

Electronic Supplementary Material

Visible-light-driven photocatalytic H₂ production from H₂O boosted by anchoring Pt and CdS nanoparticles on MoO₂

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Calculation method

The DFT calculations were performed by the Vienna ab-initio simulation package (VASP). Nuclei and core electrons were described by the projector augmented wave method, and the wavefunctions of valence electrons were expanded on a plane wave basis set with a cutoff energy of 400 eV. Perdew-Burke-Ernzrhof functional was used to evaluate the nonlocal exchange-correlation energy. A $2 \times 2 \times 1$ k -point grid determined by the Monkhorst-Pack method was applied. The structures were optimized by using conjugate gradient algorithm or quasi-Newton scheme until the forces on unconstrained atoms were less than 0.03 eV/Å. In all calculations, the bottom two layers of the slab were frozen, whereas the top four layers together with the Pt4 cluster and reaction species were optimized. Transition states for the reactions were determined through the following steps: (i) the nudged elastic band method was used to find the possible transition states, (ii) the possible transition states were relaxed by the quasi-Newton algorithm. Frequency analyses were used to validate the optimized transition state structures.

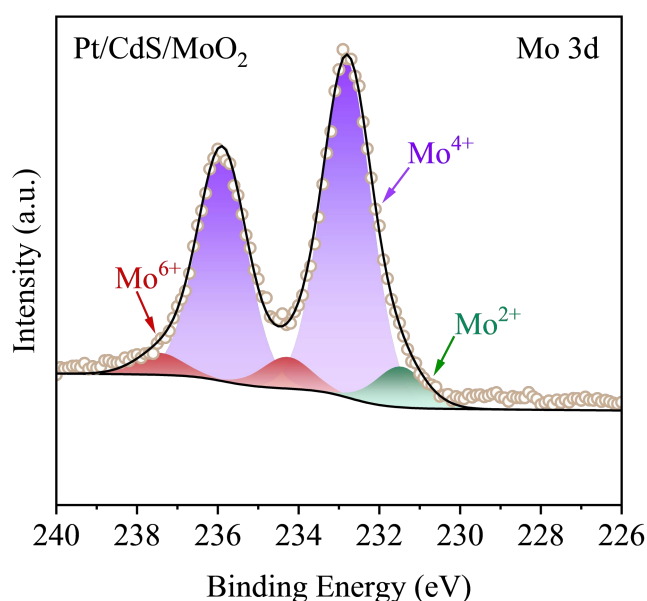


Fig. S1 Mo 3d XPS spectra

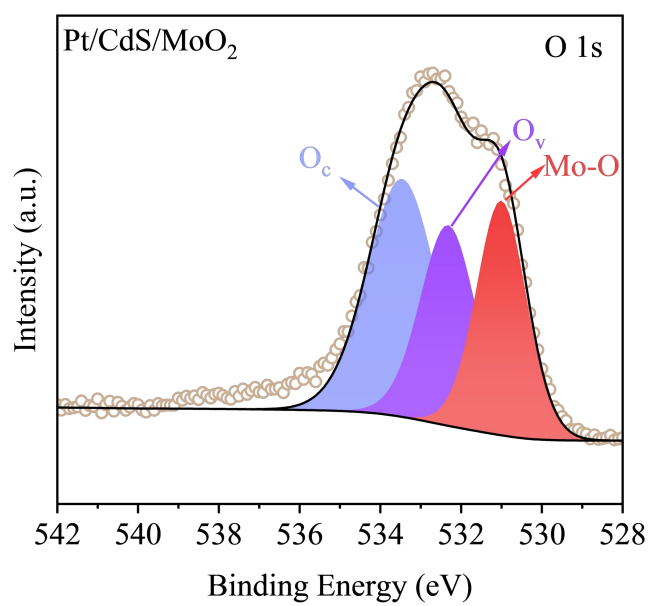


Fig. S2 O 1s XPS spectra

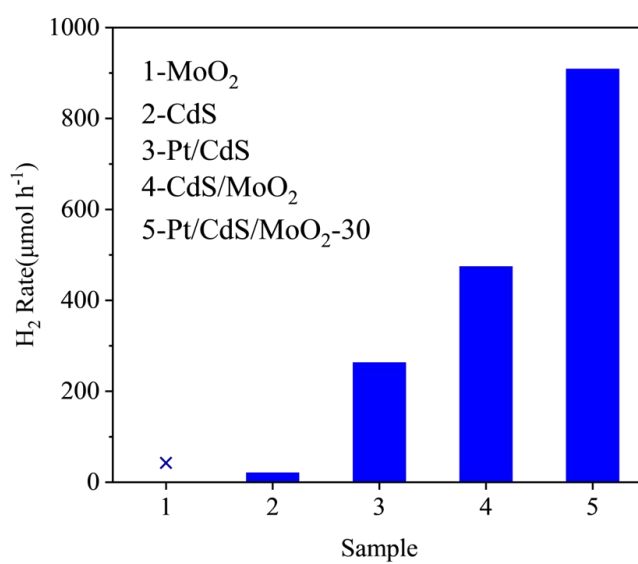


Fig. S3 H₂ rate of different samples

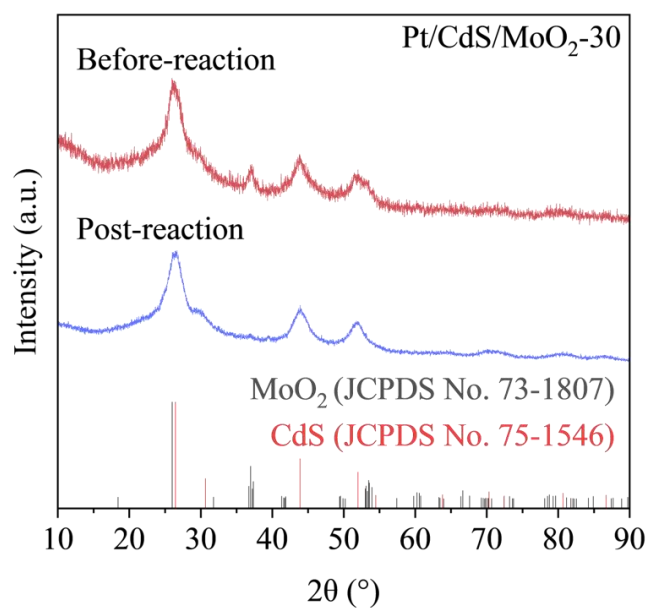


Fig. S4 XRD of Before-reaction and after-reaction

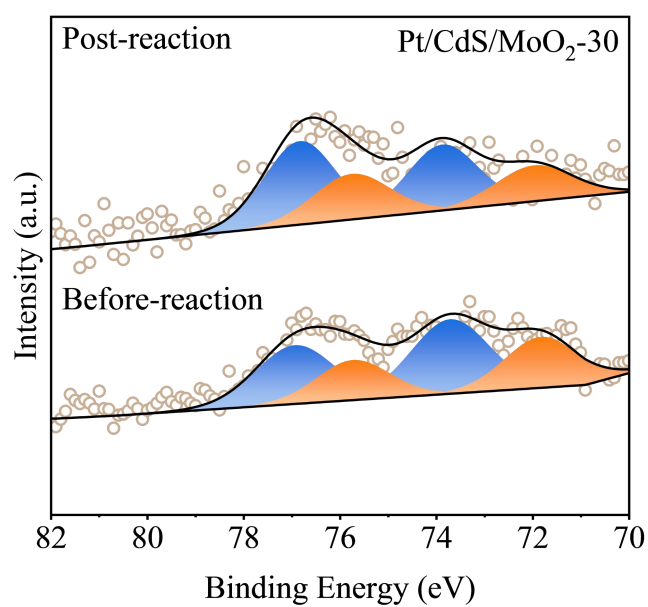


Fig. S5 Pt XPS of Before-reaction and after-reaction

Table S1 The relative concentration of Pt^{2+} derived from deconvolution results of XPS (sample: Pt/CdS/MoO_2).

Sample	Reduction times (min)	$\text{Pt}^{2+}/(\text{Pt}^{2+}+\text{Pt}^{4+}+\text{Pt}^0)$ ratio(%)	H_2 rate ($\mu\text{mol h}^{-1}$)
0-Pt/CdS/MoO ₂	0	25.98	207.98
5-Pt/CdS/MoO ₂	5	33.76	511.80
15-Pt/CdS/MoO ₂	15	46.54	806.88
30-Pt/CdS/MoO ₂	30	49.30	909.75
45-Pt/CdS/MoO ₂	45	24.39	339.3

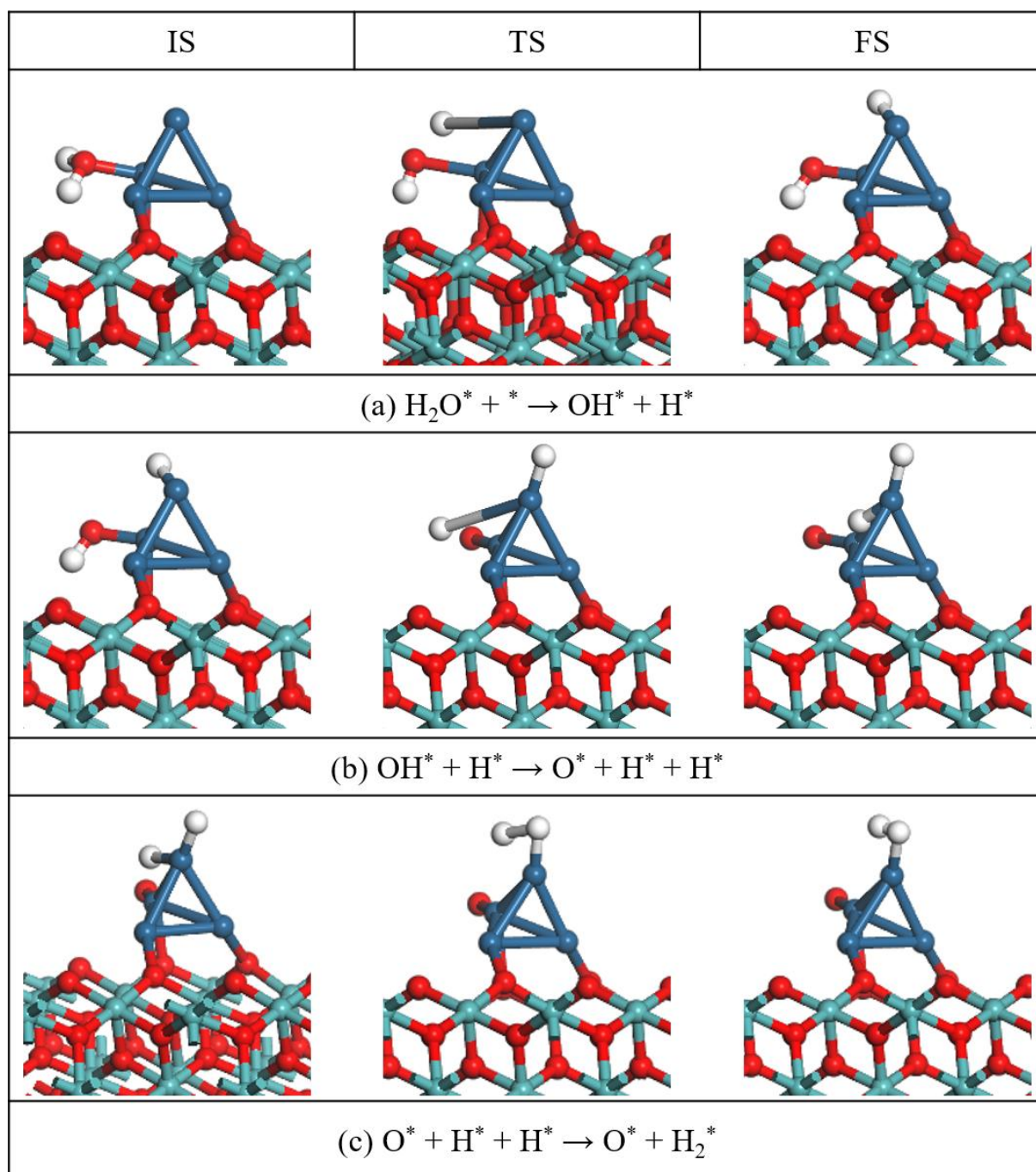


Fig. S6 The major elementary steps that are considered in the process of H_2 production from H_2O on MoO_2 (011) surface. Pt: blue; Mo: green; O: red; H: gray. The distance unit is Å.

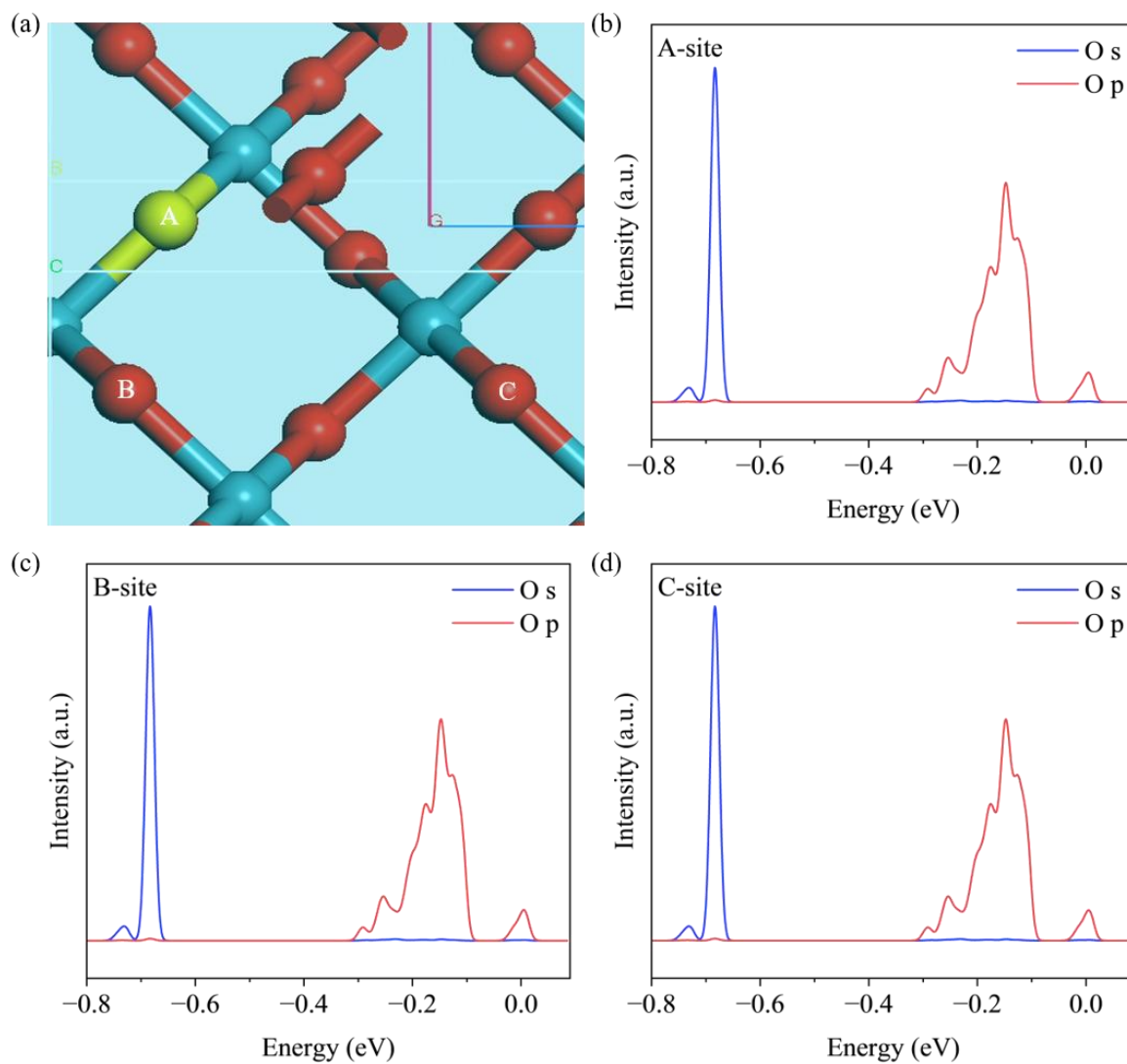


Fig. S7 MoO_2 and PDOS of MoO_2

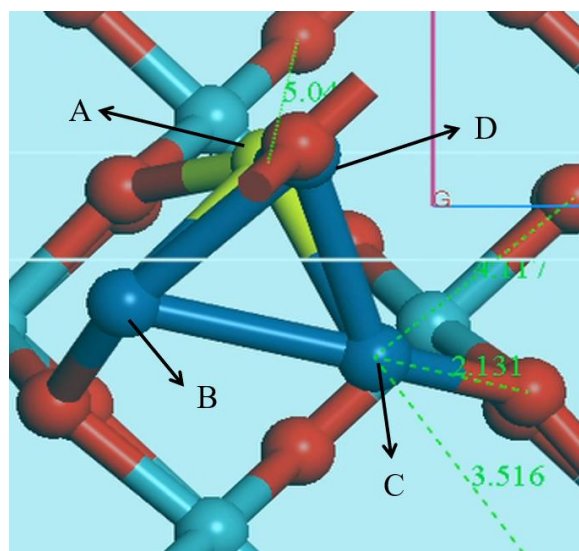


Fig. S8 Pt_4/MoO_2

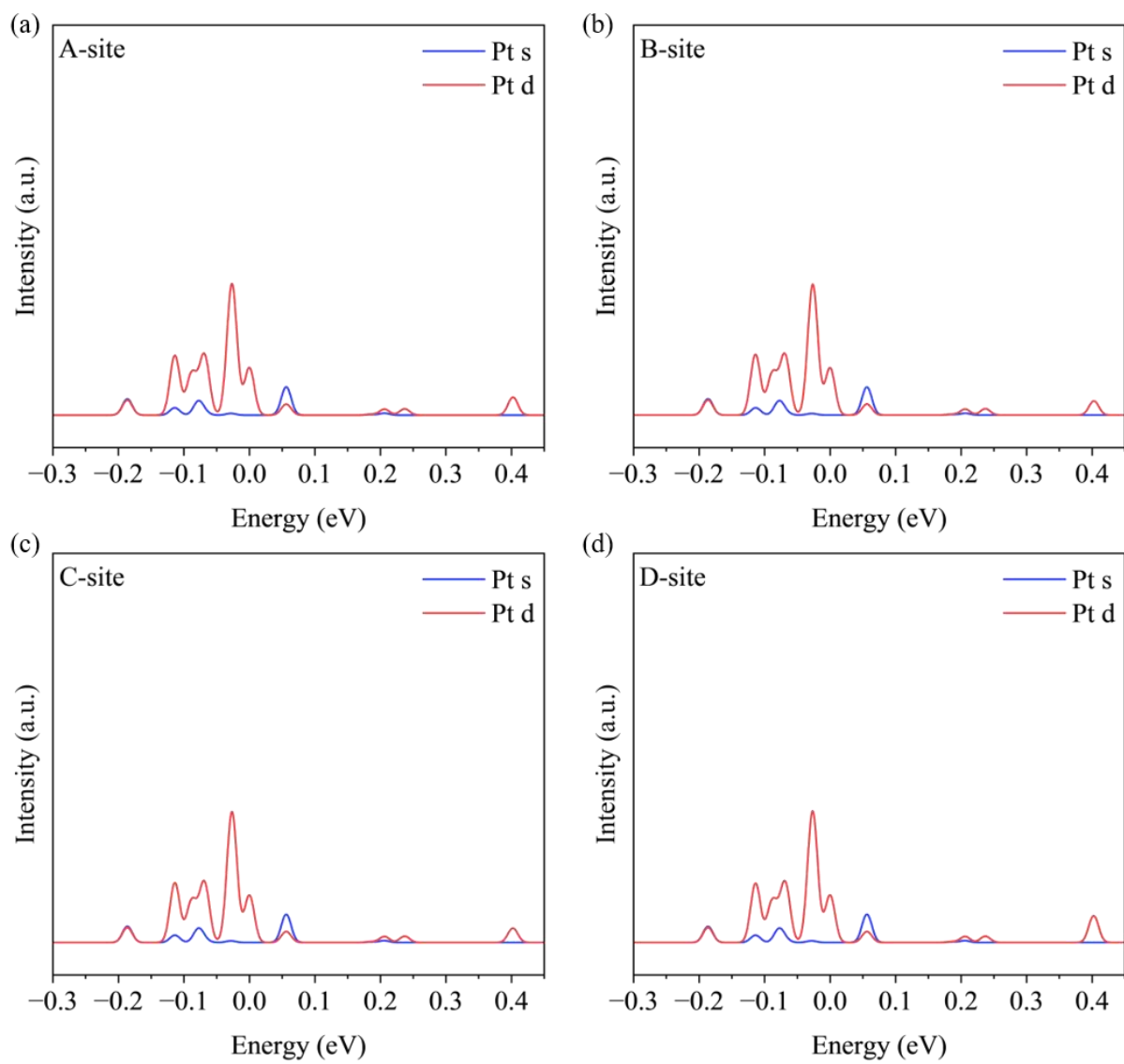


Fig. S9 PDOS of Pt₄

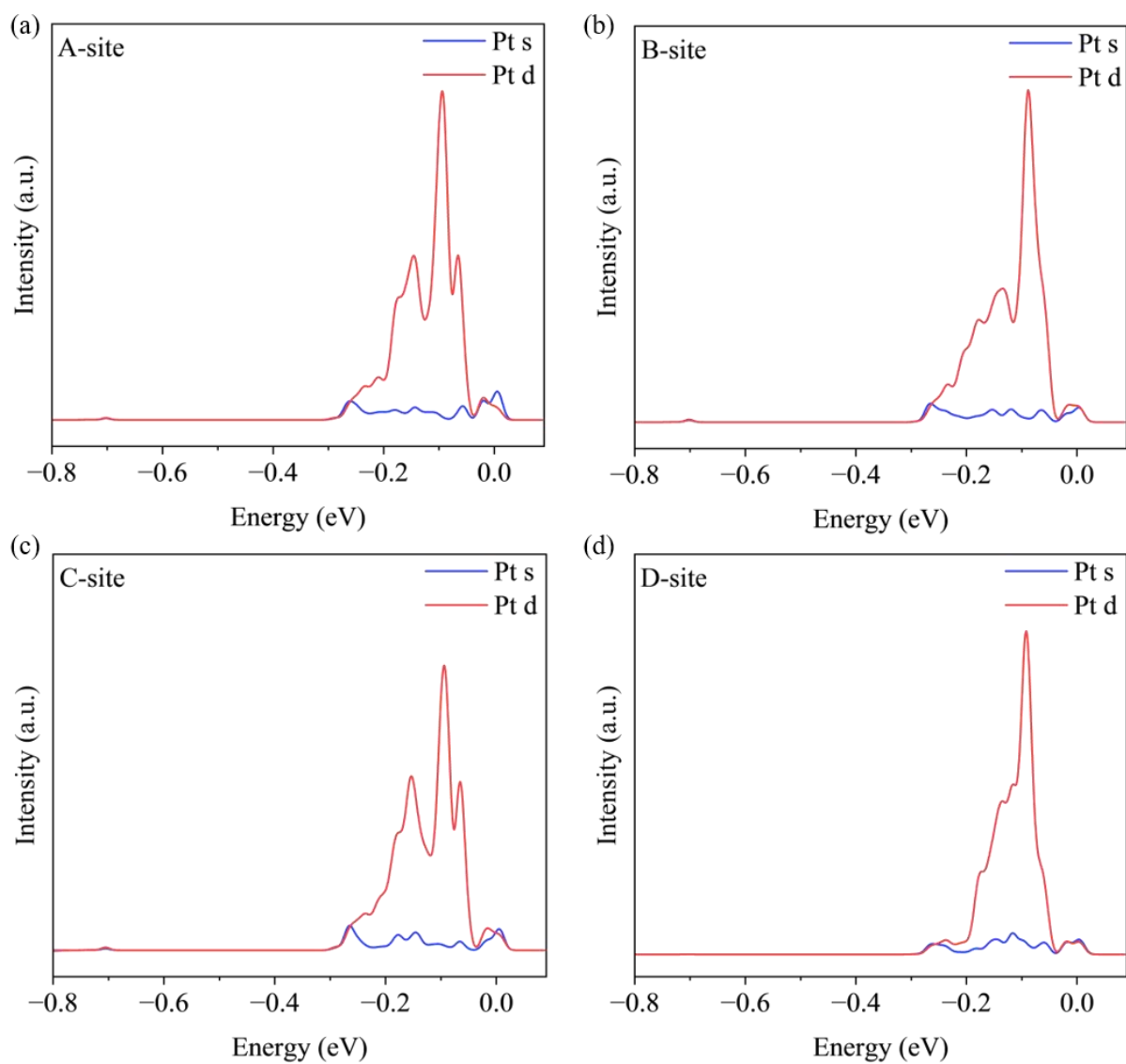


Fig. S10 PDOS of Pt₄/MoO₂

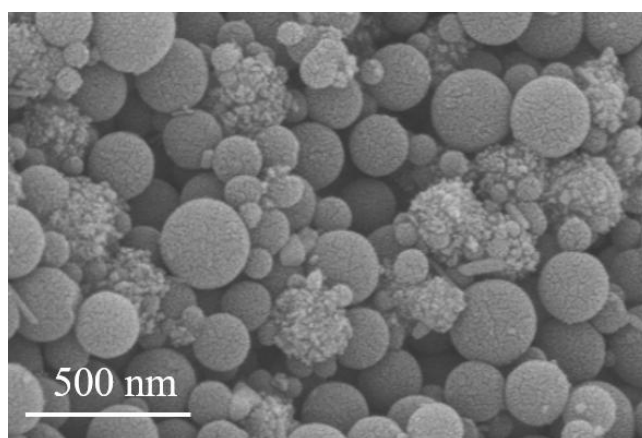


Fig. S11 SEM of MoO₂

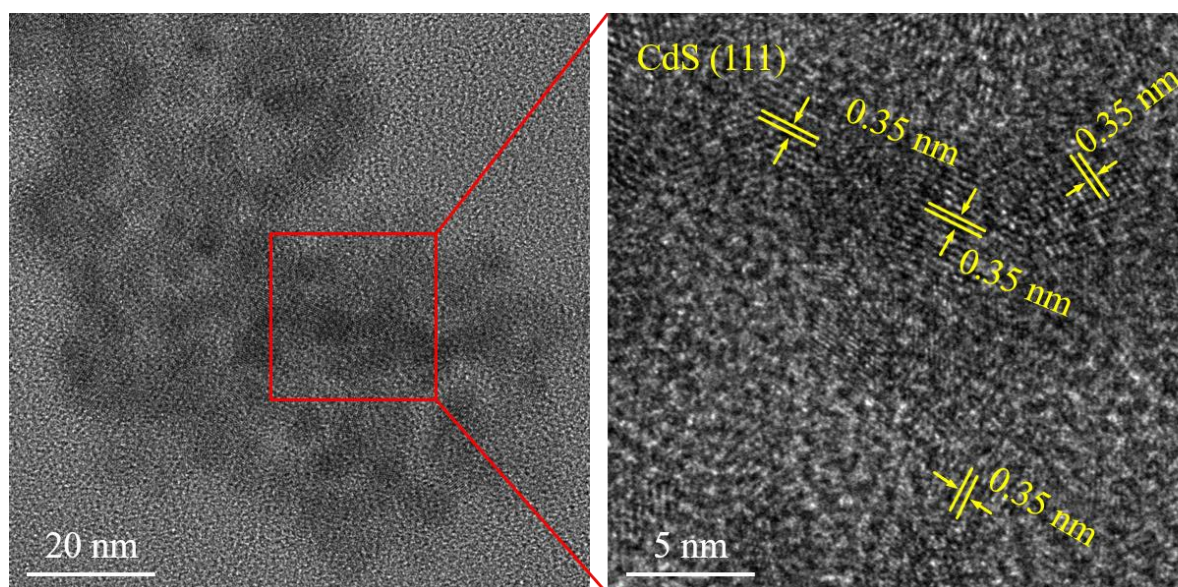


Fig. S12 TEM of CdS

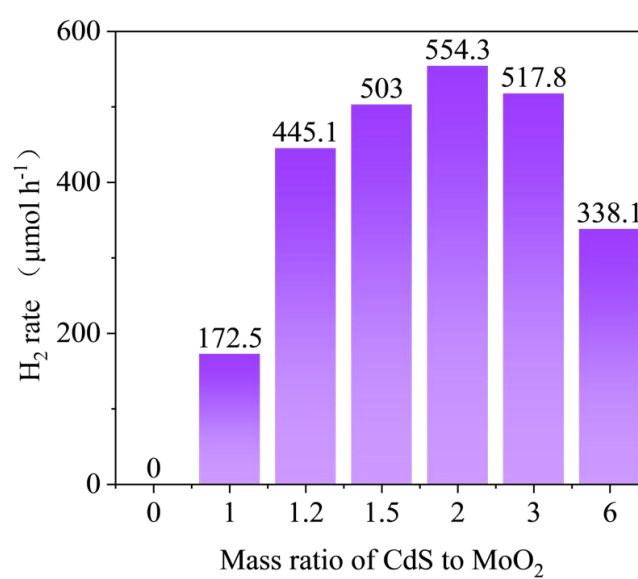


Figure S13. Influence of the mass ratio of CdS to MoO₂ used for preparing CdS/MoO₂ on the H₂ evolution rate.