

Supporting Information

Core-Shell InN/PM6 Z-scheme Heterojunction Photoanodes for Efficient and Stable Photoelectrochemical Water Splitting

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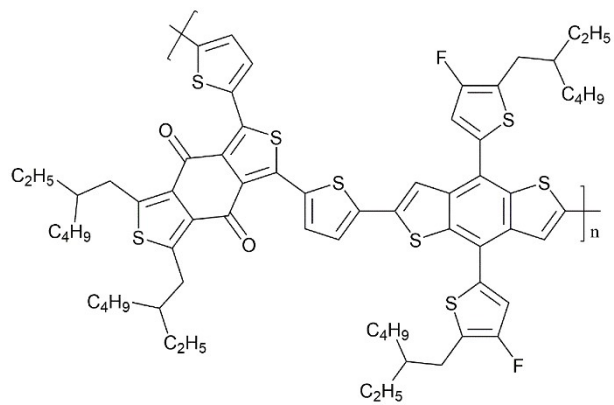


Fig. S1. Chemical structures of PM6.

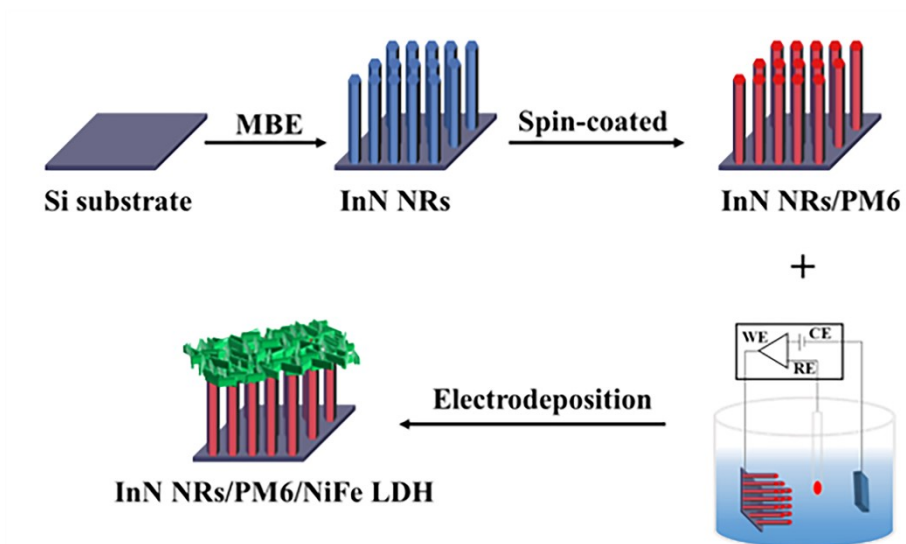


Fig. S2. Schematic diagram for the preparation of the InN/PM6/NiFe LDH photoelectrode.

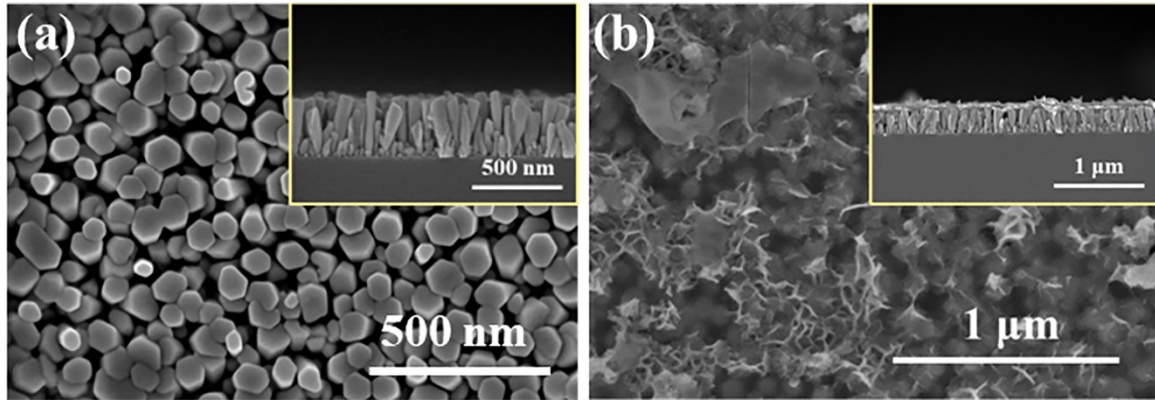


Fig. S3. The top view of SEM image of (a) InN NRs and (b) InN/PM6/NiFe LDH photoelectrode. The inset is the corresponding side view of SEM image.

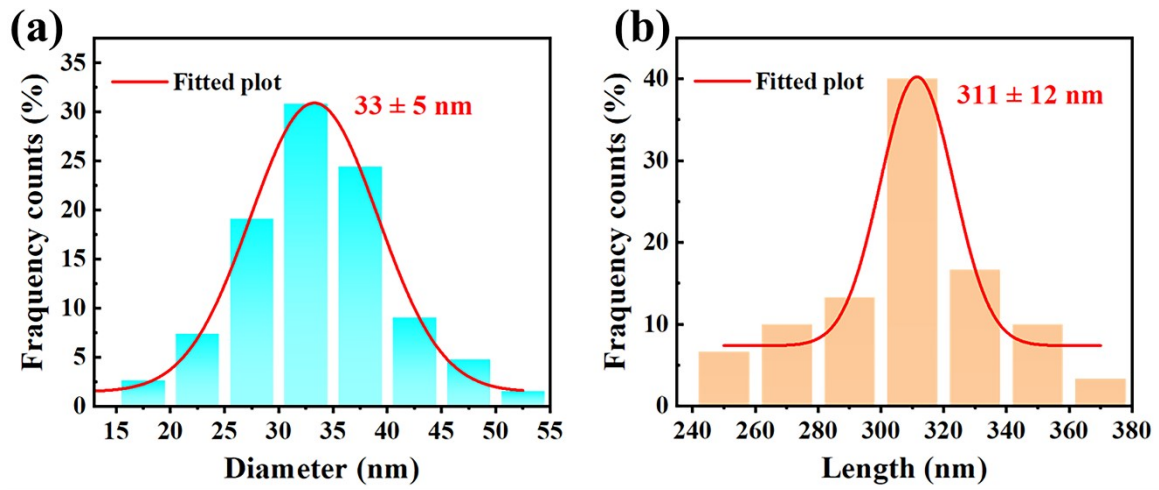


Fig. S4. The diameter (a) and length distribution (b) of the InN NRs.

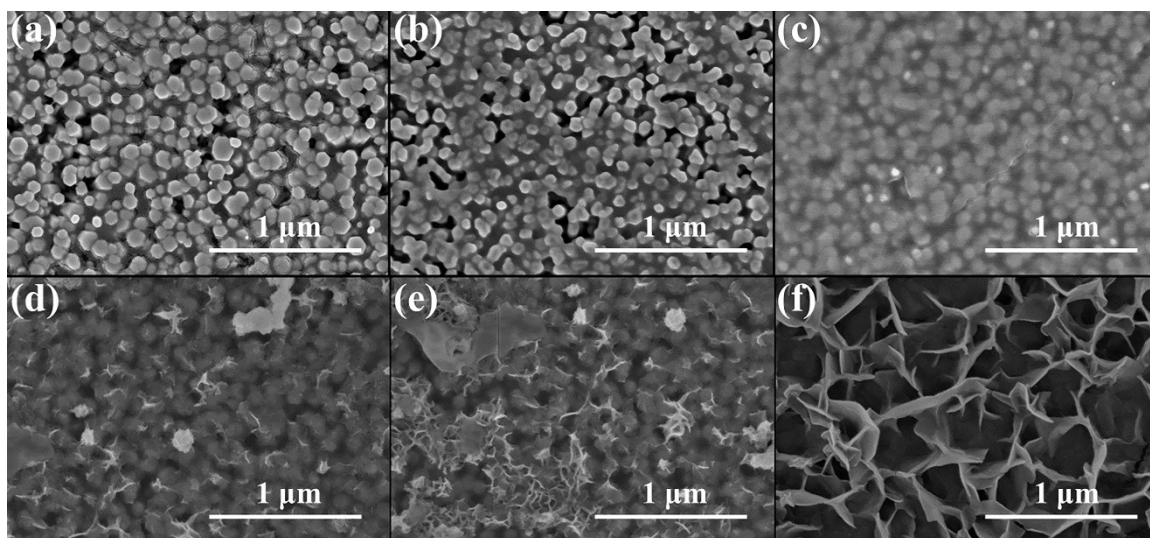


Fig. S5. (a-c) The top-view SEM images of InN/PM6-3000, InN/PM6-4000, and InN/PM6-5000. (d-f) The top-view SEM images of InN/PM6/NiFe LDH-60, InN/PM6/NiFe LDH-120, and InN/PM6/NiFe LDH-180.

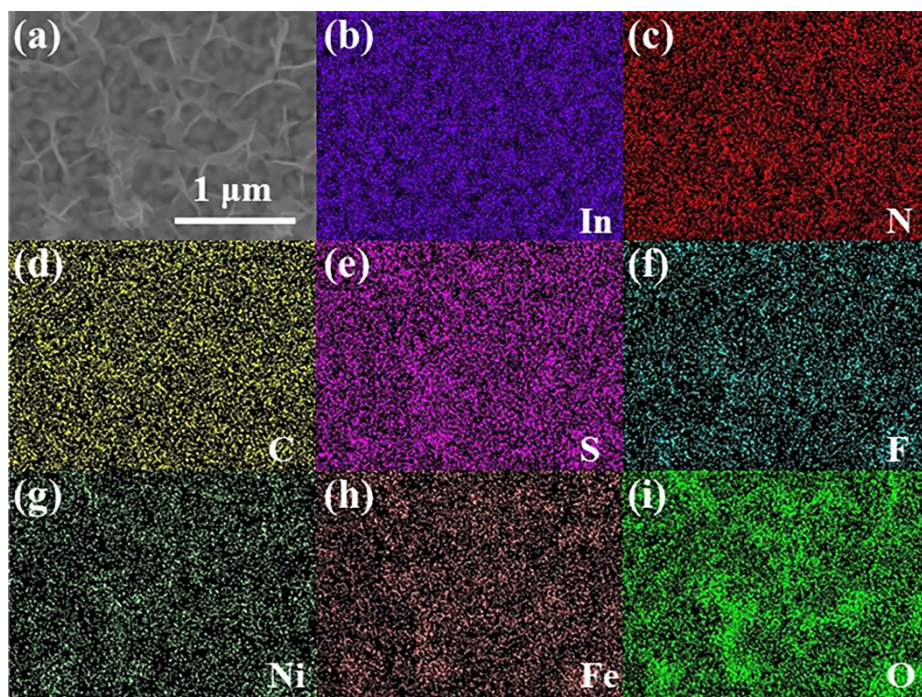


Fig. S6. (a) SEM top view images and (b-i) the corresponding elemental mapping images of the InN/PM6/NiFe LDH photoelectrode.

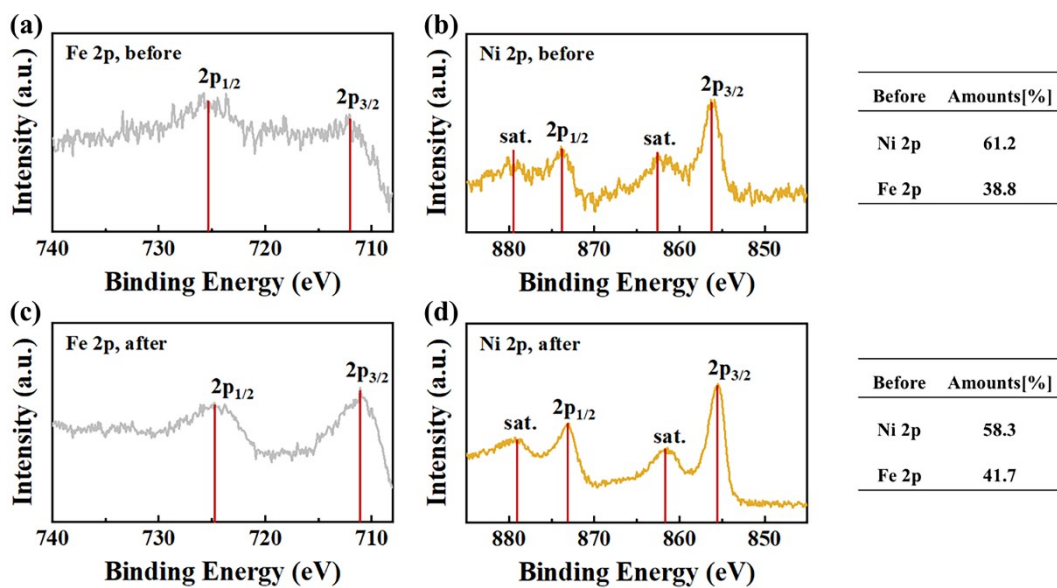


Fig. S7. XPS characterization of the InN/PM6/NiFe LDH photoelectrode before and after the PEC test and changes in Ni and Fe amounts. (a), (c) Fe 2p and (b), (d) Ni 2p XPS spectrum of the InN/PM6/NiFe LDH before and after the PEC test.

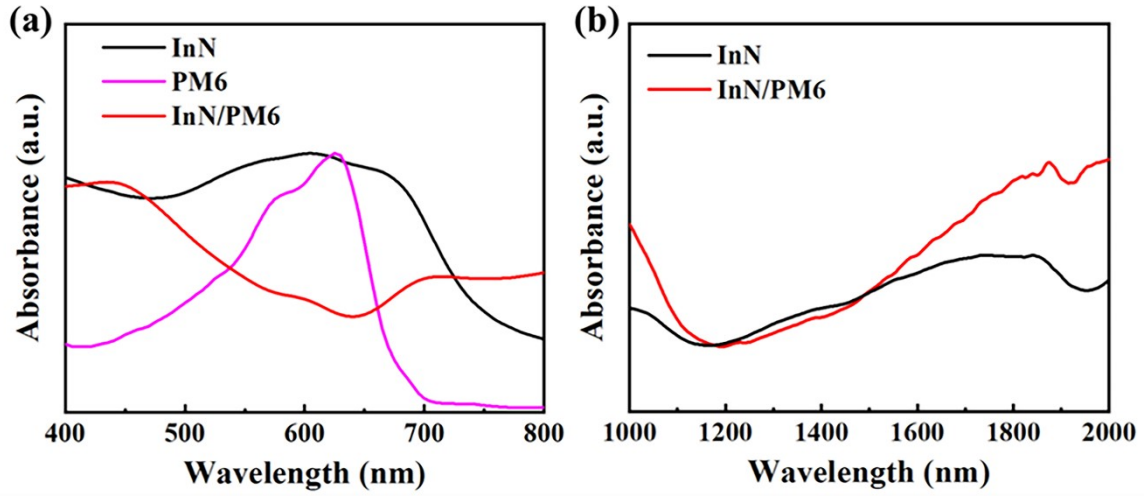


Fig. S8. (a) UV-vis absorption spectroscopy of bare InN NRs, PM6, and InN/PM6 in the visible light region, (b) bare InN NRs and InN/PM6 in the infrared region.

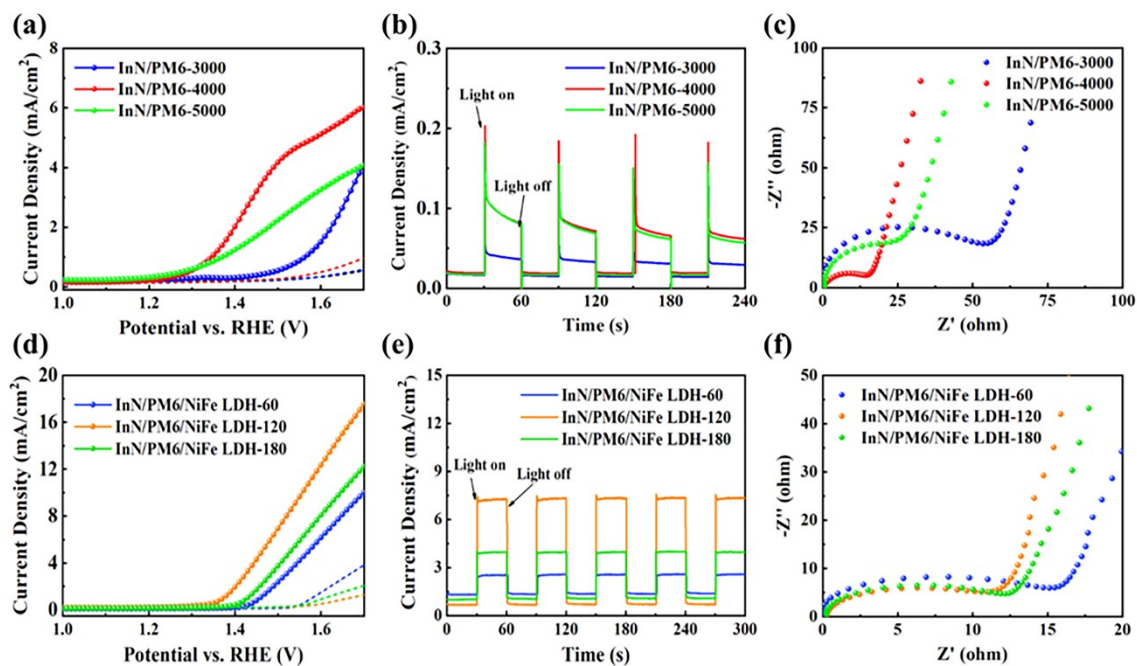


Fig. S9. PEC properties of InN-based photoanode. LSV curves of (a) the InN/PM6 and (d) InN/PM6/NiFe LDH photoanode in 0.1 M KOH solution (pH 13) under 1 sun illumination, Transient photocurrent curves of (b) the InN/PM6 and (e) InN/PM6/NiFe LDH photoanode at 1.45 V vs. RHE, EIS spectra of (c) the InN/PM6 and (f) InN/PM6/NiFe LDH photoanode at 1.2 V vs. RHE.

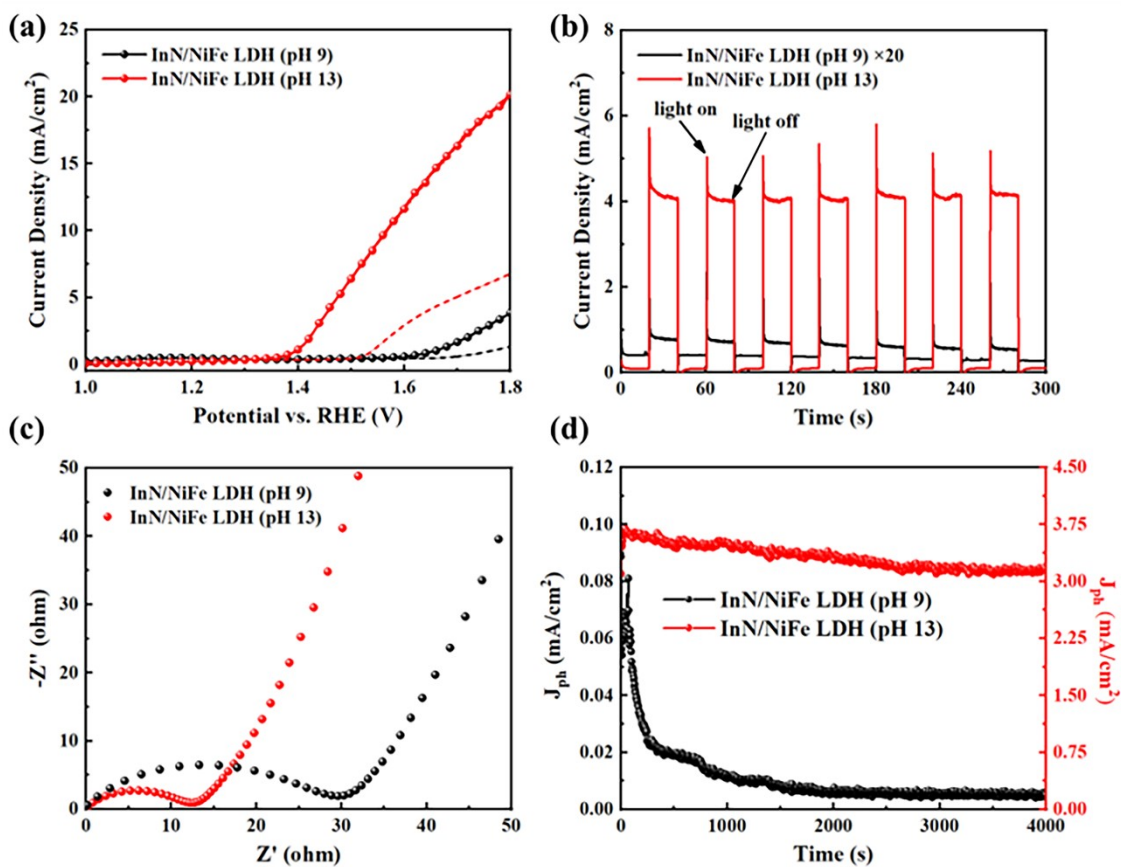


Fig. S10. (a) LSV curves of the InN/NiFe LDH photoanode in 0.2 M Na₂HPO₄ solution (pH 9) and 0.1 M KOH solution (pH 13) under 1 sun illumination. (b) Transient photocurrent curves of the InN/NiFe LDH photoanode at 1.45 V vs. RHE, (c) EIS spectra of the InN/NiFe LDH photoanode at 1.2 V vs. RHE, (d) the J-t curves of the InN/NiFe LDH photoanode in the different pH value of electrolytes at 1.45 V vs. RHE.

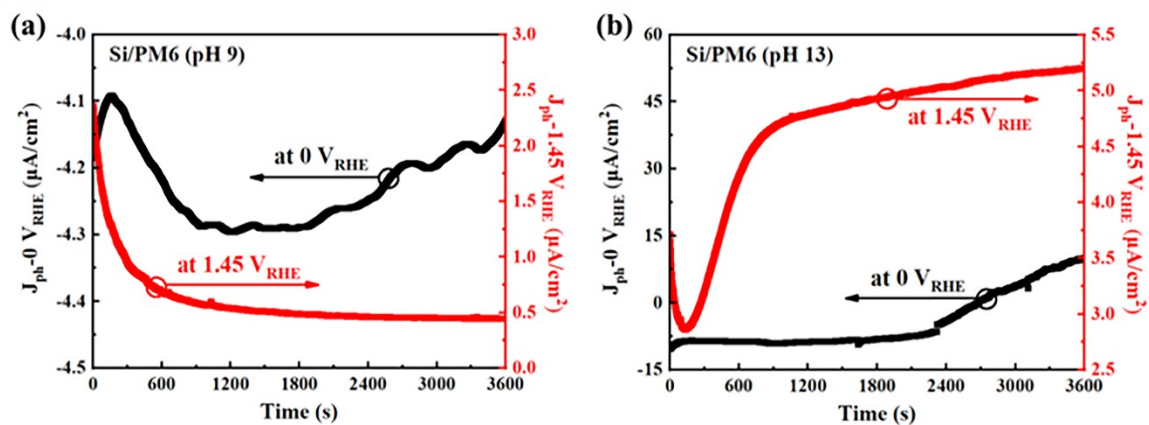


Fig. S11. J-t curves of Si/PM6 photoanodes at 0 V vs. RHE and 1.45 V vs. RHE under 1 sun illumination in 0.2 M Na₂HPO₄ solution (pH 9) and 0.1 M KOH solution (pH 13).

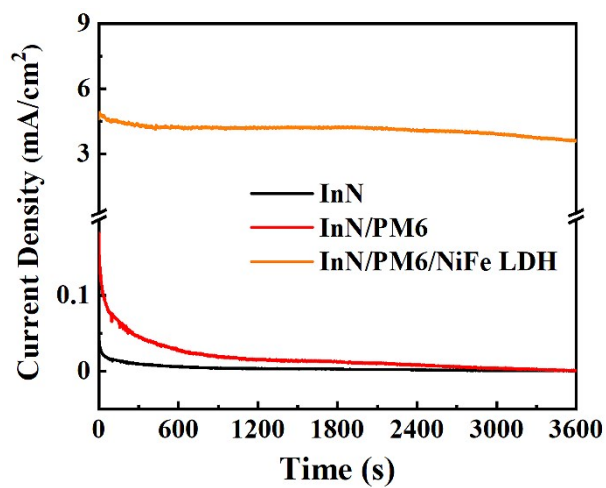


Fig. S12. J-t curves of InN-based photoanodes at 1.45 V vs. RHE under 1 sun illumination in 0.1 M KOH solution (pH 13).

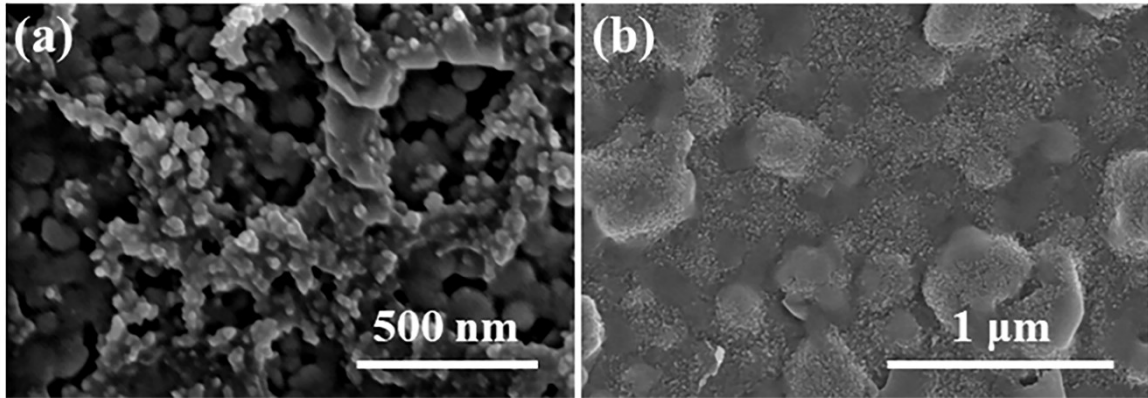


Fig. S13. SEM image of (a) InN/PM6 and (b) InN/PM6/NiFe LDH photoanode after illumination under three-electrodes system.

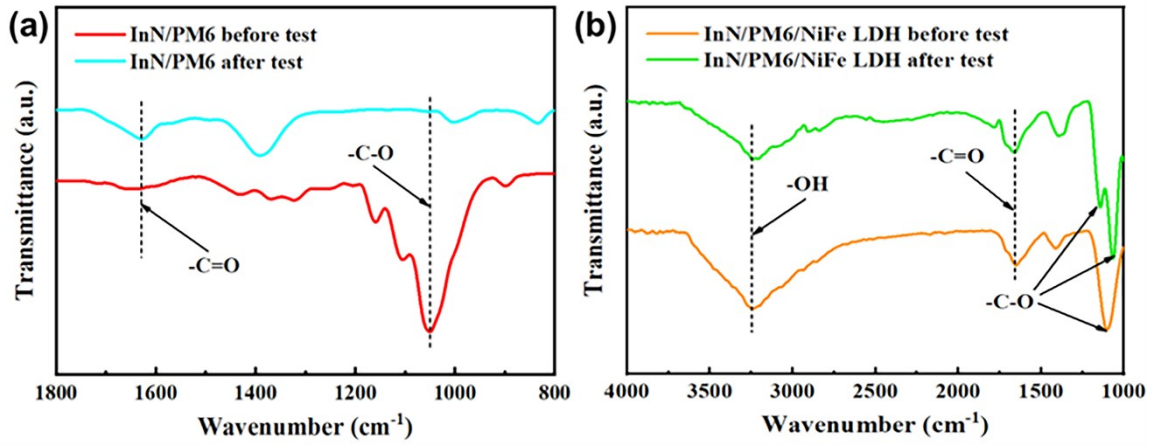


Fig. S14. FT-IR spectrum of (a) InN/PM6 and (b) InN/PM6/NiFe LDH photoanode before and after PEC testing.

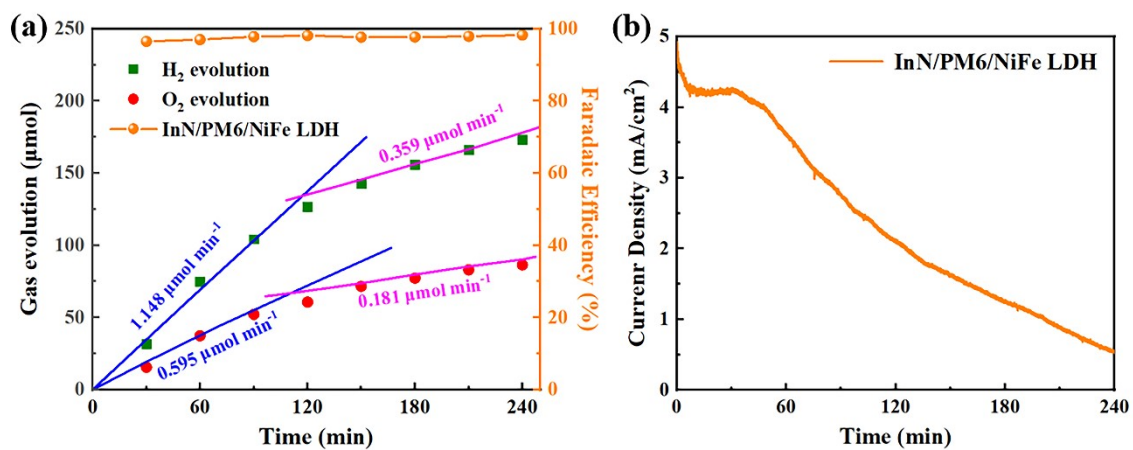


Fig. S15. (a) Gas evolution curves and faradaic efficiency measured under AM 1.5G continuous illumination (b) J-t curves of InN/PM6/NiFe LDH photoanode at 1.45 V vs. RHE under 1 sun illumination in 0.1 M KOH solution (pH 13) for 4 h.

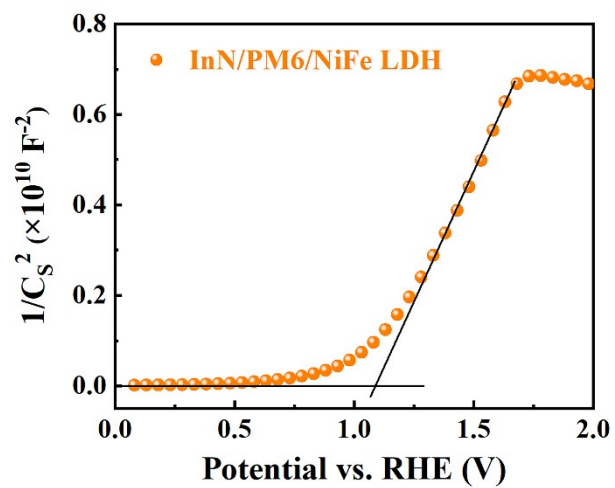


Fig. S16. M-S plots of the InN/PM6/NiFe LDH heterojunction measured in the dark.

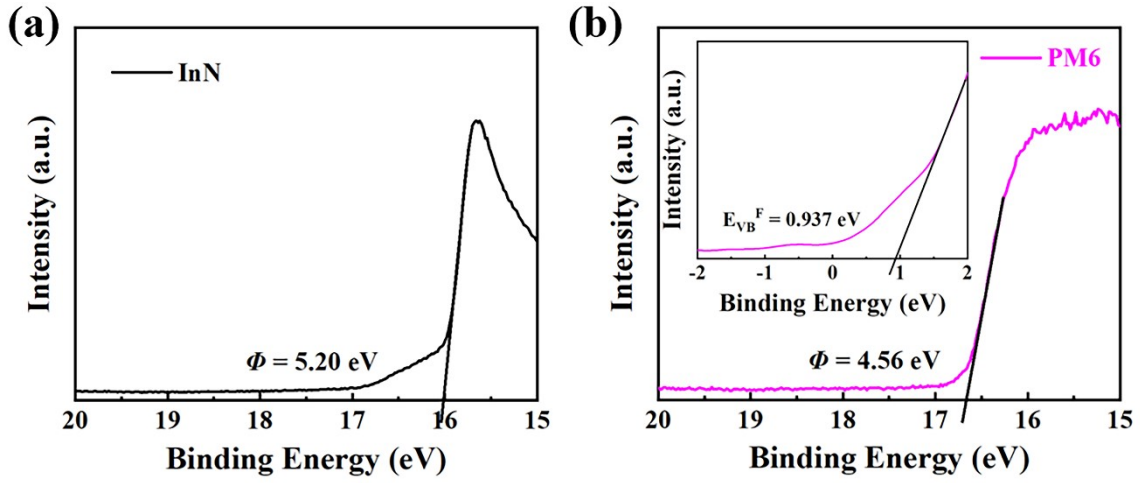


Fig.

S17. UPS spectra of (a) InN and (b) PM6. The inset is the corresponding E_{VB}^F of PM6.

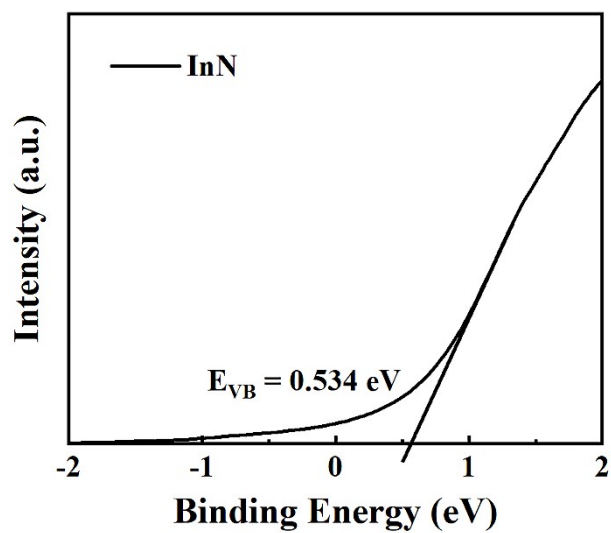


Fig. S18. XPS valence band spectra of the bare InN NRs.

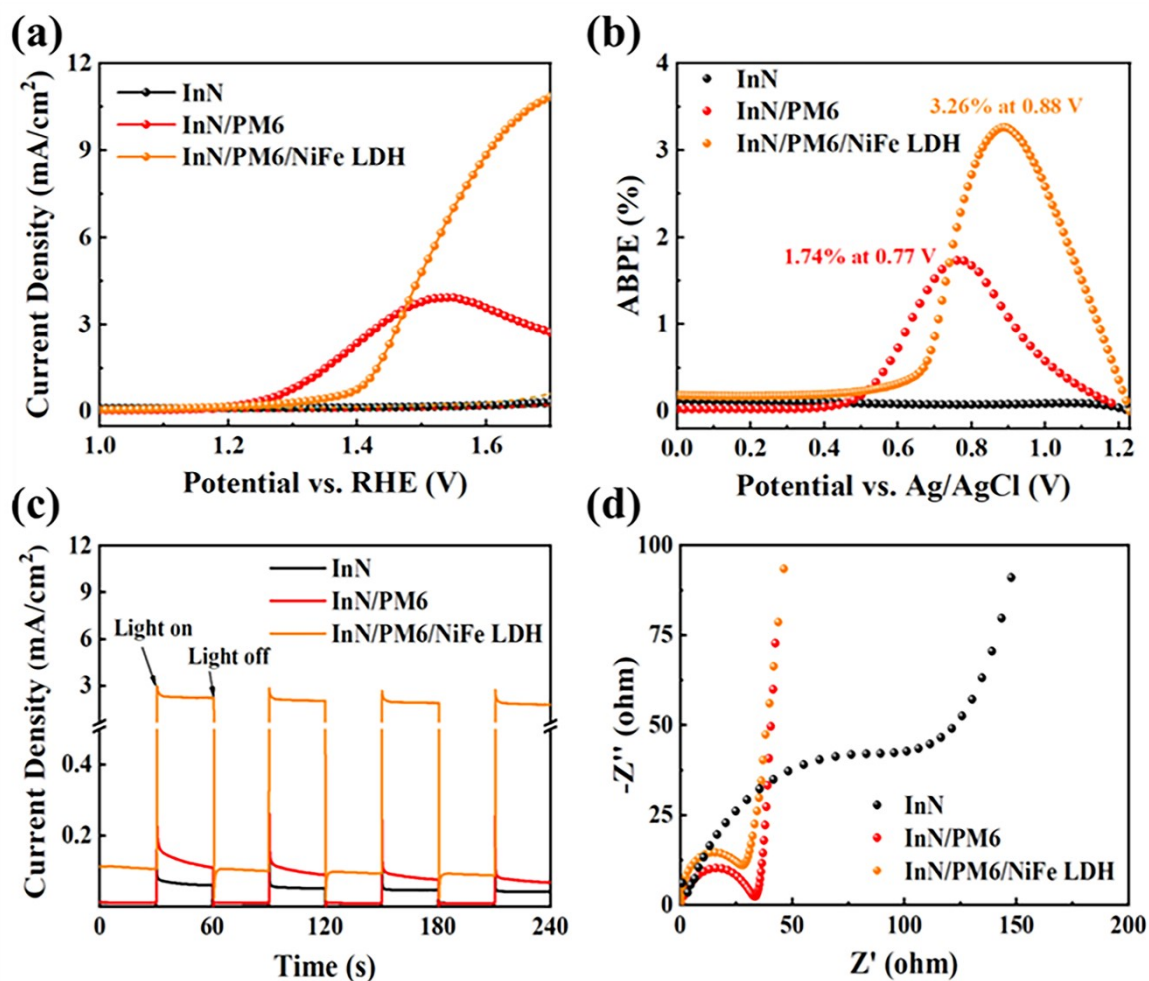


Fig. S19. PEC properties of InN-based photoanode. (a) LSV curves and (b) ABPE curves of the pristine InN NRs, InN/PM6, and InN/PM6/NiFe LDH photoanodes in 0.2 M Na₂HPO₄ solution (pH 9) under 1 sun illumination, (c) Transient photocurrent curves of the different photoanodes at 1.45 V vs. RHE, (d) EIS spectra of all photoanodes at 1.2 V vs. RHE.

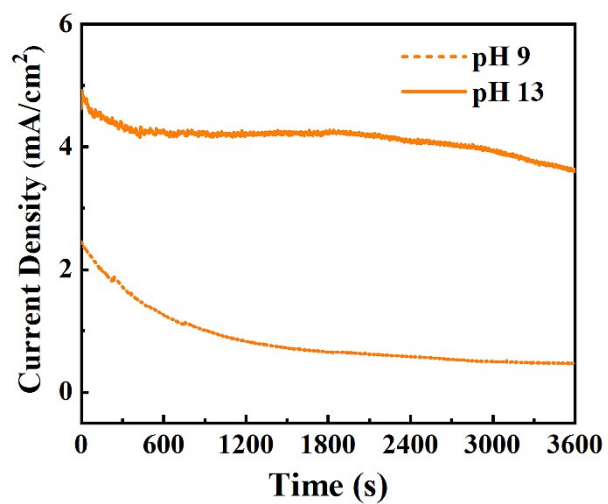


Fig. S20. Chronoamperometry curves of the InN/PM6/NiFe LDH photoanode at 1.45 V vs. RHE under 1 sun illumination in 0.2 M Na₂HPO₄ solution (pH 9) and 0.1 M KOH solution (pH 13).

Table 1. Summary of the PEC performance of InN-based photoanodes under illumination of 100 mW cm⁻² with AM 1.5G filter.

Photoanode	Electrolyte	Photocurrent density	Reference
InN NRs/PM6	0.1 M KOH	3.21 mA cm ⁻² at 1.45 V _{RHE}	This work
InN NRs/PM6/NiFe LDH	0.1 M KOH	4.82 mA cm ⁻² at 1.45 V _{RHE}	This work
InN NRs/NiFe LDH	0.1 M KOH	3.64 mA cm ⁻² at 1.45 V _{RHE}	This work
InN NW/Si	1 M NaOH	0.06 mA cm ⁻² at 1.2 V _{RHE}	Ref. ¹
In ₂ O ₃ /InN	0.1 M PBS	0.795 mA cm ⁻² at 1 V _{Ag/AgCl}	Ref. ²
In ₂ O ₃ /InN	0.1 M PBS	0.966 mA cm ⁻² at 1 V _{Ag/AgCl}	Ref. ³
InN/ZnO	0.1 M Na ₂ SO ₄	0.02 mA cm ⁻² at 1.4 V _{RHE}	Ref. ⁴
ZnO: InN	0.5 M Na ₂ SO ₄	0.015 mA cm ⁻² at 1 V _{Ag/AgCl}	Ref. ⁵
Al-rich InAlN	0.1 M PBS	1.2 mA cm ⁻² at 1 V _{Ag/AgCl}	Ref. ⁶

Table S2. The energy band parameters of all photoelectrodes obtained from the UPS and XPS valence band spectra.

Photoelectrodes	$E_{\text{VBM}}/E_{\text{HOMO}}$ (eV)	$E_{\text{CBM}}/E_{\text{LUMO}}$ (eV)	E_{g} (eV)
InN NRs	-5.734	-5.094	0.64
PM6	-5.497	-3.677	1.82

References

- 1 J. Kamimura, P. Bogdanoff, M. Ramsteiner, L. Geelhaar and H. Riechert, *Semicond. Sci. Technol.*, 2016, **31**, 6.
- 2 A. Saroni, S. A. Rahman and B. T. Goh, *7th Asian Conference on Colloid and Interface Science (ACCIS)*, 2017, **5**, S186-S190.
- 3 A. Saroni, M. Alizadeh, S. A. Rahman, W. Meevasana and B. T. Goh, *J. Power Sources*, 2020, **480**, 10.
- 4 H. Q. Liu, X. Z. Ma, Z. X. Chen, Q. G. Li, Z. Y. Lin, H. Liu, L. Y. Zhao and S. Chu, *Small*, 2018, **14**, 9.
- 5 S. S. Menon, H. Y. Hafeez, B. Gupta, K. Baskar, G. Bhalerao, S. Hussain, B. Neppolian and S. Singh, *Renewable Energy*, 2019, **141**, 760-769.
- 6 M. Alizadeh, G. B. Tong, M. S. Mehmood, K. W. Qader, S. A. Rahman and B. Shokri, *Sol. Energy Mater. Sol. Cells*, 2018, **185**, 445-455.