Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Enhanced photocatalytic activity and easy recovery of visible light active $MoSe_2/BiVO_4$ heterojunction immobilized on *Luffa Cylindrica- Experimental and DFT study*

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Supplementary Information

S1: UV-vis. spectra of MB (20mgL^{-1}) and Phenol absorption (50mgL^{-1})

The maximum absorption peak for MB and Phenol was obtained at 622 nm and 270 nm

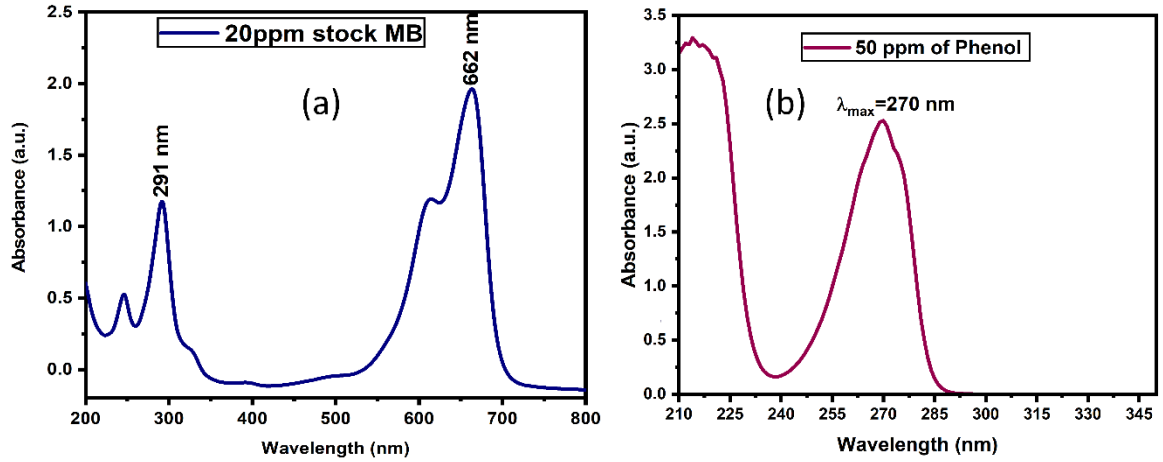

Figure S.1 UV-vis. spectra of (a) MB absorption with concentration of 20 mgL^{-1} and (b) Phenol absorption 50 mgL^{-1}.

respectively. This was recorded on Schimazdu-1800 UV-Vis. spectrophotometer.

S2: Comparison of atomic % data of XPS and EDX

The compositions obtained by the XPS and EDX for the catalysts were listed in the table **S.1** for comparison. The XPS analysis revealed the composition only of the surface within a several nano-meter range. Whereas, the EDX covers the whole catalyst since the nanoparticle diameter, 200-300 nm, was in the range of the X-ray penetration depth. A comparison of these compositions clarified the features of the surface structure of the 0.15$MoSe_2$@$BiVO_4$. First,

Bismuth content at surface of catalyst (XPS data) is comparatively very low in comparison with core (EDX) of catalyst. The vanadium and oxygen content shows higher percentage at surface in comparison with core. Molybdenum and Selenium shows higher content at core in comparison with surface. Presence of carbon shows deposition of CO_2 at time of XPS analysis. This shows Mo and Se are majorly present in inner layers than on surface [1].

Table S.1 Comparison of atomic percent thus obtained from XPS and EDX Analysis

Element	XPS	EDAX
Vanadium	15.49	6.654182
Selenium	9.06	12.94405
Molybdenum	2	5.748133
Bismuth	11.22	74.65364
Oxygen	36.96	0
Carbon	25.27	0

S3: Immobilization of 0.15$MoSe_2$@$BiVO_4$ on *Luffa cylindrica*

The *Luffa* was washed with water then double distilled water (D.I.) and ethanol to remove all impurities attached to it. Again, it was washed with D.I. water and kept for overnight drying at 60 ℃. Then, the weight of completely dried luffa was taken. It measured 11.5585g. Then, around 1.15 g of catalyst was dispersed in ethanol: water (1:1). Now, the catalyst was immobilized using dip-coating method. After complete immobilization, the luffa was dried in oven at 60℃ overnight. Next day the luffa was washed several times with ethanol and water to remove loosely held particles till clear solution was obtained. Again, Luffa was kept at 60℃ till complete drying. The dried luffa was weighed. It measured 12.5585g there by implying immobilization of 1g of 0.15$MoSe_2$@$BiVO_4$ on *Luffa cylindrica*. The weight of Luffa remained same after usage for 5 continuous cycles also.

S4: Band Positions Calculations

For a semiconductor, valance band energy potential can be calculated at zero charge point using the following empirical formula:

$$E_{VB} = X - E_e + 0.5E_g \quad (1)$$

here E_{VB} is valance band potential; X is the absolute electronegativity of respective semiconductors, and it is defined as geometric mean of all constituent atoms of the respective semiconductors; E_g is the obtained band gap from diffuse reflectance spectra; E_e is the energy of free electrons on hydrogen scale (Ca. 4.5 eV). The conduction band (CB) energy potential is calculated as follows:

$$E_{CB} = E_{VB} - E_g \quad (2)$$

From above equations, CB and VB positions of $BiVO_4$ and $MoSe_2$ were calculated and are summarised in **Table S2** below and accordingly heterojunction was elucidated **(Figure S2)**

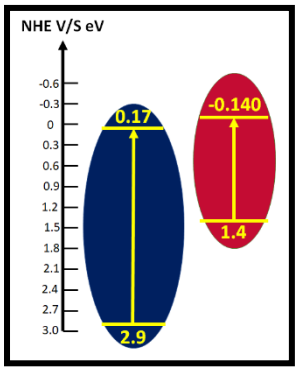

Figure S.2 The CB and VB position comparisons of $BiVO_4$ and $MoSe_2$

Table S.2 Band energy positions of $BiVO_4$ and $MoSe_2$

Semiconductor	Absolute Electronegativity (eV)	E_g (eV)	Bandgap (eV)	CB Position (eV)	VB Position (eV)
$BiVO_4$	6.04	4.5	2.73	0.175	2.905
$MoSe_2$	5.13	4.5	1.54	-0.140	1.40

S5: 20 ppm MB degradation

Samples	Concentration (mgL^{-1})	Time taken (in min.)	% Degradation	Pollutant	References

Table S.3 Degradation of MB and Phenol using various bismuth based photocatalyst

BiOCl-G	50	300	82	Phenol	[2]
$BiVO_4$-Al_2O_3	10	360	86	MB	[3]
Co-$BiVO_4$(MB)	15	300	90	MB	[4]
g-C_3N_4/Bi_2O_3/TiO_2-NTs	-	180	77.5	MB	[5]
Bi_2O_3(1.0wt.%)/C_3N_4	3.51	120	78.1	MB	[6]
FTO-$BiVO_4$	5	120	100	MB	[7]
$BiVO_4$/WO_3	10	180	94.8	Phenol	[8]
$BiVO_4$/Fe_2O	50	120	68.89	Phenol	[9]
0.15$MoSe_2$@$BiVO_4$-Luffa	50	120	96.74	Phenol	Present work
0.15$MoSe_2$@$BiVO_4$-Luffa	20	120	96.96	MB	Present work

The photoactivity of as fabricated catalysts were determined by studying photodisintegration of 20ppm MB dye. The detailed study including effect of doping, effect of concentration of pollutant, effect of pH of pollutant, effect of radical quenchers is represented in **figure S.3.**

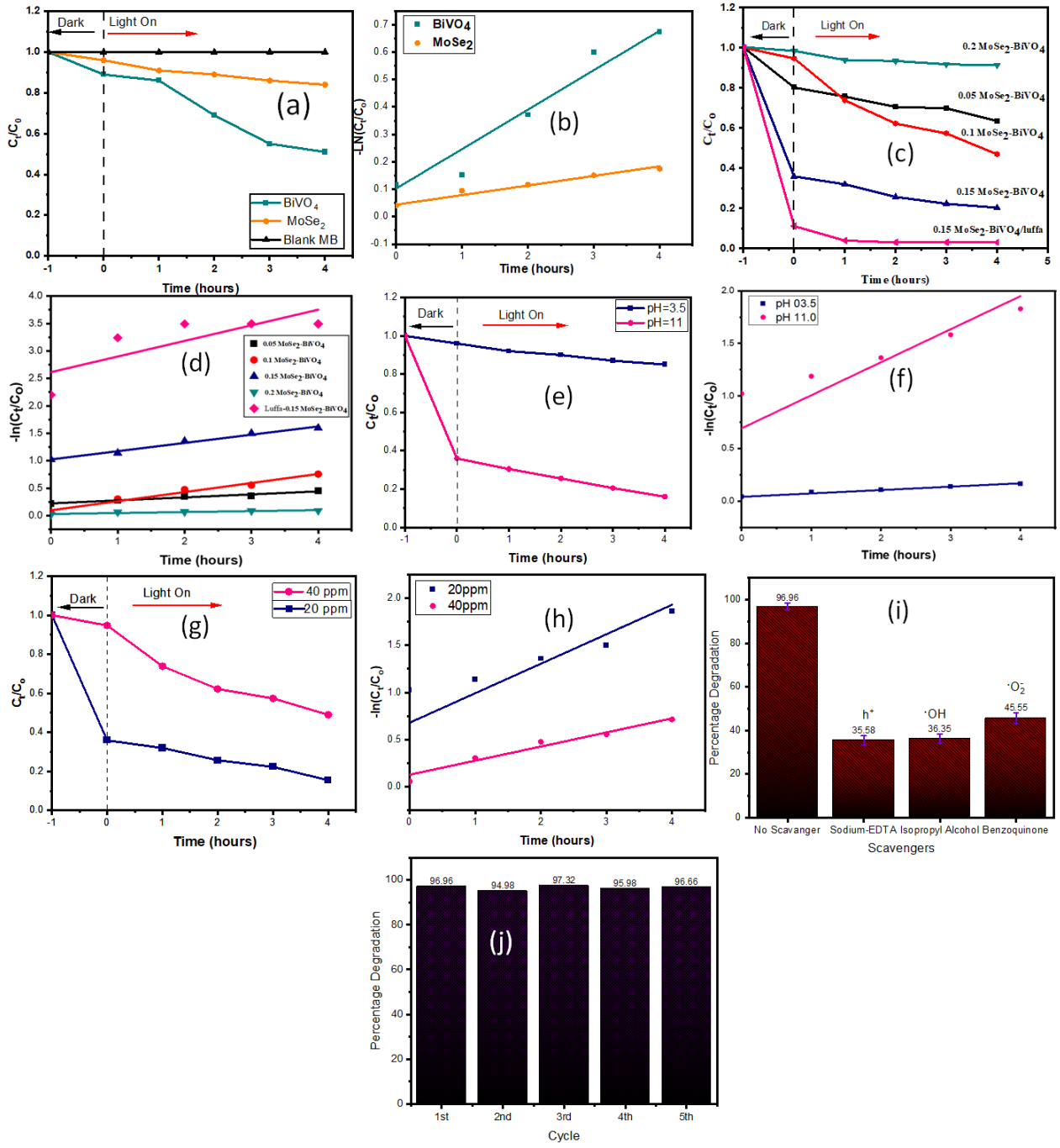

Figure S.3 Photodisintegration of (a)MB using $BiVO_4$ and $MoSe_2$, (c)MB using with $BiVO_4$ decorated with $MoSe_2$ (varying concentration of $MoSe_2$ i.e., 0.05M, 0.1M, 0.15M and 0.2M), and $0.15MoSe_2@BiVO_4$ on Luffa cylindrica (c, and d) kinetic linear simulation curves of MB with respective samples; Effect of pH(e) and initial concentration (g) on photodegradation of MB by $0.15MoSe_2@BiVO_4$-Luffa cylindrica, with their respective kinetic linear simulation curves (f, h); (i)Photodisintegration of MB by $0.15MoSe_2@BiVO_4$-Luffa in the presence of different scavengers; (j)Percentage degradation of MB for five consequent cycles of using $0.15MoSe_2@BiVO_4$-Luffa

S6: Illustrating stability of as fabricated 0.15$MoSe_2$@$BiVO_4$ and 0.15$MoSe_2$@$BiVO_4$-luffa

To illustrate the stability of as fabricated catalyst and immobilized catalyst after five continuous cycles of degradation of phenol, XRD of used catalyst and Luffa with immobilized catalyst was carried out. The XRD **[figure. S4 (a)]**showed a little decrease in intensity of peaks which can due to continuous usage but the all the diffraction pattern were thus obtained. The SEM image showed that particles are still impregned on Luffa fibres **[figure. S4 (b)]**. Also, after complete washing and drying the weight of 0.15$MoSe_2$@$BiVO_4$-Luffa remained constant thereby implying stability of particles on *Luffa cylindrica.*

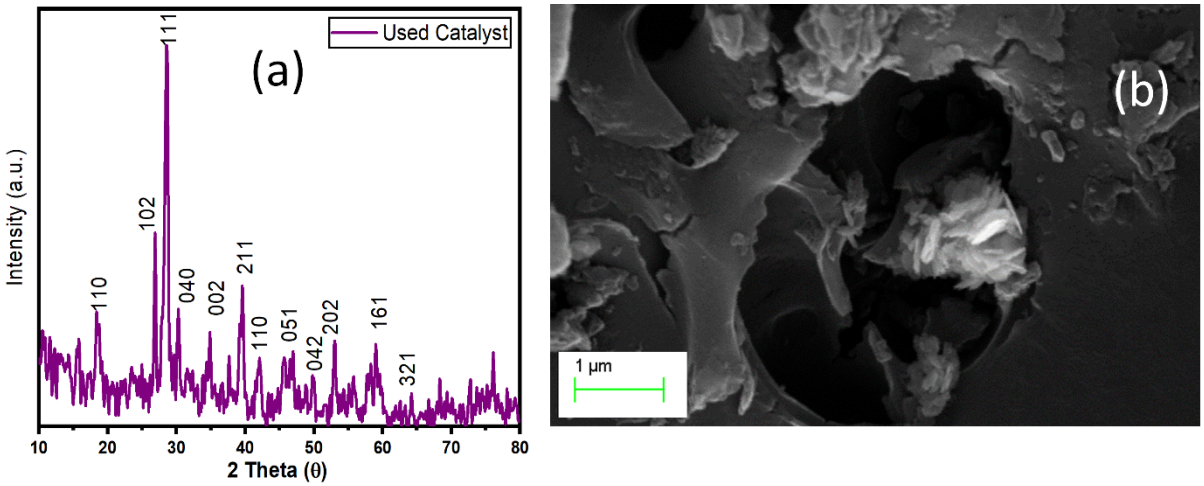

Figure S.4 XRD of used 0.15$MoSe_2$@$BiVO_4$ and (b) SEM image of used 0.15$MoSe_2$@$BiVO_4$-*Luffa*

S7: Adsorption of MB and Phenol on catalyst in dark and photodegradation after visible light irradiation

S7 (a). This study was carried out in dark for confirming the time required for adsorption-desorption equilibrium for blank luffa, 0.15$MoSe_2$@$BiVO_4$ and, 0.15$MoSe_2$@$BiVO_4$-*Lufa.*

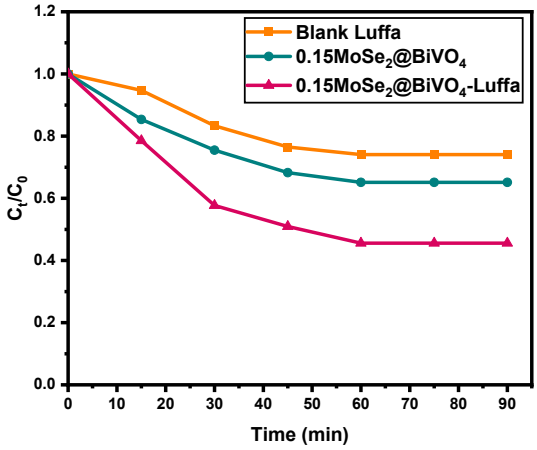

Figure S.5 Adsorption of phenol in dark using blank Luffa (orange), 0.15$MoSe_2$@$BiVO_4$ (teal), and 0.15$MoSe_2$@$BiVO_4$-Luffa

The study was carried out using 50ppm phenol. The samples were kept under ultra-sonification and after every 15 mins., the 3.5 mL of sample was collected and UV-Vis. spectra was recorded. The obtained spectra showed that after 60 mins adsorption-desorption equilibrium was established and further no adsorption was obtained.

S7 (b). To check the photoactivity of blank Luffa on MB and Phenol, blank Luffa cylindrica was implement for 60 min in dark and then kept in visible light irradiation till 90 mins. The results showed that blank luffa is only capable of adsorption of pollutants and not degradation.

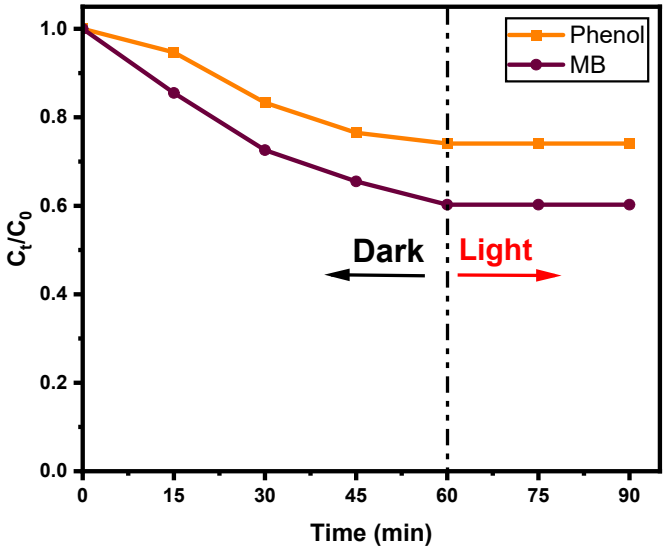

Figure S.6 Adsorption in dark for 60 mins and then exposed to visible light using blank Luffa cylindrica [phenol (orange), MB (wine)]