

Electronic Supplementary Information (ESI)

Hydrogenated MoS₂ QDs- TiO₂ Heterojunction Mediated Efficient Solar Hydrogen Production

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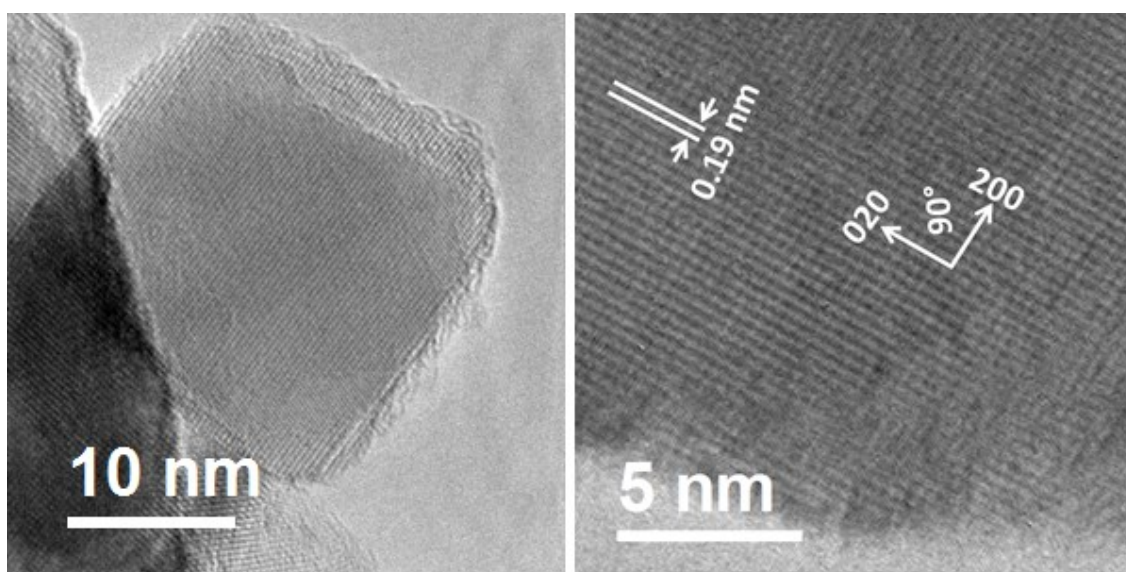


Fig. S1 TEM and HR-TEM image of the square shaped hydrogenated TiO₂ particles (T-H₂), viewed through [001] zone axes.

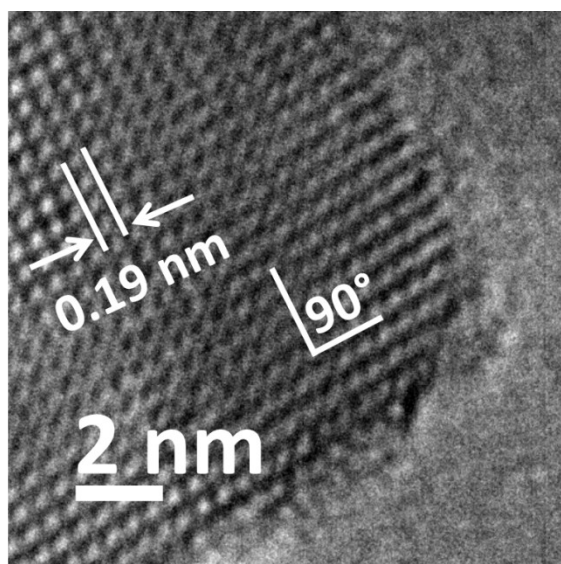
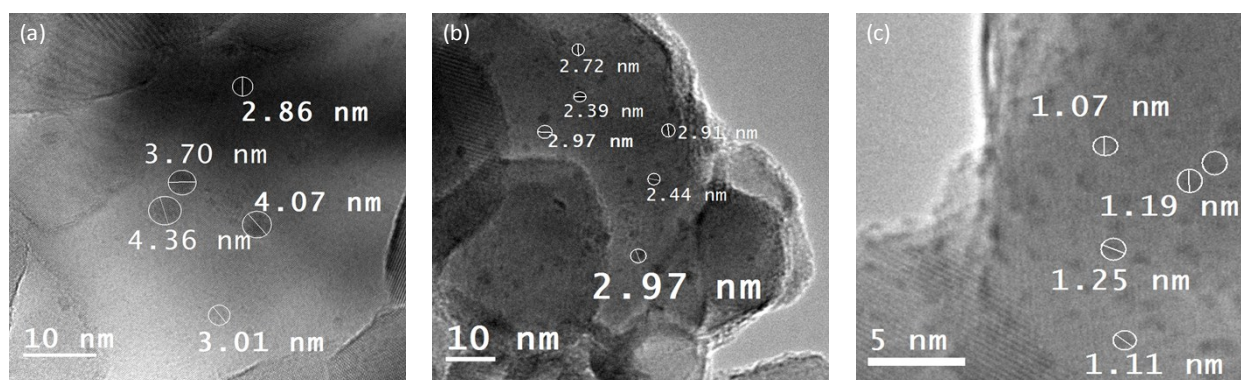


Fig. S2 HR-TEM image of the square shaped TiO_2 particles calcined at air (T-air), viewed through $[001]$ zone axes.



Size of the QDs' decreases and Number of QDs increases

Fig. S3 HR-TEM Images of (a) HMT-0.5, (b) HMT-1, and (c) HMT-1.5 displaying size variation of the MoS_2 QDs in different samples.

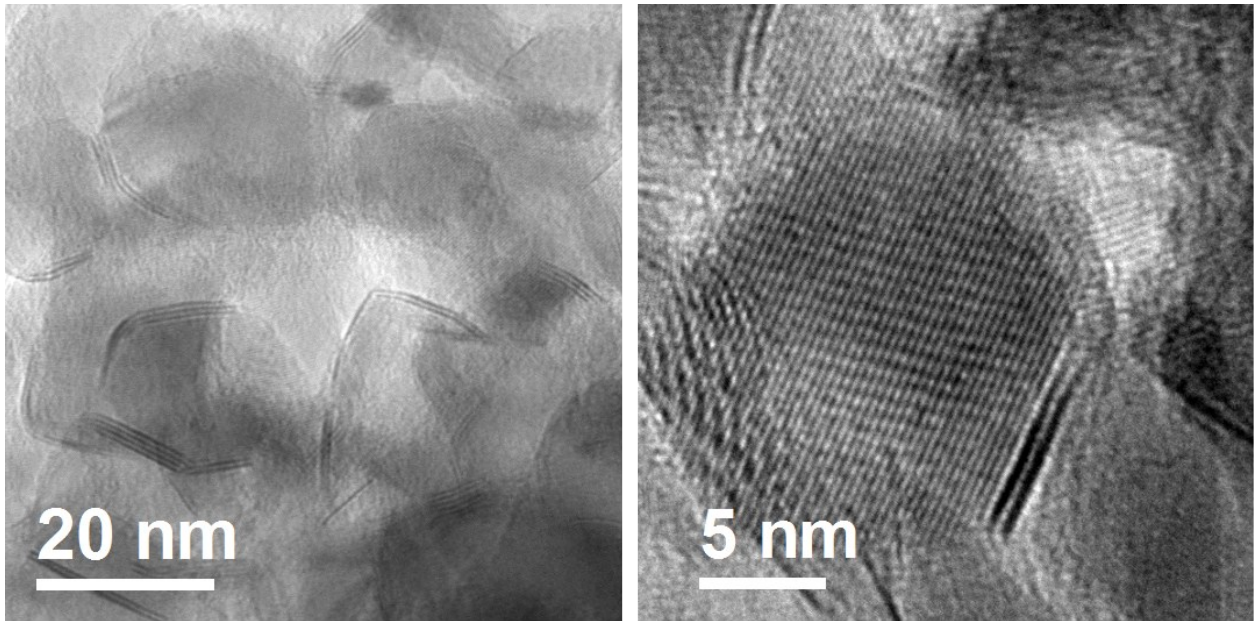
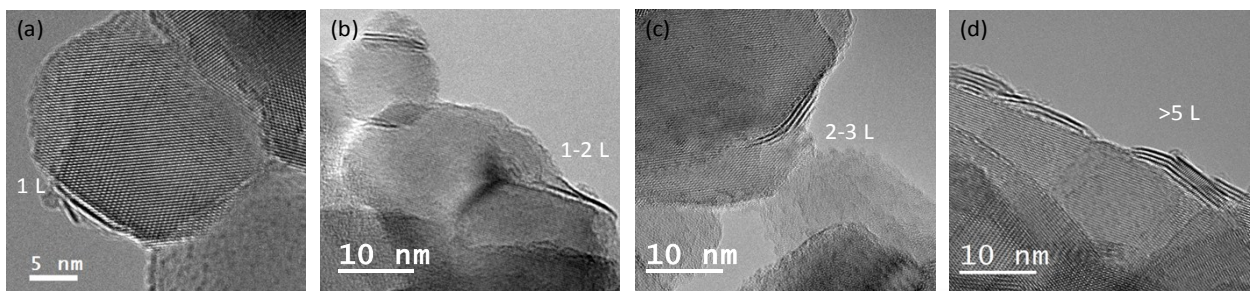


Fig. S4 TEM and HR-TEM images of HMT-5.



Number of layers as well as length of the sheets' increases

Fig. S5 HR-TEM Images of (a) HMT-1.5, (b) HMT-2.5, (c) HMT-5 and (d) HMT-10 displaying size variation of the MoS₂ sheets in different samples.

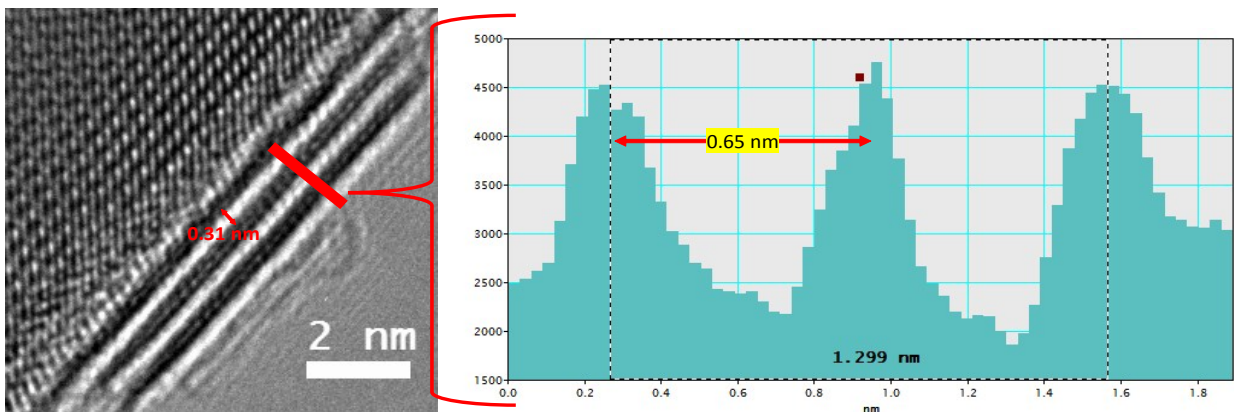


Fig. S6 HR-TEM images of HMT-2.5 showing the 3 layers of MoS₂ sheet on TiO₂.

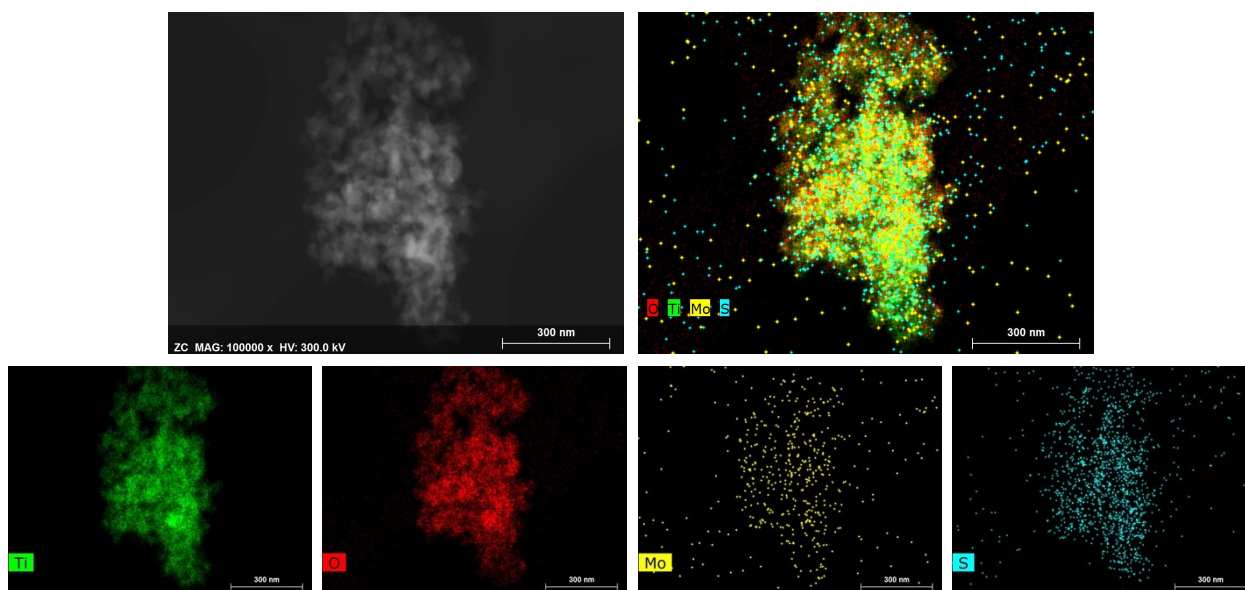


Fig. S7 Elemental mapping analysis of HMT-1 showing the presence of Mo, S, Ti, and O.

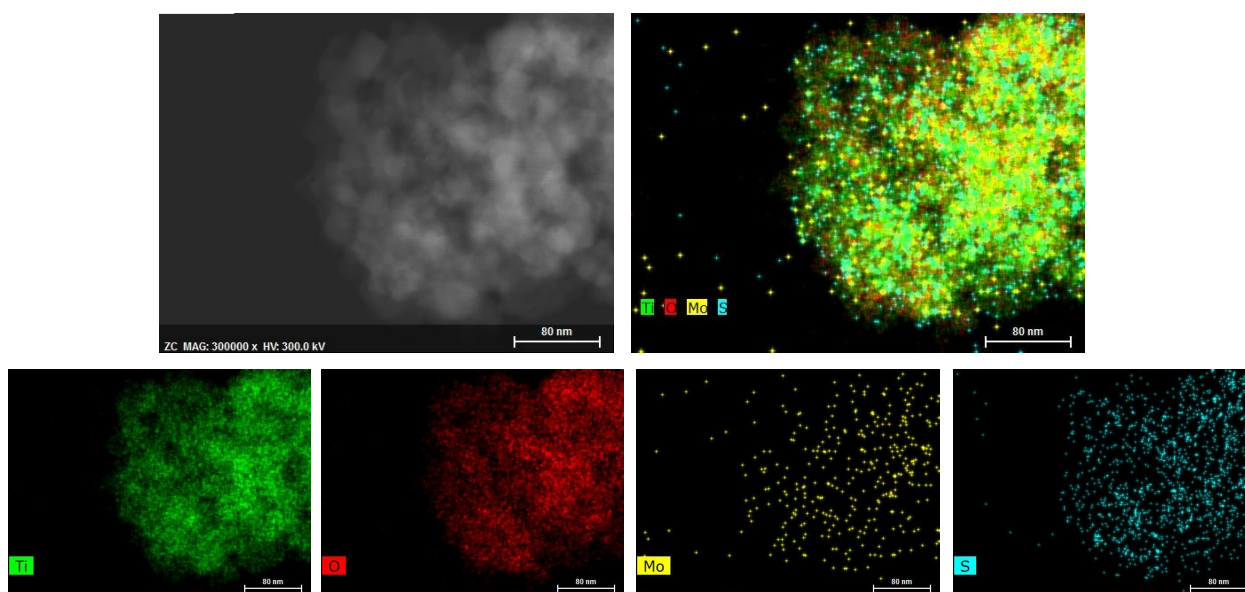


Fig. S8 Elemental mapping analysis of HMT-1.5 showing the presence of Mo, S, Ti, and O.

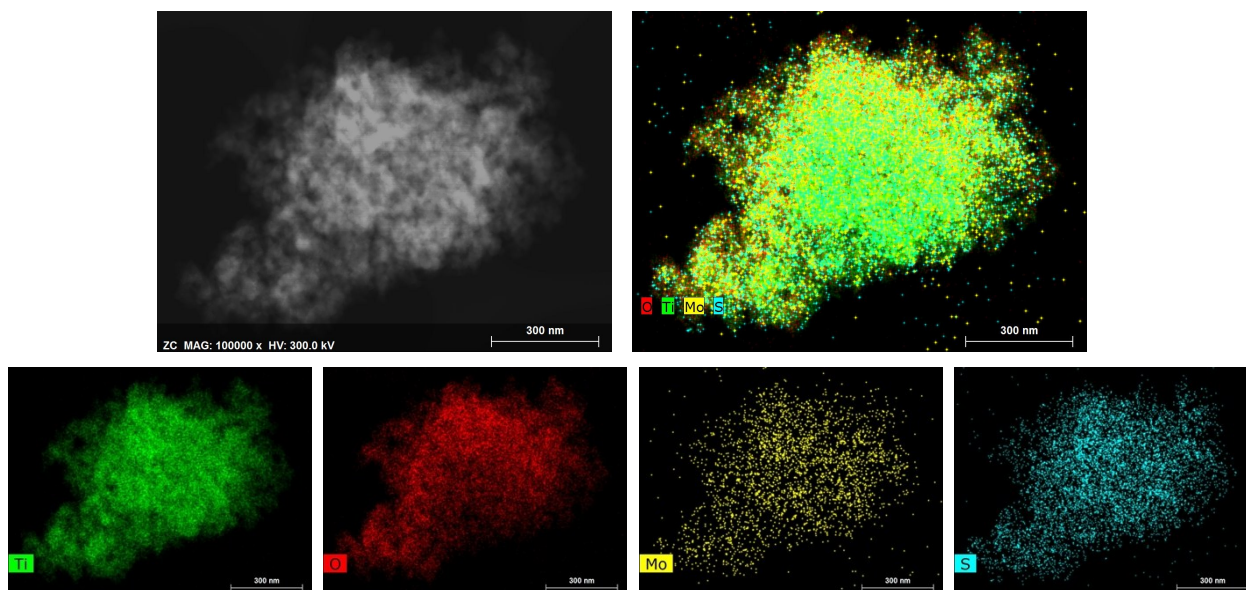


Fig. S9 Elemental mapping analysis of HMT-2.5 showing the presence of Mo, S, Ti, and O.

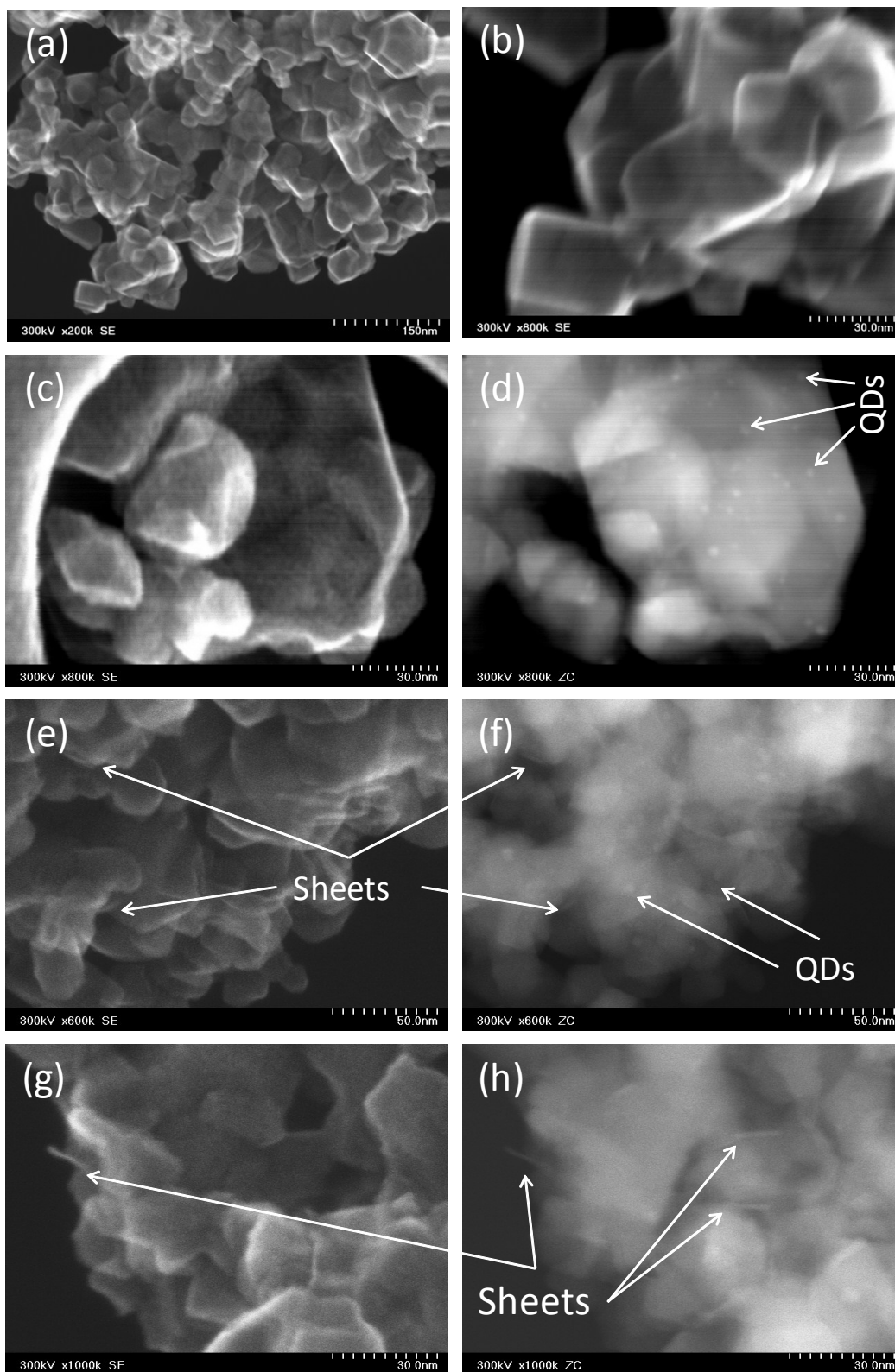


Fig. S10 (a-b) HR-SEM images of T-H₂. HR-SEM and corresponding HAADF-STEM images of (c-d) HMT-1, (e-f) HMT-1.5, (g-h) HMT-2.

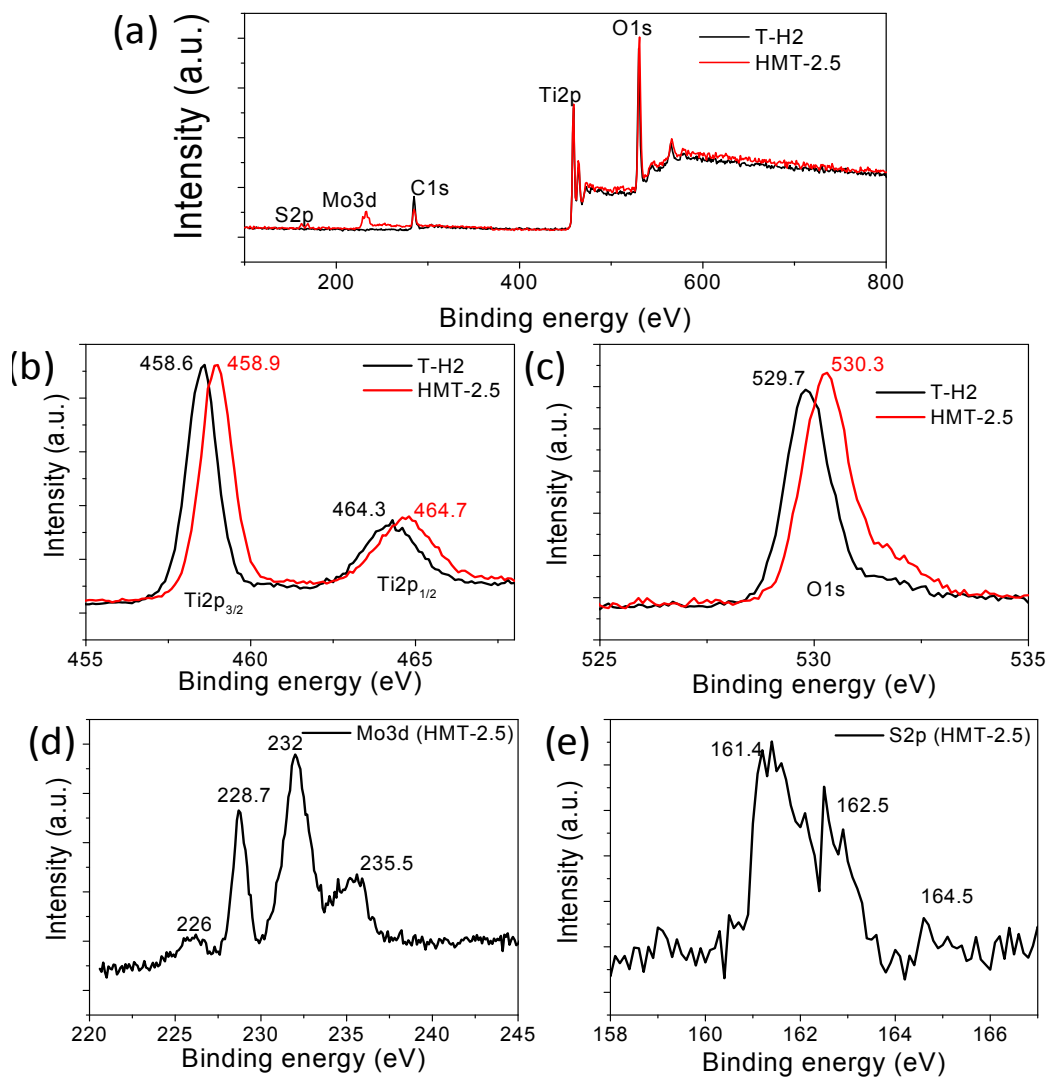


Fig. S11 X-ray photoelectron spectra for T-H₂ and HMT-2.5.

Table S1. CHNS analysis of HMT samples

Sample	Before annealing				After annealing			
	%C	%H	%N	%S	%C	%H	%N	%S
HMT-0.5	0.10	1.518	0.00	0.66	0.10	0.193	0.00	0.16
HMT-1	0.22	1.340	0.00	0.84	0.12	0.160	0.00	0.27
HMT-1.5	0.22	1.220	0.00	1.16	0.18	0.147	0.00	0.64
HMT-2	0.08	0.467	0.00	1.28	0.19	0.135	0.00	0.79
HMT-2.5	0.09	0.204	0.00	1.82	0.08	0.116	0.00	1.19

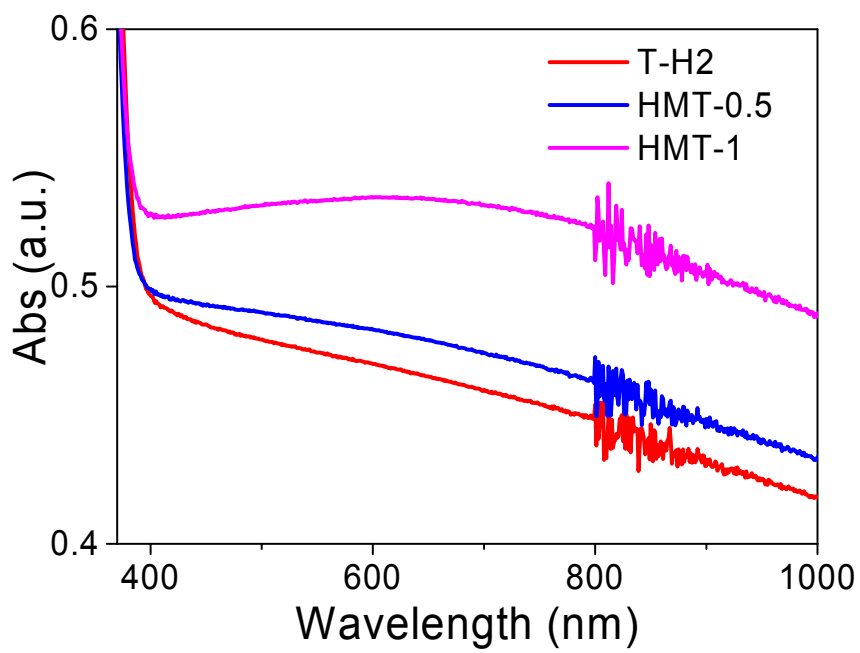


Figure S12. Absorption spectra of different samples.

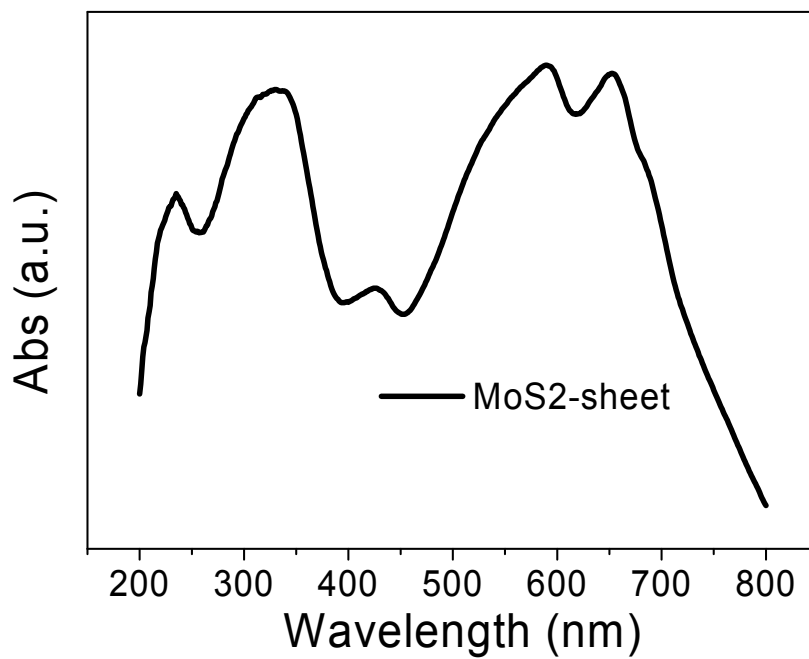


Fig. S13 Absorption spectra of the bulk MoS₂ sheet.

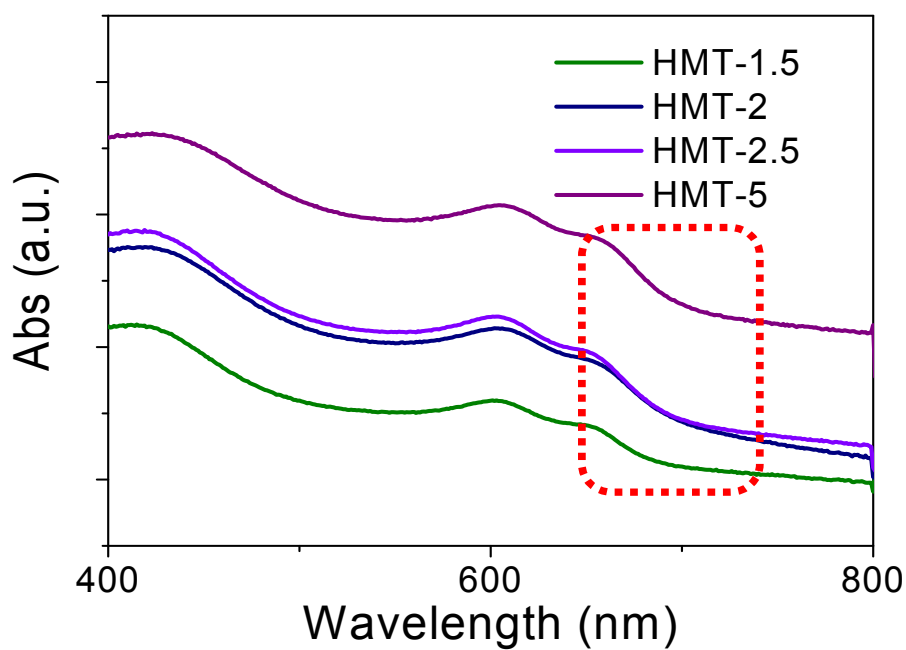


Fig. S14 Intensity normalized absorption spectra for different HMTs. The highlighted part indicating the shifting of absorption edge.

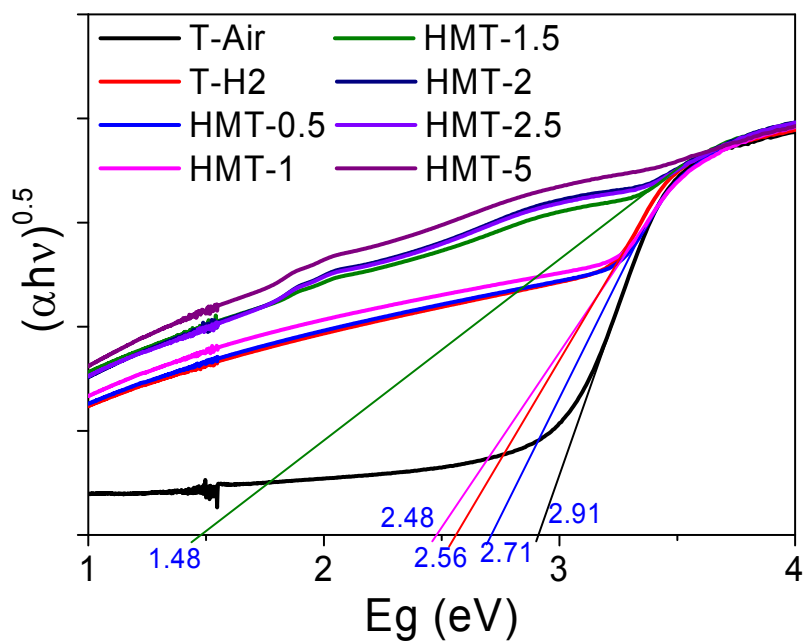


Fig. S15 Tauc plots for different HMTs obtained from UV-VIS (Figure 3c) results.

Table S2. Comparison with reported activity

Photocatalyst	Solution	Light source	H ₂ production rate (mmolg ⁻¹ h ⁻¹)	Reference
MoS₂ - Hydrogenated / Black TiO₂				
MoS₂ QD/ hydrogenated TiO₂(001)	20% methanol- water	1 sun, Simulated sunlight (AM 1.5G)	3.1	Present work
MOS₂ sheet/ hydrogenated TiO₂(001)	20% methanol- water	1 sun, Simulated sunlight (AM 1.5G)	1.5	Present work
Mesoporous Black TiO ₂ /MoS ₂ /TiO ₂ Nanosheets	20% methanol- water	300 W Xeon-lamp with a 420 nm cutoff filter.	0.56	1
MoS₂ - Normal (white) TiO₂				
2D MoS ₂ sheets / 2D anatase (001) TiO ₂ nanosheets	15% methanol- water	300 W Xe-arc lamp	2.1	2
MoS ₂ -TiO ₂ after ball- milling	20% methanol- water	300 W Xe lamp (PLS- SXE300 CUV) equipped with a UV optical filter (250–380 nm)	0.75	3
Chemically exfoliated metallic MoS ₂ nanosheets/TiO ₂	25% methanol- water	300 W Xe lamp with a 400 nm short-wave-pass cut-off filter (i.e., $\lambda < 400$ nm).	2	4
Few-layered MoS ₂ Nanosheets Wrapped Ultrafine TiO ₂ Nanobelts	20% methanol- water	1 sun	0.075	5

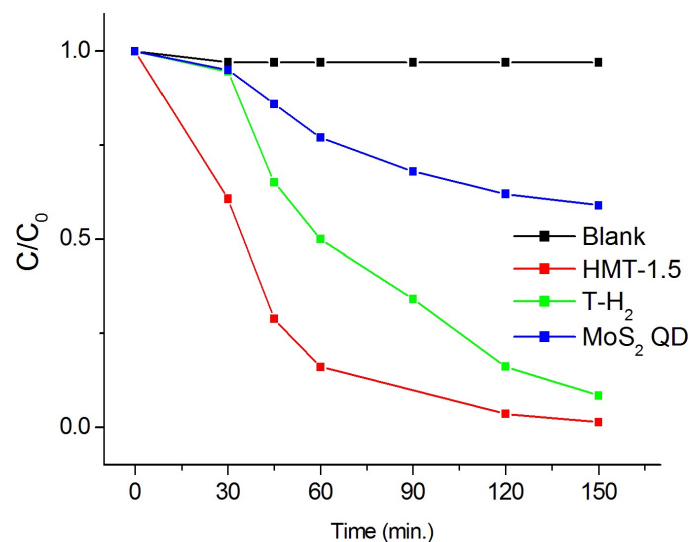


Fig. S16 Photocatalytic degradation rate of organic dye methyl orange (MO) under sunlight over synthesized HMT-1.5, HMT-0 (T-H₂) and MoS₂-QD.

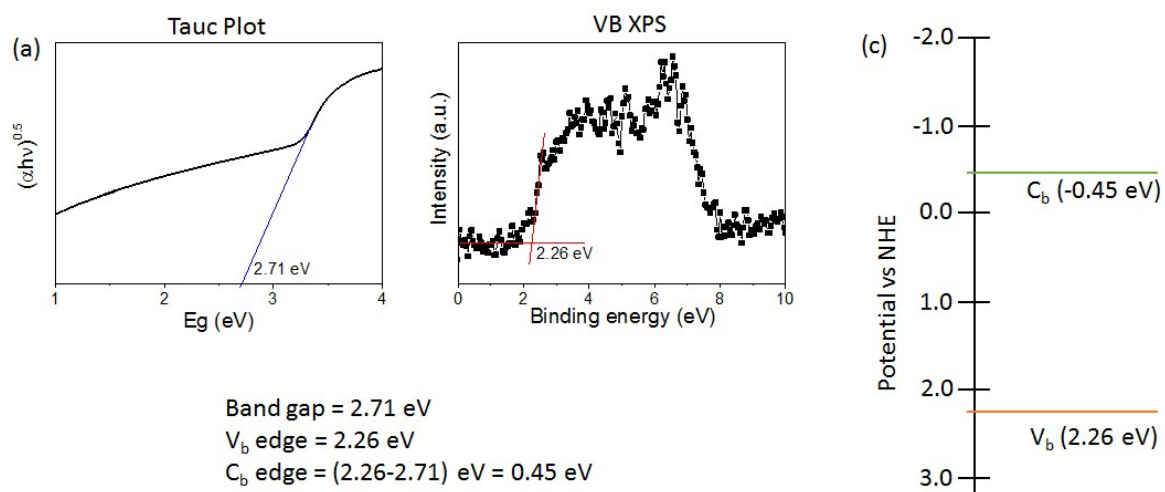


Fig. S17 (a) Tauc plot, (b) VB XPS and (c) depicted probable band energy diagram for T-H₂

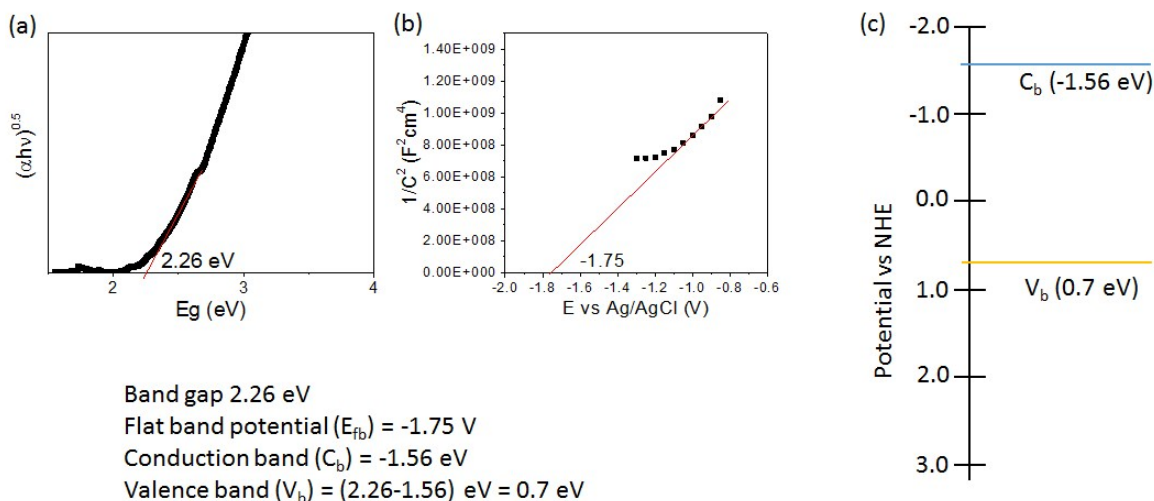


Fig. S18 (a) Tauc plot, (b) Mott-Schottky plot obtained in 1M Na₂SO₄ and (c) depicted probable band energy diagram for MoS₂-QD

References.

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