Plasmonic Mo-doped HNb_3O_8 nanosheets with tunable energy band structures for photothermal catalytic H_2 evolution in Full Solar Spectrum

Junli Chen,[a]* Xinyi Jin[a], Xinli Yang,[b] Lei deng,[b] Zhiqiang Zhang,[a] Lifeng Han,[a] Feilong Gong,[a] Yonghui Zhang[a]*

[a]School of Materials and Chemical Engineering, Collaborative Innovation Center of Environmental Pollution Control and Ecological Restoration, Zhengzhou University of Light Industry, Zhengzhou 450001, China.

[b]College of Chemistry, Chemical and Environmental Engineering, Henan University of Technology, Zhengzhou 450000, China

*Corresponding Author. Tel/Fax: +86-371-8660 9676.

E-mail: chenjunli@zzuli.edu.cn, yonghui.zhang@zzuli.edu.cn

Table S1. Atomic compositions of Mo-doped HNb_3O_8.

Catalysts	At. Comp.[a]	At. Comp.[b]	At. Comp. [wt%][c]		
	$n_{Mo}/(n_{Mo}+n_{Nb})$ (%)	(%)	Mo	Nb	$n_{Mo}/(n_{Mo}+n_{Nb})$ (%)
HNb_3O_8	0.00	0.00	0.00	66.4	0.00
MoNb-1	0.98	-	0.7	65.3	1.04
MoNb-5	4.96	4.91	3.4	64.8	4.84
MoNb-10	9.87	9.82	7.0	61.4	9.94
MoNb-15	14.6	14.8	10.5	57.9	14.9

[a]Mole content of Mo calculated by EDX.

[b]Surficial content of Mo calculated by XPS.

[c]Measured by ICP.

Table S2 Free-carrier densities of HNb_3O_8 and Mo-doped HNb_3O_8.

Catalysts	LSPR peak [nm]		Free-carrier density [cm^{-3}]	
			[a]	[b]
HNb_3O_8	-	-	-	-
MoNb-1	473	1005	4.00×10^{22}	1.12×10^{22}
MoNb-5	432	952	4.42×10^{22}	1.20×10^{22}
MoNb-10	416	952	4.50×10^{22}	2.90×10^{22}
MoNb-15	407	889	5.67×10^{22}	2.01×10^{22}

[a] calculated by LSPR peak at about 400 nm

[b] calculated by LSPR peak at about 900 nm

Table S3 the fitting parameters of the equivalent circuit for HNb_3O_8 and Mo-doped HNb_3O_8.

Catalysts	R_1	R_2	CPE1-P	W1-P
HNb_3O_8	33.98	878.7	0.9388	0.1899
MoNb-1	41.58	429.4	0.0136	0.1579
MoNb-5	47.75	201.0	1.009	0.1437
MoNb-10	47.14	45.34	0.8743	0.3979
MoNb-15	41.91	628.5	0.9678	0.2308

Table S4 Decay parameters of HNb_3O_8 and Mo-doped HNb_3O_8.

Catalysts	A_1	τ_1	R^2
HNb_3O_8	583.6	0.9060	0.9739
MoNb-1	556.9	0.6763	0.9807
MoNb-5	558.9	0.6922	0.9772
MoNb-10	542.2	0.5463	0.9726
MoNb-15	579.0	0.7618	0.9685

Table S5 Photocatalytic H_2 activities of different catalysts and a comparison with other published studies

Host Materials	Modified Method	Dopant/ cocatalysts	Light source	Activity (unit)	Ref
N , rNb co-doped $[Nb_3O_8]^-$		Pt (0.5 wt.%)	300 W Xe	449.9 μmol $g^{-1}h^{-1}$ 589.2 μmol g^{-1} h^{-1}	[1]
$Cu_{0.5}Nb_3O_8$	N/A	N/A	200 W UV	830.4 μmol g^{-1} h^{-1}	[2]
HNb_3O_8 NSs	$CuCl_2$	Cu (0.5wt.%)	300 W Xe	591 μmol g^{-1} h^{-1}	[3]
$HNb_{0.7}Ta_{0.3}WO_6$ NSs	N/A	Pt(1.0wt.%)	300 W Xe	1320.0 μmol g^{-1} h^{-1}	[4]
hy-Nb-TEOA	N/A	GR, MoS_2	500W UV	212 μmol g^{-1} h^{-1}	[5]
HNb_3O_8 NSs	N/A	Pt (1wt.%)	125W Hg	600 μmol $g^{-1}h^{-1}$	[6]
HNb_3O_8	N/A	Pt (1wt.%)	300 W Xe	193 μmol h^{-1}	
HNb_3O_8 NSs	$Ni(OH)_2$	Ni^{2+} (1wt.%)	300 W Xe	237.8μL h^{-1}	
HNb_3O_8 nanobelts	Cu ions	Pt (1wt.%)	300 W Xe	2.5 mmol $g^{-1}h^{-1}$	[7]
$HSr_2Nb_3O_{10}$	$PtCl_4$	Pt (1wt.%)	300 W Xe	530.2 μmol g^{-1} h^{-1}	[8]
$H_4Nb_2O_7$	N/A	Pt (0.5wt.%)	UV	1240 μmol g^{-1} h^{-1}	
D-HNb_3O_8		Pd (1 wt.%)	Full	3657 μmol g^{-1} h^{-1}	[9]
Mo-doped HNb_3O_8	N/A		Uv-vis	180.3 μmol g^{-1} h^{-1} 220.4 μmol g^{-1} h^{-1}	This Work
		Pt (1 wt.%)	Full	6698.7 μmol g^{-1} h^{-1}	

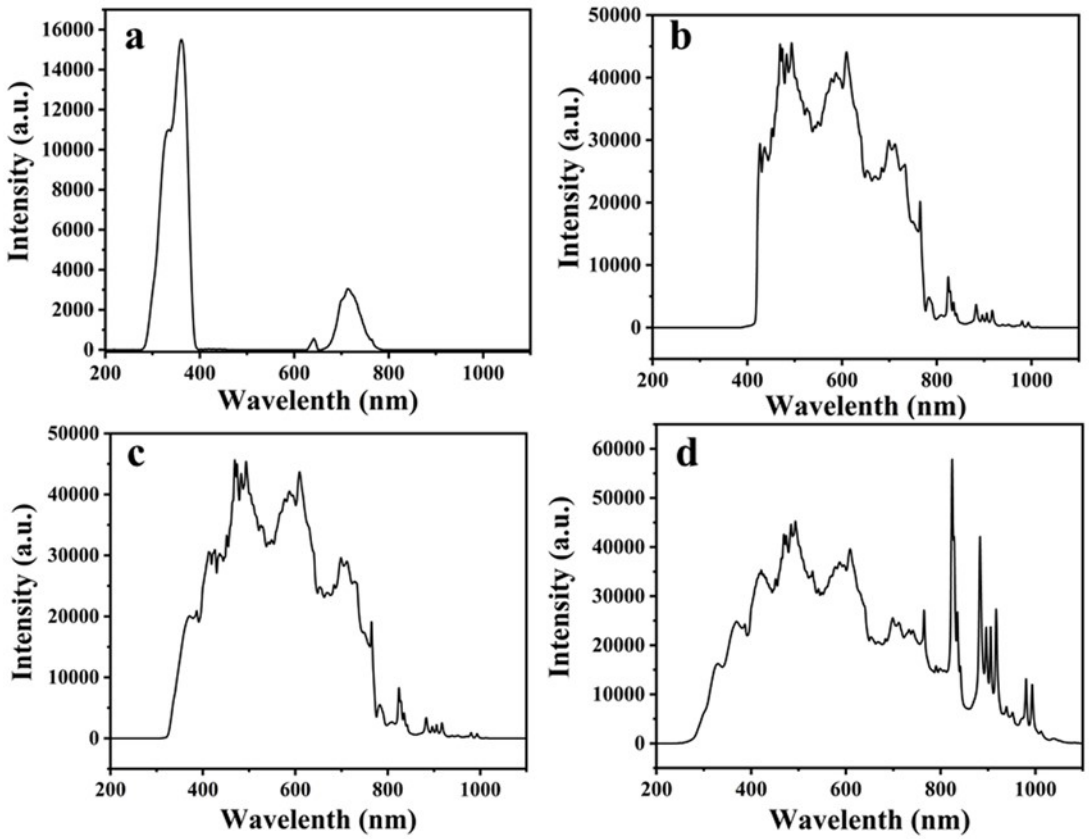

Fig. S1 The spectra of Xenon lamp. (a) Uv, (b) Visible light, (c) Uv-vis, (d) Full spectrum.

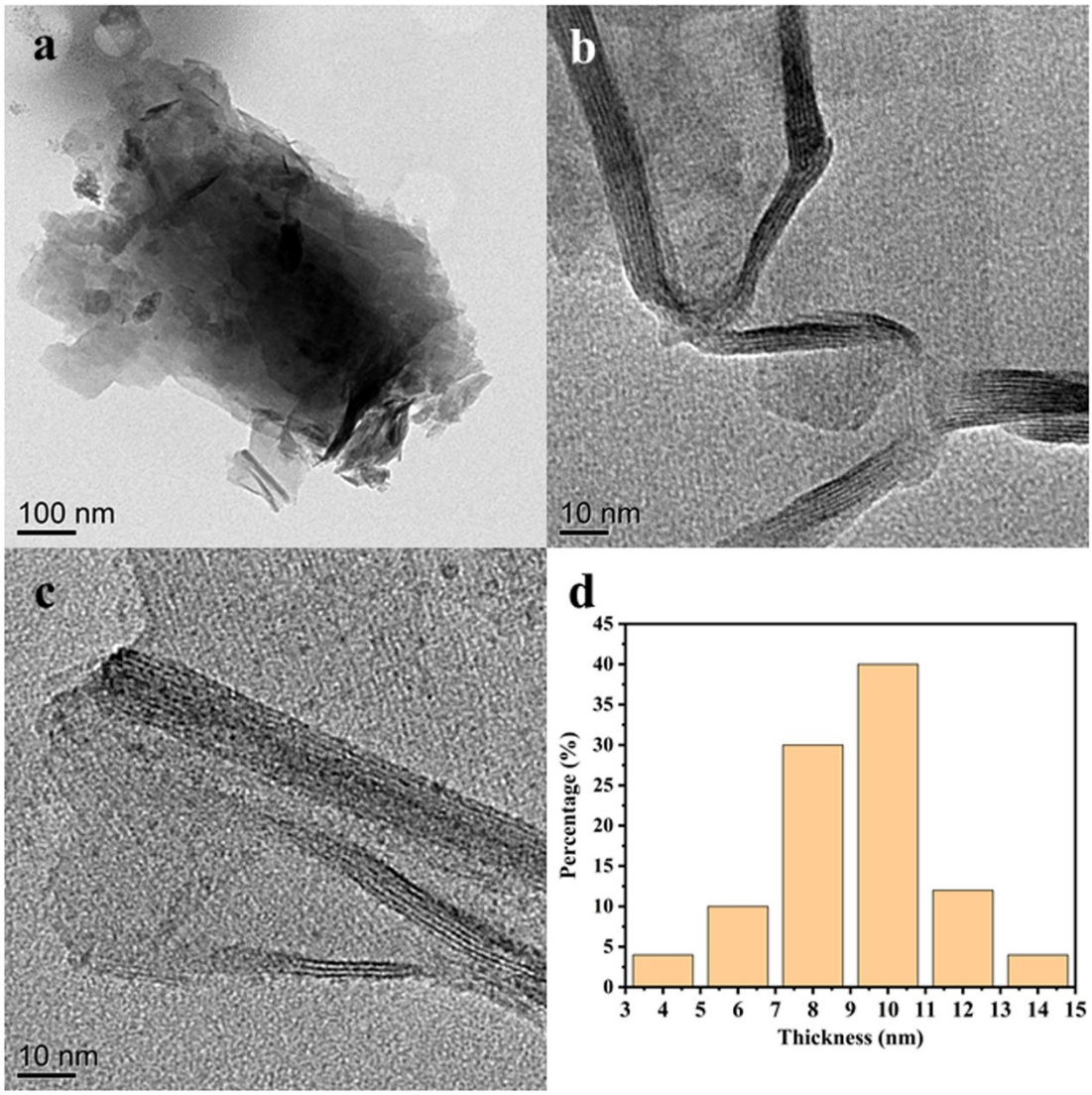

Fig. S2 Typical TEM images of (a, b, c) and the thickness distribution of MoNb-10 nanosheets

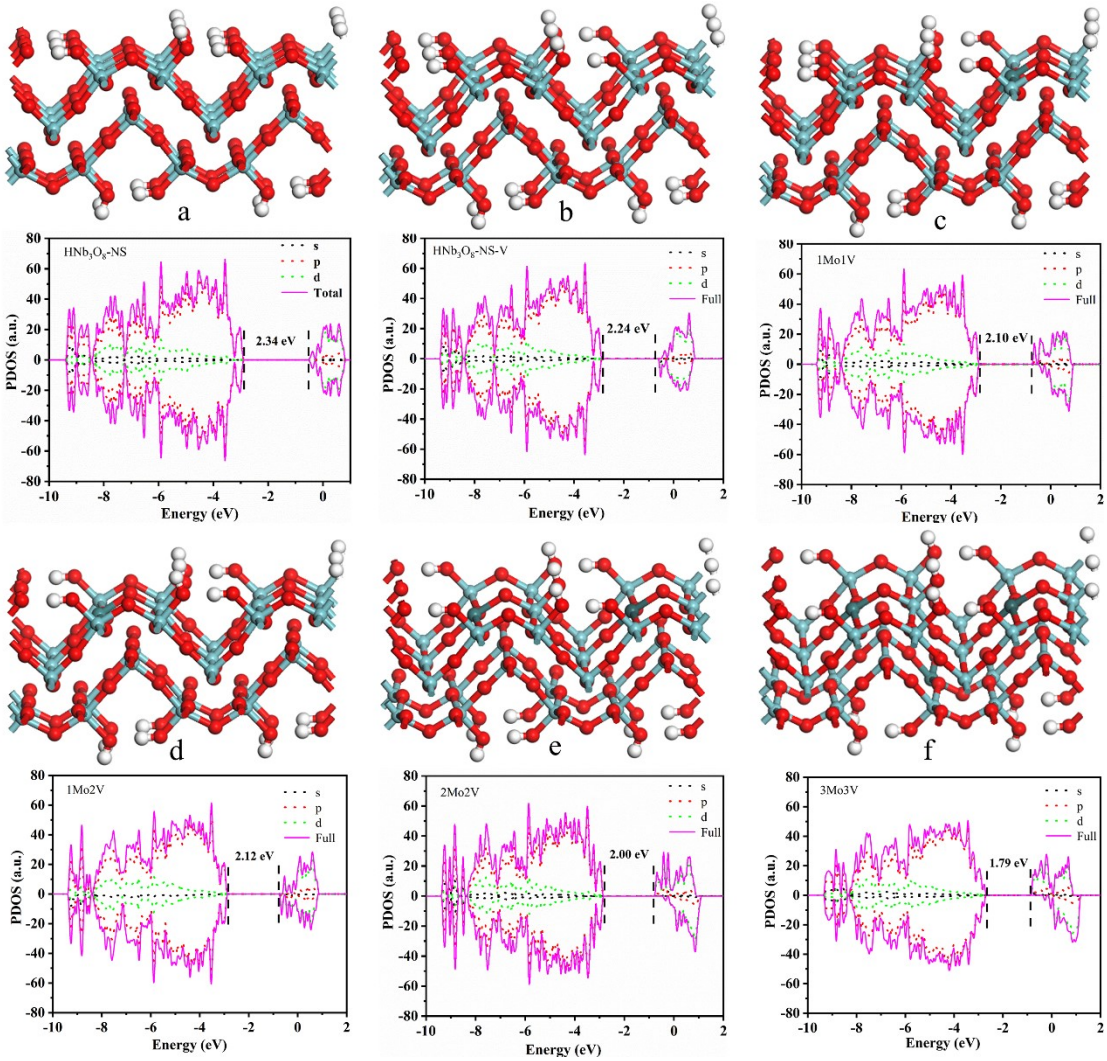

Fig. S3 The optimized configurations and the corresponding projected densities of states (PDOS) of the HNb_3O_8 nanosheet (a), HNb_3O_8-NS with oxygen vacancies (HNb_3O_8-NS-V, b), and Mo-doped HNb_3O_8-NS.

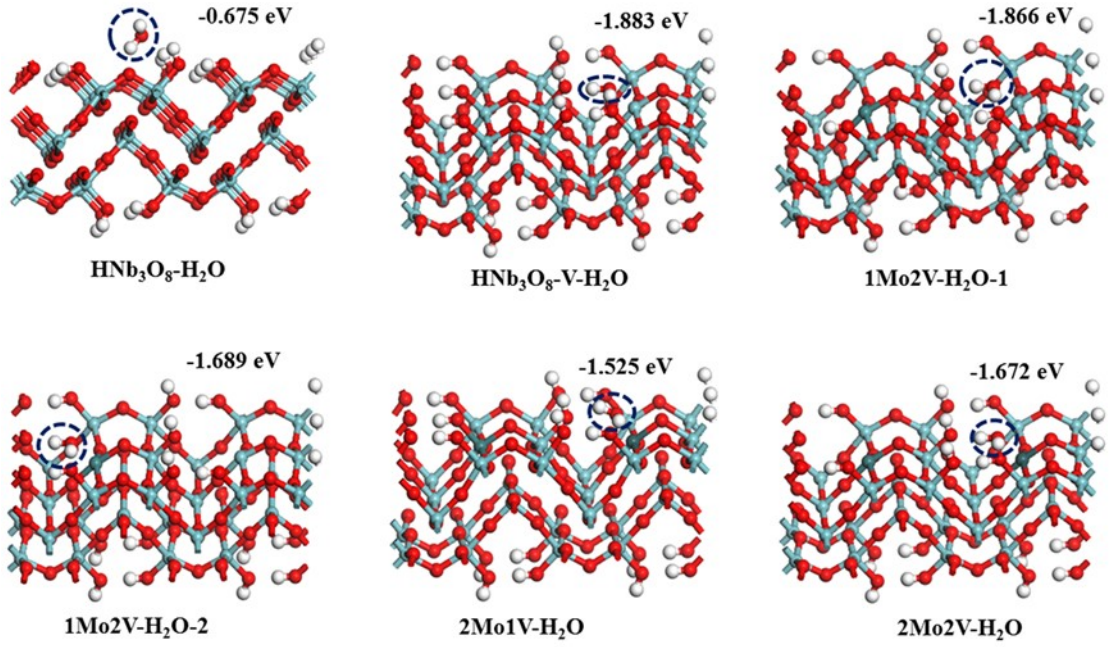

Fig. S4 The optimized adsorption configurations of H_2O on HNb_3O_8 nanosheet and Mo-doped samples.

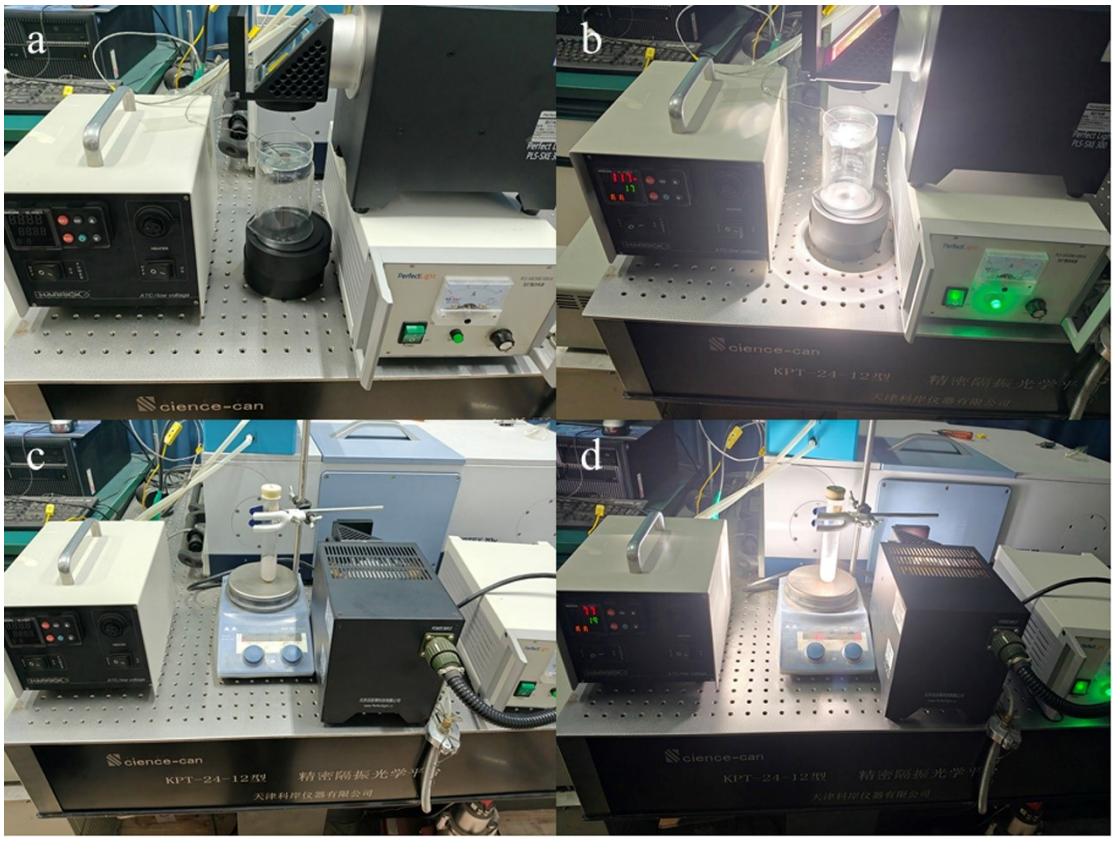

Fig. S5 The home-made equipment for measuring the temperature of the surface of catalysts and the solutions under Xe lamp irradiation.

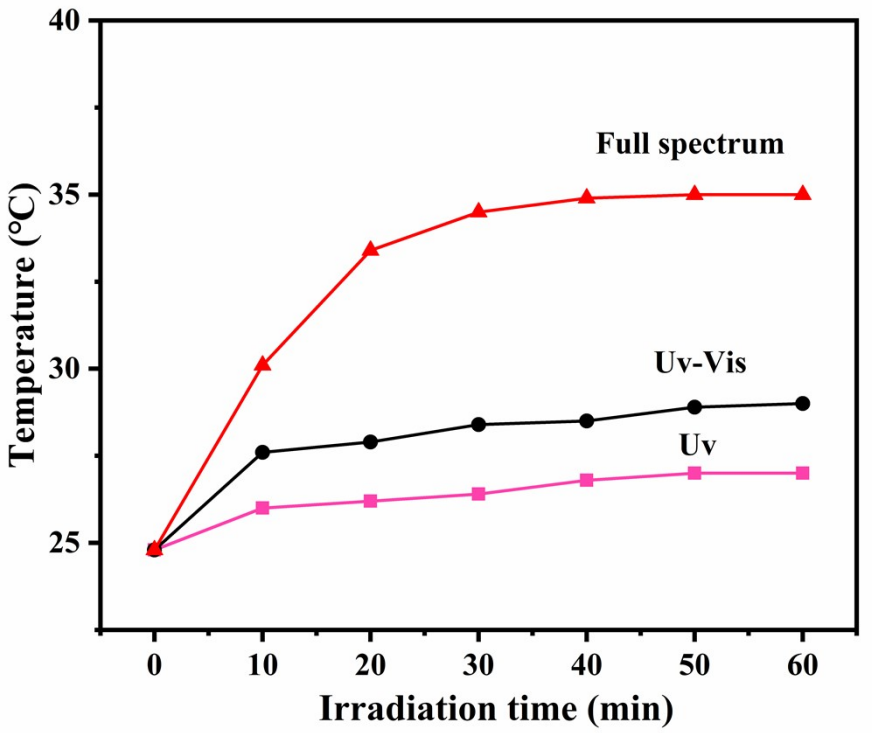

Fig. S6 Temperature evolution of the blank solution under Uv (300 - 400 nm), Uv-vis (300 – 780 nm) and full spectrum irradiation.

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