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Electronic Supplementary Information

Developing an Efficient NiCo₂S₄ Cocatalyst for Improving Visible Light H₂ Evolution Performance of CdS Nanoparticles

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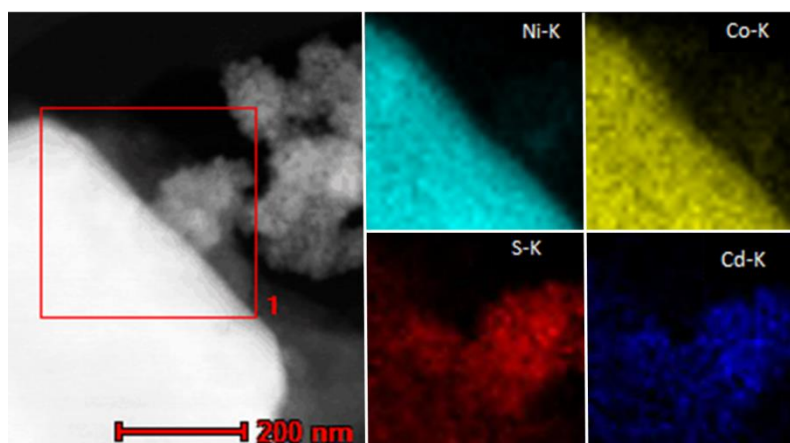


Fig. S1 EDX mappings of the NiCo₂S₄/CdS sample

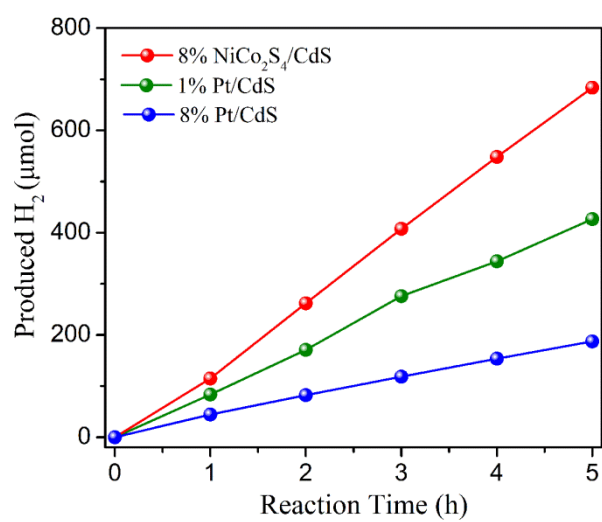


Fig. S2 Evolution of H₂ over the 8%NiCo₂S₄/CdS composite materials and Pt/CdS composite materials with different Pt content.

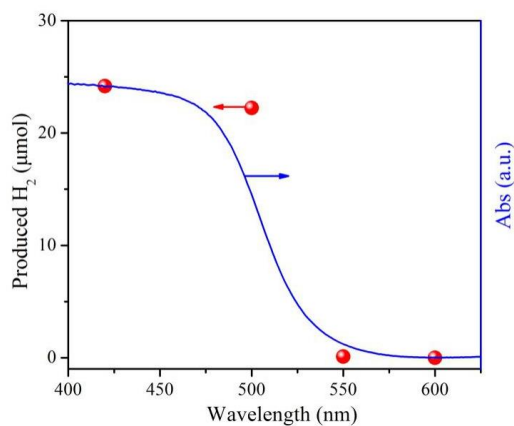


Fig. S3 Wavelength dependence of H₂ evolution over NiCo₂S₄/CdS sample.

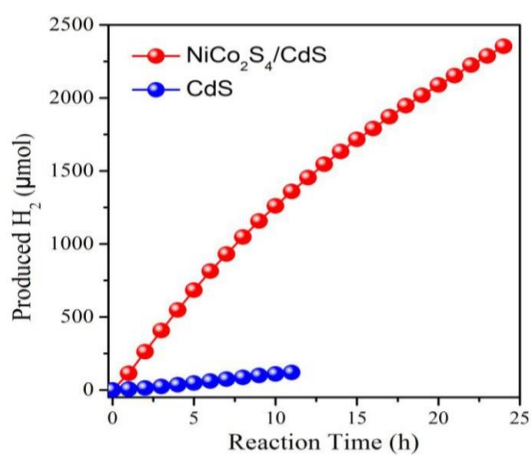


Fig. S4 Long term stability test of H₂ production over NiCo₂S₄/CdS and CdS samples under visible light irradiation.

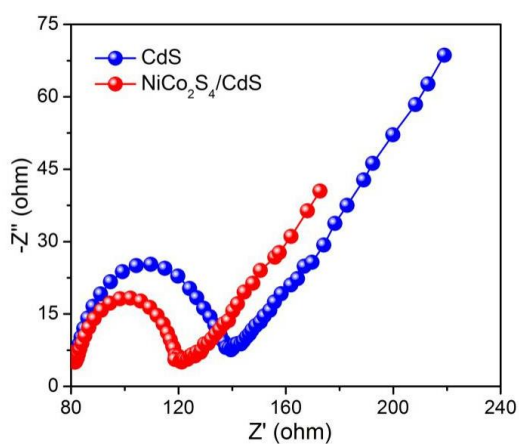


Fig. S5 Nyquist plots of CdS and NiCo₂S₄/CdS material electrodes.

Determinations of conduction and valence band potentials of NiCo₂S₄ and CdS.

In the NiCo₂S₄/CdS hybrid system, NiCo₂S₄ holds an appropriate band structure with a suitable potential relative to CdS according to the theoretical calculation. The valence band potentials of a semiconductor from the absolute electronegativity follow the empirical formulas:^[1]

$$E_{CB} = X - E_C + 0.5E_g$$

$$E_{VB} = E_{CB} + E_g$$

E_g is the band gap energy of the semiconductor, the values for NiCo₂S₄ and CdS are 2.5 eV and 2.4 eV, respectively ^[2,3]. E_{VB} is the valence band (VB) edge potentials, E_{CB} is the conduction band (CB) edge potentials, X is the electronegativity of the semiconductor that is the geometric mean of the electronegativity of the constituent atoms (the electronegativity of an atom is the arithmetic mean of the atomic electron affinity and the first ionization energy), and E_C is the energy of free electrons on the hydrogen scale (about 4.5 eV). The X values for NiCo₂S₄ and CdS are estimated to be 5.33 and 5.19 eV, respectively. Thus, the E_{CB} values of NiCo₂S₄ and CdS are calculated to be -0.42 and -0.51 eV, respectively. The E_{VB} values of NiCo₂S₄ and CdS is estimated to be 2.08 and 1.89 eV, respectively.

References

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