

S1: EDX image of Aeroxide TiO₂ and MS-TiO₂

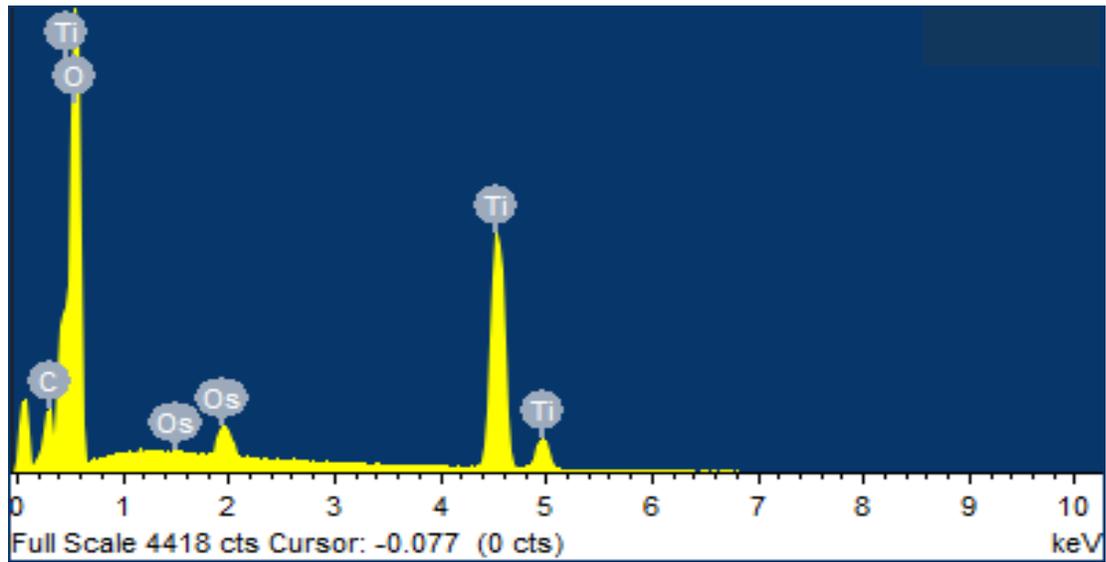


Figure S1: Aeroxide TiO₂

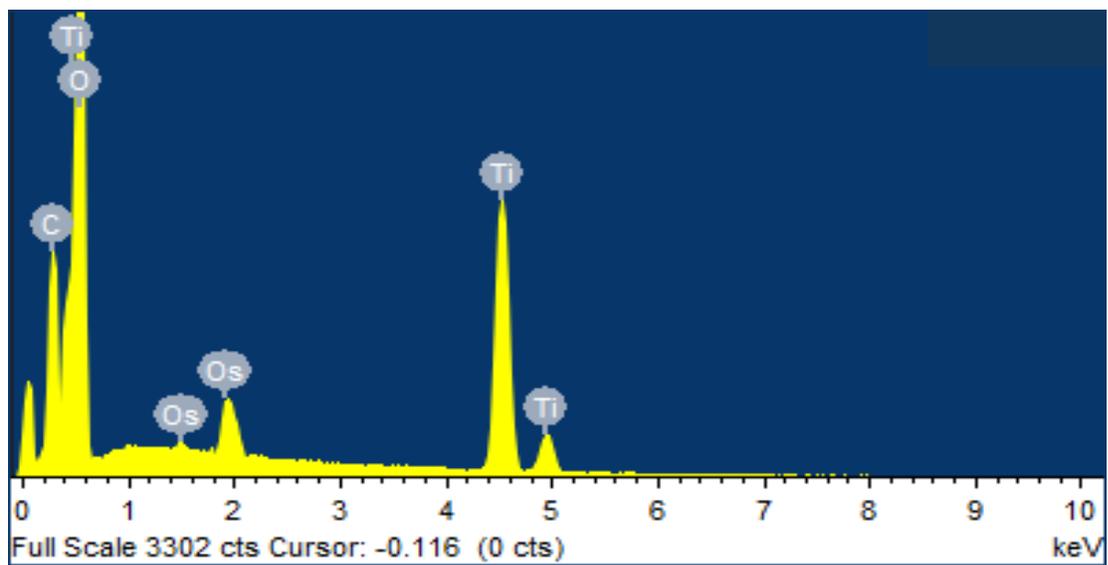


Figure S2: MS-TiO₂

S2: UV-Vis Spectrophotometer data of MS-TiO₂

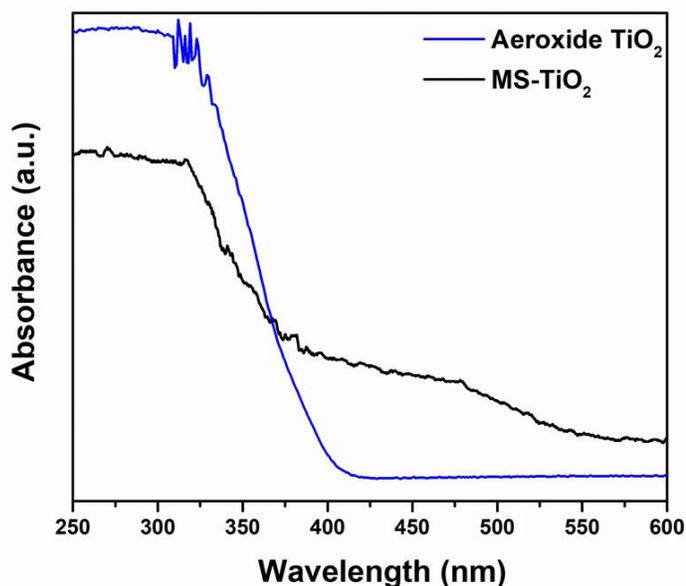


Figure S3: Diffuse Reflectance Spectra for Aeroxide-TiO₂ and MS-TiO₂

The band gap is calculated as follows (also mentioning this in SI):

The energy of a photon is given by the Planck Einstein relation: $E = h\nu = \frac{hc}{\lambda}$

where, h =Planck's constant= 6.626176×10^{-34} Js; c =velocity of light= 3×10^{10} m/s; λ =wavelength in m.

From the diffuse reflectance spectra λ (max) is calculated from the slope and then using other known constants, the energy E is calculated (eV), which is basically band gap.

In case of Aeroxide-TiO₂: $\lambda_{\text{max}} = 406.66$ nm and $E=3.05$ eV;

In case of MS-TiO₂: $\lambda_{\text{max}} = 420.13$ nm and $E=2.95$ eV;

S3: Univariate Parametric Studies

At first, the effect of catalyst dosage was studied on the degradation of MB. Five different catalyst dosages were studied ($0.25 - 1.25$ g L⁻¹), keeping all other reaction parameters constant (pH=6, light intensity = 60 mW cm⁻², initial concentration of MB = 20 mg L⁻¹). The result is shown in the below figure [Fig S1]. From the result, it is evident that as the catalyst dosage is increased from $0.25 - 0.75$ g L⁻¹, degradation of MB also increases. However, it reaches a plateau when the catalyst dosage is further increased from $0.75 - 1.25$ g L⁻¹. Initially, with increasing catalyst dosage, the amount of active site also increases, thereby increasing the degradation. However, further increasing catalyst amount results in agglomeration of catalyst, thereby decreasing the amount of active site and hindering penetration of incident light [1, 4].

As a result, the degradation of MB reaches a plateau. Hence for further studies, catalyst dosage has been chosen in the range of 0.25 – 0.75 g L⁻¹.

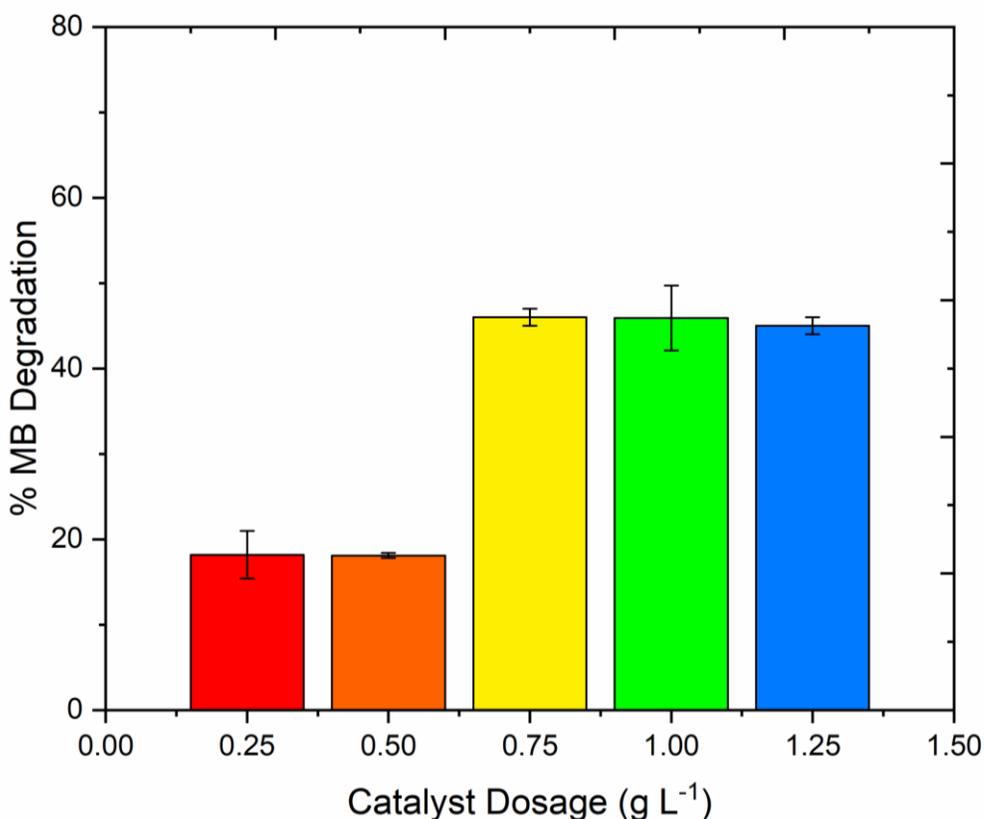


Figure S4: Effect of catalyst dosage on % degradation of MB; Experimental condition: pH 6, light intensity 60 mW cm⁻², initial concentration of MB 20 mg L⁻¹

The effect of initial concentration of MB on its degradation was studied with four different concentrations (5, 10, 15 and 20 mg L⁻¹), keeping all other reaction parameters constant (pH = 6, light intensity = 60 mW cm⁻², catalyst dosage = 0.75 g L⁻¹). The result is shown in the figure below [Fig S2]. It was observed that as the initial concentration of MB was increased, the % degradation of MB gradually decreases; however, it remains almost the same for initial concentrations 15 and 20 mg L⁻¹. This phenomenon can be recognized by the fact that as the initial concentration of MB increases, the requirement of catalyst surface for adsorption also increases. However, since the amount of catalyst remains the same for each case, the degradation decreases [31]. Also, as the initial MB concentration increases, the penetration of the light decreases, resulting in lower degradation of MB [31]. For further studies, the initial concentration was chosen to be 20 mg L⁻¹.

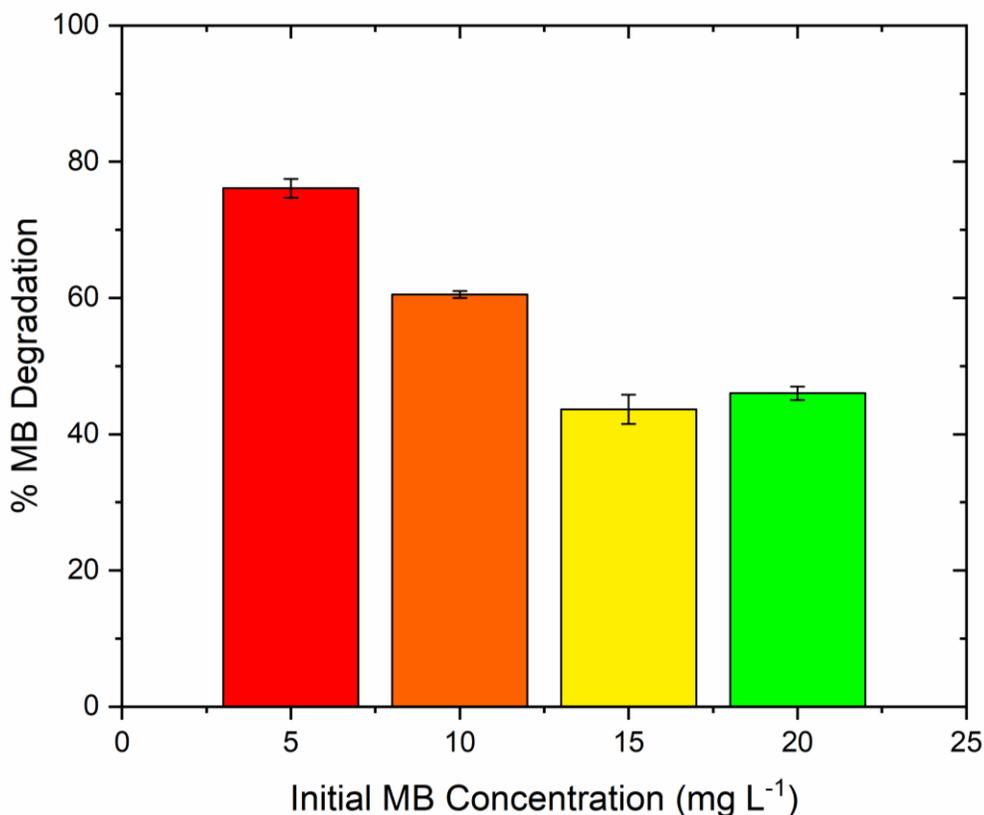


Figure S5: Effect of the initial concentration of MB on % degradation of MB; Experimental condition: pH 6, light intensity 60 mW cm^{-2} , catalyst dosage 0.75 g L^{-1}

Finally, the effect of light intensity was studied on the degradation of MB. Five different light intensities were studied ($20 - 100 \text{ mW cm}^{-2}$), keeping all other parameters constant (pH = 6, light intensity = 60 mW cm^{-2} , catalyst dosage = 0.75 g L^{-1}). The results are shown in the below figure [Fig S3]. It was observed that as the light intensity is increased from $20 - 60 \text{ mW cm}^{-2}$, the degradation also increases. However it reaches a plateau when light intensity is further increased. This may be due to the fact that with further increase in light intensity, the generation of the active site does not increase on the catalyst surface and hence the degradation remains unchanged. Hence, for further studies, light intensity has been studied in the range of $60 - 100 \text{ mW cm}^{-2}$ to see if, with increasing catalyst dosage, the effect of higher light intensity changes.

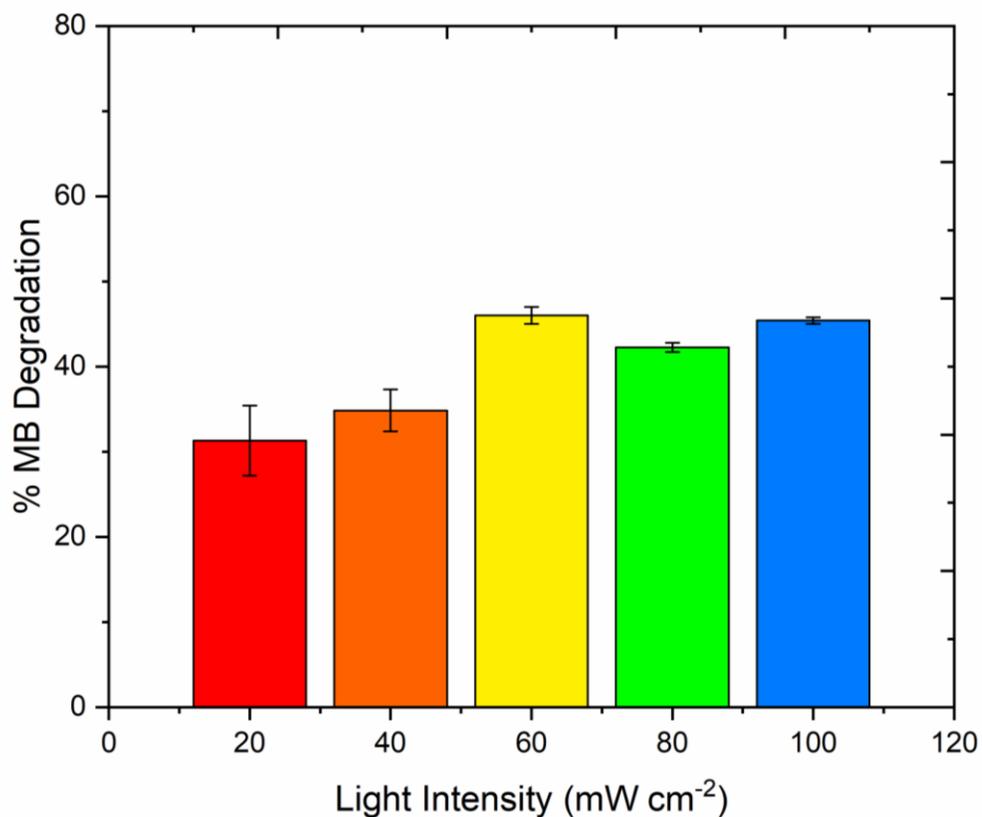


Figure S6: Effect of light intensity on % degradation of MB; Experimental condition: pH 6, catalyst dosage 0.75 g L⁻¹, initial concentration of MB 20 mg L⁻¹

The pH for further studies has been chosen in the range of 4 – 6. Since, in any parametric studies, the range of parameters should be decided considering economic viability and practical applications, the pH range in this study is chosen closest to the natural pH possible [31].

S4: Data used for model validation

pH	Catalyst Dosage (g L⁻¹)	% MB removal (experimental)	% MB removal (model predicted)
6.3	0.75	42.4	49.4
5.7	0.75	40	42.8
6.6	0.75	54	52.7
5.4	0.75	35.3	39.5
6	0.79	47.9	48.3
6	0.83	53.4	50.6