

Supporting Information

A Novel Architecture of Dandelion-like Mo₂C/TiO₂ Heterojunction Photocatalysts: Towards High-Performance Photocatalytic Hydrogen Production from Water Splitting

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Fig. s and Tables

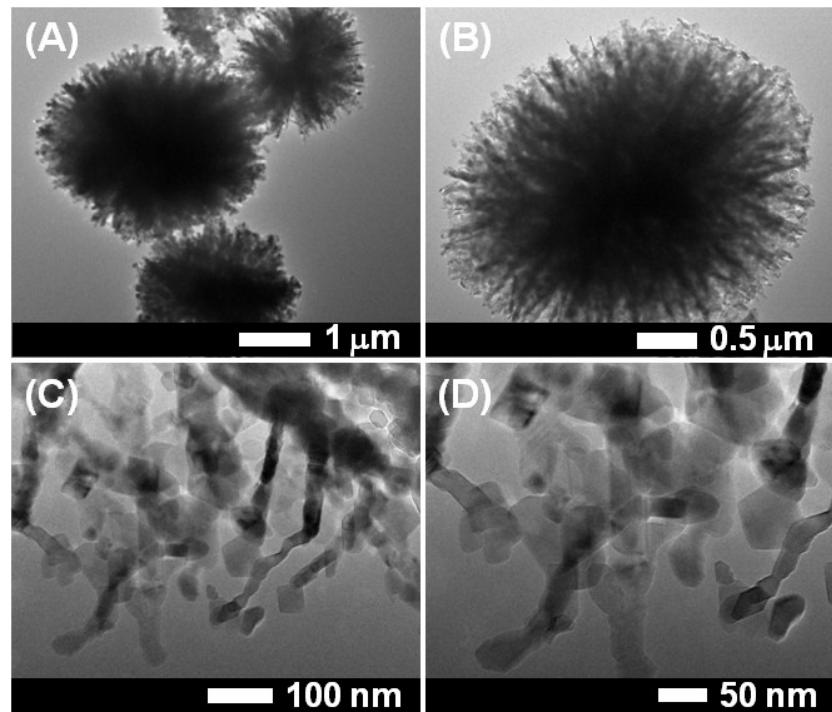


Fig. S1 TEM images of pure TiO_2 of low-resolution (A,B) and high-resolution (C,D).

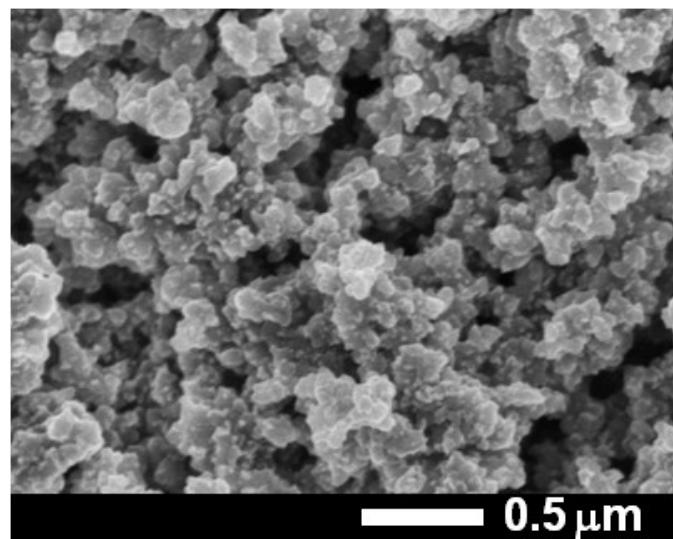


Fig. S2 SEM images of pure Mo_2C .

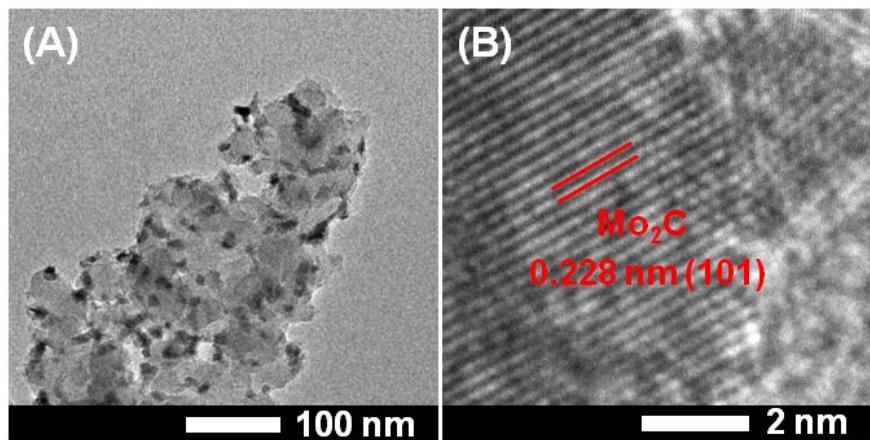


Fig. S3 A) TEM, and B) HRTEM images of pure Mo₂C.

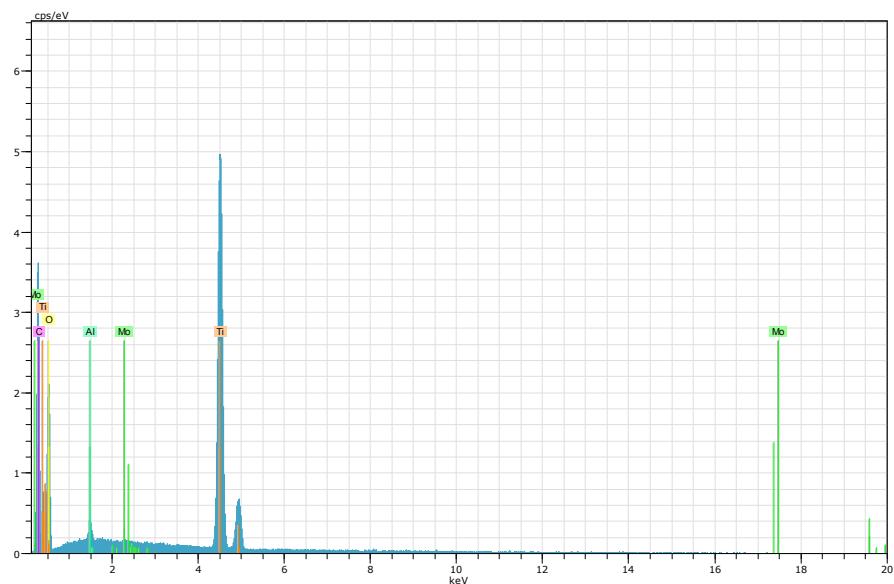


Fig. S4 EDX analysis of 1 wt% Mo₂C/TiO₂ sample.

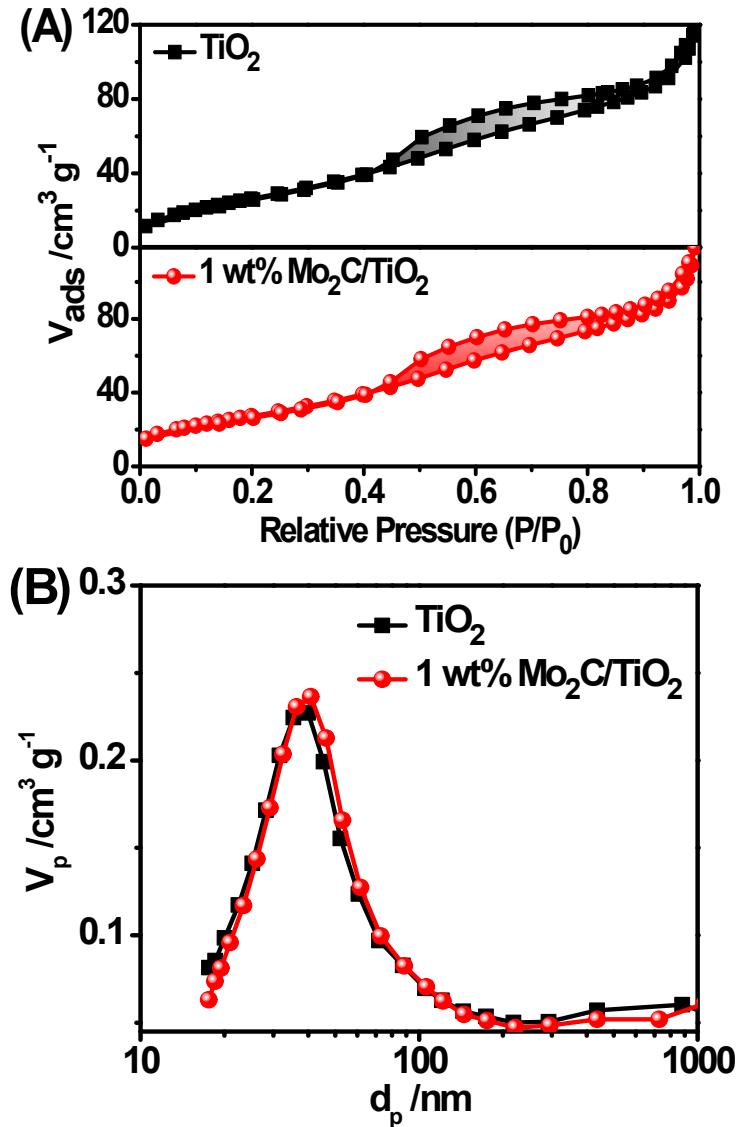


Fig. S5 (A) BET adsorption-desorption isotherms, and (B) BJH pore size distribution of the bare TiO_2 and 1 wt% $\text{Mo}_2\text{C}/\text{TiO}_2$ samples.

Nitrogen adsorption-desorption isotherms were performed to investigate the Brunauer-Emmett-Teller (BET) surface areas and porous structures of TiO_2 and 1 wt% $\text{Mo}_2\text{C}/\text{TiO}_2$. As shown in Fig. S5, the isotherms of the two present samples exhibit H3-type hysteresis behavior according to the classification of IUPAC, indicating the presence of mesopores and macropores.^{S1} The specific surface areas of TiO_2 and 1 wt% $\text{Mo}_2\text{C}/\text{TiO}_2$ are 104.0 and 105.6 $\text{m}^2 \text{g}^{-1}$, suggesting that Mo_2C 's loading is not improve the surface area of TiO_2 .

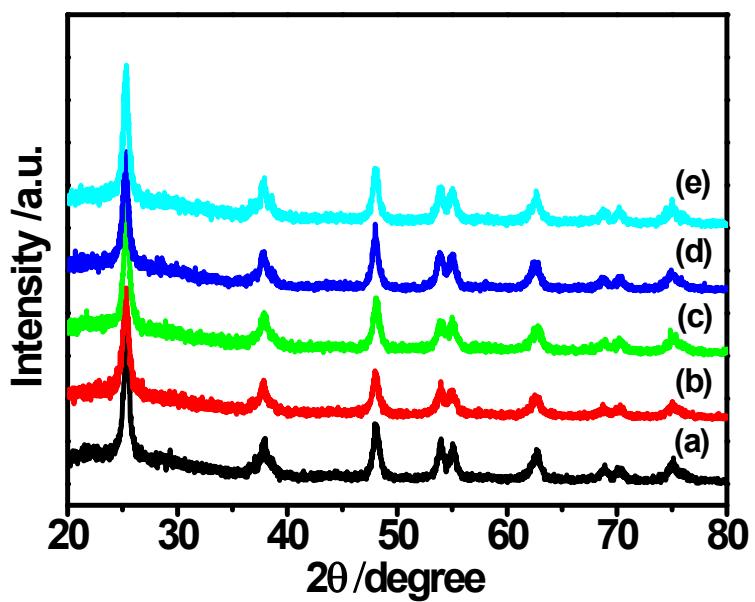


Fig. S6 XRD patterns of Mo₂C/TiO₂ hybrid with varying Mo₂C contents: (a) 0.25 wt%, (b) 0.5 wt%, (c) 1 wt%, (d) 2 wt%, and (e) 4 wt%.

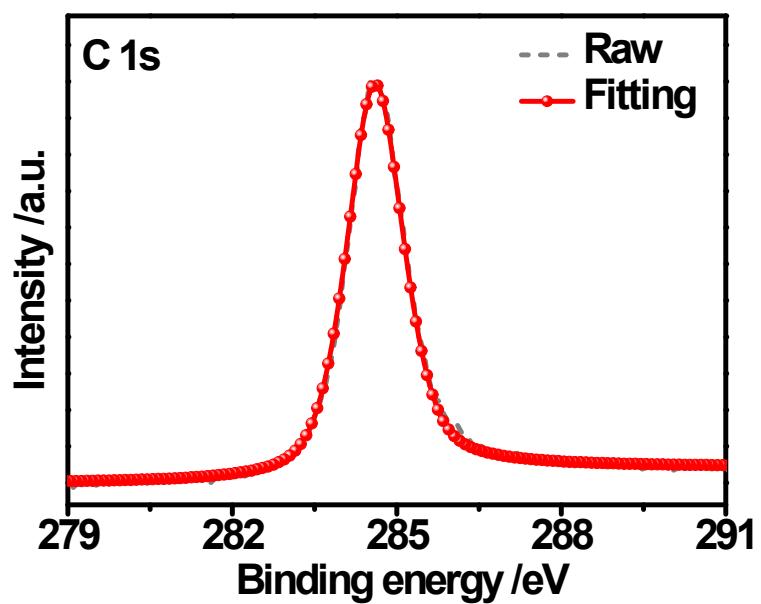


Fig. S7 XPS spectrum of C 1s for pure Mo₂C sample.

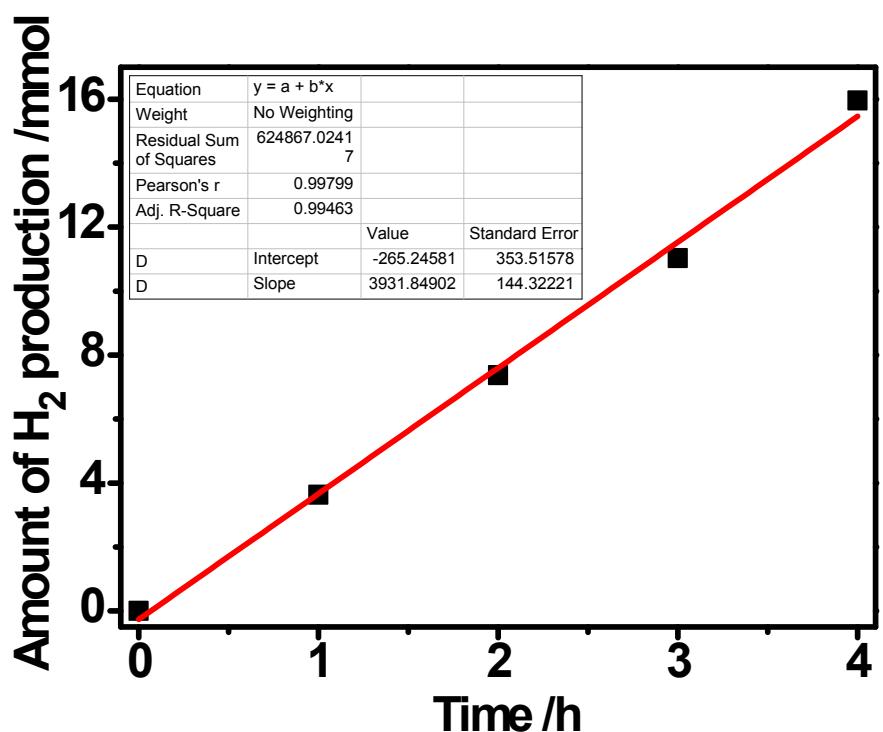


Fig. S8 Photocatalytic H₂ production measured for 1 wt% Mo₂C/TiO₂ under monochromatic light of 365 nm in 10 vol% triethanolamine aqueous solution.

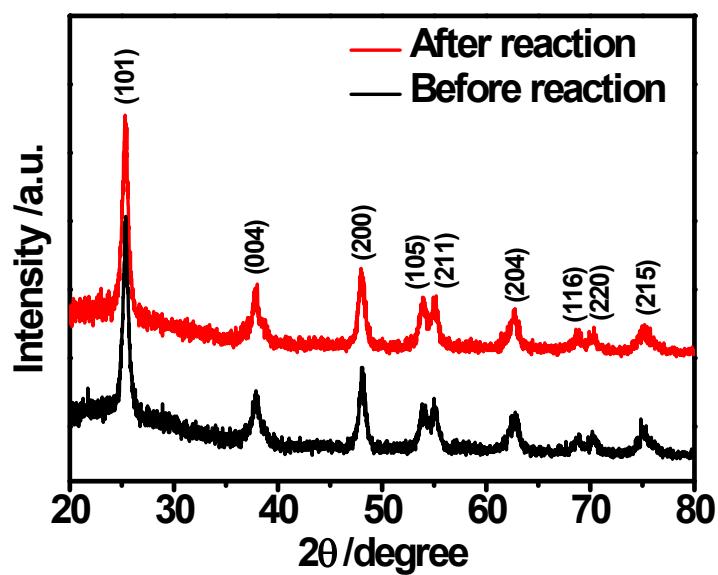


Fig. S9 XRD patterns of 1 wt% Mo₂C/TiO₂ before and after the recycling experiments.

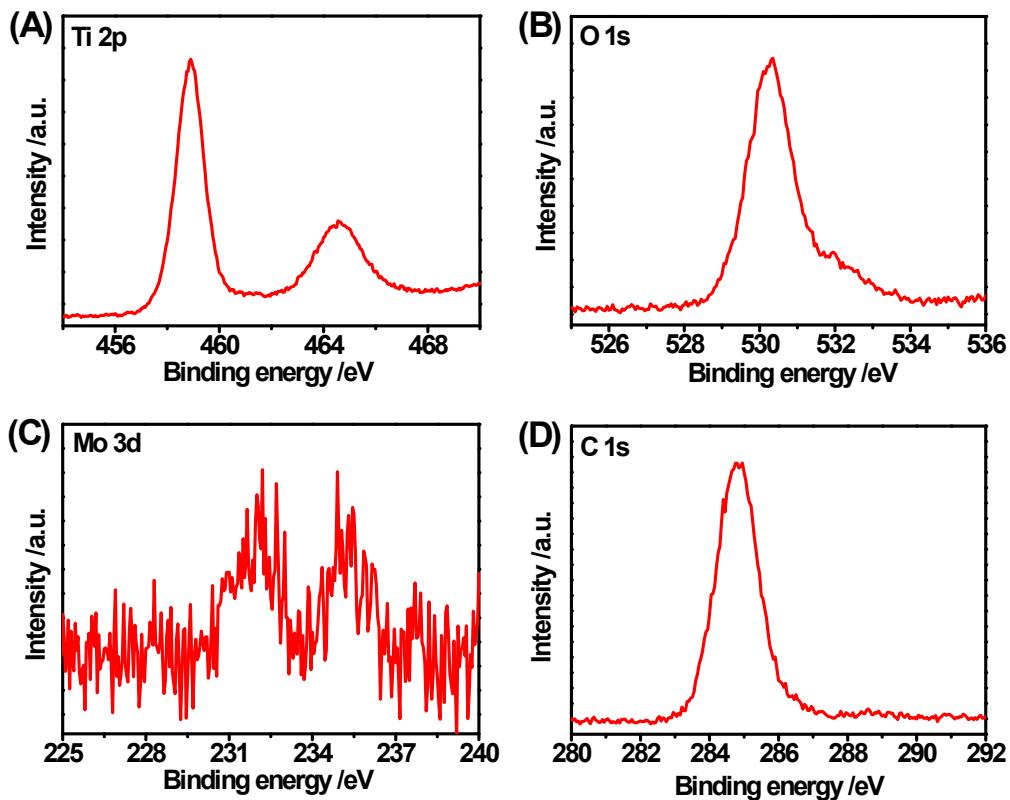


Fig. S10 The high-resolution XPS profiles of 1 wt% Mo₂C/TiO₂ after the recycling experiments for A) Ti 2p, B) O 1s, C) Mo 3d, and D) C 1s, respectively.

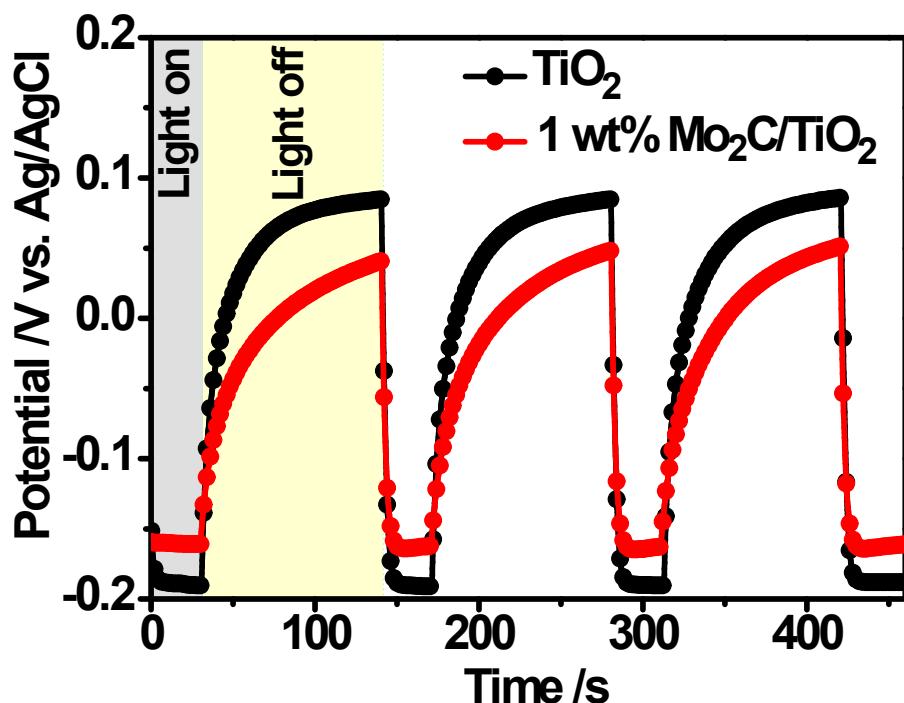


Fig. S11 OCP as a function of time under simulated solar light irradiation.

The open circuit photovoltage (OCP) decay curves were recorded under simulated solar light irradiation with on-off switches, as shown in Fig. S11. Generally, OCP decay kinetics reflects the surface charge recombination in the electrode, because bulk recombination usually occurs in the scale of nanosecond/microsecond.⁵¹

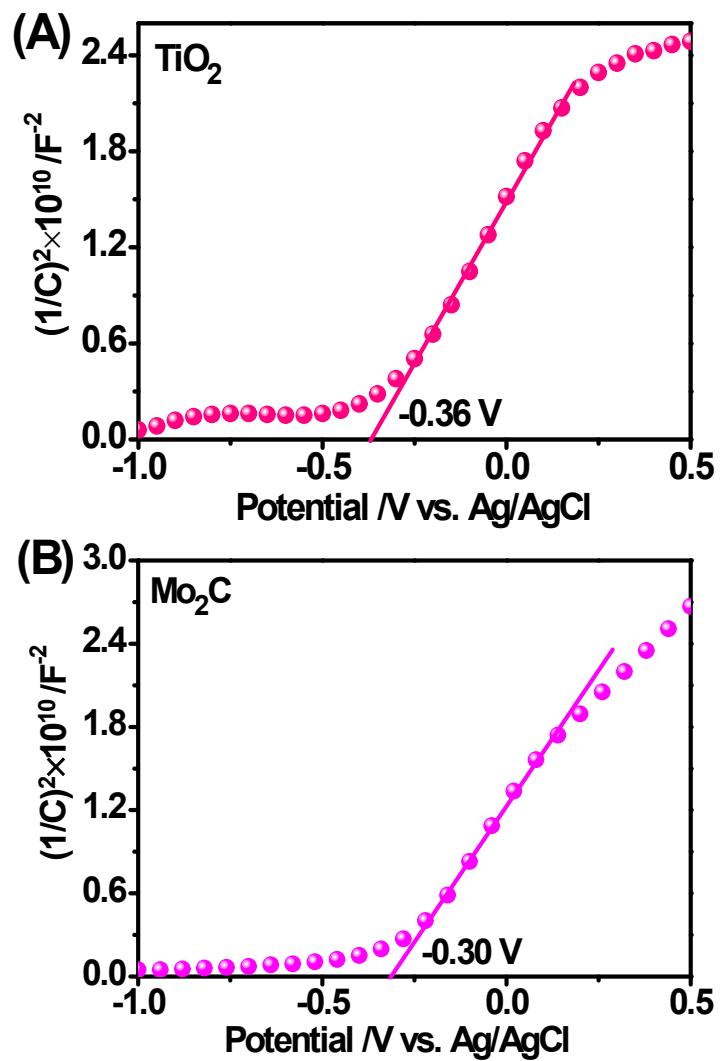


Fig. S12 M-S plots for A) TiO_2 , and B) Mo_2C in 0.5 M Na_2SO_4 solution ($\text{PH} = 7$).

Table S1. The band gap energy, energy levels of calculated conduction band edge and valence band edges for Mo₂C and TiO₂.

Semiconductors	Band gap energy E _g /eV	Conduction band edge (V vs. NHE)	Valence band edge (V vs. NHE)
Mo ₂ C	1.10	-0.30	0.80
TiO ₂	3.27	-0.36	2.91

Table S2. Comparison of photocatalytic hydrogen production performances for Mo₂C/TiO₂ system with other promising photocatalysts.

Photocatalyst	Light source	H ₂ (μmol h ⁻¹ g ⁻¹)	Ref.
FeP/TiO ₂	200 W Hg	1900	ACS Nano 2014, 8 , 11101 ²¹
Cu/TiO ₂	UV-LED (365 nm)	5104	Nano Lett. 2015, 15 , 4853 ^{S2}
MoS ₂ /RGO/TiO ₂	350 W Xe	2066	J. Am. Chem. Soc. 2012, 134 , 6575 ^{S3}
GO/TiO ₂	300 W Hg	1930	ChemSusChem 2014, 7 , 618 ^{S4}
Cu(OH) ₂ /TiO ₂	UV-LED (365 nm)	3418	Energy Environ. Sci., 2011, 4 , 1364 ^{S5}
Prorous TiO ₂	300 W Xe	23740	J. Mater. Chem. A, 2015, 3 , 3710 ^{S6}
Ni(OH) ₂ /TiO ₂	UV-LED (365 nm)	3056	J. Phys. Chem. C 2011, 115 , 4953 ^{S7}
Au/B-TiO ₂	300 W Xe	2740	ACS Catal. 2014, 4 , 1451 ^{S8}
Au@TiO ₂ /CdS	300 W Xe	1970	ACS Appl. Mater. Interfaces 2013, 5 , 8088 ^{S9}
PdAu/TiO ₂	UV-LED (365 nm)	19600	ACS Nano 2014, 8 , 3490 ¹³
PtO/TiO ₂	300 W Xe	4400	Nat. Commun. 2013, 4 , 2500 ^{S10}
CNT/TiO ₂	200 W Hg	2940	Appl. Catal. B Environ. 2015, 179 , 574 ^{S11}
MoS ₂ /TiO ₂	300 W Xe	1600	Small 2013, 9 , 140 ¹¹
Au/TiO ₂	300 W Xe	6900	Nat. Chem. 2011, 3 , 489 ¹²
Mo₂C/TiO₂	300 W Xe	39400	This work

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