Supplementary Information

Noble-metal-free hexagonal wurtzite CdS nanoplates with exposed (110) and (112) crystal facets for efficient visible-light H_2 production

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Instrumentations and characterizations

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The morphologies of samples were observed by Scanning electron microscopy (SEM, Hitachi S-4800) and Transmission Electron Microscopy (TEM, JEM 2100F, JEOL). 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 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/P_0 =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.

The apparent quantum yield test

The apparent quantum yield (AQY) of H_2 production of all samples was tested by the same photocatalytic condition except cut-off filters was replaced by bandpass filters (420 ± 10 nm). The intensity of light is about 1322 mW/cm^2. The value of AQY was calculated by the following formula:

$$\mathrm{AQY}(\%) = \frac{2 \times \text{ number of evolved } H_2 \text{ molecules}}{\text{number of incident photons}} \times 100$$

Computational methods

The calculations in this paper was performed using the first principles density functional theory (DFT), which was based on Quantum Espresso (QE) procedure. This software contained several quantum mechanics computing modules. Among them, we used the PWscf module. The calculation employed a PBE-type ultra-soft functional of GGA-PBE, which is based on the generalized gradient approximation (GGA) exchange correlation approximation. During structural optimization process, the plane wave cutoff energy was set to be 50 Ry. The convergence precision of iterative process (SCF) was 10^{-6}. The convergence index of the maximum atomic displacement was 0.01nm. The maximum force of convergence on an atom was 0.01 eV per atom. The thickness of the vacuum layer is 12 angstrom.

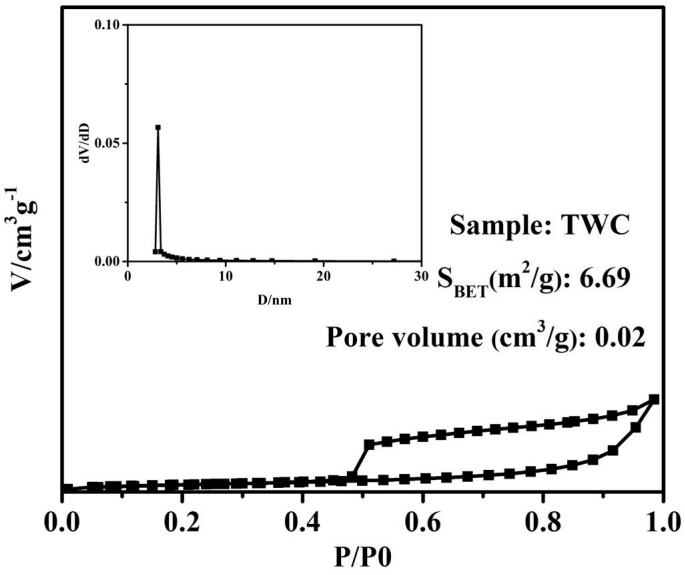

Fig. S1 N_2 adsorption-desorption isotherms of TWC.

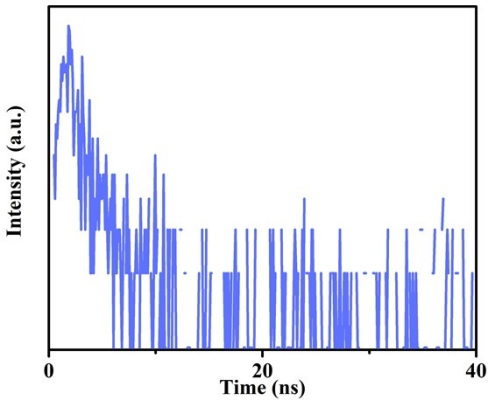

Fig. S2 The steady-state photoluminescence (PL) peak intensity of HWCs.

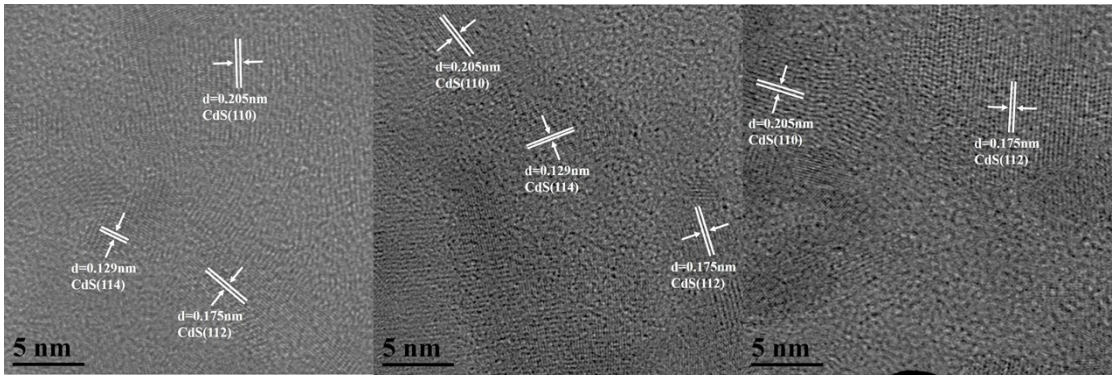

Fig. S3 HRTEM images of HWCs.