Biomass derived graphene modified γ-Fe₂O₃/N,Fe-TiO₂@GO – A prolific photoactive material with extended visible to near IR harvesting

Manpreet Kaur,^a Abhishek Charak,^b Sofia Sandhu^a, Amrit Pal Toor^{c,d} Vasundhara Singh^a*

^a Department of Applied Sciences, Punjab Engineering College (Deemed to be University), Sector-12, Chandigarh, India

^bDepartment of Industrial and Production Engineering, Punjab Engineering College (Deemed to be University), Sector-12, Chandigarh, India

°Dr. SSB, University Institute of Chemical Engineering & Technology, Panjab University, Chandigarh, India

^dEnergy Research Centre, Panjab University, Chandigarh, India

*Email: vasun7@yahoo.co.in; vasundhara@pec.edu.in



Fig S1- UV-Vis spectra of synthetic dye solution at different interval degradation time

		Factor 1	Factor 2	actor 2 Factor 3 Factor 4 Response 1		Response 2	
Std	Run	A:Initial Concentr ation	B:Catalyst Loading	C:pH D:H2O2 Degradation		COD Reduction	
		mg/L	g/L	g/L ml/L %		%	
1	14	20	0.6	2	0.5	80.3	61.5
2	5	60	0.6	2	0.5	73.2	46
3	24	20	1.2	2	0.5	84.5	63
4	3	60	1.2	2	0.5	79	54
5	10	20	0.6	8	0.5	62	46
6	22	60	0.6	8	0.5	75.6	56
7	4	20	1.2	8	0.5	74.5	53
8	1	60	1.2	8	0.5	87.9	69
9	15	20	0.6	2	1.5	85.6	66
10	29	60	0.6	2	1.5	85.6	63
11	26	20	1.2	2	1.5	80.3	57
12	2	60	1.2	2	1.5	78.3	61.5
13	6	20	0.6	8	1.5	56.3	32
14	16	60	0.6	8	1.5	78	54
15	25	20	1.2	8	1.5	58	27.5
16	11	60	1.2	8	1.5	79.3	57
17	13	60	0.9	5	1	89.4	77
18	20	80	0.9	5	1	63.5	52
19	18	40	0.3	5	1	84.3	65
20	21	40	1.5	5	1	89	69
21	17	40	0.9	8	1	88.5	71
22	7	40	0.9	11	1	72.5	41
23	28	40	0.9	5	0	78.6	57.5
24	30	40	0.9	5	2	72.3	49.5
25	27	40	0.9	5	1	100	85
26	9	40	0.9	8	1	86.4	71
27	8	40	0.9	5	1.5	91.1	74
28	23	40	0.9	5	1	100	84.5
29	19	40	0.9	5	1	100	85.5
30	12	40	0.9	2	1	97.3	80

Table S1. The 3-factor face centered composite design matrix and the value of response function.

Table S2- ANOVA for Quadratic model Response 1: Degradation

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	3862.93	14	275.92	111.25	< 0.0001	significant
A-Initial Concentration	181.40	1	181.40	73.14	< 0.0001	
B-Catalyst Loading	49.88	1	49.88	20.11	0.0004	
С-рН	456.55	1	456.55	184.07	< 0.0001	

D-H2O2	35.11	1	35.11	14.16	0.0019	
AB	0.0625	1	0.0625	0.0252	0.8760	
AC	447.32	1	447.32	180.35	< 0.0001	
AD	44.22	1	44.22	17.83	0.0007	
BC	57.76	1	57.76	23.29	0.0002	
BD	123.21	1	123.21	49.68	< 0.0001	
CD	106.09	1	106.09	42.77	< 0.0001	
A ²	1590.63	1	1590.63	641.30	< 0.0001	
B ²	198.18	1	198.18	79.90	< 0.0001	
C ²	233.42	1	233.42	94.11	< 0.0001	
D ²	797.15	1	797.15	321.39	< 0.0001	
Residual	37.20	15	2.48			
Lack of Fit	35.00	12	2.92	3.97	0.1416	not significant
Pure Error	2.20	3	0.7350			
Cor Total	3900.13	29				

Final Equation of Degradation in Terms of Coded Factors

Degradation= 98.12+3.24A+1.11B-4.82C-1.19D-0.0625AB+5.29AC+1.66AD+1.90BC-2.77BD-

10.07A²-2.71B²-4C²-5.51D² (S1)

Table S3- ANOVA for Quadratic model Response 2: COD Reduction

Source	Sum of Squares	Df	Mean Square	F-value	p-value	
Model	6145.25	14	438.95	1486.70	< 0.0001	significant
A-Initial Concentration	194.08	1	194.08	657.33	< 0.0001	
B-Catalyst Loading	27.09	1	27.09	91.77	< 0.0001	
C-pH	453.45	1	453.45	1535.83	< 0.0001	
D-H2O2	96.13	1	96.13	325.60	< 0.0001	
AB	47.27	1	47.27	160.09	< 0.0001	
AC	631.27	1	631.27	2138.08	< 0.0001	
AD	165.77	1	165.77	561.45	< 0.0001	
BC	23.77	1	23.77	80.49	< 0.0001	
BD	107.64	1	107.64	364.58	< 0.0001	
CD	365.77	1	365.77	1238.84	< 0.0001	
A ²	1499.57	1	1499.57	5079.02	< 0.0001	
B ²	504.56	1	504.56	1708.95	< 0.0001	
C ²	1040.00	1	1040.00	3522.45	< 0.0001	
D ²	1559.04	1	1559.04	5280.44	< 0.0001	
Residual	4.43	15	0.2952			
Lack of Fit	3.93	12	0.3274	1.96	0.3165	not significant
Pure Error	0.5000	3	0.1667			
Cor Total	6149.68	29				

Final Equation of COD Reduction in Terms of Coded Factors

COD Reduction=84.36 +3.35A +106B -4.81C -1.97D +1.72AB +6.28AC +3.22AD +1.22BC-2.59BD - 4.78CD +9.78A² -4.32B² -8.45C² -7.71D² (S2)



Fig S2- Normal vs predicted graph of Response 1 degradation



Fig S3- Response surface plot of response 1, degradation of mixed dyes



Fig S4- Normal vs predicted graph of Response 2 COD reduction



Fig. S5 Response surface plot of response 2, COD reduction



Fig S6- LC chfromatogram of Mixed disperse dye after 120 min of degrdataion



Fig S7. MS spectra of the mixture of disperse dye by □Fe₂O₃/N,Fe-TiO₂@1.5%GO after 120 min of degradation at RT-0.67, m/z=131.03



Fig S8. MS spectra of the mixture of disperse dye by \Box Fe₂O₃/N,Fe-TiO₂@1.5%GO after 120 min of degradation at RT-0.88, m/z=147.24