

Supporting Information

A hollow core-shell structure material NiCo₂S₄@Ni₂P with uniform heterojunction for efficient photocatalytic H₂ evolution reaction

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1.

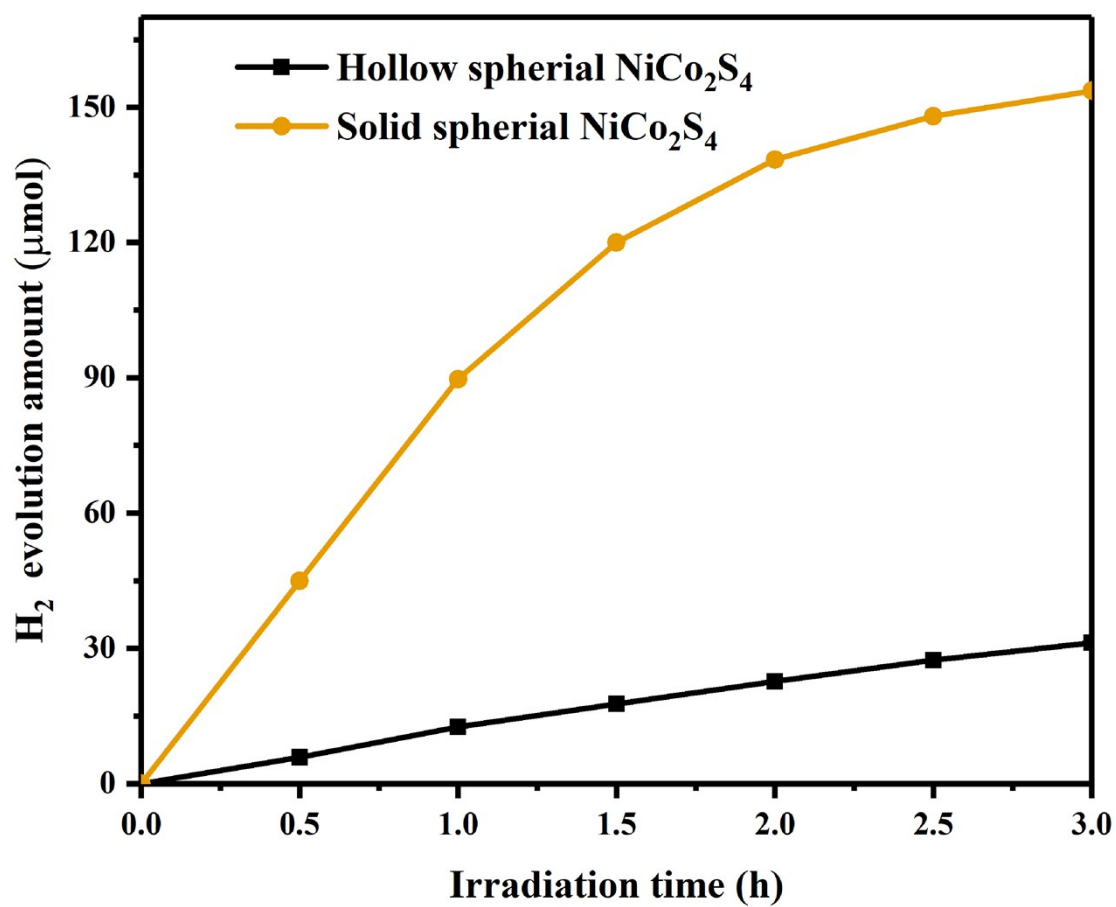


Fig. S1 H_2 evolution curves of solid spherical NiCo_2S_4 and hollow spherical NiCo_2S_4 .

2.

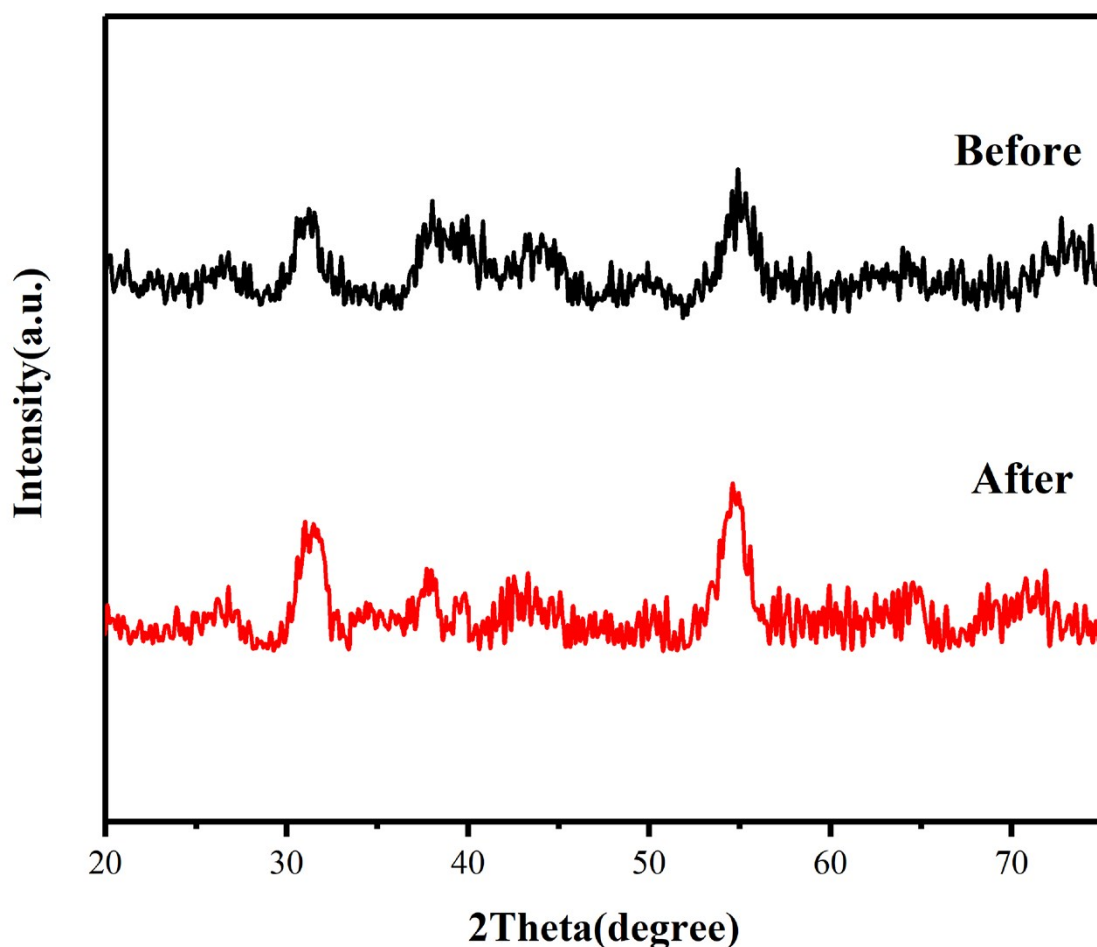


Fig. S2 XRD patterns of NiCo₂S₄@Ni₂P 10% before and after before and after stability tests (12h).

3. Band potential calculation

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

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

In the above formulas, X is the absolute electronegativity of the calculated material; E_g is the band gap width of the material; E_{CB} and E_{VB} and the conduction band and valence band potential (VS.NHE) of the corresponding materials respectively; E_c is the difference value from standard hydrogen electrode and vacuum level (about 4.5eV). E_g value of NiCo₂S₄ is derived from the UV-vis DRS tests. A number of previous reports have shown that the E_g value of Ni₂P is about 1.0eV.

Pearson Absolute Electronegativity of different elements comes from the following

database:

http://www.knowledgedoor.com/2/elements_handbook/pearson_absolute_electronegativity.html#opennewwindow?tdsourcetag=s_pcqq_aiomsg

NiCo₂S₄:

$$X = [x(\text{Ni}) * x(\text{Co})^2 * x(\text{S})^4]^{1/7} = [x(4.40) * x(4.30)^2 * x(6.22)^4]^{1/7} = 5.32 \text{ eV}$$

$$E_g = 2.49 \text{ eV}$$

$$E_{\text{CB}} = X - E_c - 0.5E_g = 5.32 - 4.5 - 0.5 * 2.49 = -0.42 \text{ eV}$$

$$E_{\text{VB}} = E_{\text{CB}} + E_g = -0.42 + 2.49 = 2.07 \text{ eV}$$

Ni₂P:

$$X = [x(\text{Ni})^2 * x(\text{P})]^{1/3} = [x(4.40)^2 * x(5.62)]^{1/3} = 4.77 \text{ eV}$$

$$E_g = 1.00 \text{ eV}$$

$$E_{\text{CB}} = X - E_c - 0.5E_g = 4.77 - 4.5 - 0.5 * 1.00 = -0.23 \text{ eV}$$

$$E_{\text{VB}} = E_{\text{CB}} + E_g = -0.23 + 1.00 = 0.77 \text{ eV}$$