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Supporting Information

The doping of B in ZnO/CdS for enhanced visible-light H_2 production

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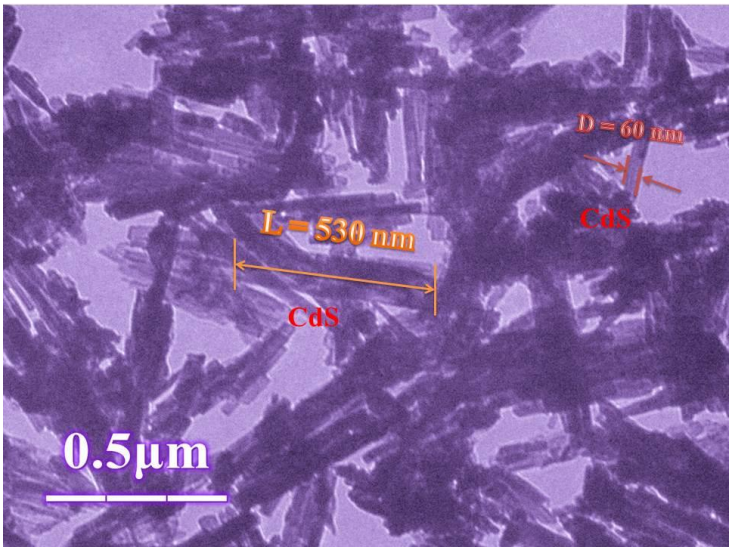

Fig. S1. TEM images of composite (b) B-ZnO/CdS-2

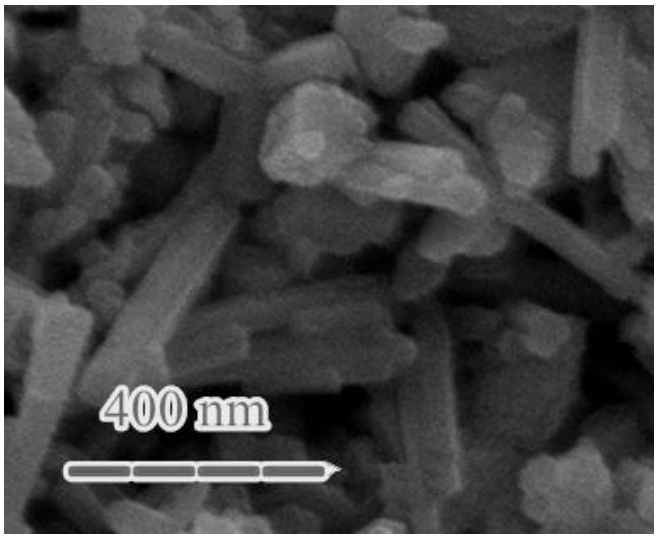

Fig. S2. SEM images of B-ZnO/CdS-2

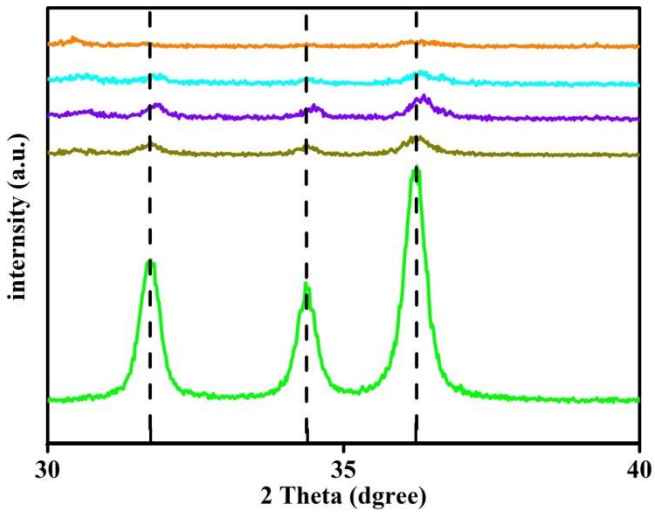

Fig. S3. Magnified XRD patterns of the series of B-ZnO/CdS samples

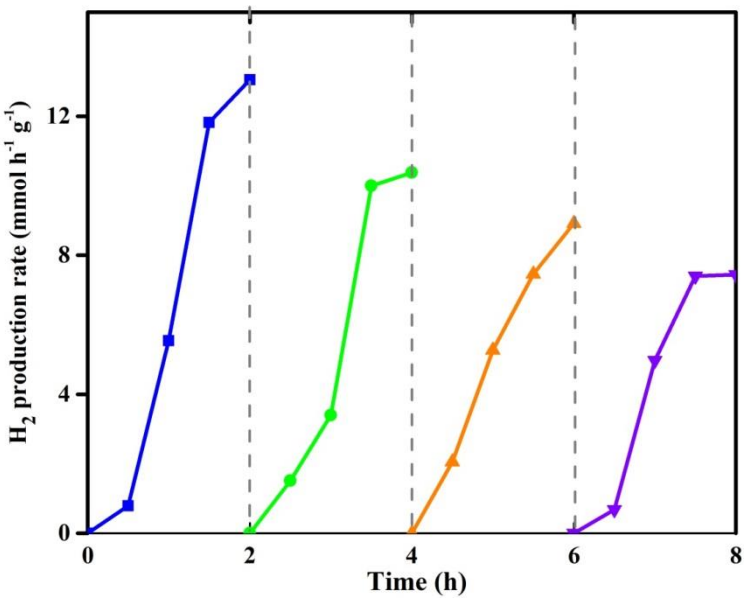

Fig. S4. The H_2 evolution stability test of B-ZnO/CdS sample.

Chemical and material.

All chemicals were of analytical grade without further purification. All experiments used deionized (DI) water.

Table.1. List of experimental chemicals

chemical	standard	manufacturer
$CdSO_4$	AR	Shanghai Macklin Biochemical Co., Ltd.
CH_4N_2S	AR	Yanbtai far east fine chemical Co.,Ltd
NaOH	AR	Shanghai Macklin Biochemical Co., Ltd.
$NaBH_4$	AR	Shanghai Macklin Biochemical Co., Ltd.
$ZnCI_2$ $6H_2O$	AR	Tianjin fuyu fine chemical Co., Ltd.
C_2H_5OH	AR	Yanbtai far east fine chemical Co.,Ltd
CH_4N_2S	AR	Shanghai Macklin Biochemical Co., Ltd.
deionized water	AR	Materials Department, Qingdao University of Science and Technology

Material characterization

The morphologies of samples were observed by Scanning electron microscopy (SEM, Hitachi S-4800). Transmission electron microscopy (TEM) and high-resolution TEM (HRTEM) measurements were performed on JEM-2100UHR with operating at 200 kV. The crystal structure of all samples was recorded by X−ray diffraction (XRD) on ULTIMA IV (Rigaku Corporation) with Cu-Kα radiation, the range of 2 Theta from 10 to 90 °, 40 kV of rated voltage and 40 mA of rated current. The Fourier transform infrared spectra (FT-IR) researched the chemical structure and performed on Nicolet IS10 (America). The X-ray photoelectron spectra (XPS) measurements were carried out using Thermo ESCALAB 250 instruments (USA) with non-monochromatic Al Kα 1486.6 radiation. The photoluminescence (PL) spectroscopy was measured using fluorescence spectrometer (Shimadzu RF-5301) at the excitation wavelength of 320 nm. The specific surface area was determined from the linear part of the BET equation (P/P0 =0.05–0.25). The pore size distribution was derived from the desorption branch of the N_2 isotherm using the Barrett–Joyner– Halenda (BJH) method. UV-vis absorption spectra analysis was performed using a Shimadzu UV 3600 spectrometer. In photoelectrochemical measurements, $MgSO_4$ solution was used as electrolyte and the tests were performed by switching visual light ON/OFF with a duration of 30 s in a typical three-electrode cell.

DFT calculations detail

The density functional theory (DFT) calculation was carried out using the Cambridge serial total energy package (CASTEP) code, in which a plane wave basis set was used. The model was established by the generalized gradient approximation (GGA) and the Perdew-Burke-Ernzerhof (PBE) functional. The cutoff energy of the OTFG ultrasoft pseudopotential was 571.40 eV. The Brillouin zone integration was performed using 3×2×1 k-point sampling through all the computational process. Geometric convergence tolerances with maximum force and maximum displacement was 0.03 eV/Å and 10^{-3} Å. Self-consistent field (SCF) tolerance with high accuracy of 10^{-6} eV/atom for energy convergence. The d band center (ε) was calculated based on the following equation: where ρ(x) is the PDOS at the energy of x. The detailed information about the structural model used in the DFT calculations as follow:

$$\varepsilon = \frac{\int_{-\infty}^{\infty} \rho(x) x dx}{\int_{-\infty}^{\infty} \rho(x) dx}$$

Where ρ(x) is the PDOS at the energy of x.

1. CdS was cut with (002) surface, and ZnO was cut with (101) surface.

2. The lattice parameters of fencelike CdS/ZnO

   a 12.8828Å, b 15.1800Å, c 30.0000Å.

   α 90°, β 90°, γ 90 °.

3. The thickness of slab are 2 layers.