

SUPPORTING INFORMATION

**Robust Route to Photocatalytic Nitrogen Fixation Mediated by
Capitalizing on Defect-Tailoring InVO₄ Nanosheets**

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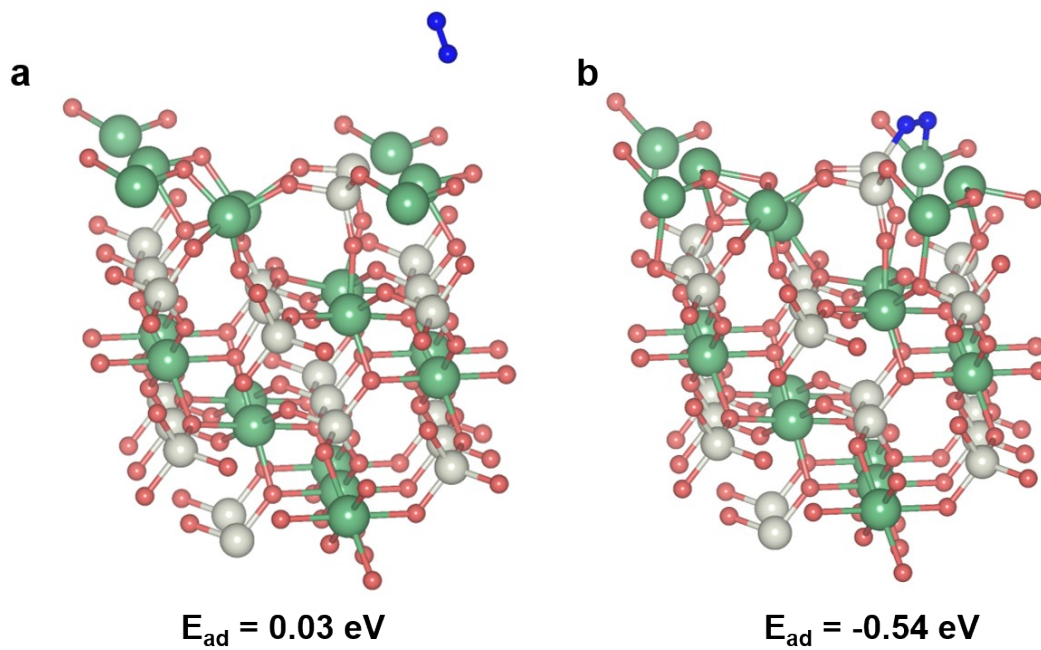


Figure S1. Calculated model and corresponding energy of a N_2 molecule adsorbed on (a) the top site of In atom and (b) the bridge site between In and V atom.

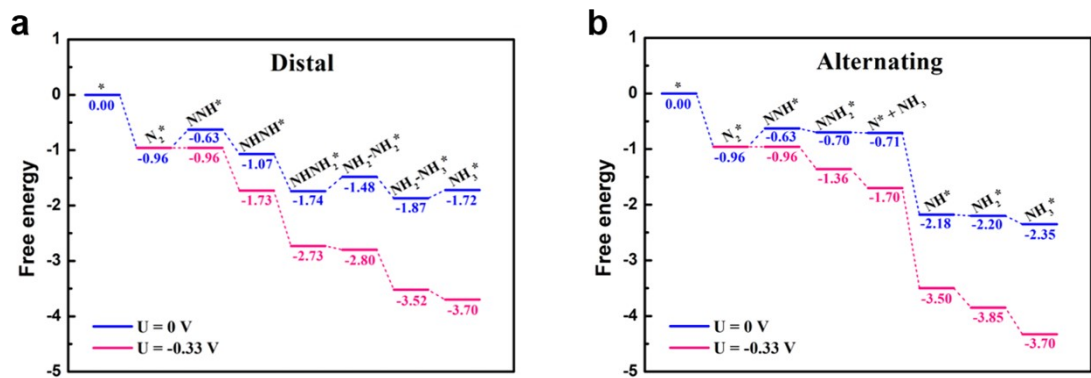


Figure S2. Free energy diagrams for N₂ reduction through (a) distal, (b) alternating mechanisms at U = 0 V and -0.33 V, respectively.

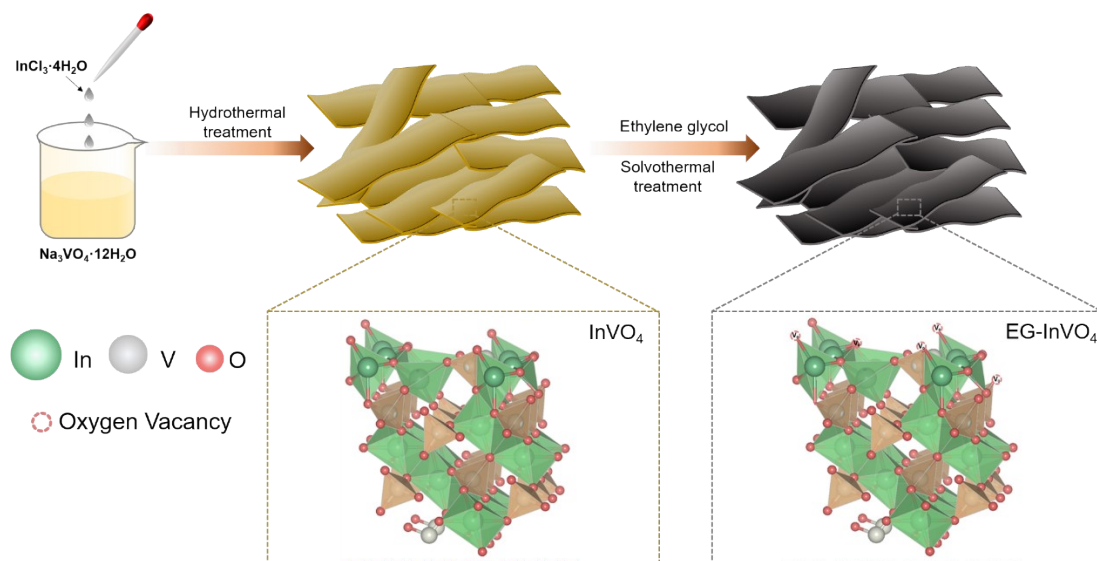


Figure S3. Schematic synthetic route of InVO₄ and EG-InVO₄ nanosheets. InVO₄ nanosheets were synthesized via a mild hydrothermal method. Then the obtained samples were dispersed in the reducing agent (i.e., ethylene glycol). At last, the InVO₄ photocatalysts rich in oxygen vacancies could be obtained after a solvothermal treatment.

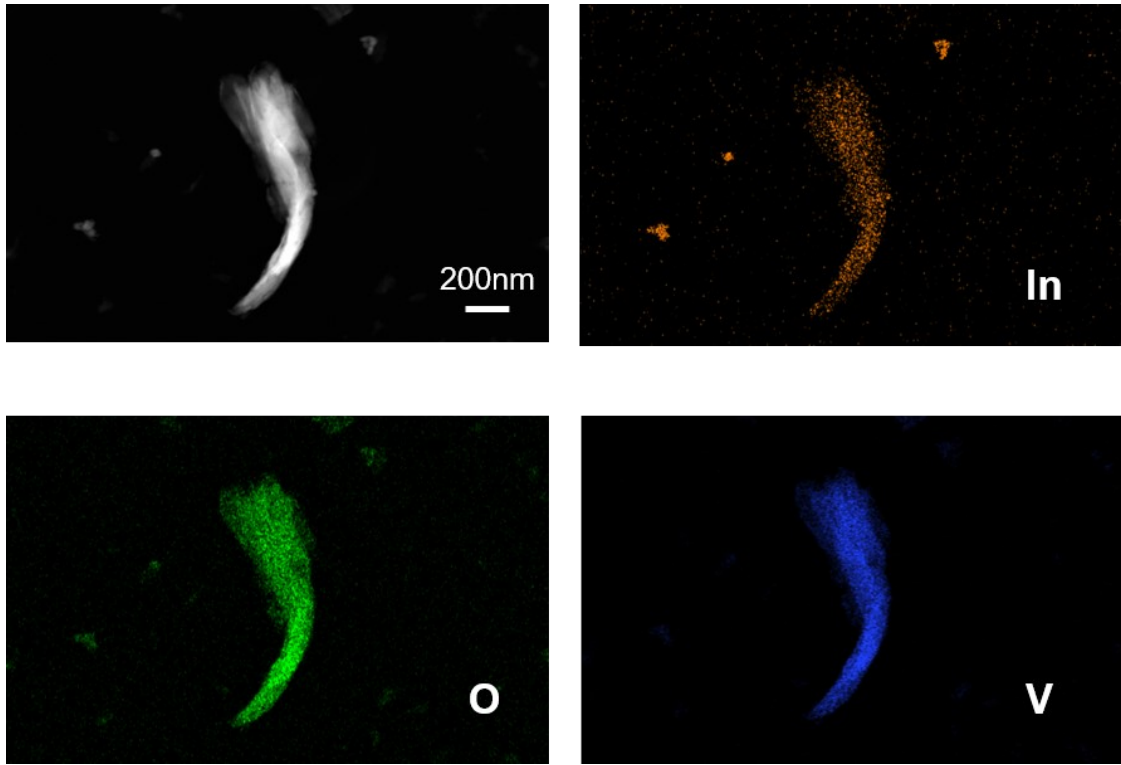


Figure S4. STEM image and EDS element mapping profiles of InVO_4 with In, O, and V distribution.

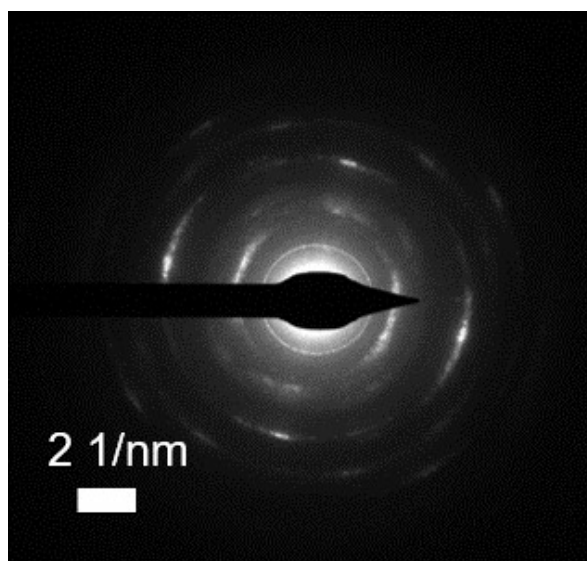


Figure S5. SAED patterns of EG10h-InVO₄

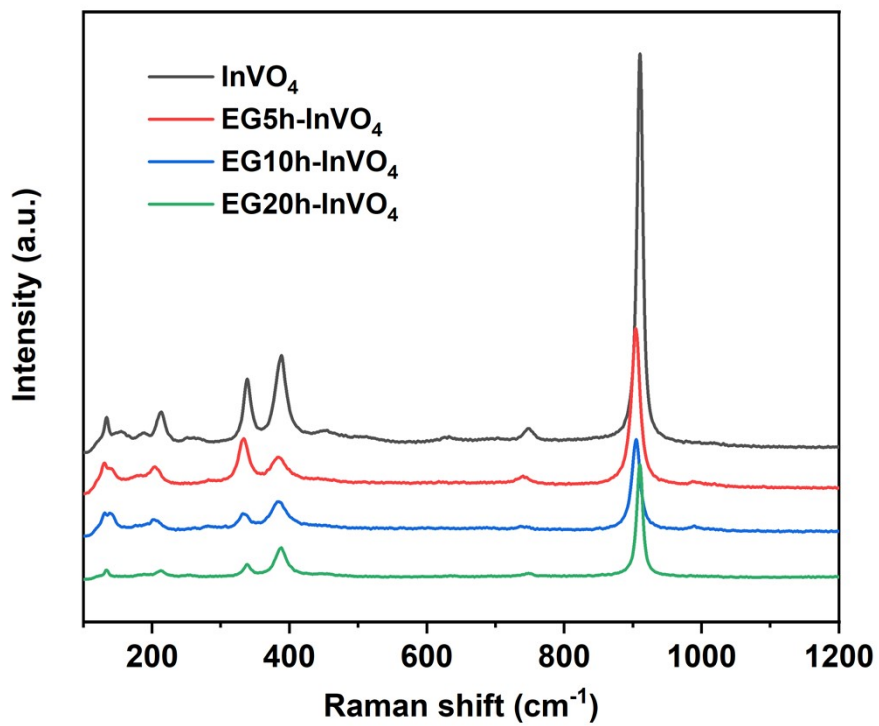


Figure S6. Raman patterns of InVO₄ with different solvothermal treatment times. The Raman peaks for all the samples can be well indexed to the InVO₄, indicating that the introduction of oxygen vacancies does not alter the crystal phase.

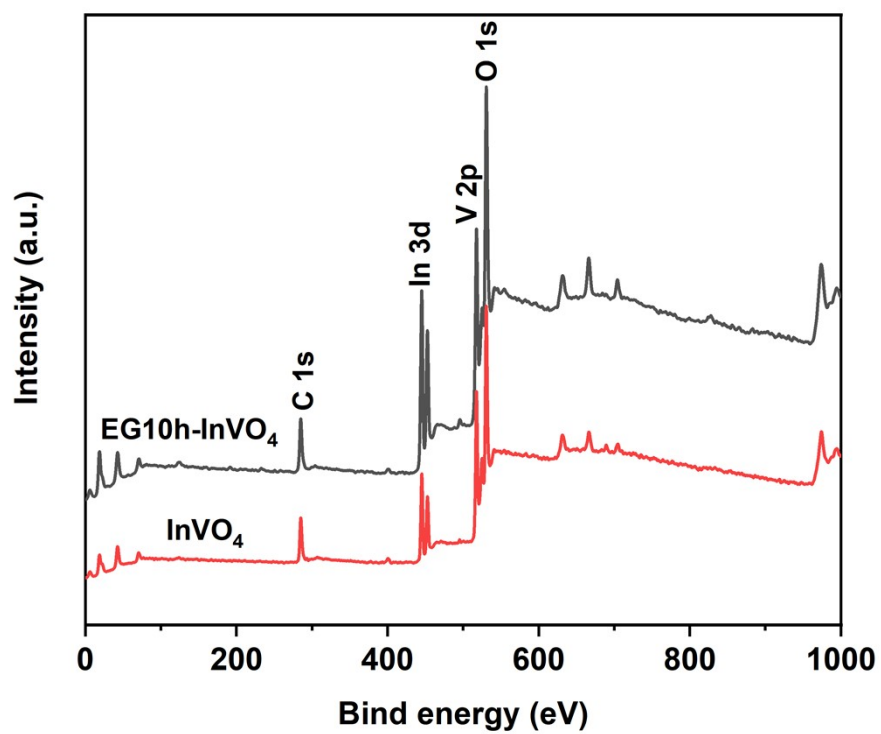


Figure S7. XPS survey spectra of InVO₄ and EG10h-InVO₄.

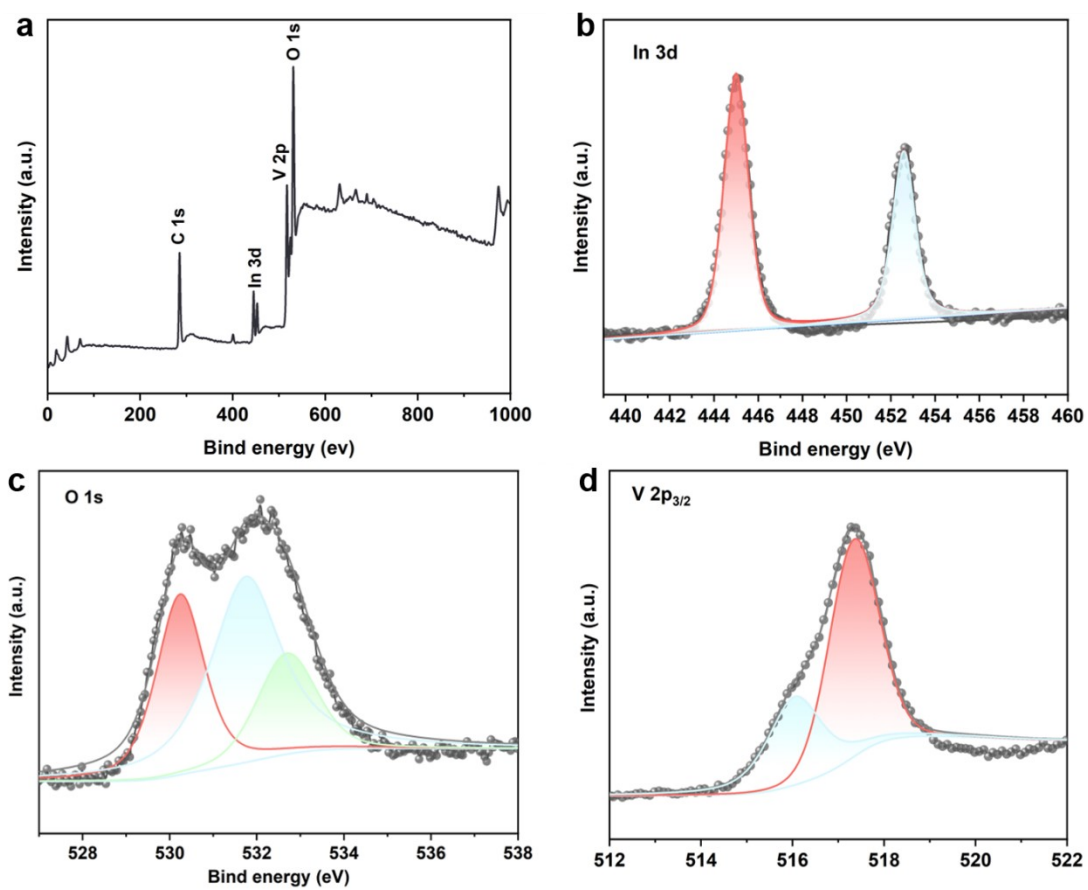


Figure S8. (a) XPS survey spectra of EG20h-InVO₄. High-resolution XPS spectra of (b) In 3d, (c) O 1s, and (d) V 2p_{3/2} of EG20h-InVO₄.



Figure S9. Digital image of (a) InVO_4 and (b) EG10h-InVO_4 .

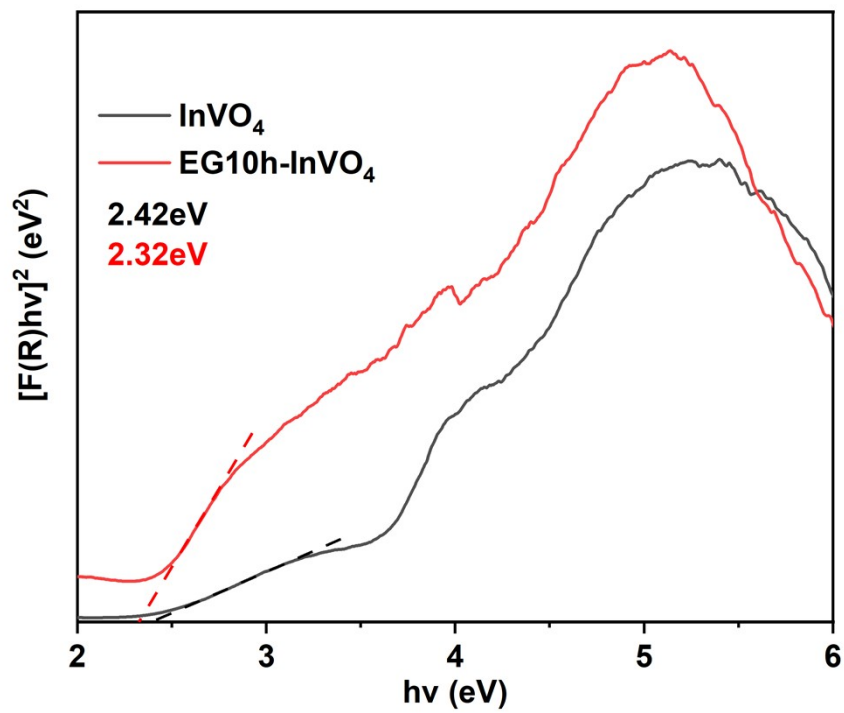


Figure S10. Tauc plots of InVO_4 and EG10h-InVO_4 .

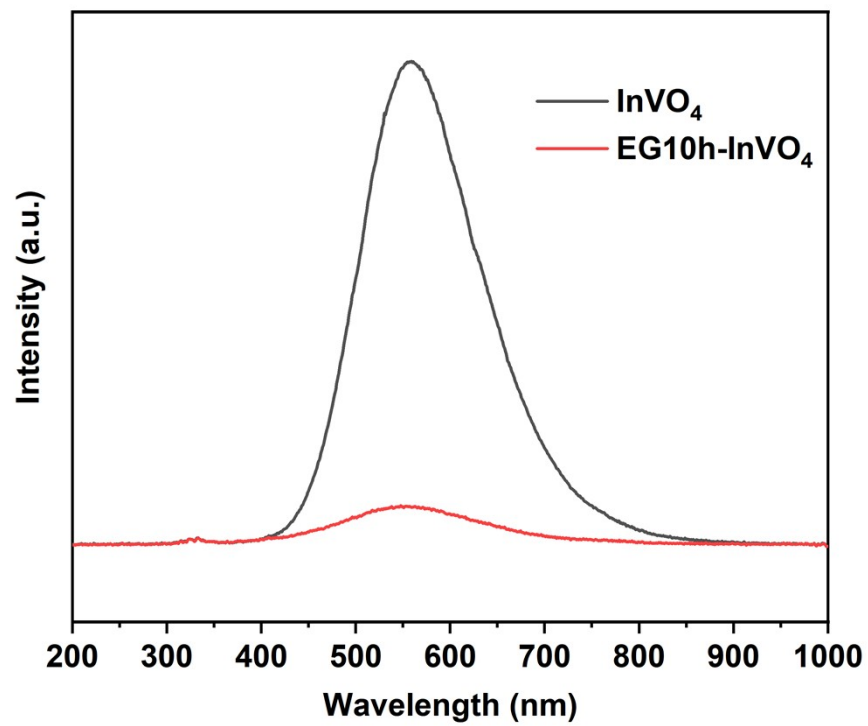


Figure S11. PL spectra of pristine InVO₄ and EG10h-InVO₄.

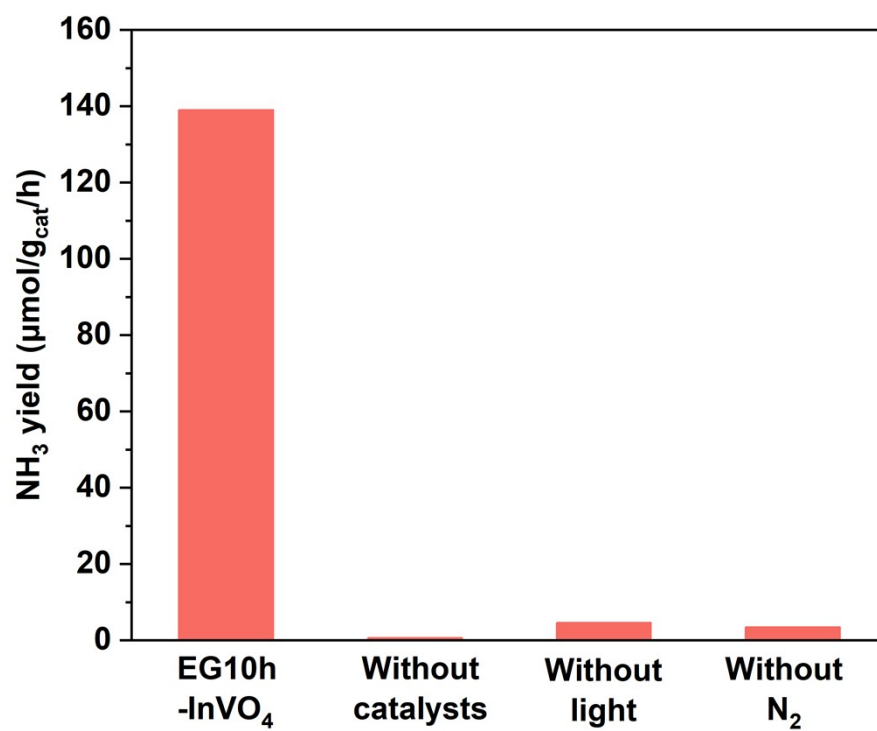


Figure S12. Control experiments under different conditions.

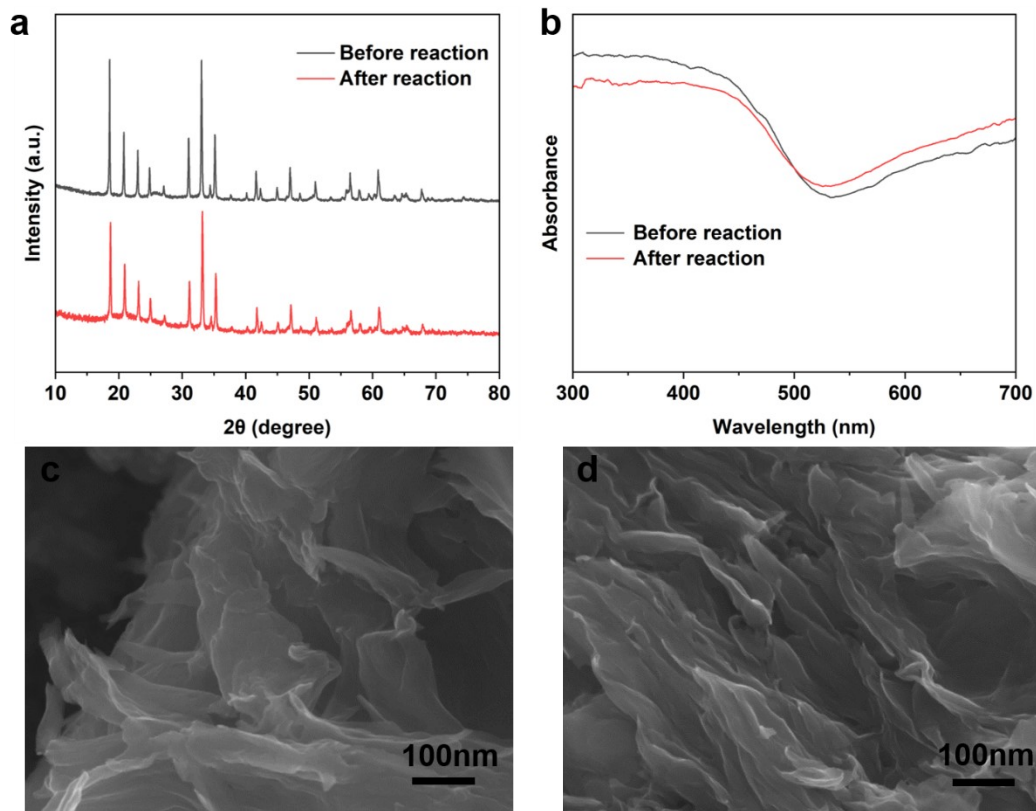


Figure S13. (a) XRD patterns, (b) UV-vis absorption spectra of EG10h-InVO₄ before and after the photocatalytic reaction. SEM images of the EG 10h-InVO₄ nanosheets (c) before and (d) after the photocatalytic reaction.

Table S1. Specific surface areas of different samples

Samples	Specific Surface Area (m ² /g)
InVO ₄	2.3271
EG5h-InVO ₄	3.0307
EG10h-InVO ₄	5.2493
EG20h-InVO ₄	2.6351

Table S2. The ratio of V⁵⁺, V⁴⁺ and different types of oxygen in InVO₄, EG10h-InVO₄ and EG20h-InVO₄ reckoned by XPS.

	V ⁵⁺	V ⁴⁺	lattice oxygen	oxygen vacancy	surface oxygen
InVO ₄	83.46%	16.54%	92.04%	4.78%	3.18%
EG10h-InVO ₄	65.13%	34.87%	62.05%	26.41%	11.54%
EG20h-InVO ₄	74.94%	25.06%	30.2%	50.64%	19.16%