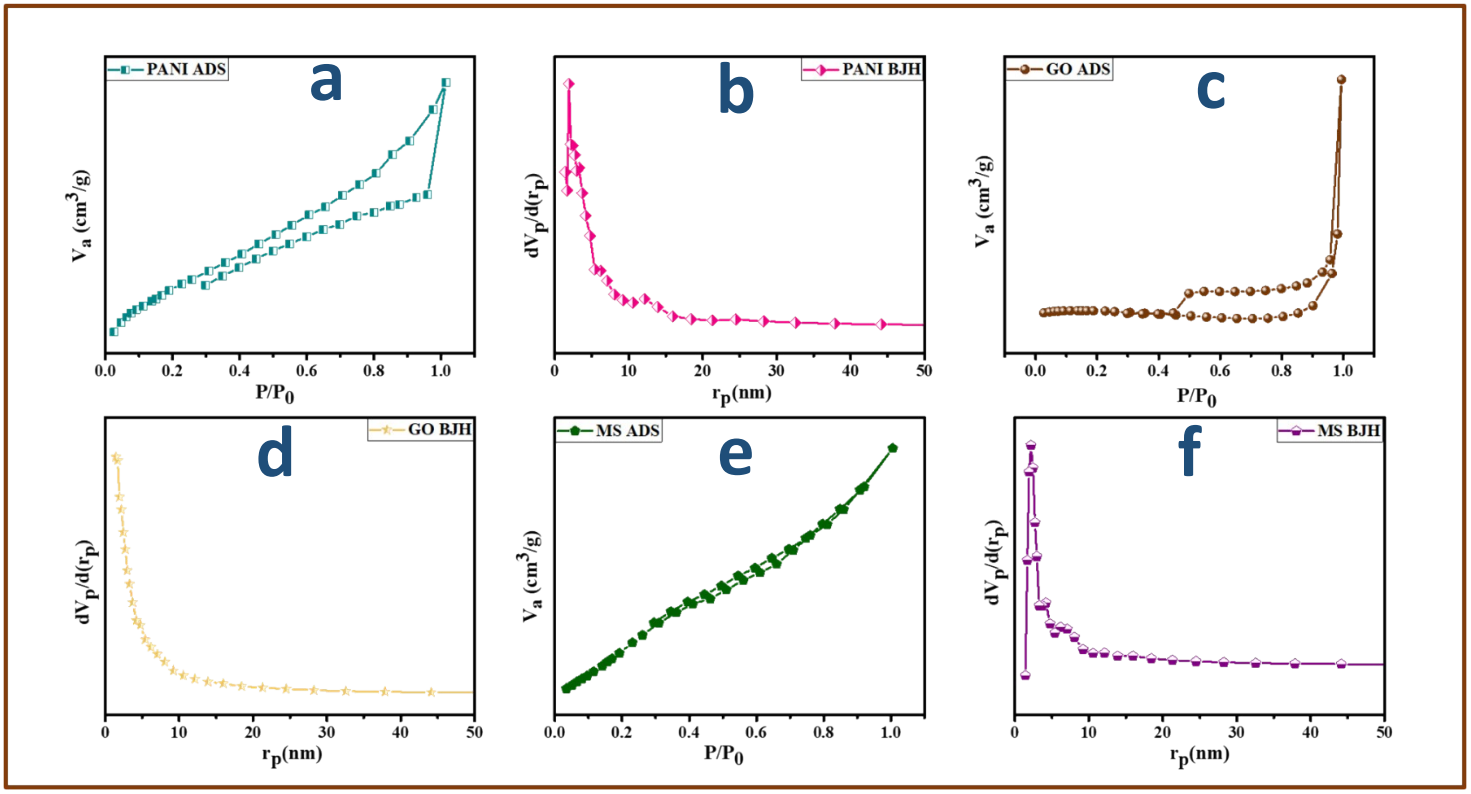


Fig. S4: a, c, and e are adsorption-desorption curves of PANI, GO, and MS respectively, whereas b, d and f are BJH plots of PANI, GO, and MS respectively.

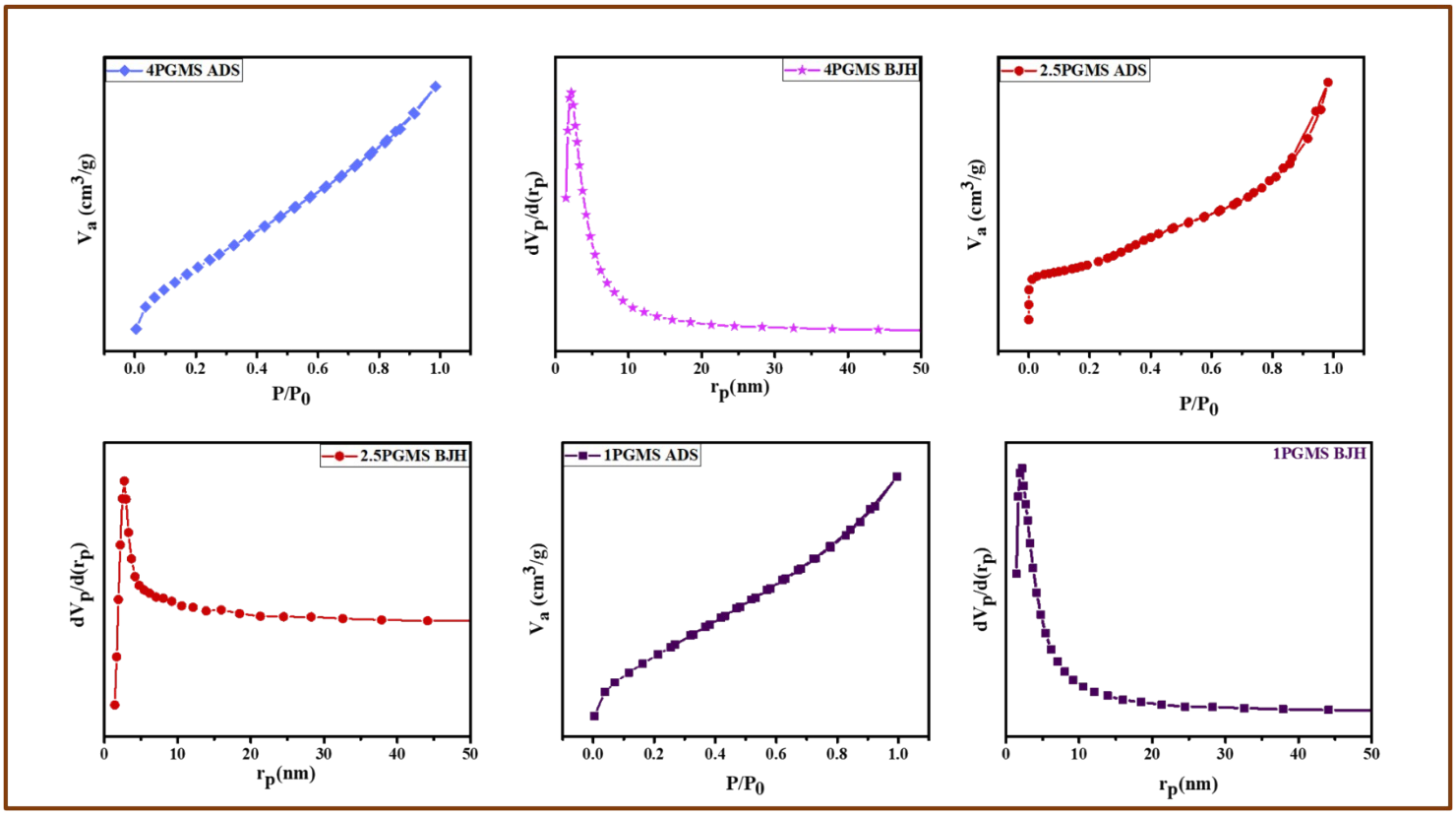
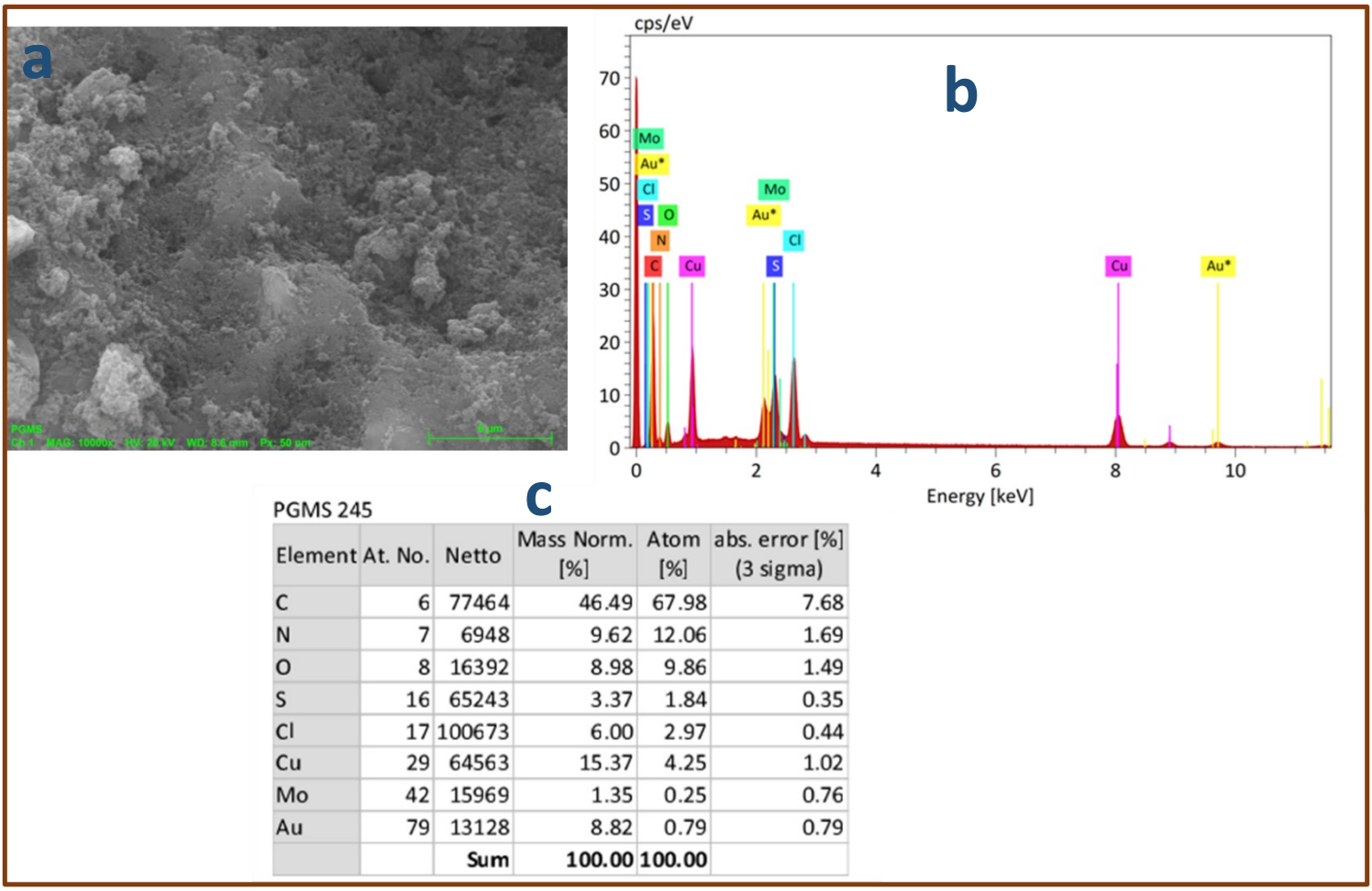


Fig. S5: a, c, and e are adsorption-desorption curves 4PGMS, 2.5 PGMS, and 1PGMS

Respectively, whereas b, d, and f are BJH plots of 4PGMS, 2.5 PGMS, and 1PGMS respectively.



PGMS 245

Element	At. No.	Netto	Mass Norm. [%]	Atom [%]	abs. error [%] (3 sigma)
C	6	77464	46.49	67.98	7.68
N	7	6948	9.62	12.06	1.69
O	8	16392	8.98	9.86	1.49
S	16	65243	3.37	1.84	0.35
Cl	17	100673	6.00	2.97	0.44
Cu	29	64563	15.37	4.25	1.02
Mo	42	15969	1.35	0.25	0.76
Au	79	13128	8.82	0.79	0.79
		Sum	**100.00**	**100.00**	

Fig. S6: (a) FESEM image of 2.5PGMS (b,c) EDS spectrum of 2.5PGMS.

Table S1: GC-TCD results for standard sample gases, with the sacrificial agent, acidic condition, basic condition, only catalyst (neutral condition), and Mineralization of methyl orange solution.

Samples	**Gases**	**Peak area**
Standard	H_2	2.084
With sacrificial agent	H_2	6.150
Acidic condition	H_2	4.068

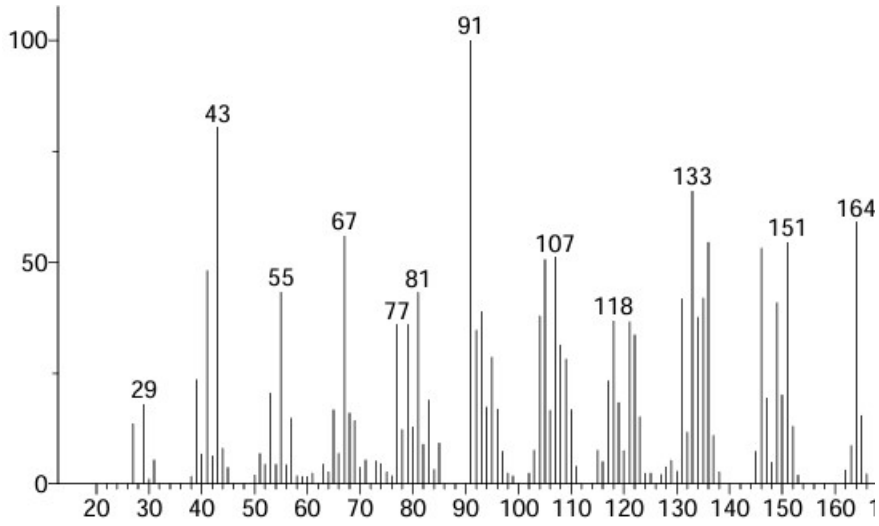
Basic condition	H_2	3.33
Only catalyst	H_2	1.66

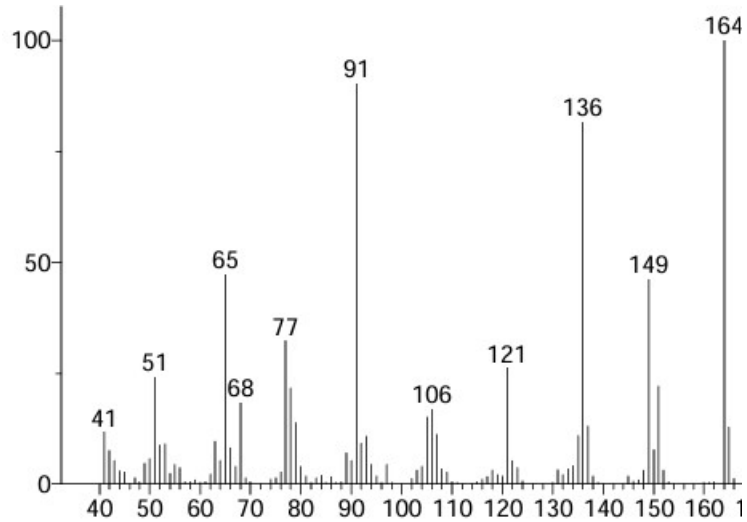
Concentration $=$

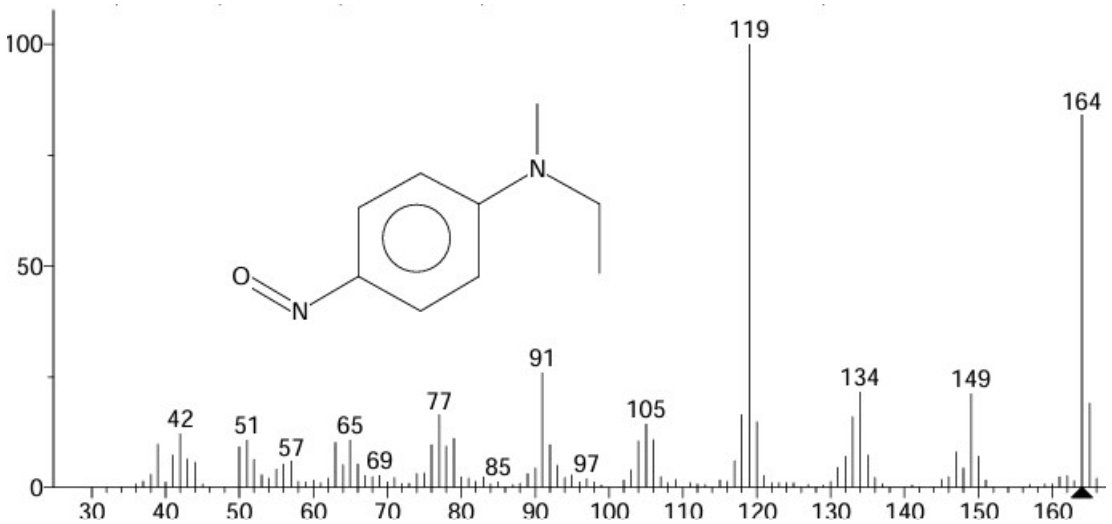
$$\frac{(standard\ concentration \times sample\ area)}{standard\ area} \times \frac{standard\ injection\ volume}{sample\ injection\ volume} \times \frac{gas\ volume\ generated}{sample\ taken\ (lit.)}$$

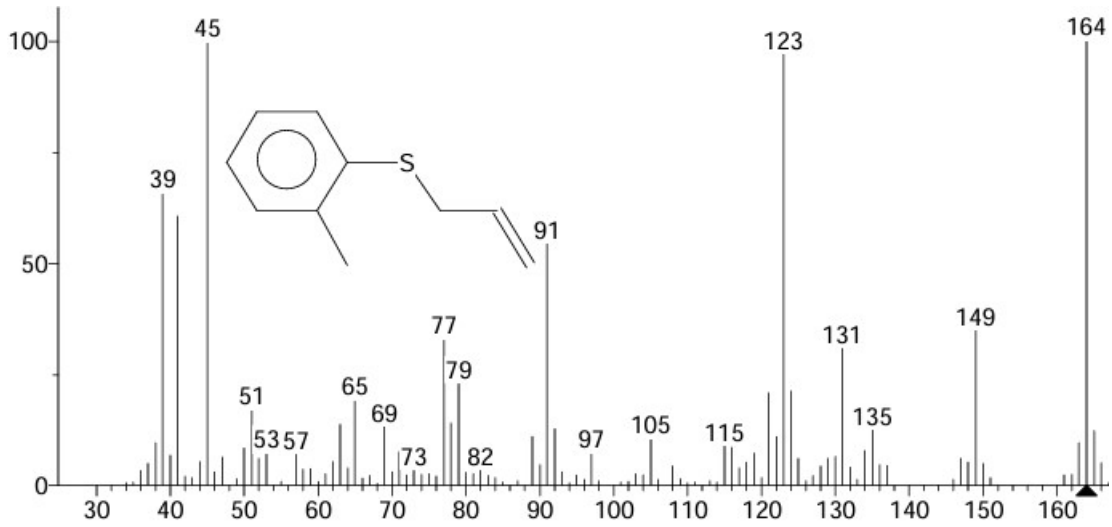
Standard concentration 505 ppm.

S3. GC-MS data after degradation of methyl orange






100
50
0
119
164
91
134
149
42
51
57
65
69
77
85
97
105
O
N
N
30 40 50 60 70 80 90 100 110 120 130 140 150 160


100
50
0
45
123
164
39
S
91
77
79
131
149
51
65
69
53
57
73
82
97
105
115
135
30 40 50 60 70 80 90 100 110 120 130 140 150 160

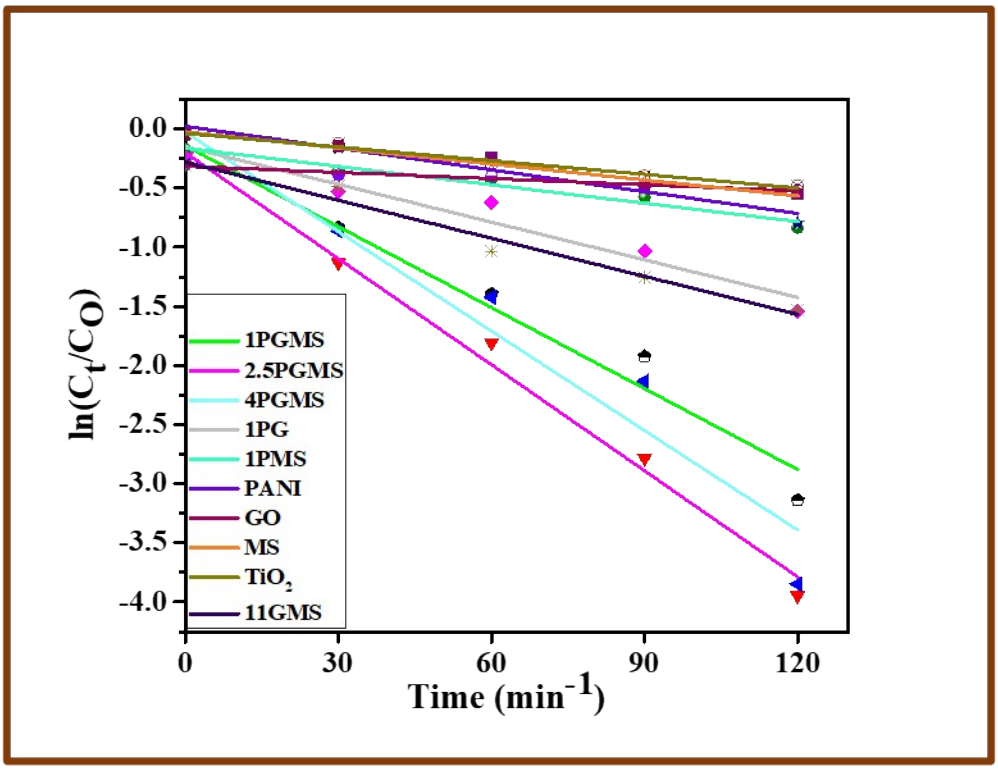


Fig. S7: Kinetic graph.

Table S2: Comparison with different photocatalyst materials for photocatalytic degradation.

Photocatalyst	Catalyst amount (mg)	% degradation	Time (min)	References
PANI-TiO_2	10	89.7	120	[1]
PANI/TiO_2/Cotton	-	87.7	180	[2]
PANI/TiO_2/SiO_2	-	87	120	[3]
PANI/Fe-TiO_2	-	28	150	[4]
Ag-Ag_2O/TiO_2@PPY	100	100	175	[5]
PEDOT/GO/MnO_2	20	92.7	420	[6]
RGO/mesoTiO_2/AuNP	10	-	240	[7]
PANI@GN/TiO_2	50	87	180	[8]

Ag_2O/TiO_2@PPY	50	100	240	[9]
PANI/TiO2	5	99	360	[10]
Ag-ZnO/PANI	200	98.6	120	[11]
PANI/GO/MoS_2 (2.5%)	2	99	120	Present work

References

1 H. M. El-Bery, M. R. Salah, S. M. Ahmed and S. A. Soliman, *RSC Adv.*, 2021, **11**, 13229–13244.

2 J. Ma, J. Dai, Y. Duan, J. Zhang, L. Qiang and J. Xue, *Renew. Energy*, 2020, **156**, 1008–1018.

3 A. Li, W. Zhu, C. Li, T. Wang and J. Gong, *Chem. Soc. Rev.*, 2019, **48**, 1874–1907.

4 J. Kröger, A. Jiménez-Solano, G. Savasci, P. Rovó, I. Moudrakovski, K. Küster, H. Schlomberg, H. A. Vignolo-González, V. Duppel, L. Grunenberg, C. B. Dayan, M. Sitti, F. Podjaski, C. Ochsenfeld and B. V. Lotsch, *Adv. Energy Mater.*, 2021, **11**, 2003016.

5 R. Kumar, R. El-Shishtawy and M. Barakat, *Catalysts*, 2016, **6**, 76.

6 L. Zhang, R. Jamal, Q. Zhao, M. Wang and T. Abdiryim, *Nanoscale Res. Lett.*, 2015, **10**, 148.

7 Y. Yang, Z. Ma, L. Xu, H. Wang and N. Fu, *Appl. Surf. Sci.*, 2016, **369**, 576–583.

8 R. Kumar, M. O. Ansari, N. Parveen, M. Oves, M. A. Barakat, A. Alshahri, M. Y. Khan and M. H. Cho, *RSC Adv.*, 2016, **6**, 111308–111317.

9 R. Kumar, *J. Colloid Interface Sci.*, 2016, **477**, 83–93.

10 Y.-J. Lee, H. S. Lee, C.-G. Lee, S.-J. Park, J. Lee, S. Jung and G.-A. Shin, *Appl. Sci.*, 2020, **10**, 6710.

11 F. Habtamu, S. Berhanu and T. Mender, *J. Chem.*, 2021, **2021**, 1–12.