Electronic Supplementary Information

MoS_2 nanosheets incorporated α-Fe_2O_3/ZnO nanocomposite with enhanced photocatalytic dye degradation and hydrogen production ability

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Table S1 Atomic coordinates, constituent crystallographic phases (in wt%) of synthesized nanomaterials and reliability (R) factors obtained from Rietveld refined powder spectra. Numbers in the parentheses indicate errors in the last significant digit.

Sample	Atomic Coordinates	Crystallographic Phase (in wt%)	R Factor
α-Fe_2O_3	Fe (0,0, 0.3557) O (0.3176,0,0.25)	Trigonal (100%)	$R_{wp} = 2.83$ $R_p = 2.25$ $R_{Exp} = 2.90$ $\chi^2 = 0.953$
α-Fe_2O_3/ZnO	Fe (0,0, 0.3556) O (0.3052,0,0.25) Zn (0.33333,0.66667,0) O (0.33333,0.66667, 0.3919)	Trigonal (80%) Hexagonal (20%)	$R_{wp} = 3.01$ $R_p = 2.41$ $R_{Exp} = 2.94$ $\chi^2 = 1.00$
NMS inc. α-Fe_2O_3/ZnO	Fe (0,0, 0.3563) O (0.3067,0,0.25) Zn (0.33333,0.66667,0) O (0.33333,0.66667, 0.3663) Mo (0.33333,0.66667,0) S (0.33333,0.66667, 0.6243)	Trigonal (17%) Hexagonal (83%)	$R_{wp} = 4.34$ $R_p = 3.27$ $R_{Exp} = 3.27$ $\chi^2 = 1.77$
UMS inc. α-Fe_2O_3/ZnO	Fe (0,0, 0.3547) O (0.3121,0,0.25) Zn (0.33333,0.66667,0) O (0.33333,0.66667, 0.3508) Mo (0.33333,0.66667,0) S (0.33333,0.66667, 0.6243)	Trigonal (24%) Hexagonal (76%)	$R_{wp} = 2.73$ $R_p = 2.19$ $R_{Exp} = 2.67$ $\chi^2 = 1.05$

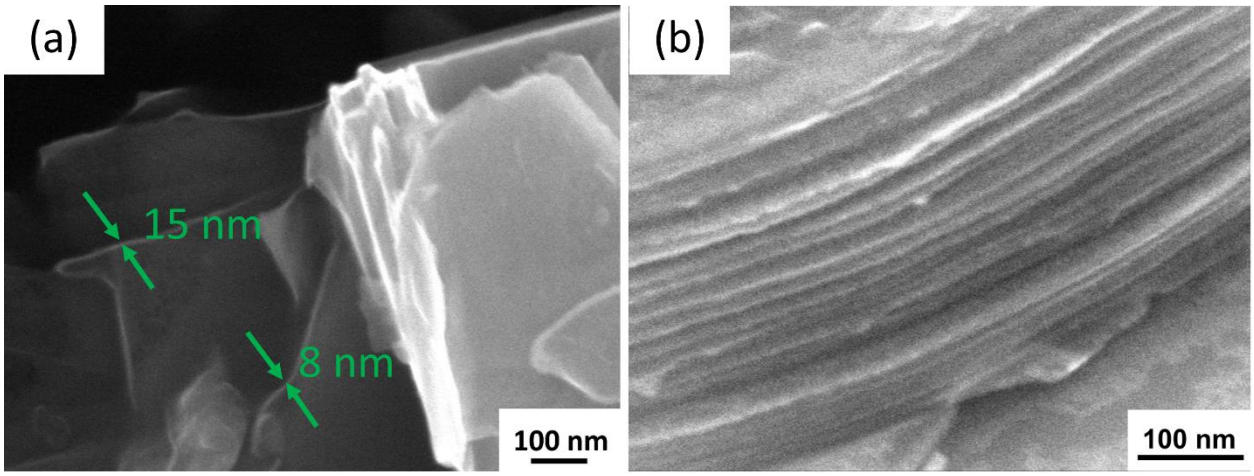

Fig. S1 FESEM images of ultrasonicated few-layer MoS_2 nanosheets with two different magnifications. The layer thickness of two nanosheets is marked in (a) and an overall view of successfully delaminated few-layer nanosheets of MoS_2 is demonstrated in (b).

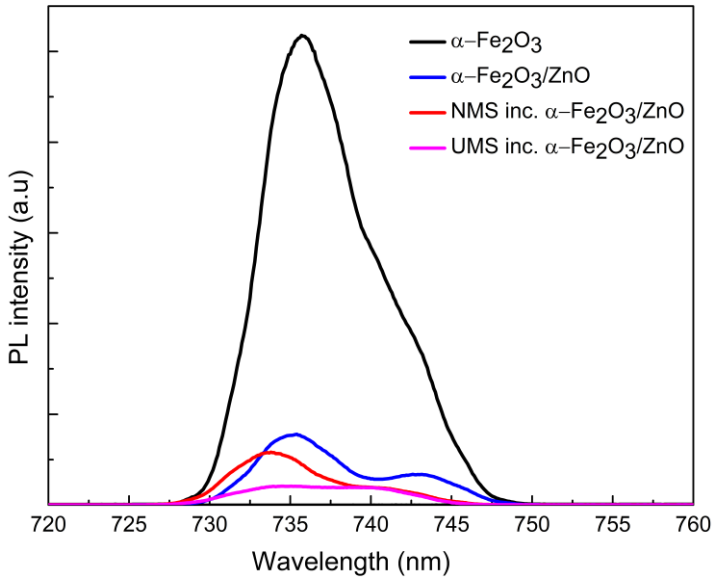

Fig. S2 (a) Steady-state photoluminescence intensity spectra of synthesized α-Fe_2O_3 nanoparticles, α-Fe_2O_3 /ZnO, non-ultrasonicated MoS_2 incorporated α-Fe_2O_3 /ZnO and ultrasonicated MoS_2 incorporated α-Fe_2O_3 /ZnO nanocomposites.

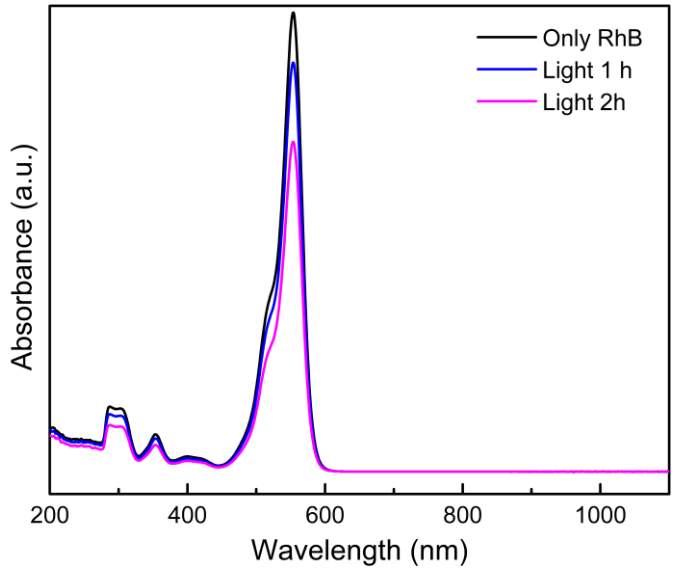

Fig. S3 Absorption spectra of RhB dye solution before and after being photodegraded by ultrasonicated MoS_2 incorporated α-Fe_2O_3/ZnO under UV-visible light irradiation.

Table S2 Amount of produced hydrogen gas by as-synthesized ultrasonicated MoS_2 incorporated α-Fe_2O_3/ZnO and other analogous nanocomposites

Photocatalyst	**Light Source**	**Amount of produced hydrogen gas after 4 hours of irradiation (µmol H_2 /g catalyst)**	**Reference**
UMS inc. α-Fe_2O_3/ZnO	500 W Hg-Xe lamp	~614	Present work
MoS_2/RGO	300 W Xe lamp	~190	[1]
WO_3/g-C_3N_4	Artificial solar light	~250	[2]
TiO_2/$MoSe_2$	300 W Xe lamp	~20	[3]

Calculation of Conduction Band Minima (CBM) and Valence Band Maxima (VBM)

The Fermi energy (E_F) of a semiconductor material can be calculated theoretically using the empirical formula[4]:

$$E_F = \chi - E_c \qquad (1)$$

Here, χ is the absolute electronegativity and E_c is the free electron energy on hydrogen scale (approximately 4.5 eV). For compound semiconductors, χ is calculated using the geometric mean of constituent atoms' absolute electronegativity.[5] Usually for semiconductor, Fermi energy denotes the

midlevel of the gap between CBM and VBM. Hence, the CBM and VBM of a semiconductor can be calculated using the following equations:

$CBM = E_F - 0.5E_g$ (2)

$VBM = E_F + 0.5E_g$ (3)

Here, E_g denotes the bandgap energy.

The calculated values of χ, E_F, CBM and VBM for α-Fe_2O_3, ZnO and MoS_2 nanosheets are presented in Table S3. For α-Fe_2O_3, the experimentally obtained bandgap (E_g) value is used whereas for ZnO and few-layer MoS_2 nanosheets, we have considered the bandgap values as reported by previous investigations.[6,7]

Table S3 Obtained values of absolute electronegativity (χ), bandgap energy (E_g), Fermi energy (E_F), CBM and VBM of α-Fe_2O_3, ZnO and few-layer MoS_2 nanosheets.

Material	**χ (eV)**	**E_g(eV)**	**E_F (eV)**	**CBM (eV)**	**VBM (eV)**
α-Fe_2O_3	5.88618	1.87	1.386	0.451	2.321
ZnO	5.79250	3.37	1.293	-0.393	2.978
MoS_2 Nanosheets	5.32372	1.25	0.824	0.199	1.449

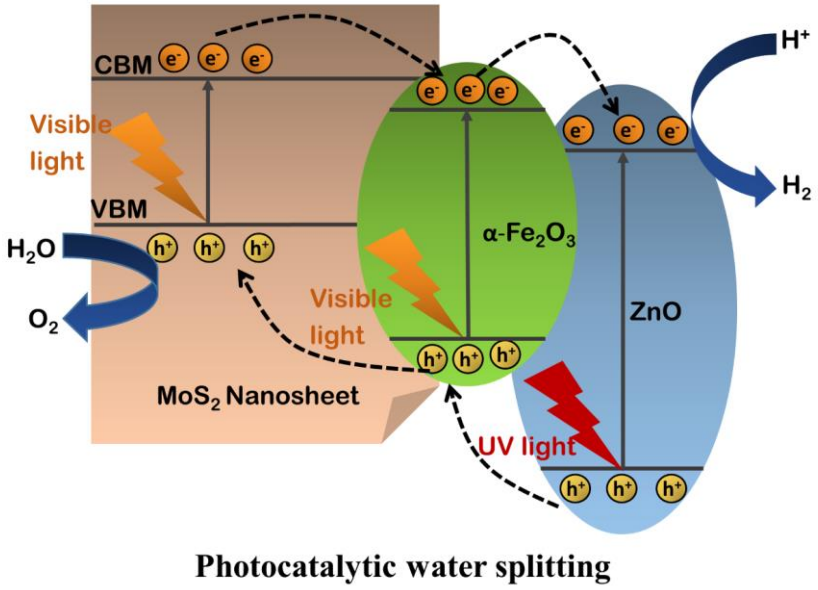

Fig. S4 Schematic of proposed photocatalytic water splitting mechanism using ultrasonicated MoS_2 incorporated α-Fe_2O_3/ZnO nanocomposite as catalyst under solar light irradiation

References

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