Supplementary Information

Synergistic Effects of Fe and Ag Doping on The Structural and Optical Properties of TiO_2 Thin Film: Dual Functions Platform for Hydrogen Generation and Dye Degradation

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S1: Characterization Techniques

To examine the structural properties and the crystallite size of the developed thin films, diffraction peaks analysis performed with Cu- Kα radiation (λ = 1.54Å) using X-ray powder diffraction from PAN analytical. A scan rate of 1 min^{-1} was applied to record a pattern in 2θ range of 10-60°. Optical characteristics of developed thin films were examined by using Shimadzu 1800, Japan UV-Vis spectrophotometer. Morphological properties study of the developed thin films was explored by scanning electroscopic microscope (SEM) (Supra 40) from Carl-Zeiss, Germany. FT-IR spectra were recorded by using Perkin Elmer PE- 1600 model spectrometer using KBr pellet with the resolution of 4cm^{-1}.

S2: Calculations for Structural Parameters

The average crystal size and Microstrain of the TiO_2 nanostructures were determined using XRD data. The Debye-Scherrer formula was applied to calculate the average crystallite size, as shown in Eqn 2.

$$D=k\lambda/\beta Cos\theta \qquad (2)$$

where k = crystal shape constant having value 0.94, λ = X-ray wavelength, β = full-width at half maxima and θ = Bragg's diffraction angle. The Microstrain is evaluated by using Eqn. 3

$$\varepsilon=\beta/4\tan\theta \qquad (3)$$

The dislocation density is also calculated by using the following Eqn. 4

$$\delta=1/D^2 \qquad (4)$$

S3: Calculations for Bandgap using Bruss formula

The average particle size (R) of TiO_2 nanoparticles was estimated using Bruss Equation as follows:

$$E_g = E + h^2/8R^2 \, [1/(m_{e*}) + 1/(m_{h*})] - 1.8e^2/\varepsilon R \qquad (5)$$

Where, Eg = band gap of synthesized nanoparticles, E = bulk band gap of TiO_2 (3.2 eV), R=radius of particle, m_{e*}=effective mass of the electron, m_{h*}=effective mass of hole (for TiO_2, it is 0.8 m_o), ε = dielectric constant of the material, h is Planck's constant. The fundamental absorption due to electronic excitation from the valance band (VB) to the conduction band is decidedly useful to determine the nature and value of the optical band gap. The band gap was calculated using the formula

$$Eg = 1240/\lambda \qquad (6)$$

where, E_g = band gap of TiO_2 and λ = wavelength of absorption maxima for TiO_2.

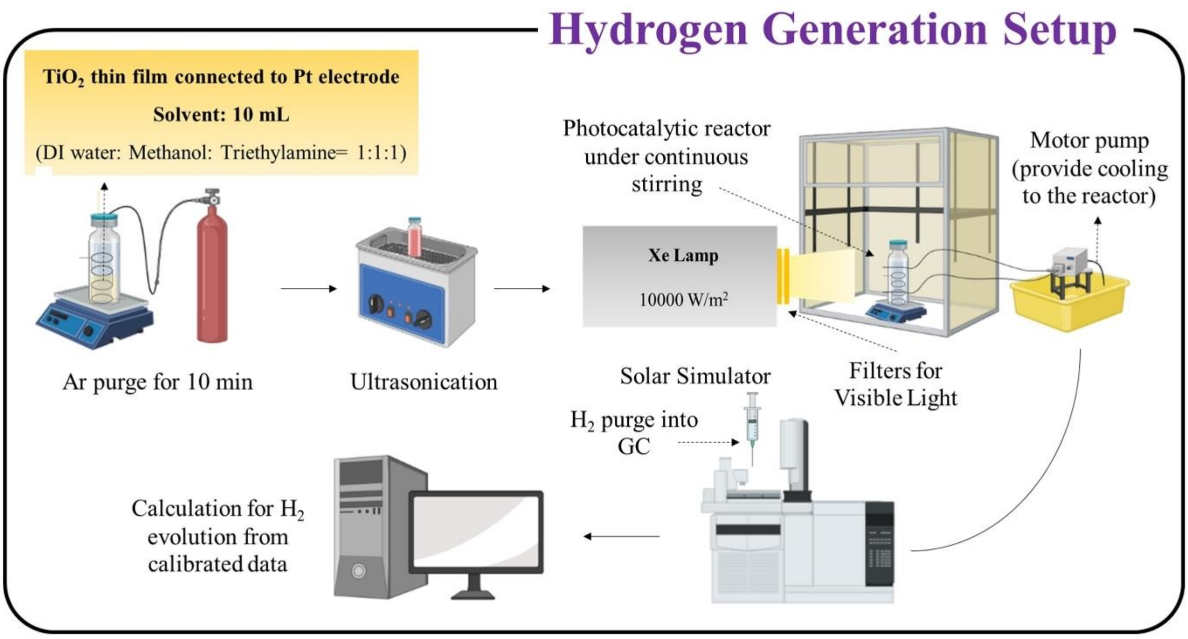


Fig. S1 shows the photocatalytic Hydrogen generation setup

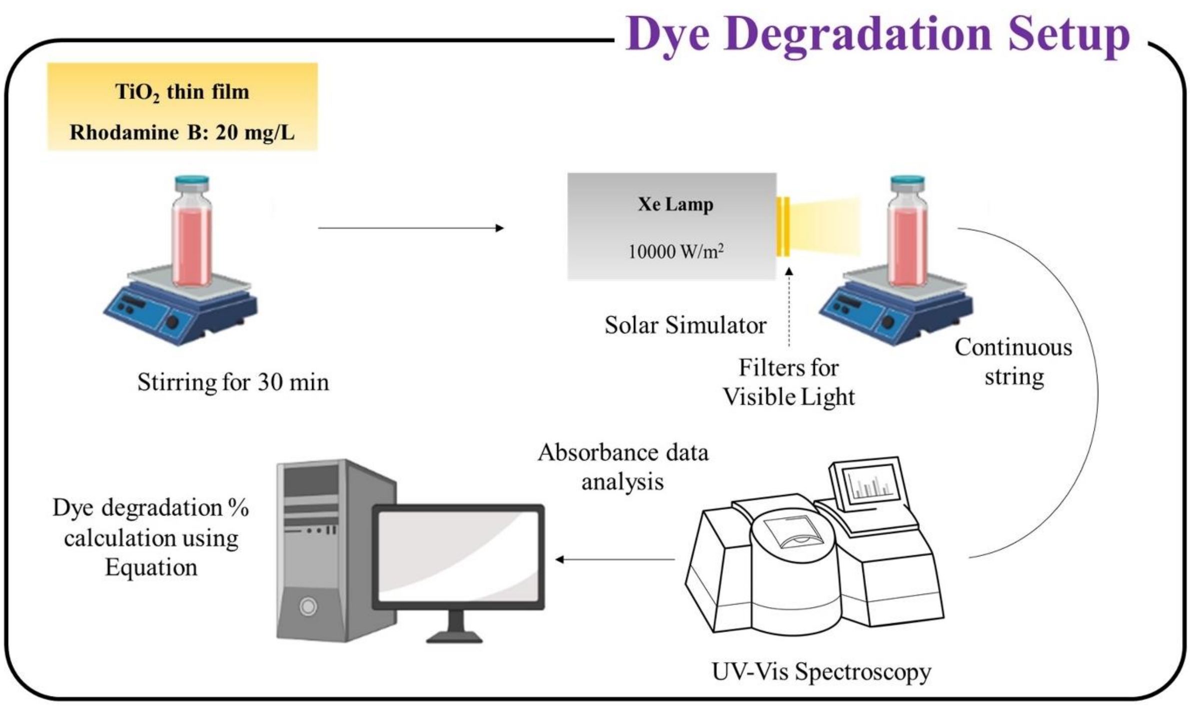


Fig. S2 shows the photocatalytic dye degradation efficiency setup

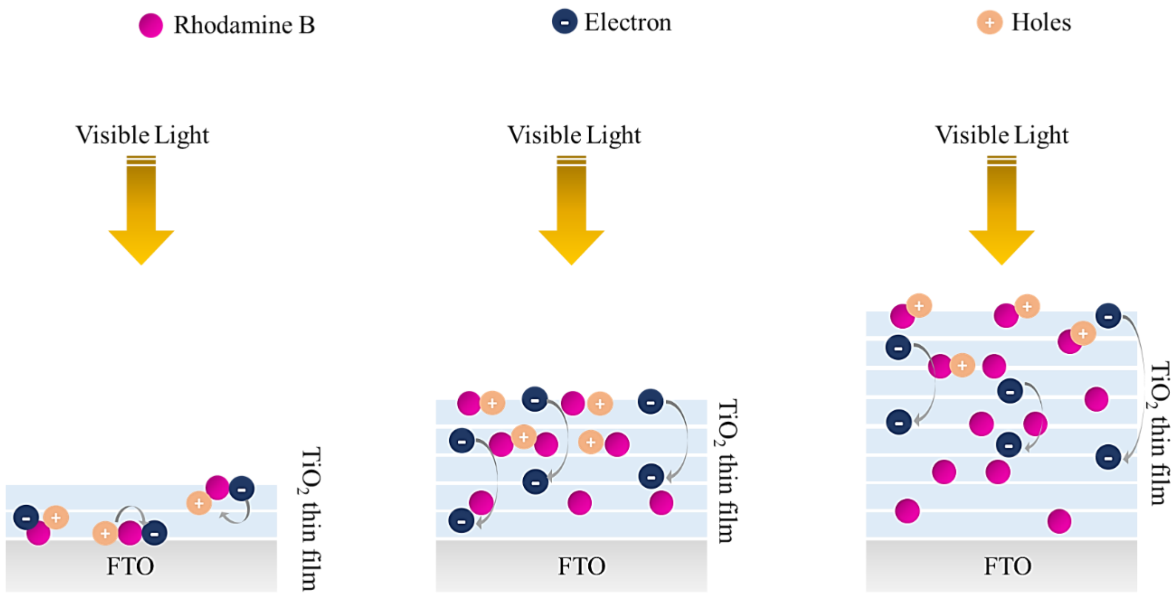


Fig. S3 shows the mechanism of TiO_2 thin film dye degradation for different layers.

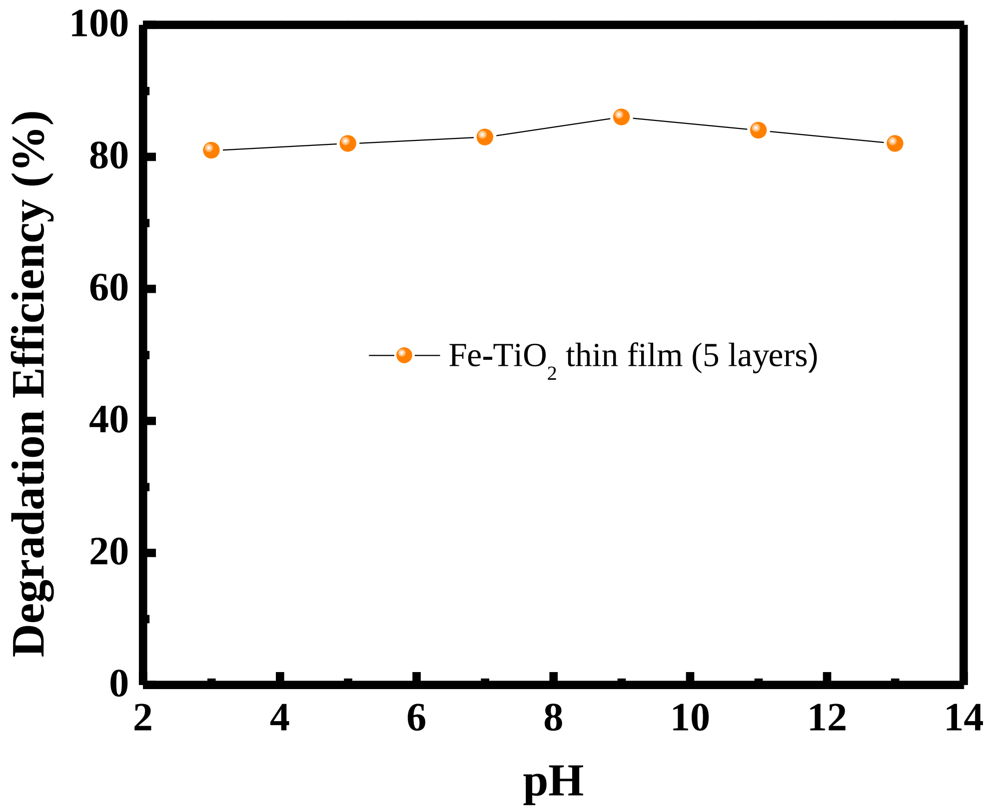


Fig. S4 shows the visible light driven Rhodamine 6G dye degradation using TiO_2-Fe_2O_3 photocatalyst in different pH conditions.

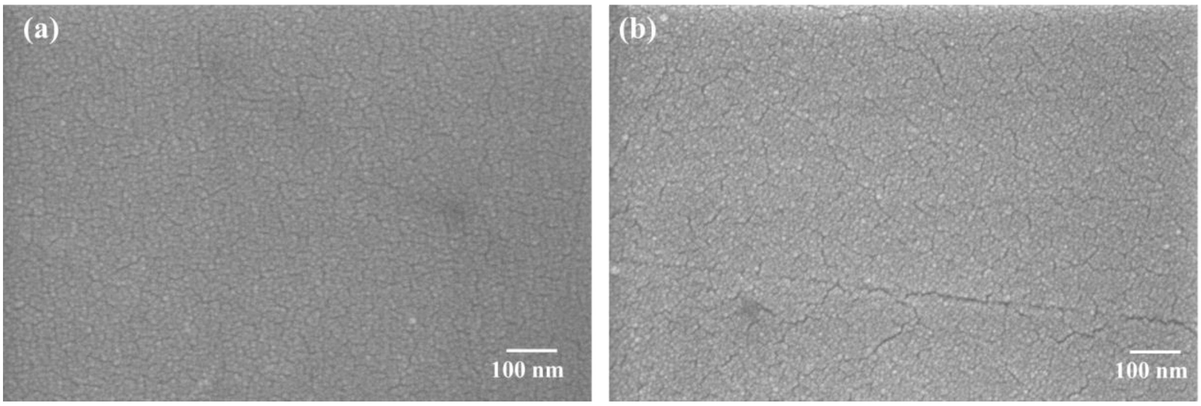


Fig. S5 shows the FESEM surface images of Ag-TiO2 (a) and Fe-TiO2 (b) thin film photocatalyst in 100 nm scale.

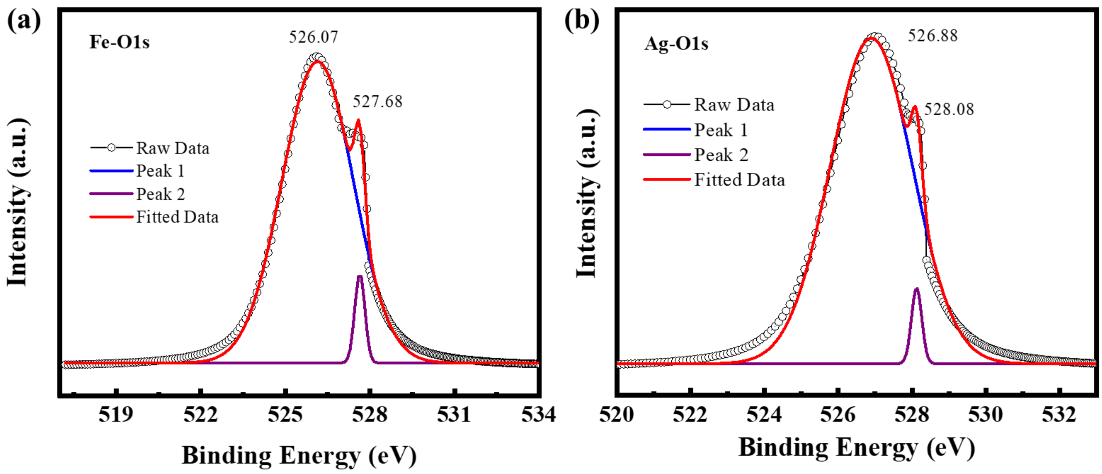


Fig. S6 shows the XPS spectrum of O1s for Fe-TiO_2 (a) and Ag-TiO_2 (b)

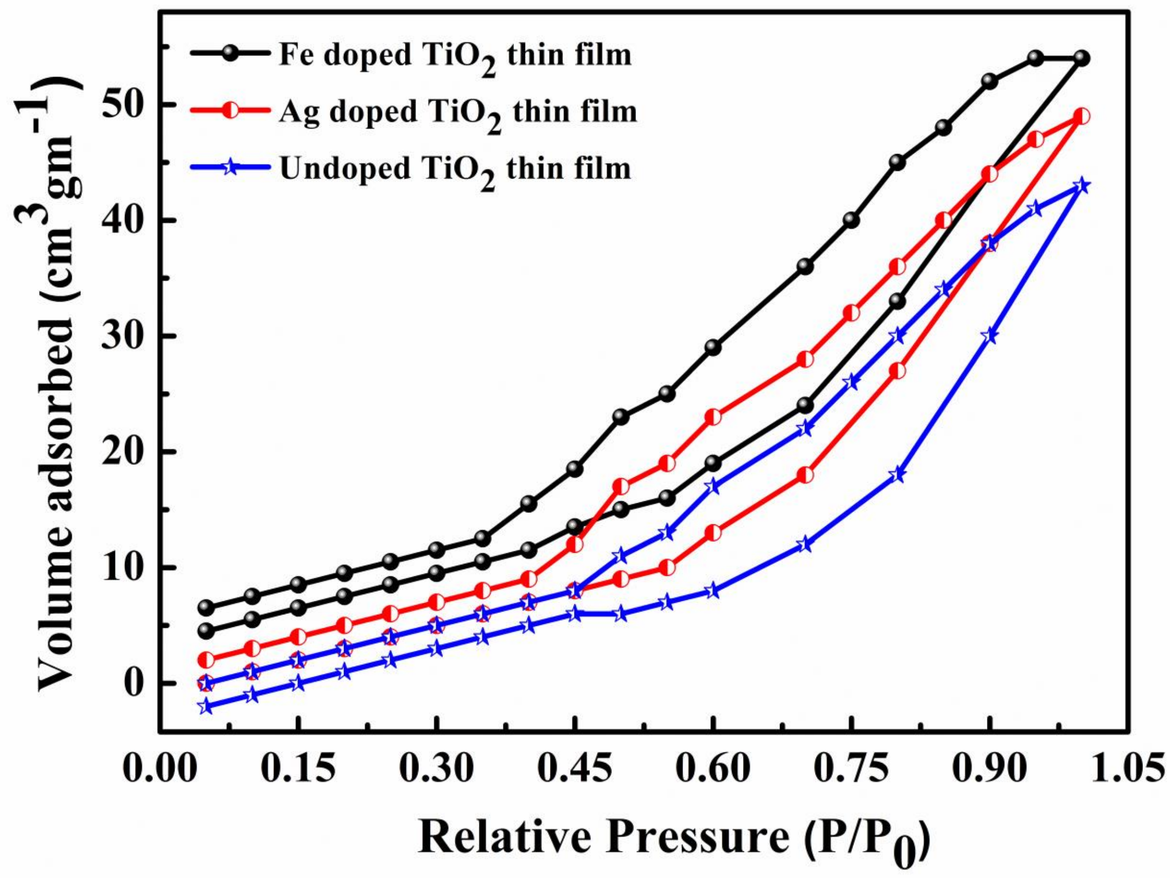


Fig. S7 shows the BET surface area for all the developed thin film samples.

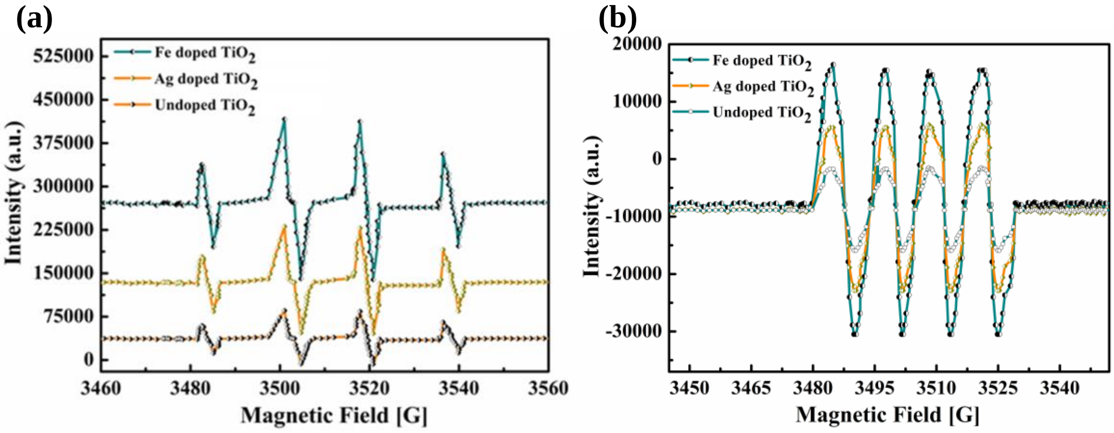
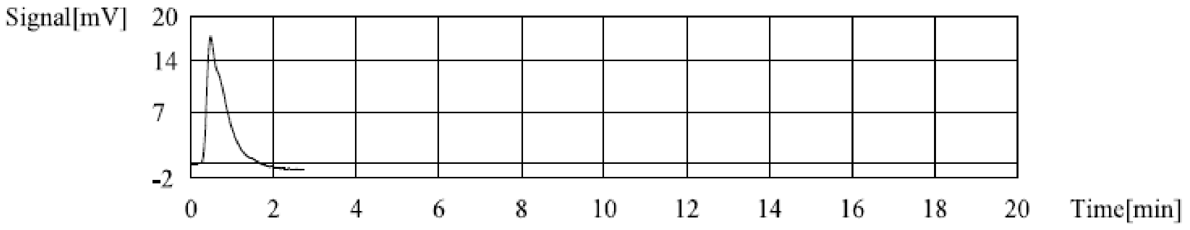


Fig. S8 shows the ESR and EPR data for all the developed thin film samples.

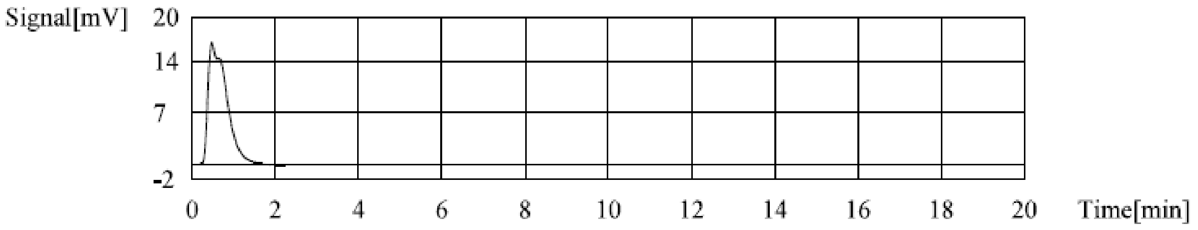
Table S1

Sample ID	Sample Details	Injection Volume(μL)	Degradation time	Mean area	TOC (ppm)
Sample 1	Original Dye	50	0 mins	55.78	27.45
Sample 2	Dye after 45 mins deg	50	45 mins	51.32	24.73
Sample 3	Dye after 75 mins deg	50	75 mins	46.34	21.28

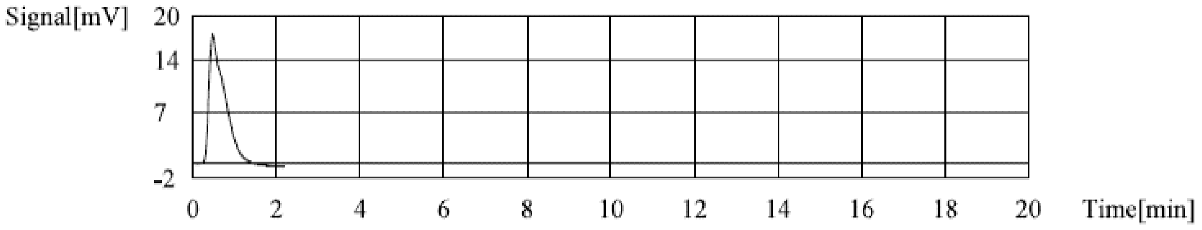
S9: Sample 1:



S10: Sample 2:



S 11: Sample 3:



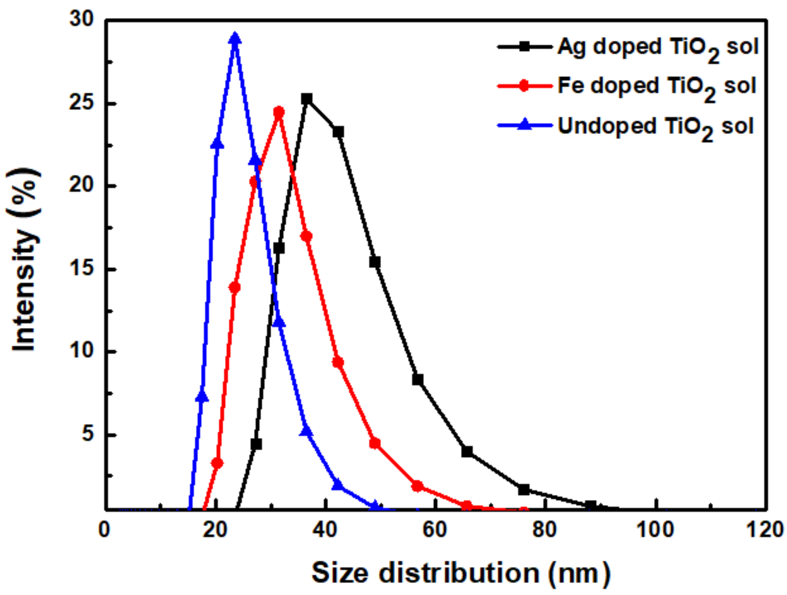


Fig. S12 DLS study of Ag-TiO_2, Ag-TiO_2, Undoped TiO_2 sol

Table S2 shows a comparative photocatalytic dye degradation efficiency of the present work on TiO_2-Fe_2O_3 thin film with other reported literatures.

Sl. No.	Photocatalyst	Photocatalyst Amt. of (mg)	Conc.(mgL^{-1}) of dye	Time (min)	Dye degradation Efficiency (%)	Ref.
1.	TiO_2-Fe_2O_3	200	25- Methylene blue	300	88	[1]
2.	TiO_2-Fe_2O_3	50	20- Orange II	180	55	[2]
3.	TiO_2-Fe_2O_3	5	10- Rhodamine B	300	60	[3]
4.	TiO_2-Fe_2O_3	200	10 and Phenol	60	17	[4]
5.	TiO_2-Fe_2O_3	30	10- Methylene Blue	150	70	[5]
6.	**TiO_2-Fe_2O_3**	**50**	**10- Rhodamine B**	**145**	**85**	**Present study**

References

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