

## Supplementary Information

### ***In-situ* grown CdS on 2D Cd-based porphyrin MOFs enhance the significant separation and transfer of charge carriers with an appropriate heterojunction during photocatalytic hydrogen evolution**

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#### **Synthesis of porphyrin ligand (TCPP)**

Firstly, methyl 4-formylbenzoate (0.086 mol, 14.41 g) was completely dissolved in propionic acid (250 mL), then pyrrole solution (6.1 mL pyrrole/20 mL propionic

acid) was added slowly, and the mixture was refluxed at 150 °C for 12 h. After the mixture was cooled, the precipitate was obtained by suction filtration and washed with a large amount of ethanol, ethyl acetate and a small amount of THF respectively. The precipitate was dried at 70 °C for 12 h to obtain the purple product, recorded as TPPCOOMe. Then, TPPCOOMe (3.0 g) was stirred in a mixture of THF (60 mL) and MeOH (60 mL), and 60 mL KOH (10.5 g) aqueous solution was added and then refluxed at 90 °C for 12 h. After the mixture was cooled, the solution was filtered and the solvent was removed by rotary evaporation. Next, adjust the filtrate with 1M HCl to pH = 2 to get the precipitate. The precipitate was filtered and washed several times with water, and dried at 80 °C for 12 h to obtain the purple product, recorded as TCPP.

### **Photoelectric test**

Working electrode: 5 mg sample was dispersed in 500 uL EtOH and then 10 uL Nafion was added as binder. After ultrasonic treatment for 30 minutes, 40 uL mixed solution was added to the conductive glass and dried at room temperature. Test conditions: The electrode system was the same as CV. A 300 W xenon lamp (FX300) was used as the light source. The photocurrent response of the sample was tested at a bias voltage of - 0.6 V and a chopping period of 5 s. At the same time, the EIS of the sample was tested at a constant voltage of 0.6 V. Mott-Schottky was measured in the open circuit voltage range of  $\pm 1$  V.

### **Characterization**

The microstructure and morphology of samples were tested by X-ray powder diffraction (XRD) (XRD-6100, Shimadzu, Japan), fourier transform infrared (FT-IR) spectra (IRPrestige-21, Shimadzu, Japan), scanning electron microscope (SEM) (Quanta 650FEG, FEI, USA), transmission electron microscope and

element mapping (TEM) (JEM-2100F, JEOL, Japan) and X-ray photoelectron spectroscopy (XPS) (ESCALAB 250Xi, Thermofisher, USA). The study of photocatalytic performance and mechanism was through ultraviolet-visible diffuse reflectance spectroscopy (UV-vis DRS) (UV-2700, Shimadzu, Japan), photoluminescence spectrum (PL spectrum) (F-7000, HITACHI, Japan), transient photocurrent response curve (PEC 1000, Perfect Light, Beijing and CHI660E, Shanghai Chenhua Co., China), Mott-Schottky (M-S) (CHI660E, Shanghai Chenhua Co., China) and electrochemical impedance spectroscopy (EIS) (CHI660E, Shanghai Chenhua Co., China).

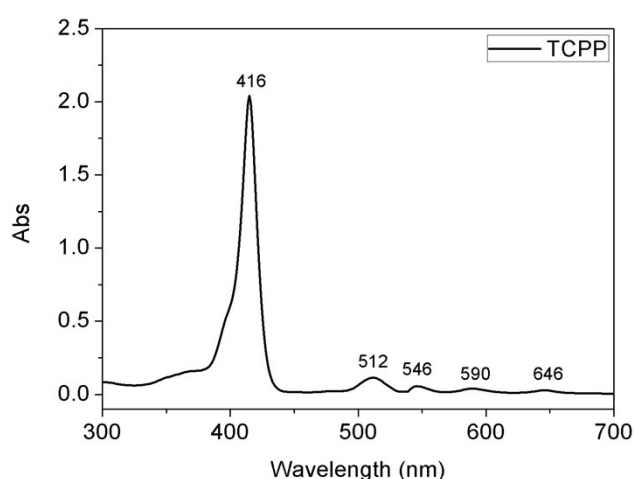


Fig. S1. Liquid UV-vis absorption spectra of TCPP.

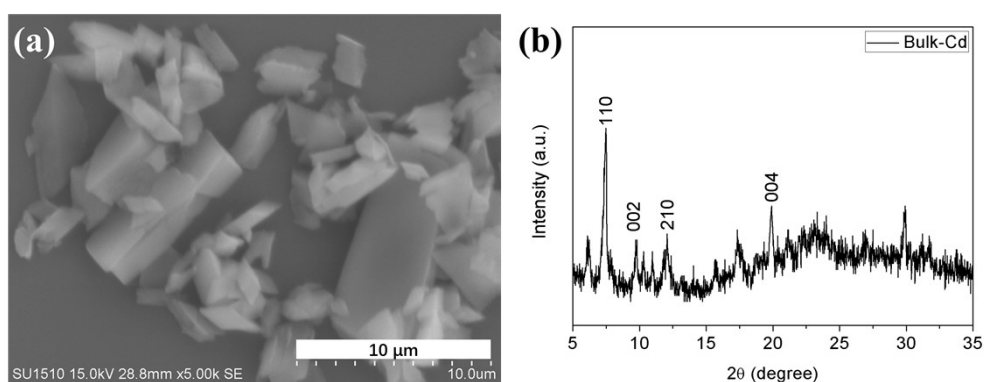


Fig. S2. SEM and XRD of Bulk-Cd.

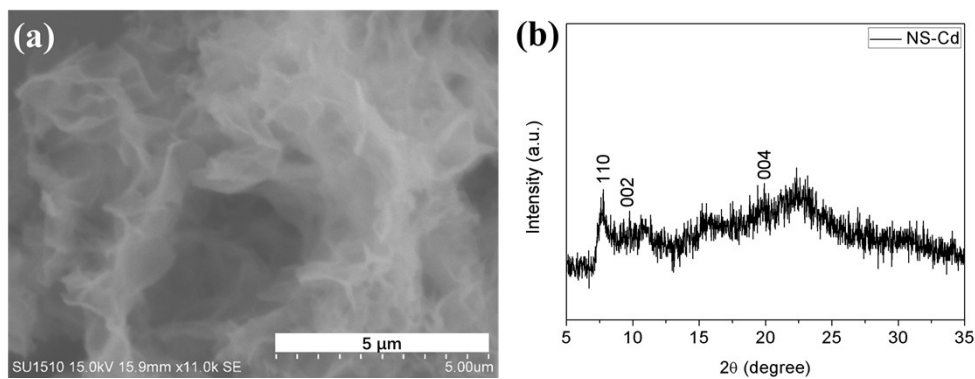


Fig. S3. SEM and XRD of NS-Cd.

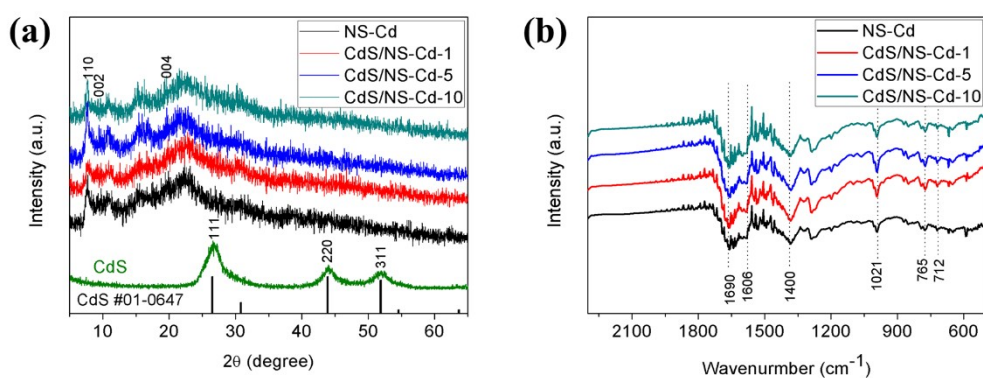


Fig. S4 (a) XRD, and (b) FT-IR of NS-Cd and CdS/NS-Cd-x (x=1, 5,10).

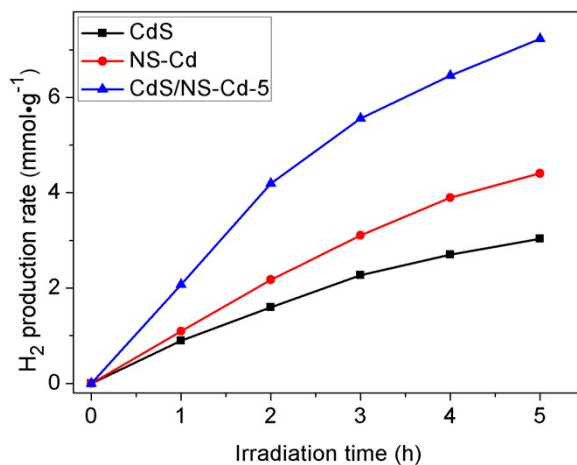


Fig. S5. Photocatalytic hydrogen production ( $\lambda \geq 420$  nm) of CdS, NS-Cd and CdS/NS-Cd-5.

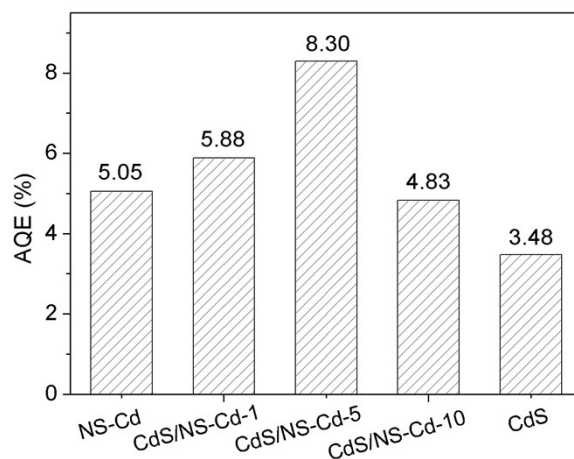


Fig. S6. AQE of NS-Cd and CdS/NS-Cd-x (x=1,5,10) ( $\lambda \geq 420$  nm).

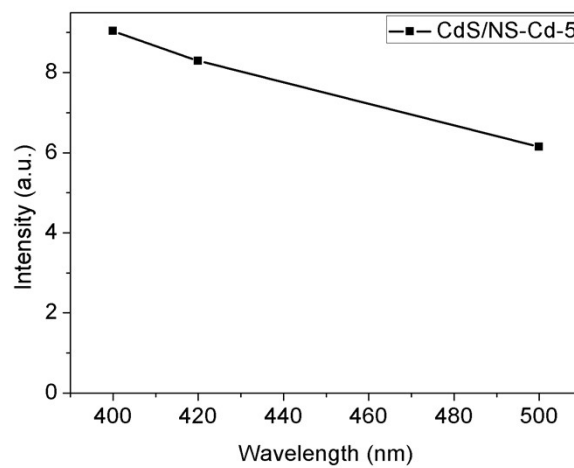


Fig.S7.AQE of CdS/NS-Cd-5 at different wavelengths.

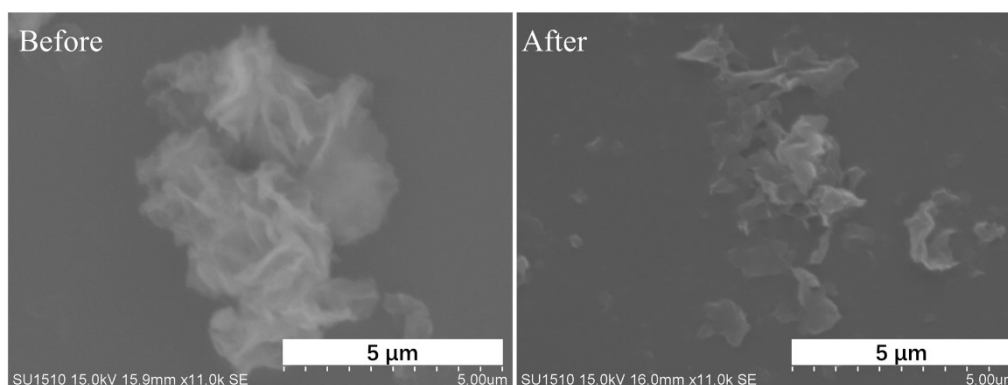


Fig. S8. SEM of CdS/NS-Cd-5 before and after photocatalytic hydrogen evolution.

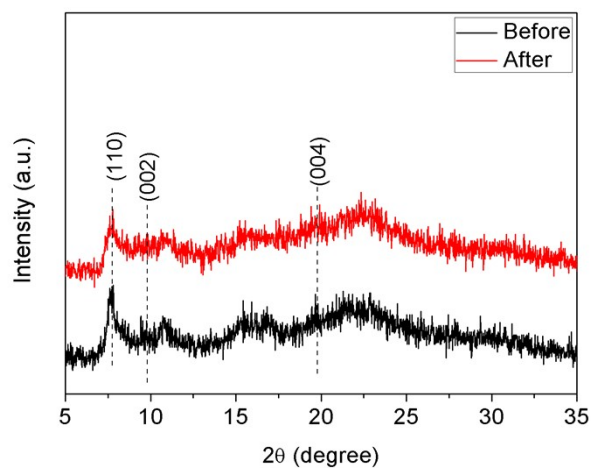


Fig. S9. The XRD of the CdS/NS-Cd-5 before and after photocatalytic hydrogen production ( $\lambda \geq 420$  nm).

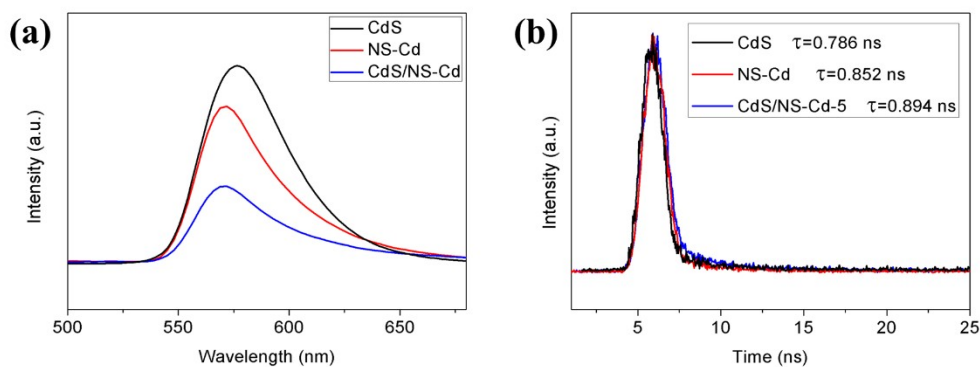


Fig. S10. (a) The PL and (b) TRPL of CdS, NS-Cd and CdS/NS-Cd-5.

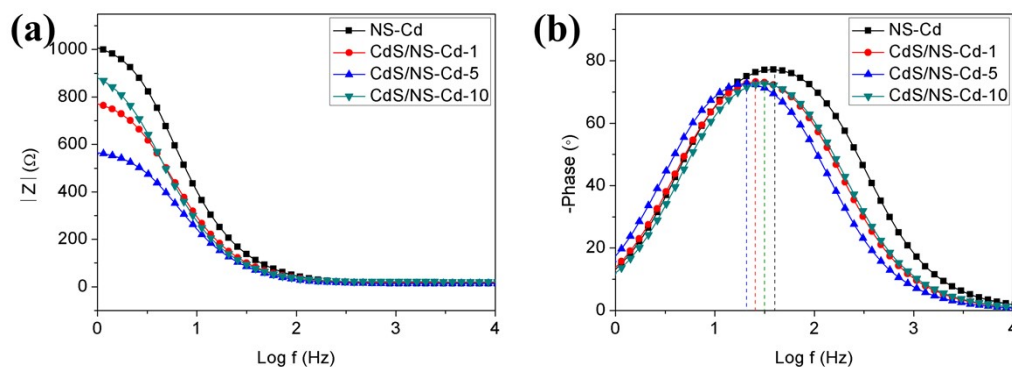


Fig. S11. Bode plots of NS-Cd and CdS/NS-Cd-x ( $x=1,5,10$ ).

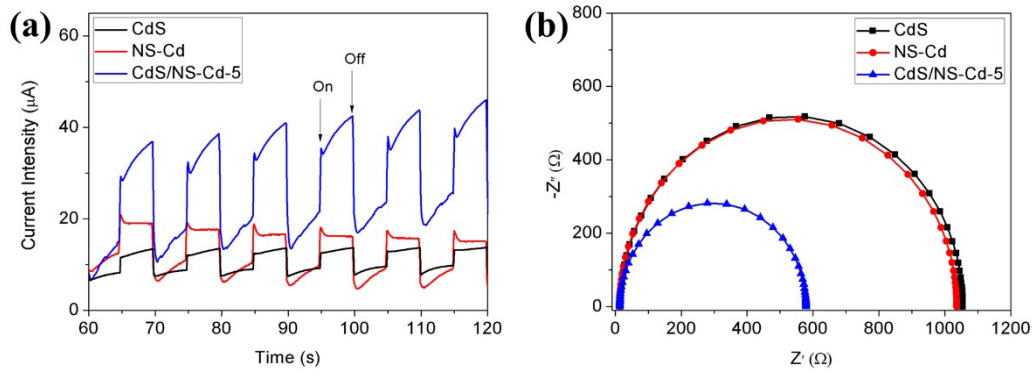


Fig. S12. (a) Photocurrent response, and (b) Nyquist plots of CdS, NS-Cd and CdS/NS-Cd-5.

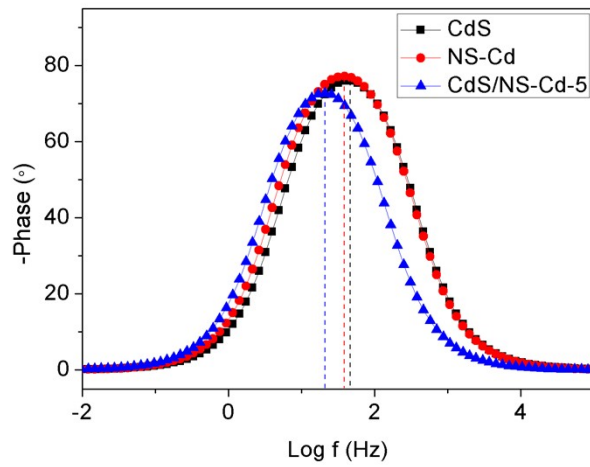


Fig. S13. The Bode plots of CdS, NS-Cd and CdS/NS-Cd-5.