Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Boosting Photocatalytic Hydrogen Evolution of Covalent Organic Frameworks by Introducing 2D Conductive Metal-organic Frameworks as Noble Metal-free Co-catalysts

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Characterization instrument

X-ray diffraction (XRD, Bruker D8 with a Cu Kα radiation, 40 KV, 40 mA, λ = 1.5418 Å), field emission scanning electron microscope (FESEM, Sigma 500, Germany), Fourier transform infrared spectrometer (FT-IR, Nicolet iS50, America), X-ray photoelectron spectroscopy (XPS, Escalab 250Xi, America), automatic Micromeritics apparatus (ASAP2460-Vapor, Micromeritics Instrument Corporation, America), ultraviolet-visible (UV-vis, UV3600, SHIMADZU, Japan), SourceMeter (2634B, KEITHLEY, America), electrochemical workstation (Autolab PGSTAT302N, Metrohm, Switzerland), gas chromatography (GC, GC-2014C, SHIMADZU, Japan, TCD detector).

The calculation of AQE (apparent quantum efficiency)

$$\mathrm{AQE} = \frac{2 \times numbers\ of\ evolved\ hydrogen\ molecules}{number\ of\ incident\ photons} \times 100\%$$

The calculation of VASP[1-5]

The electronic structures were calculated by the density functional theory (DFT) by using Vienna Ab-initio Simulation Package (VASP). The projector augmented wave (PAW) model with Perdew−Burke−Ernzerhof (PBE) function was employed to describe the interactions between core and electrons, an energy cutoff of 450 eV was used for the planewave expansion of the electronic wave function. The Brillouin zones of all systems were sampled with gamma-point centered Monkhorst-Pack grids. A 2 × 2 × 1 Monkhorst Pack *k*-point setup were used for slab geometry optimization. The force and energy convergence criterion were set to 0.02 eV $Å^{-1}$ and 10^{-5} eV, respectively.

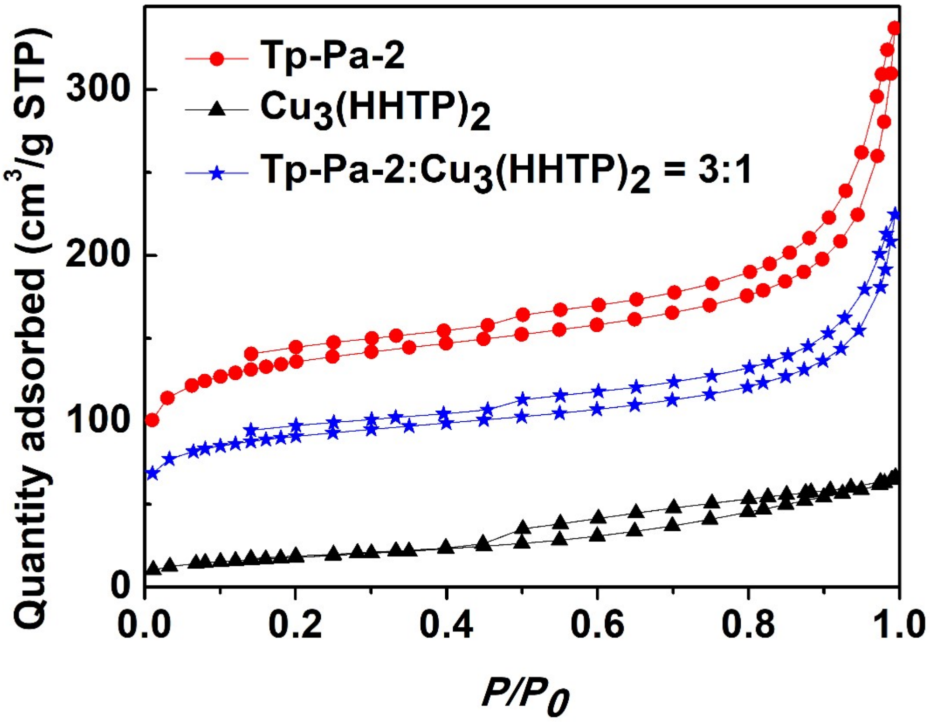

Figure S1. N_2 adsorption-desorption isotherm of Tp-Pa-2, $Cu_3(HHTP)_2$ and Tp-Pa-2/$Cu_3(HHTP)_2$ (3:1) composite.

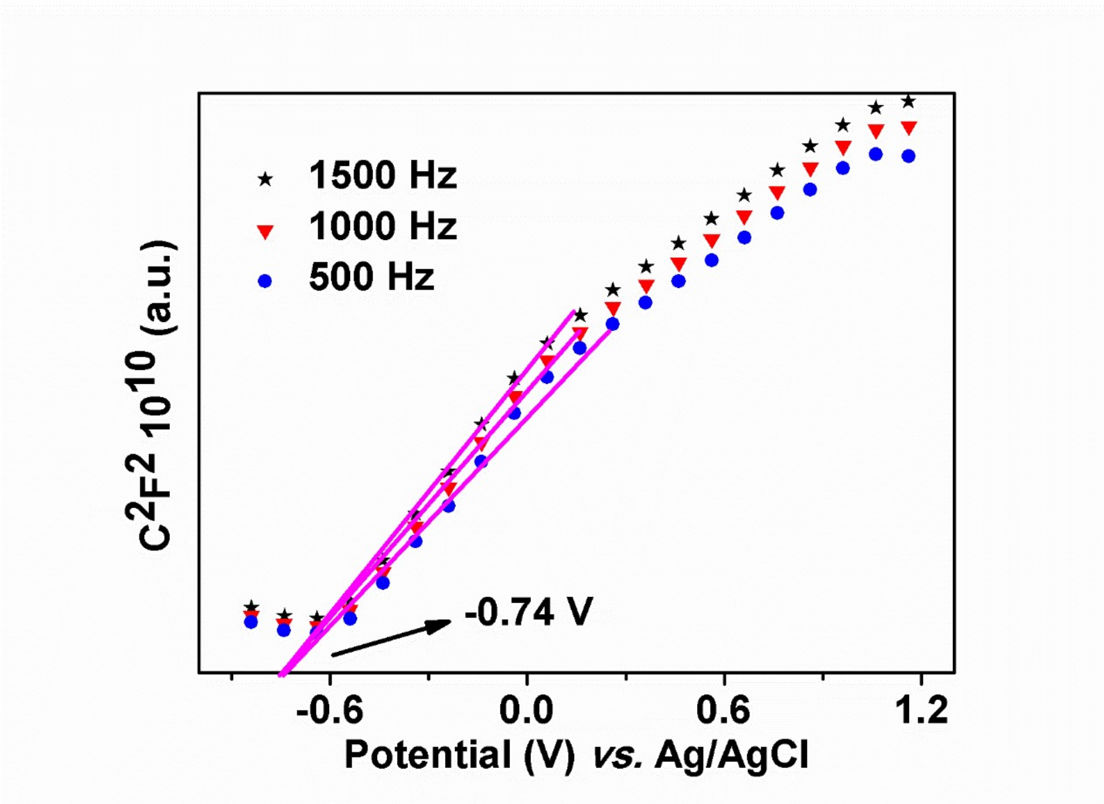

Figure S2. Mott-Schottky plot of Tp-Pa-2/$Cu_3(HHTP)_2$ (3:1) composite.

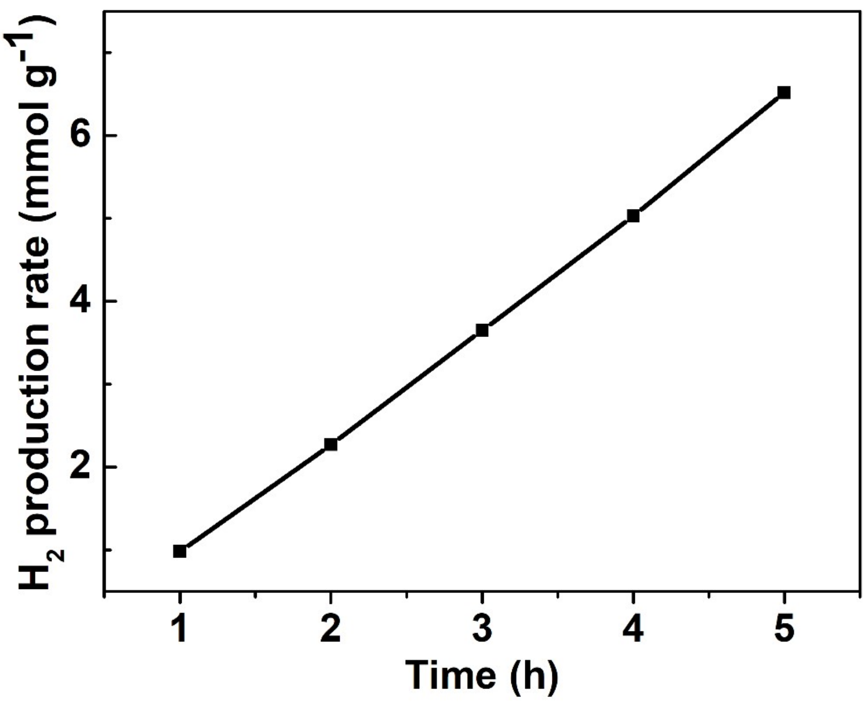

Figure S3. Photocatalytic H_2 production rate of Tp-Pa-2/$Cu_3(HHTP)_2$ (3:1) (without full griding).

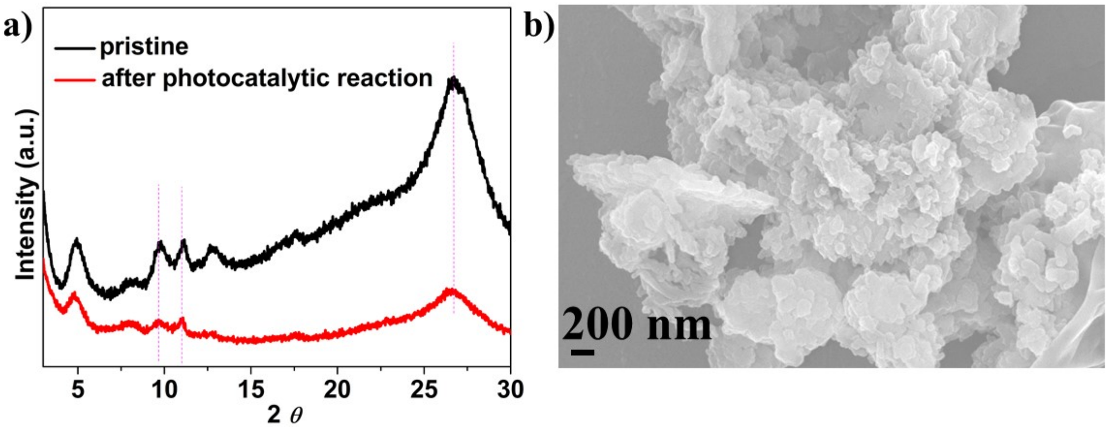

Figure S4. a) The XRD of Tp-Pa-2/$Cu_3(HHTP)_2$ (3:1) composite after photocatalytic reaction; b) SEM image of Tp-Pa-2/$Cu_3(HHTP)_2$ (3:1) composite after photocatalytic reaction.

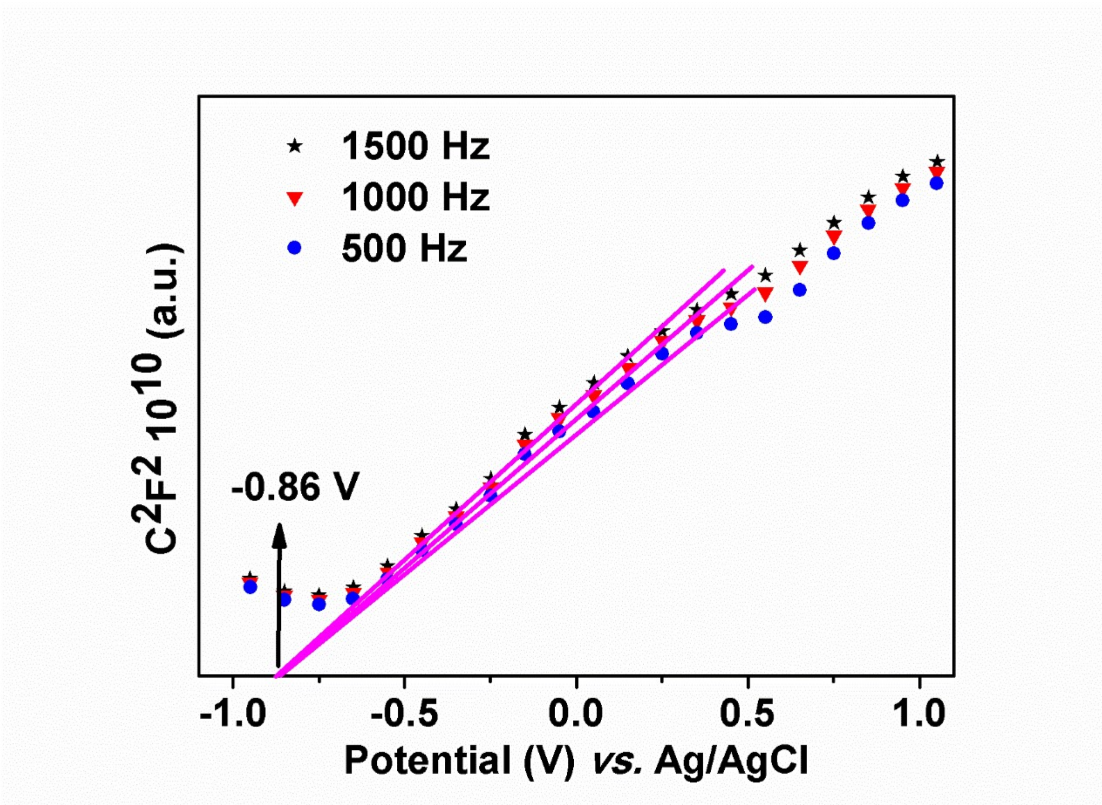

Figure S5. Mott-Schottky plot of Tp-Pa-2.

References

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