Efficient interfacial charge transfer: Establish B-Co electron bridge and heterojunction synergistic enhancement of hydrogen evolution activity between Borophene and Co_9S_8

Yan Shang, Jing Xu*

School of Chemistry and Chemical Engineering, Ningxia Key Laboratory of Solar Chemical Conversion Technology, Key Laboratory for Chemical Engineering and Technology, State Ethnic Affairs Commission, North Minzu University, Yinchuan 750021, P.R.China

* Corresponding author: Jing_XU@nmu.edu.cn

Experimental section

1. Characterization

Scanning electron microscope (SEM) and transmission electron microscope (TEM) were tested by ESCALAB 250Xi. X-ray diffractometer(XRD) was detected by Japanese instrument Rigaku RINT-2000. The crystal structure is determined by the data of azimuth and intensity distributed in space. The morphology and internal structure of the catalyst were analyzed. The specific surface area and pore size distribution were measured by N_2 adsorption-desorption curve. The degassing temperature is controlled at 50℃-350℃. X-ray photoelectron spectroscopy (XPS) is used for elemental analysis and valence identification, and the X-ray source is an X-ray tube with Al or Mg as anode. The detection wavelength range of ultraviolet-visible diffuse reflectance spectrum is 200-800nm, and its model is Shimadzu (UV-2550). Lambert-Beer law is used to describe the light absorption intensity. The electrochemistry is tested by electrochemical workstation and three-electrode system.

2. Photocatalysis experiment

A 5W LED lamp (PCX-50B Discover λ>420 nm) was used to simulate the solar light source. 10 mg of catalyst, 24 mg of Eosin Y (EY AR) and 30 ml of triethanolamine (TEOA AR,98%) were weighed for ultrasonic stirring and mixing. The reaction was carried out in a multichannel photocatalytic reaction system (PCX-50B Discover) for five hours. A sampling needle is used to

absorb 500 μL of gas every hour, and N_2 is used as the carrier gas for detection in gas chromatography (N_2 carrier gas, Tianmei GC7900, TCD, 13 column). The hydrogen production per hour was obtained by calculating the peak area.

3. Calculation details

The Cambridge structure database (CCDC) is used to search the crystal structure, and the software is transformed into XRD simulation map for comparison, and a matching crystal model is found for optimization. Using the formula $Deviation\ (\%) = \frac{Final\ volume - Initial\ volume}{Initial\ volume} \times 100$. The data error after model optimization is calculated. The appropriate k-points and energy cutoff are selected. Density functional theory (DFT) was used to calculate.

Table 1 Basic data for DFT calculations

Samples	Functional	Energy cutoff (eV)	K-point set	Deviation (%)
Borophene	GGA-PBE	400	3 × 4 × 5	0.56
Co_9S_8	GGA-PBE	350	1 × 2 × 1	0.83

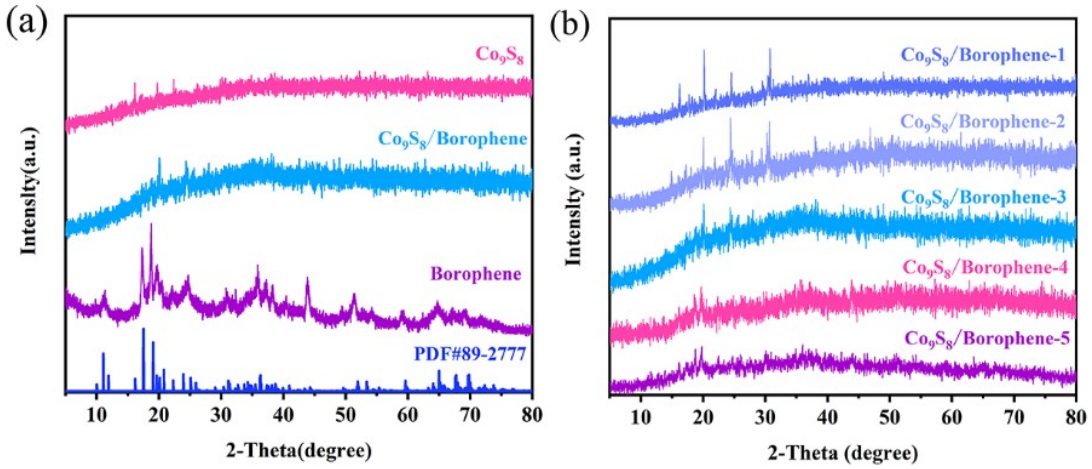
4. Photocatalytic performance

As shown in Table 2, the hydrogen production activity of Co_9S_8/Borophene was compared with that of other catalysts reported in the literature. The hydrogen production capacity of Co_9S_8/Borophene was 4271.40 μmol·g^{-1}·h^{-1}. It has excellent hydrogen production activity and great potential in the field of photocatalytic hydrogen production.

Table.2 Comparison of the hydrogen production activity of Co_9S_8/Borophene and previously reported.

Sample	Light source	Acrificial agent	Hydrogen production (μmol·g^{-1}·h^{-1})	Refs.
Co_9S_8/Borophene	5 W LED	TEOA,EY	4271.40	This work
Co_9S_8/ZnSe	300 W Xe Lamp	Na_2SO_3/Na_2S	967.80	[1]
P-Co_9S_8/g-C3N4	5 W LED	TEOA,EY	4362.00	[2]
Co_9S_8-GDY-CuI	5 W LED	TEOA,EY	1411.82	[3]
Co_9S_8/RP	5 W LED	TEOA,EY	1562.50	[4]
Co_9S_8/CdS/ZIF-67	300 W Xe Lamp	Na_2SO_3/Na_2S	1852.00	[5]

Supplemental Figure



S1 The XRD patterns of (a) Borophene， Co_9S_8 and Co_9S_8/Borophene; (b) Co_9S_8/Borophene-n (n= 1,2,3,4,5)

References

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