Supplementary information

Synergistic Effect of 2D Ti_2C and g-C_3N_4 for efficient photocatalytic hydrogen production

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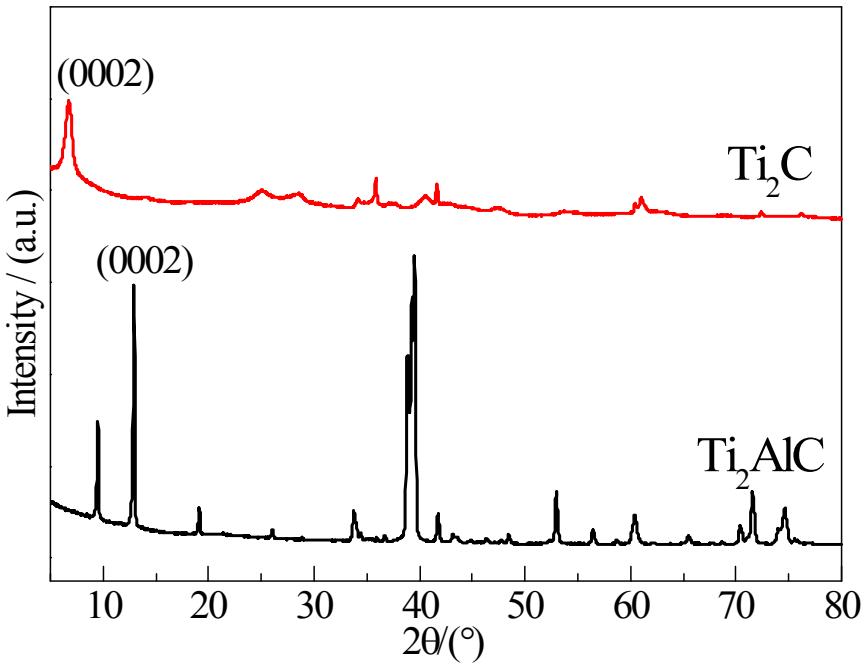

Fig. S1 XRD patterns of Ti_2C and Ti_2AlC.

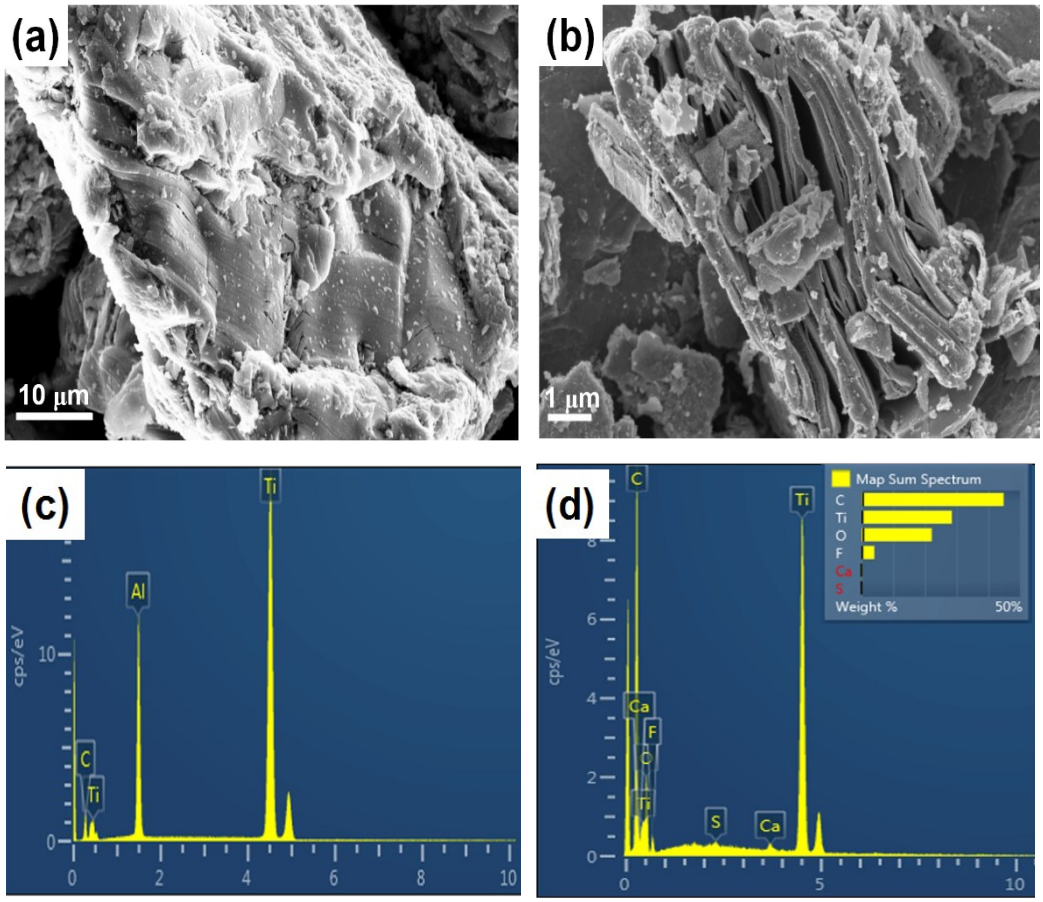

Fig. S2 SEM images of (a) Ti_2AlC and (b) Ti_2C. EDX elemental mapping for (c) Ti_2AlC and (d) Ti_2C.

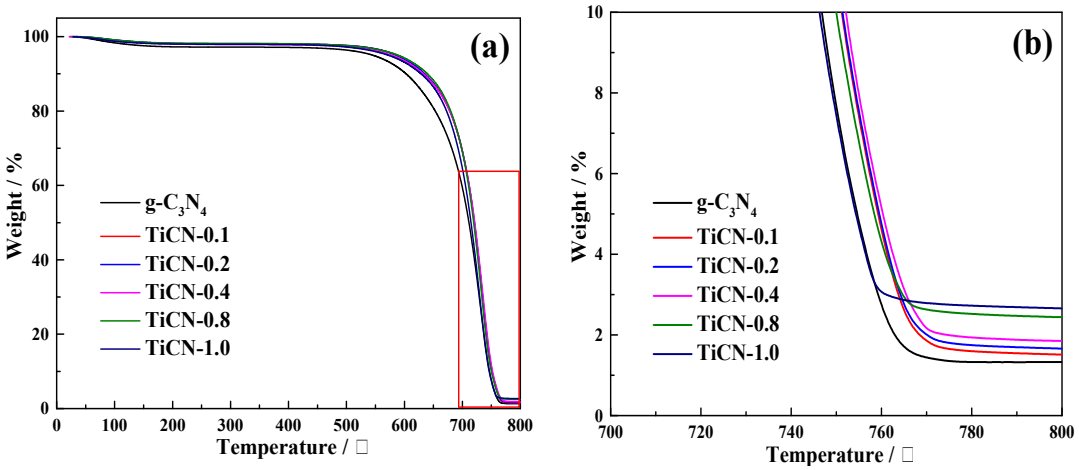

Fig. S3 (a) TG curves of g-C_3N_4 and TiCN and (b) the enlarged views of (a) in a range of 700-800 ℃.

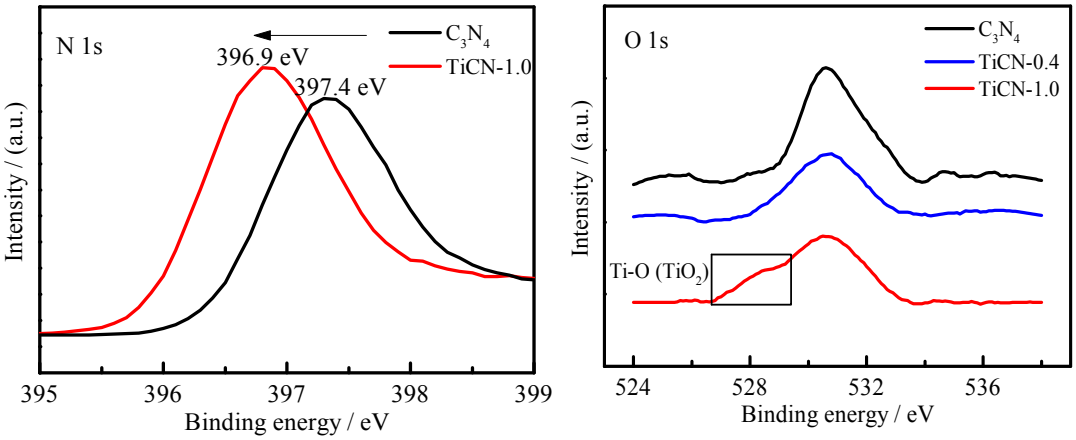

Fig. S4 XPS spectra of N 1s and O 1s for g-C_3N_4, TiCN-0.4 and TiCN-1.0.

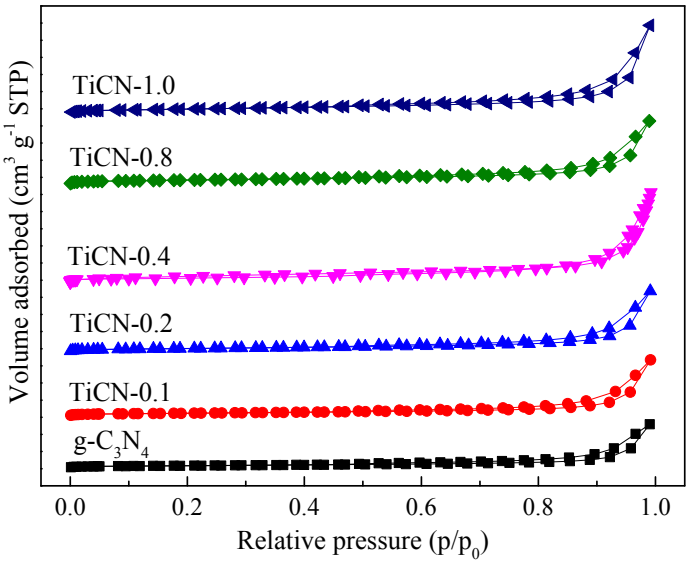

Fig. S5 N_2 adsorption-desorption isotherms of g-C_3N_4, TiCN-0.1, TiCN-0.2, TiCN-0.4,

TiCN-0.8 and TiCN-1.0.

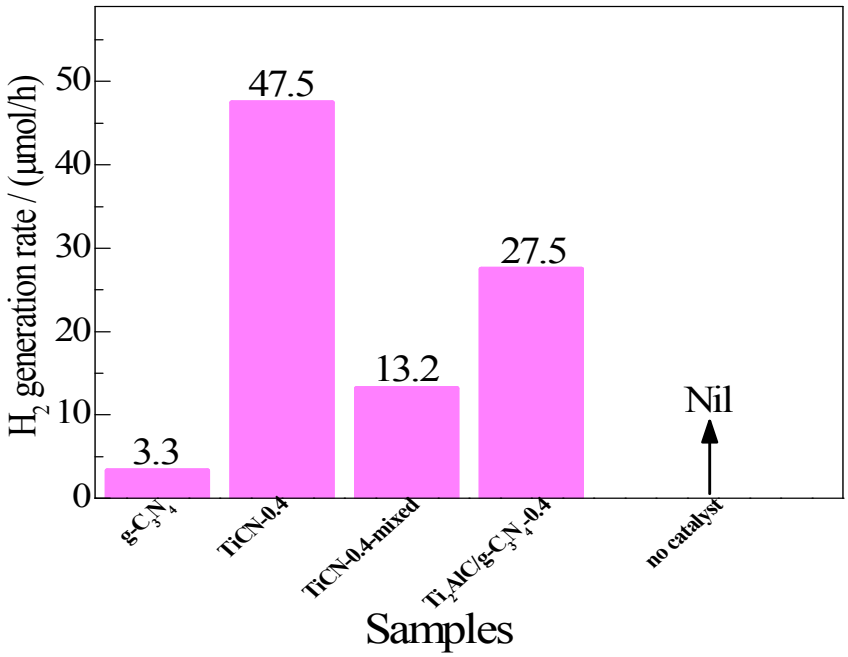

Fig. S6 Photocatalytic hydrogen production rates of g-C_3N_4, TiCN-0.4, TiCN-0.4-mixed (Ti_2C and g-C_3N_4 physical mixing), Ti_2AlC/g-C_3N_4-0.4 and no catalyst.

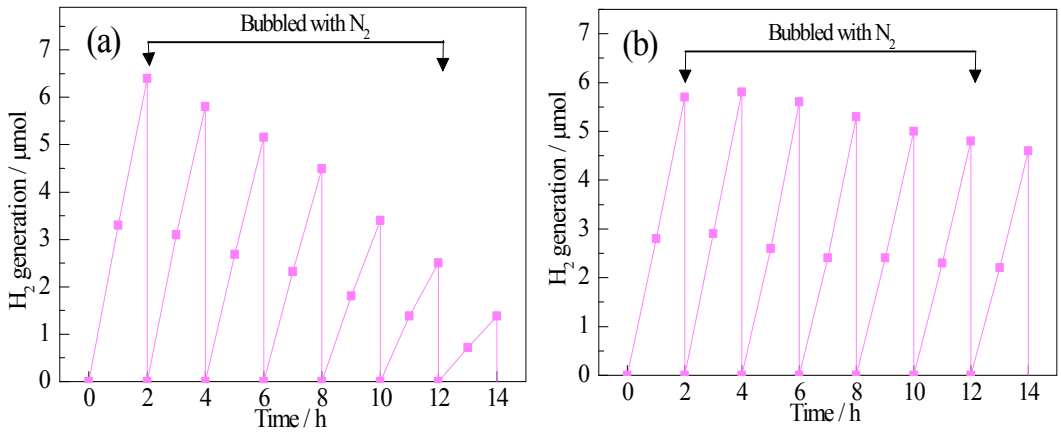

Fig. S7 Recycling studies of hydrogen production over g-C_3N_4 (a) and Ti_2C (b). The reaction system was purged with N_2 before every cycling.

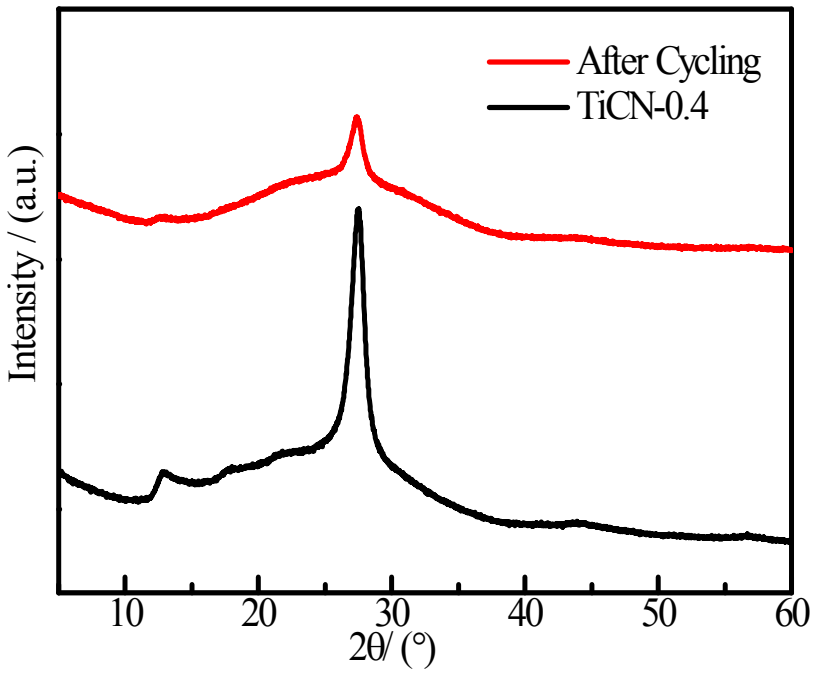

Fig. S8 XRD patterns of TiCN-0.4 and after cycling 10 times.

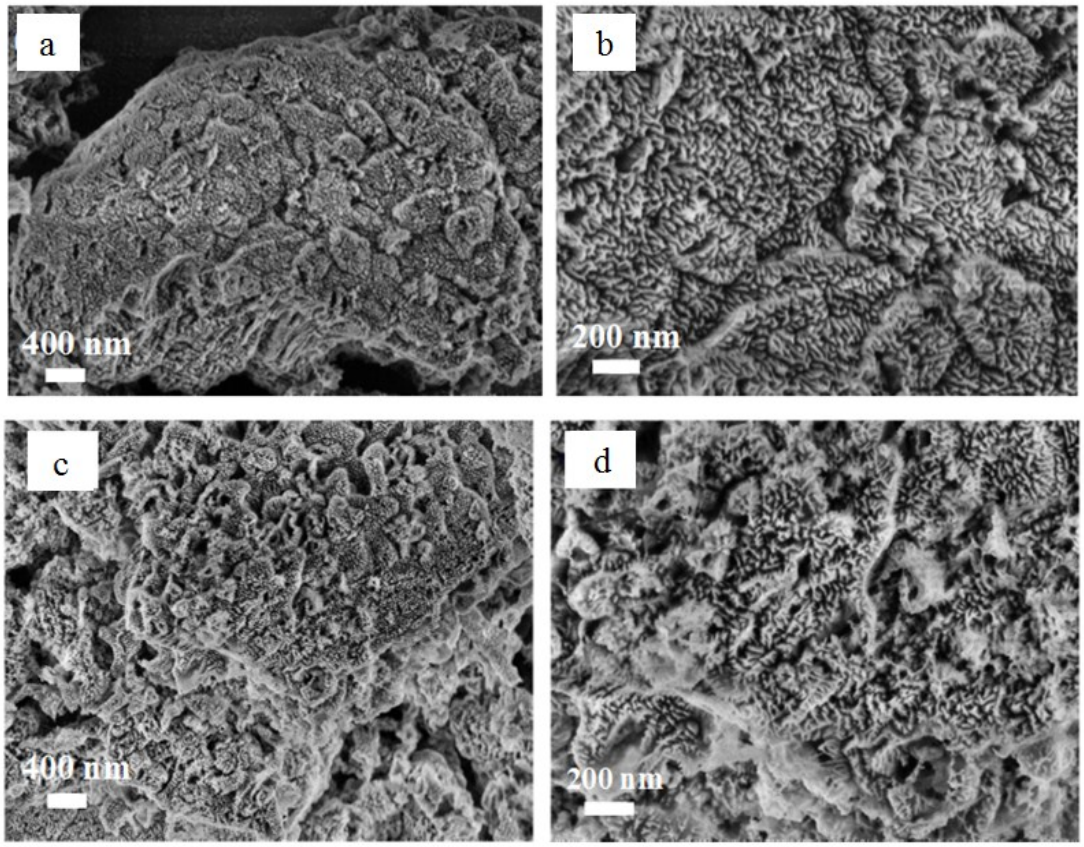

Fig. S9 SEM images of TiCN-0.4: as prepared (a, b) and after cycling 10 times (c, d).

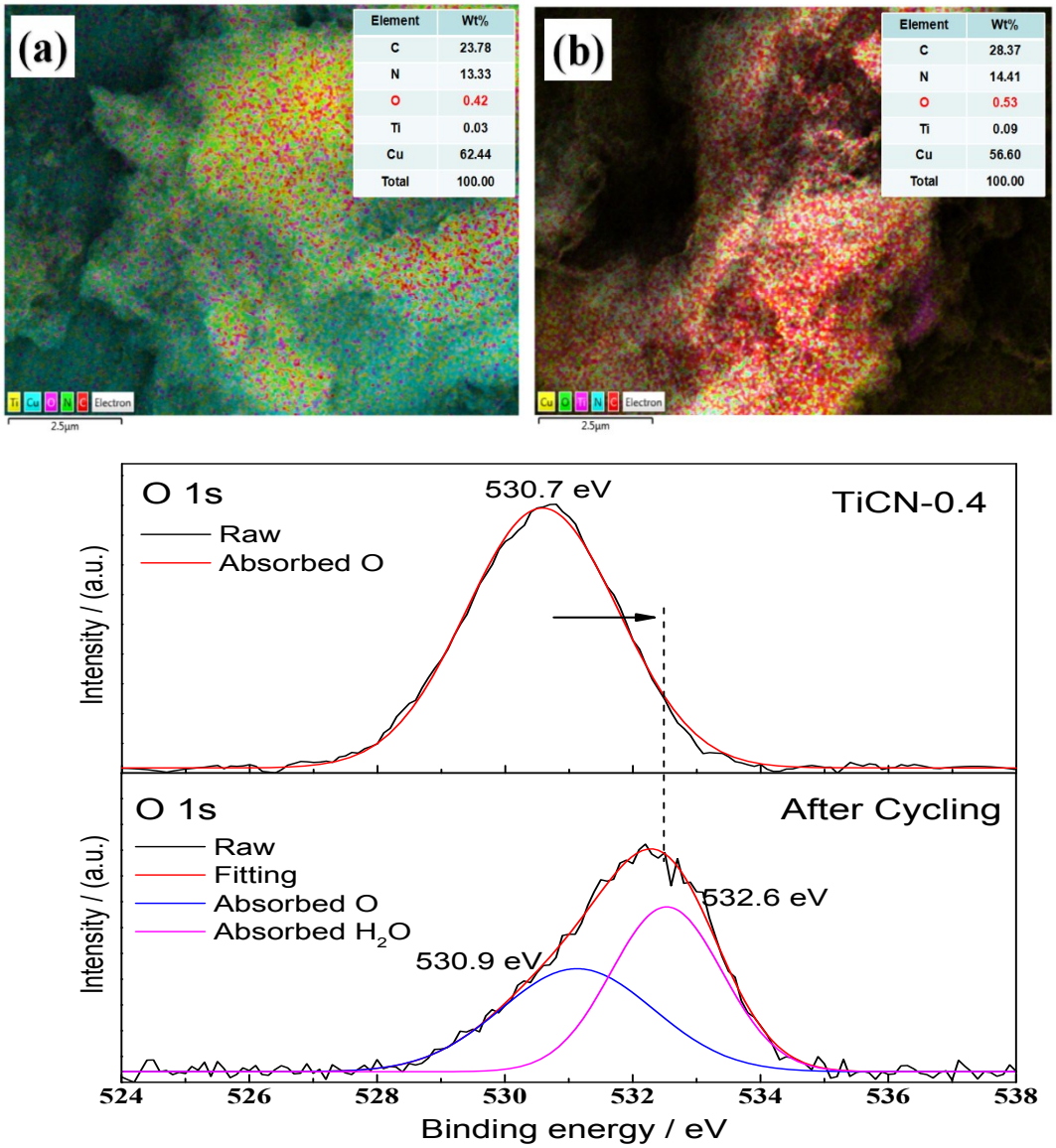

Fig. S10 EDS elemental mapping for TiCN-0.4: a) as prepared and b) after cycling 10 times; XPS spectra of O 1s for TiCN-0.4: as prepared and after cycling 10 times. Notes: the high percentage of Cu in the EDS mapping of TiCN-0.4 is attributed to the Cu substrate.

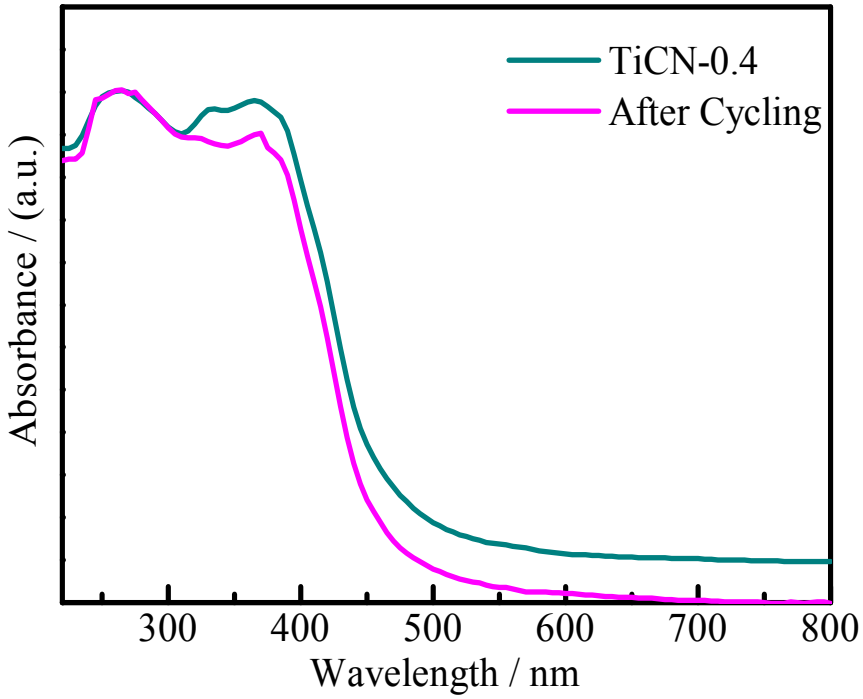

Fig. S11 UV-vis adsorption spectra of TiCN-0.4: as prepared and after cycling 10 times.

Table S1 Comparison of the photocatalytic H_2 production rate for g-C_3N_4-based photocatalysts loading different co-catalysts

Photocatalyst	Amount of photocatalyst (mg)	Co-catalyst	Loading method	Optimum loading	Light source	Hydrogen production rate (μmol/h/g)	Reference
TiCN-0.4	**50**	**Ti_2C**	**Calcination**	**0.4 wt%**	**solar simulator AM 1.5**	**950**	**This work**
Pt/g- C_3N_4	50	Pt	Adsorption-deposition	1 wt%	350 W Xe lamp	588	1
MoS_x/g-C_3N_4	50	MoS_x	Adsorption-in situ transformation	3 wt%	four low-power LEDs	273.1	2
CoP/g-C_3N_4	100	CoP	Grinding	0.25 wt%	300 W Xe lamp	474.4	3
Ni/g-C_3N_4	10	Ni	Photodeposition	7.4 wt%	300 W Xe lamp	4318	4
Cu/g-C_3N_4	50	Cu	Milling	3 wt%	Xe lamp	20.5	5
Ag_2S/g-C_3N_4	50	Ag_2S	Photodeposition	5 wt%	Four low power UV-LEDs	200	6
NiS/g-C_3N_4	100	NiS	Hydrothermal	1.1 wt%	300 W Xe lamp	482	7
Ni_2P/g-C_3N_4	20	Ni_2P	Hydrothermal	0.4 wt%	300 W Xe lamp	183.6	8
WS_2/g-C_3N_4	50	WS_2	Impregnation-sulfidation	0.3 wt%	300 W Xe lamp	240	9
Graphene/g-C_3N_4	80	Graphene	Impregnation-chemical reduction	1.0 wt%	350 W Xe lamp	451	10
Carbon nanotubes/g-C_3N_4	100	Carbon nanotubes	Heat treatment	0.5 wt%	300 W Xe lamp	42	11

Computational method

The density functional theory (DFT) calculations were performed by using the Vienna ab initio simulation package (VASP).[12,13] To describe the valence and core states, plane wave basis set and projector augmented wave (PAW) potentials were employed with a kinetic energy cutoff of 500 eV.[14] The Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA) exchange and correlation functional was used.[15] For structure relaxation, both lattice constants and atom coordinates were optimized until the forces converged to less than 0.02 eV/Å. The Monkhorsk- Pack k-point sampling of g-C_3N_4 and Ti_2C were 5 × 5 and 15 × 15, respectively. For density of states (DOS) calculations, Gaussian smearing was 0.05 eV and Monkhorsk-Pack k-point sampling of g-C_3N_4 and Ti_2Cwere 7 × 7 and 21 × 21. The vacuum layer was 20 Å in vertical direction.

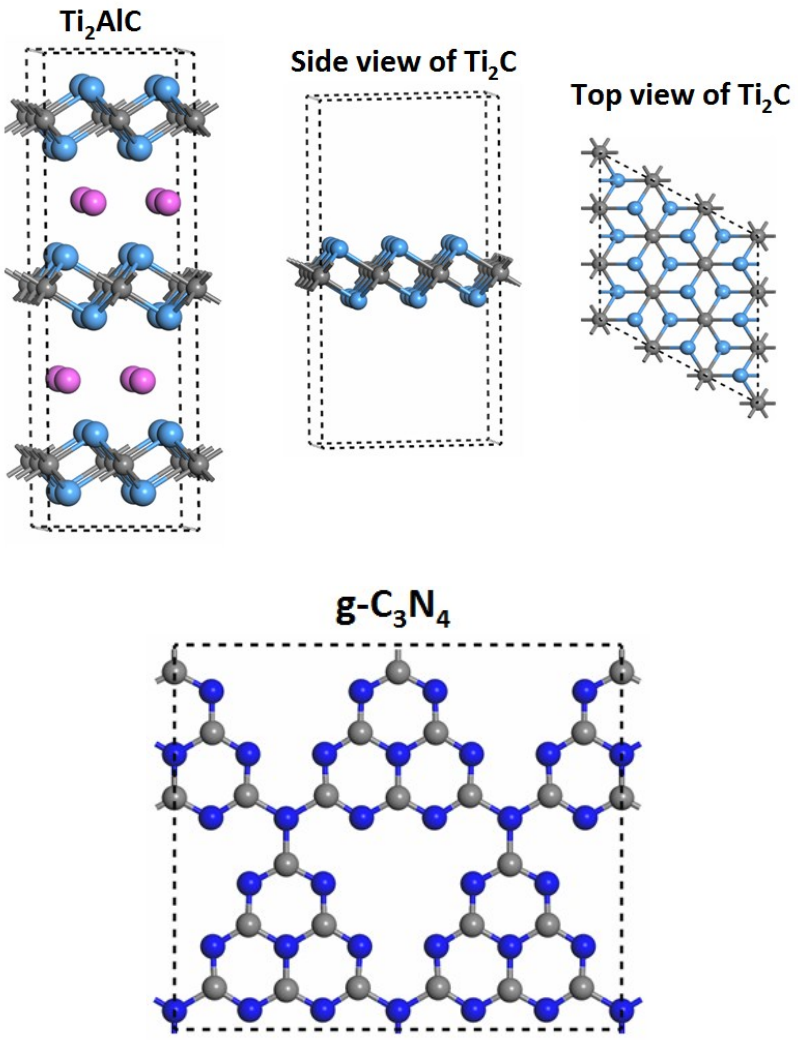

Fig. S12 The structural models of Ti_2AlC, Ti_2C and g-C_3N_4.

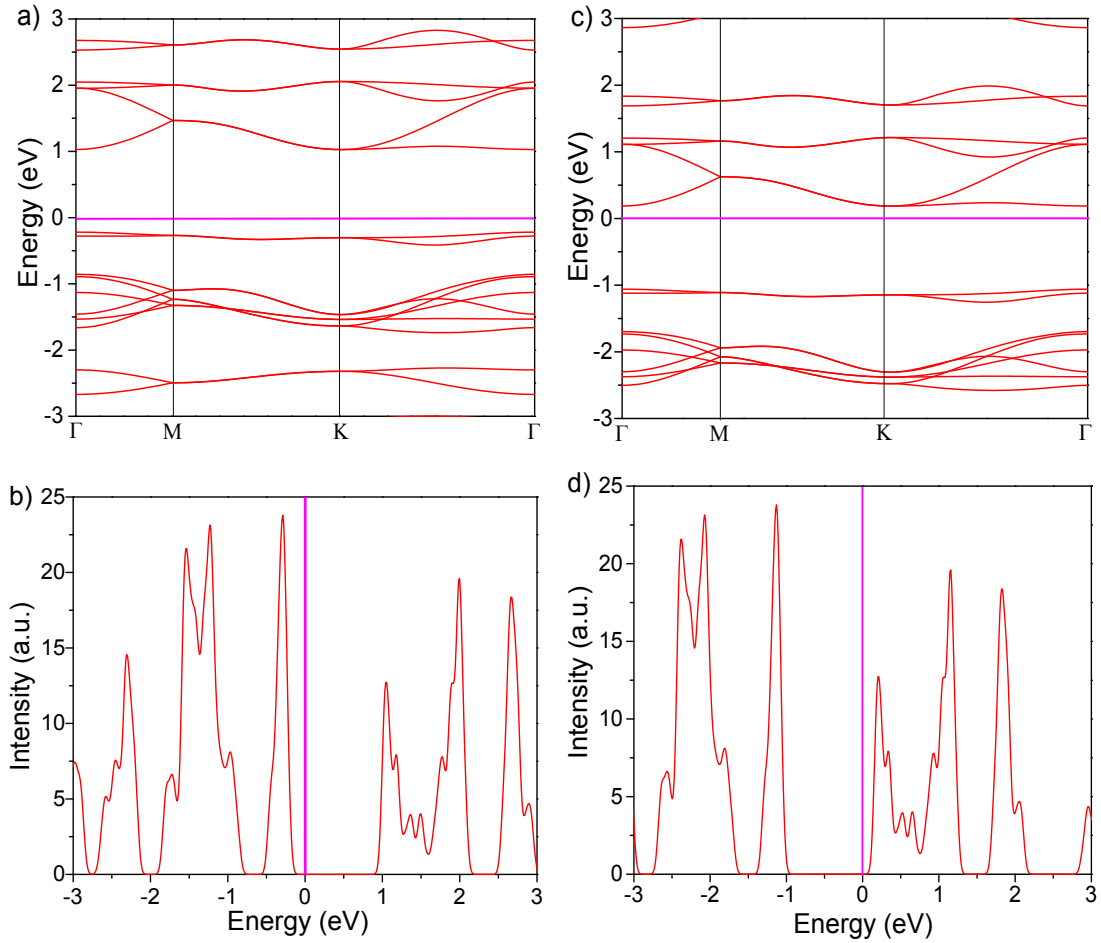

Fig. S13 The calculated band structure of (a) g-C_3N_4 and (c) TiCN; and the total density of states of (b) g-C_3N_4 and (d) TiCN.

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