EXAFS and Photocatalytic measurements of Mo inserted TiO_2 samples

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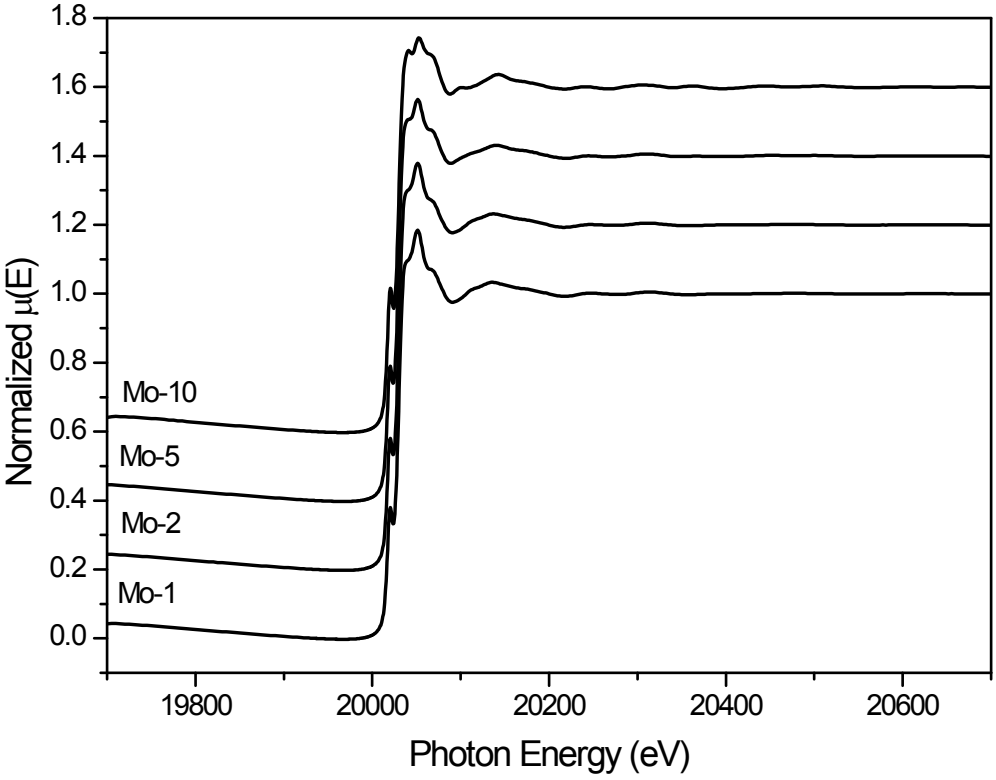
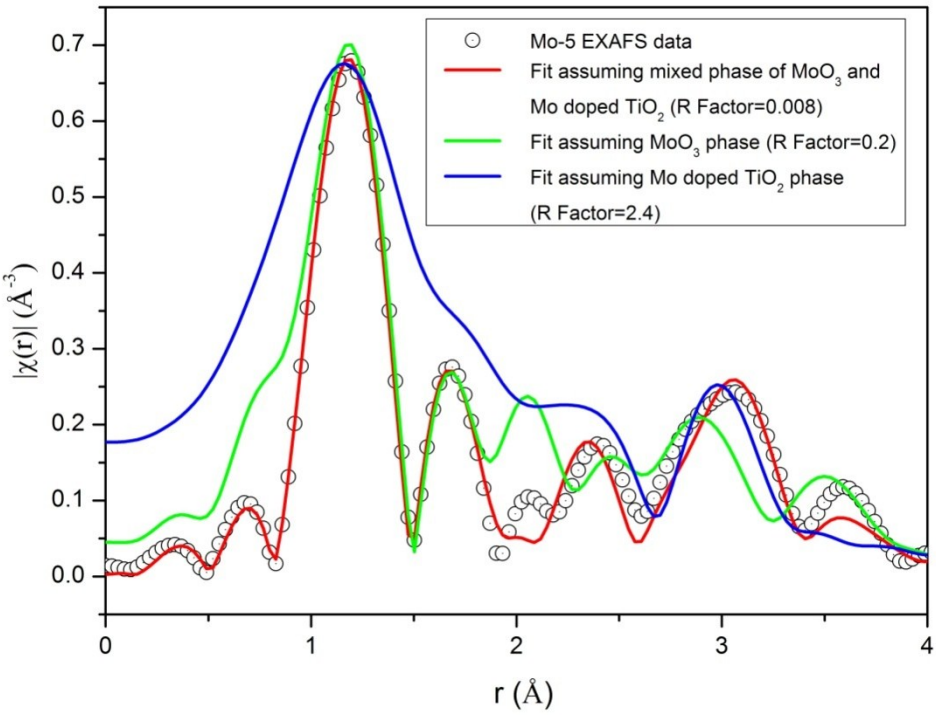
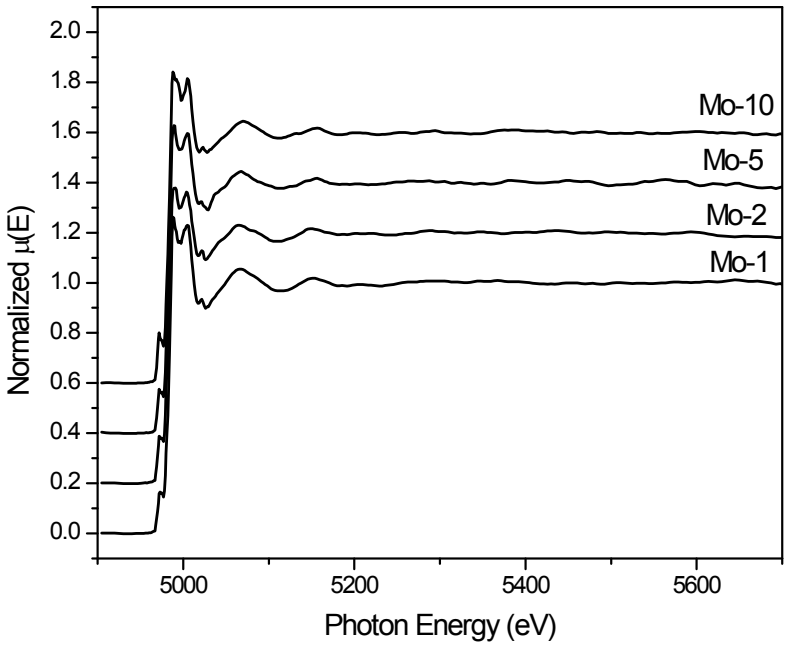
Supporting Information



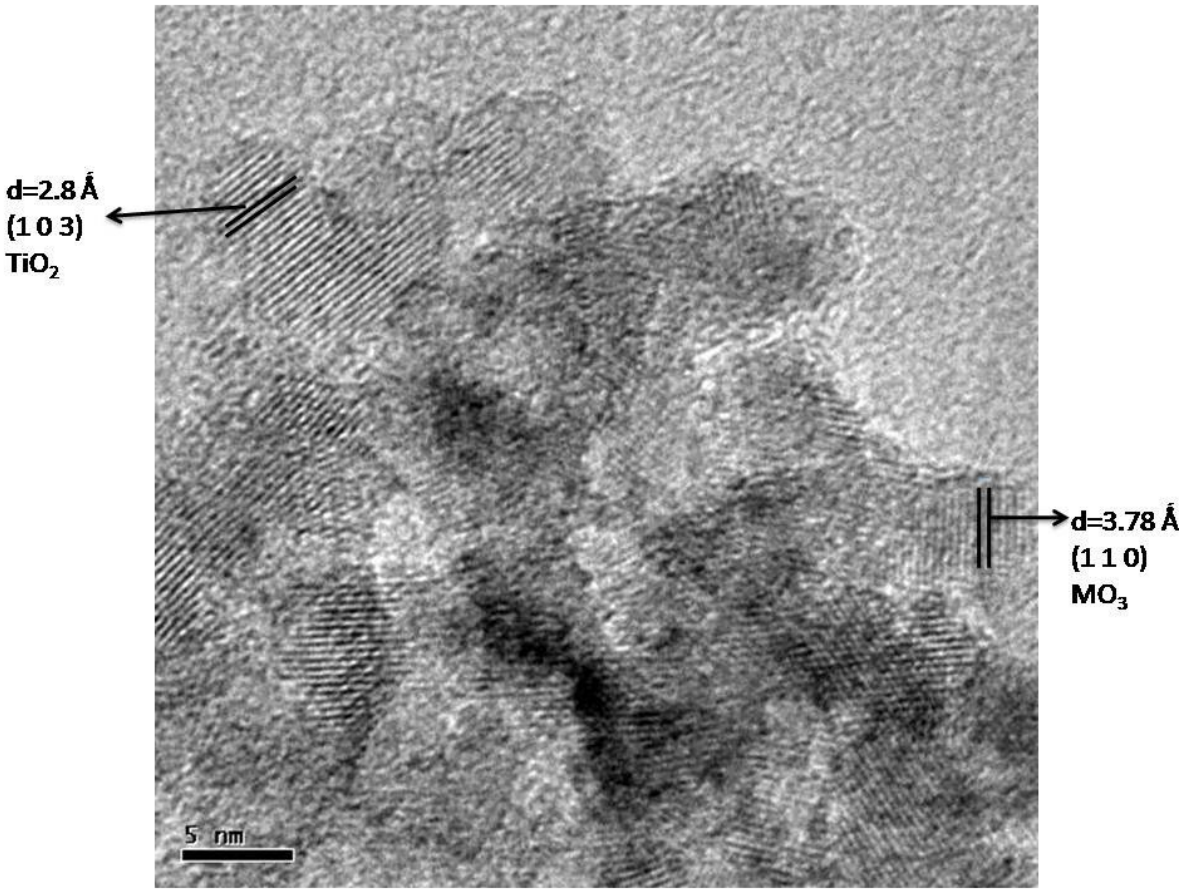
S.I.1: Absorption coefficient verses Photon Energy plot for different doping concentrations of Mo in TiO_2 at Mo K edge.



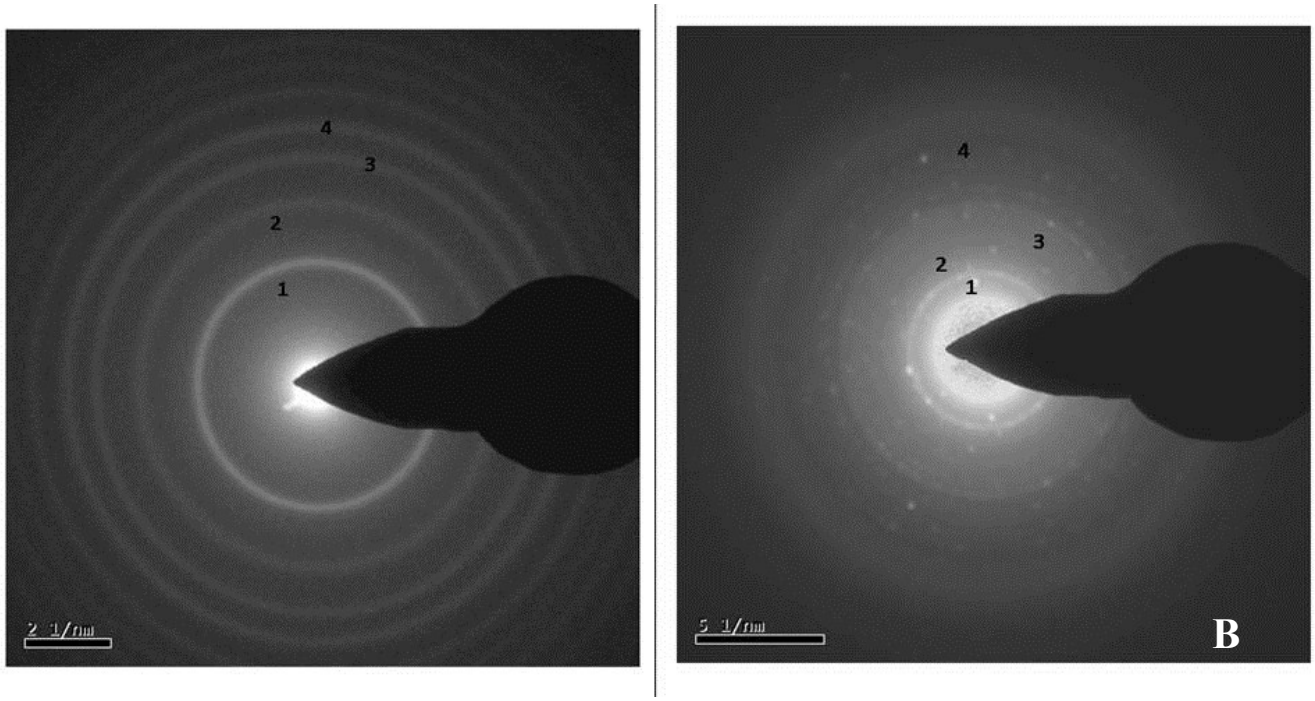
S.I. 2: Experimental χ(r) versus r spectra of Mo-5 sample along with the theoretical fits assuming different fitting models.



S.I.3: Absorption coefficient verses Photon Energy plot for different doping concentrations of Mo in TiO_2 at Ti K edge.



S.I.4: TEM Figure of Mo-2 (Fig-6 A) which is expanded for brevity. We observe both the TiO2 (1 0 3) plane and that of MoO3 (1 1 0) plane lattice fringes in the above provided image. This image is provided for the reader's discretion.



S.I. 5: **(A) SAED pattern for the Mo-2** ; **(B) SAED pattern for the Mo-10 sample**

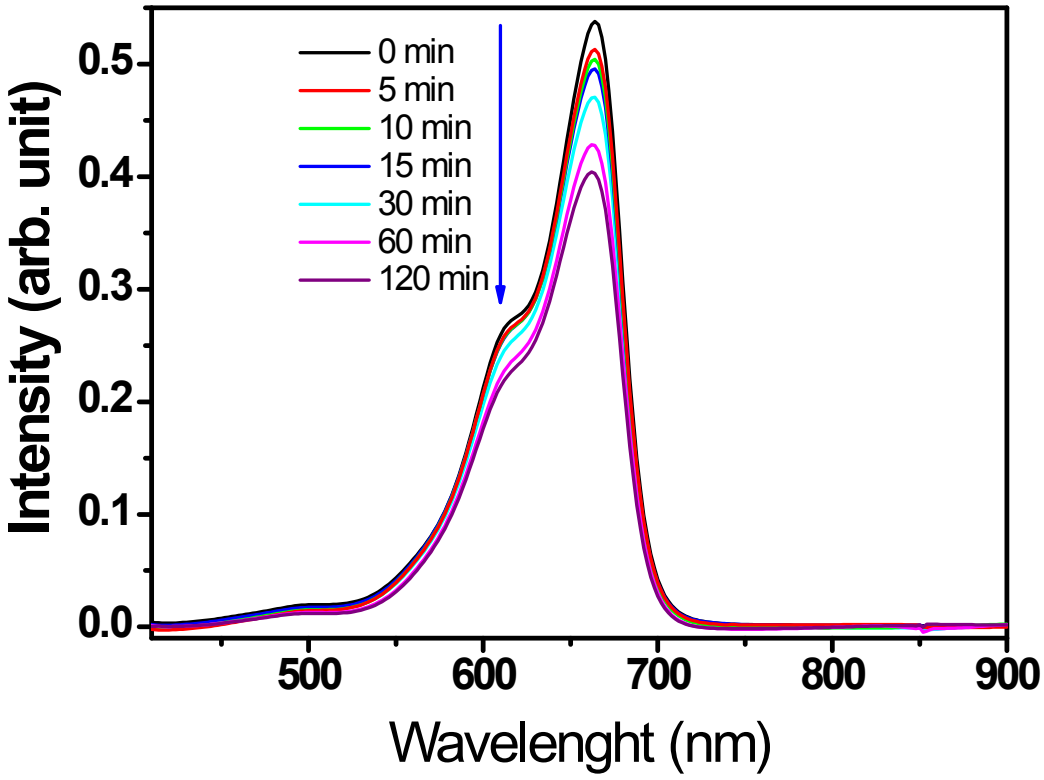
Table - (A)- Corresponds to SAED pattern of Mo-2

Circle	Calculated d-value (Å)	JCPDS d-value-(**1**) (**CAS-84-1750**) **TiO_2-Anatase**	JCPDS d-value-(**2**) (**CAS-80-0347**) **MoO_3**	Error (%) (**1**)	Error (%) (**2**)	(hkl)- plane (**1**)	(hkl)- plane (**2**)
1	3.51	3.4979	3.7075	0.51	5.3	110	020
2	2.4544	2.4531	2.661	0.053	7.7	002	022
3	1.7699	1.7489	1.7503	1.2	1.2	220	411
4	1.561	1.4815	1.5227	2.7	2.51	113	**4**22

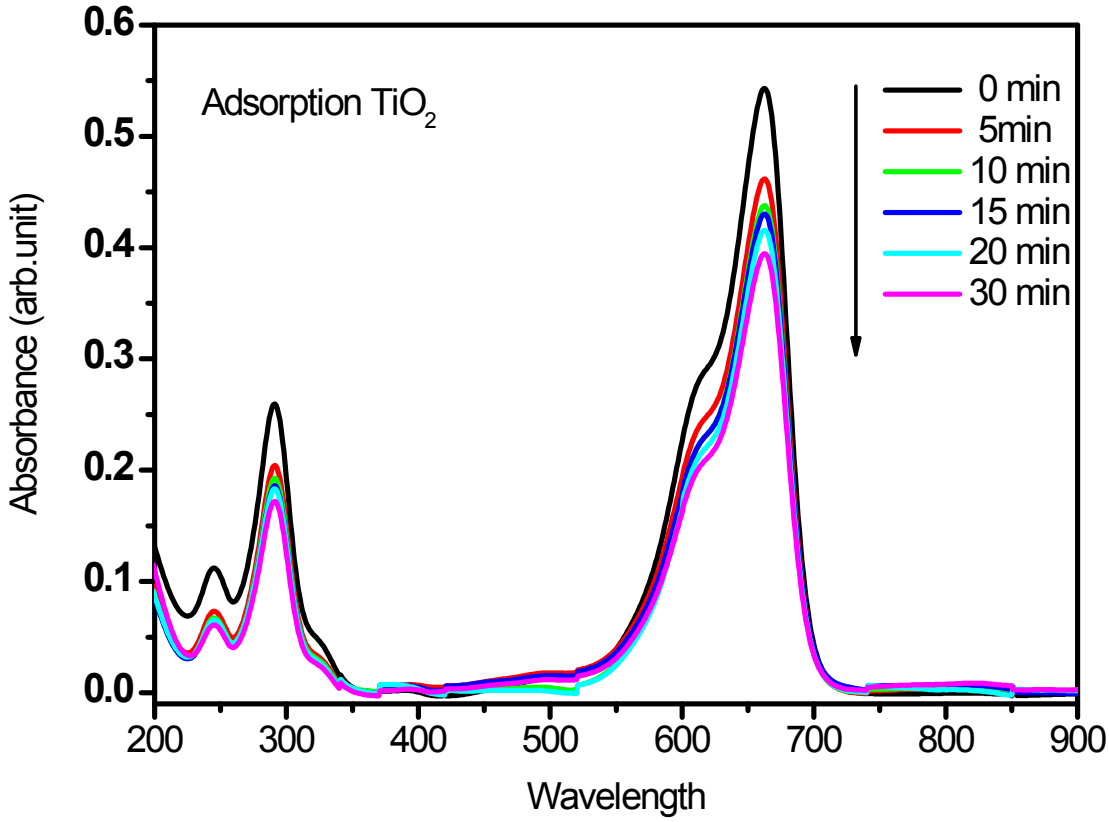
Table –(B)- Corresponds to SAED pattern of Mo-10

Circle	Calculated d-value (Å)	JCPDS d-value-(**1**) (**CAS-84-1750**) **TiO_2-Anatase**	JCPDS d-value-(**2**) (**CAS-84-1360**) **MoO_3**	Error (%) (**1**)	Error (%) (**2**)	(hkl)- plane (**1**)	(hkl)- plane (**2**)
1	3.25	3.4979	3.33	7.8	2.4	110	120
2	2.8196	2.4531	3.1043	14	9.1	002	122
3	1.755	1.7489	1.7534	0.3	0.09	220	411
4	1.4909	1.4815	1.490	0.6	0.06	113	134

In the Table-(A) it SAED pattern matches more with that of TiO_2 –Anatase whereas in Table-(B) it matches more with that of MoO_3 structure. Though the CAS value of the MoO3 are different yet both represents MoO3 with Cell parameters (a=7.424, b=7.478, c=7.689, Total Volume = 426.94- CAS- 84-1360); parameters (a=7.415, b=7.433, c=7.654, Total Volume = 4261.86- CAS- 80-0347)

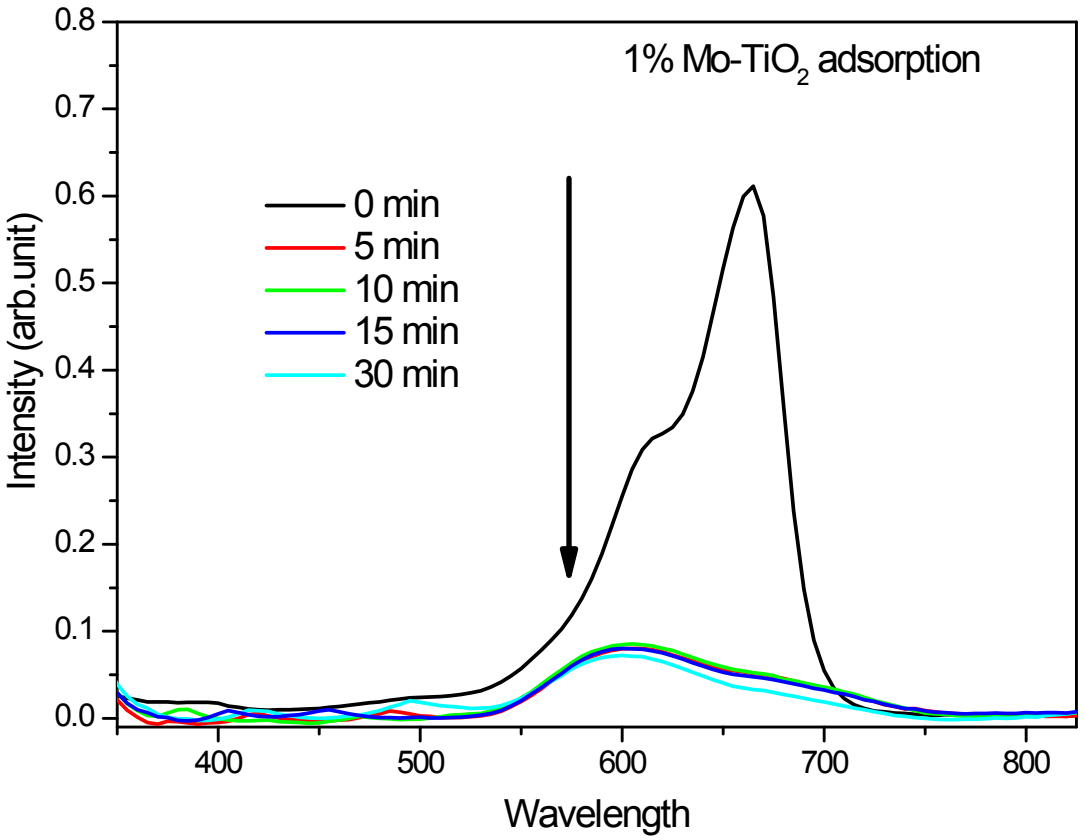


S.I.-6 : Plot of the UV-Vis absorption spectrua for the Methylene Blue dye under visible irradiation without any catalyst (blank data) at different time intervals.



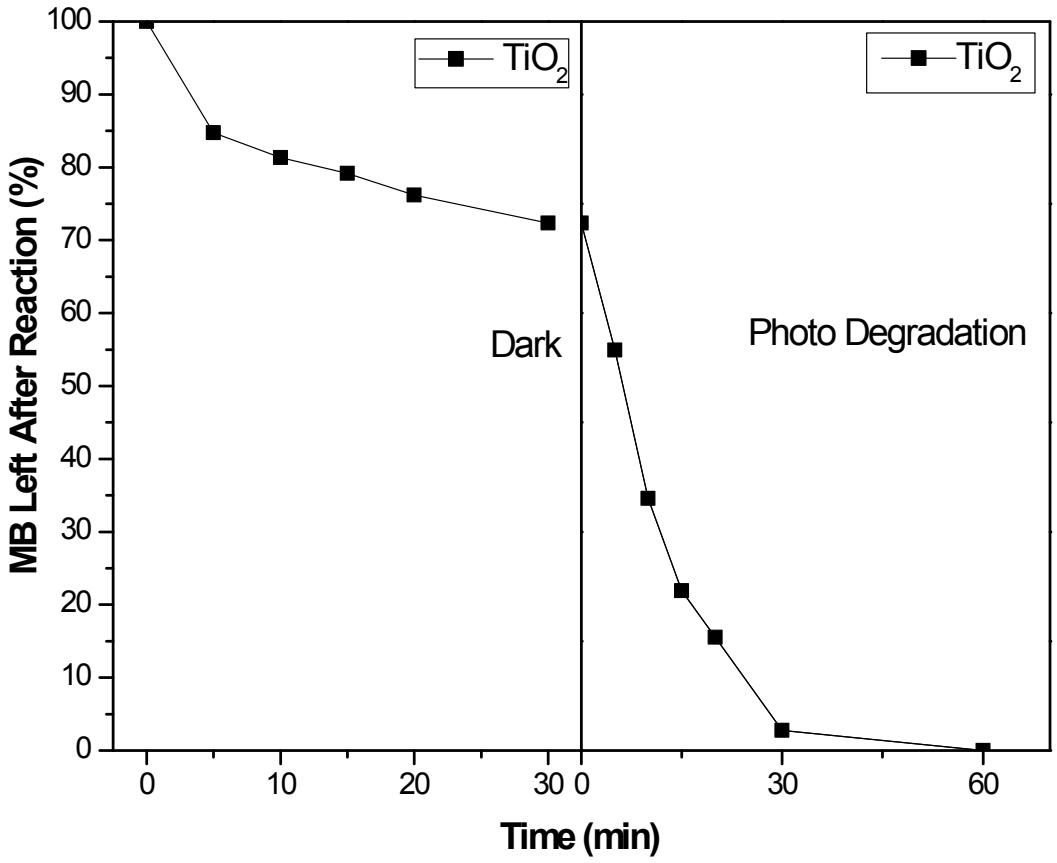
S.I. -7: Temporal profile for the UV-Vis absorption spectra of MB Dye using TiO_2 photocatalyst to study the effect of adsorption.

Adsorption studies were conducted to confirm the presence of catalytic activity. The adsorption over the TiO_2 photocatalyst shows that the effect of adsorption is not that high over the TiO2 photocatalyst like that of the Mo-TiO_2 photocatalysts.

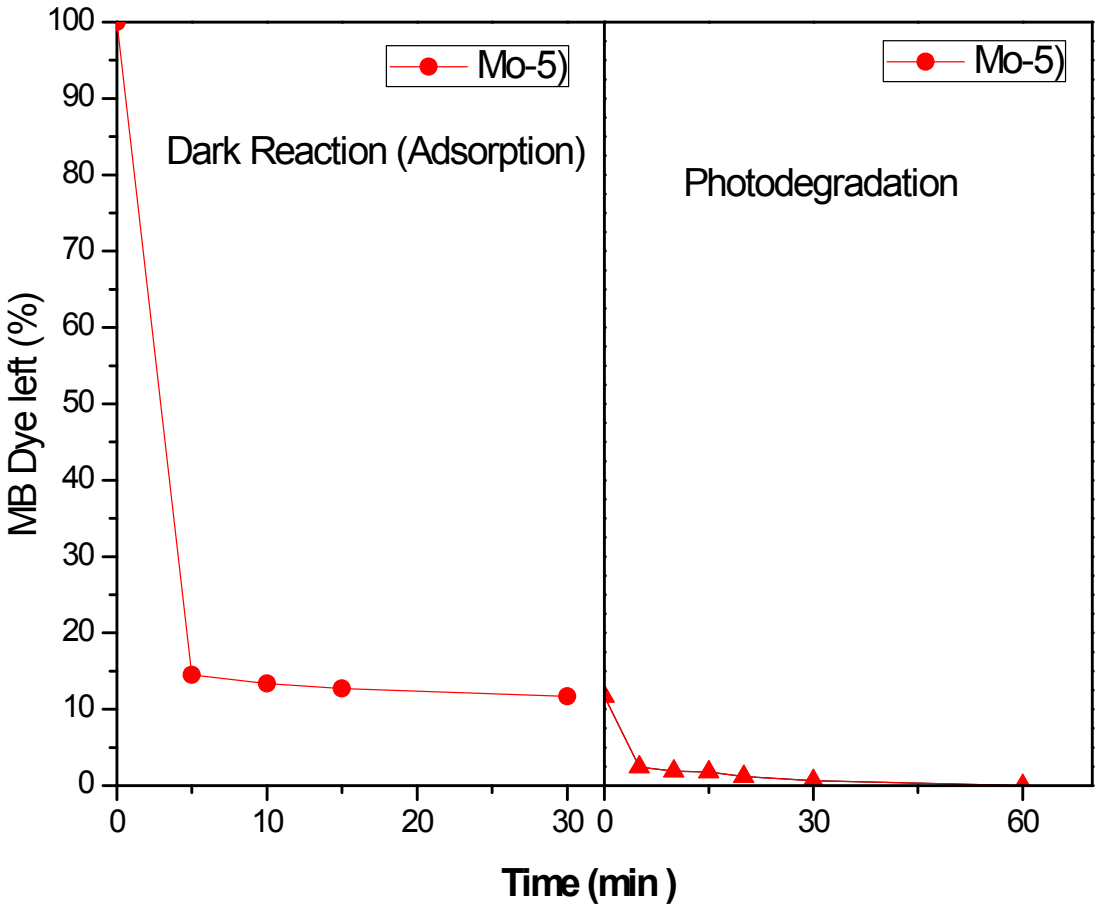


S.I. -8:Temporal profile for the UV-Vis spectra of MB Dye using Mo-1photocatalyst to study the effect of adsorption.

Adsorption studies were conducted to confirm the presence of catalytic activity. The adsorption was also very fast that almost 80% of the sample got adsorbed in the first 10 minutes which later saturated and did not degrade further. While in the case of Photocatalytic degradation almost 99 % degradation occurred in the first 15 min in the Visible light and 95% degradation in the first 30 min in presence of UV irradiation.



S.I.9: Comparative plot of the effect of Adsorption and the Photocatalytic degradation for the TiO_2 photocatalyst with UV irradiation. In the Figure 7 this photodegradation curve is same but is normalized to -100% for the dye concentration left after the process of adsorption to have a easy $t_{1/2}$ understanding. However the dye and the photocatalyst equilibrated for 30 min for a complete adsorption process and then the study of photo degradation by the same photocatalyst was initiated.



S.I.10: Comparative plot of the effect of Adsorption and the Photocatalytic degradation for the Mo-5 TiO_2 photocatalyst with UV irradiation. In the Figure 7 this photodegradation curve is derived from normalization of the dye left after adsorption effect to 100 % to have a easy $t_{1/2}$ understanding. However the dye and the photocatalyst is to equilibrate for 30 min for complete adsorption and then the photo degradation is studied to understand the effect of photocatalysis.

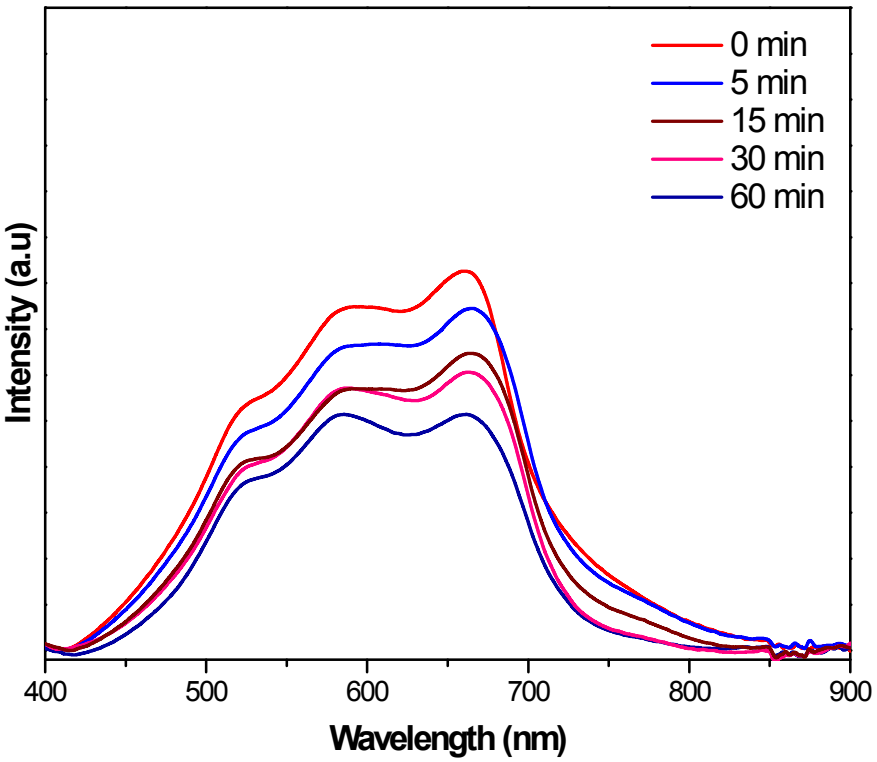


Fig. S.I. 11: The DRS temporal profile for the photo-oxidation of the MB dye adsorbed on the Mo-5 surface .

The Mo-5 surface was exposed to Methylene Blue molecule (MB) with a concentration of 50 ppm aqueous solution of MB. The photocatalyst was taken over a Whatmann-41 filter paper and 10 cc of 50 ppm was added dropwise and filtered. The subsequent photocatalyst is taken as the MB-adsorbed photocatalyst. We find that upon adsorption there is a shift in the peak of the UV-Vis absorption profile of the dye to λmax = 665 and FWHM of this peak is increased almost two fold. Along with it there are appearance two new peaks at 581 and 523 nm respectively. The formation of the new peaks, peak shift to higher entity and the increment in the FWHM value show that there is definitely a very strong electronic interaction between the Mo-5 surface and the MB dye. Therefore this process of adsorption of the MB on Mo-5 is a process of chemisorption (strong electronic interaction) rather than that of physisorption, however not to the extent of reactive chemisorption.

Further, to study photo degradation of the adsorbed dye, the photocatalyst with the MB-adsorbed on it's surface was subjected to photo-irradiation with the visible light. The DRS profile of this MB-adsoped Mo-5 dye was taken for 60 minutes during which we find that almost 37 % of the adsorbed dye is degraded. This clearly indicates that the adsorbed dye on the Mo-5 surface gets photodegraded.