

Supporting information

2D-2D Heterojunctions of Covalent Triazine Framework with Triphenylphosphine-based Covalent Organic Framework for Efficient Photocatalytic Hydrogen Evolution

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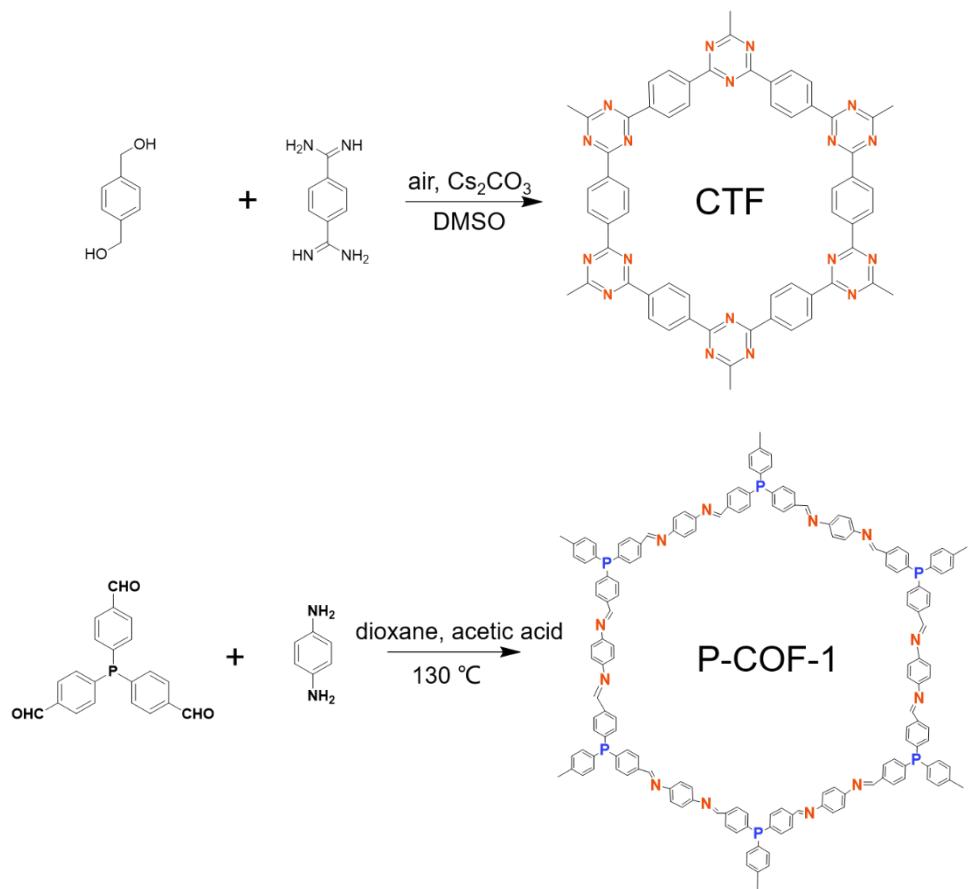


Fig. S1 Synthesis of CTF and P-COF-1 materials.

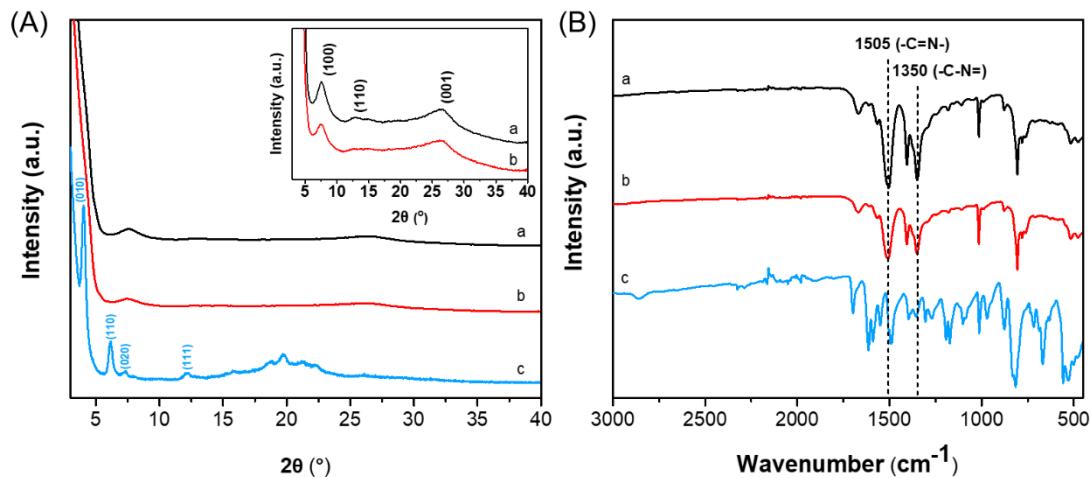


Fig. S2 XRD patterns (A) and FTIR spectra (B) of P-COF-1/CTF samples. (a) CTF, (b) 5% P-COF-1/CTF, (c) P-COF-1.

Tab. S1 Crystallographic parameters for P-COF-1¹ and CTF².

Sample	Space group	Crystal system	Lattice Parameter	Stacking arrangement
CTF	hexagonal	P6	$a = b = 14.480 \text{ \AA}$ $c = 3.622 \text{ \AA}$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$ $a = b = 32.549 \text{ \AA}$ $c = 7.9215 \text{ \AA}$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	A-A
P-COF-1	hexagonal	P6		A-A

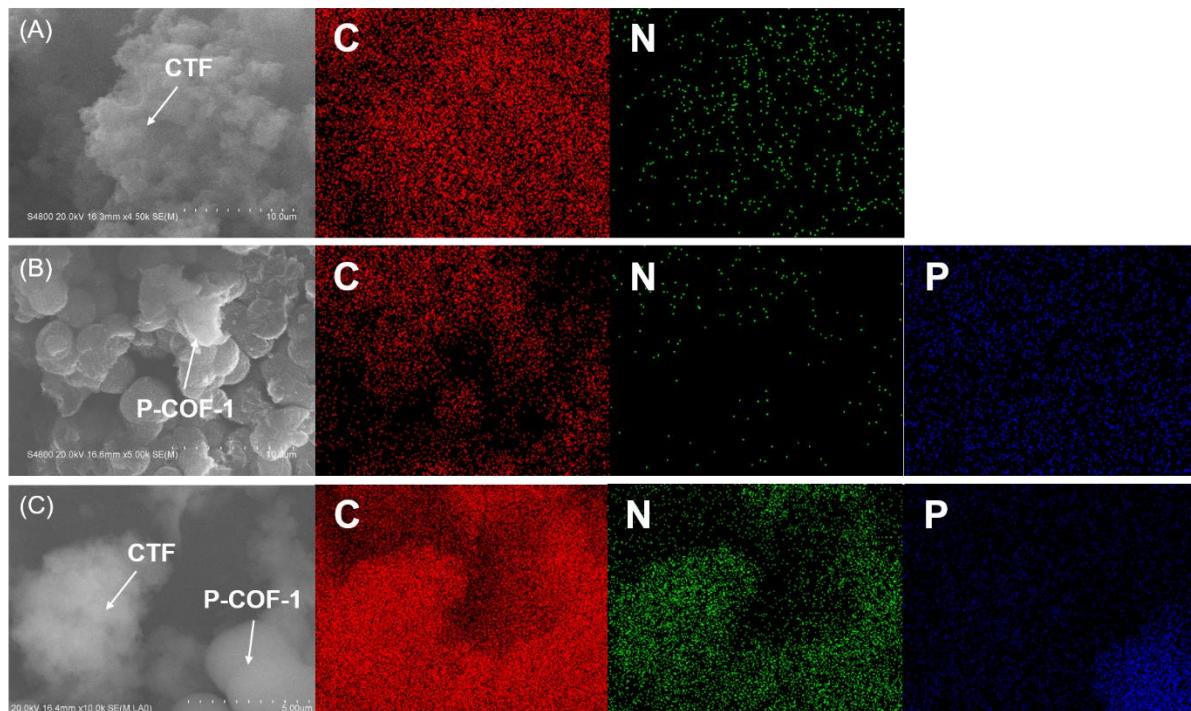


Fig. S3 SEM image and elemental mapping of CTF (A), P-COF-1 (B) and 5% P-COF-1/CTF (C).

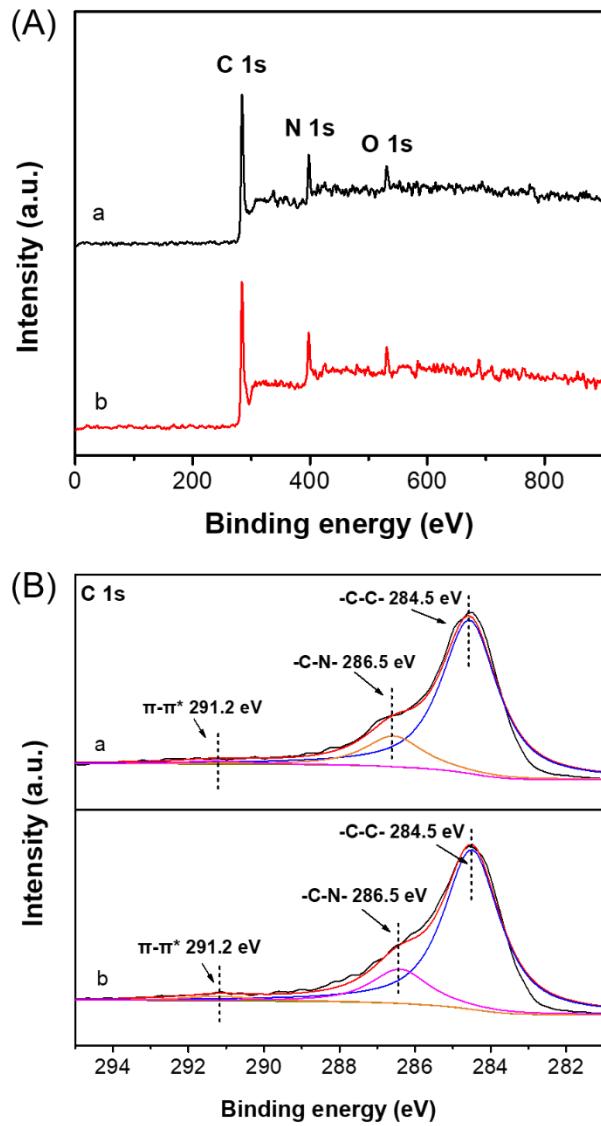


Fig. S4 XPS survey (A) and C 1s (B) spectra of P-COF-1/CTF samples. (a) CTF, (b) 5% P-COF-1/CTF.

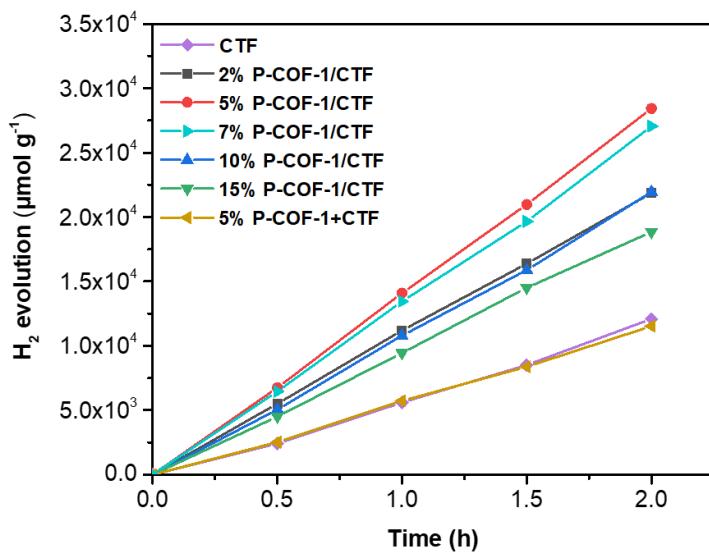


Fig. S5 The amount of hydrogen evolution over the P-COF-1/CTF with different mass ratio of P-COF-1.

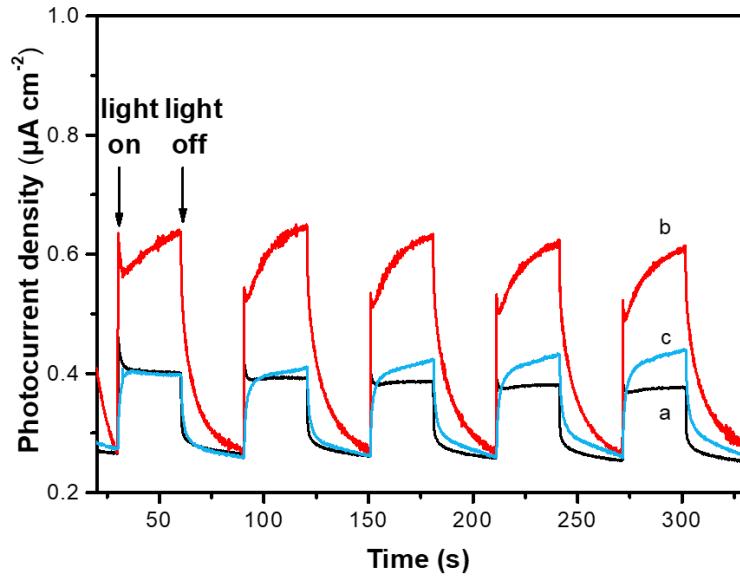


Fig. S6 Transient photocurrent spectra of P-COF-1/CTF samples. (a) CTF, (b) 5% P-COF-1/CTF, (c) P-COF-1.

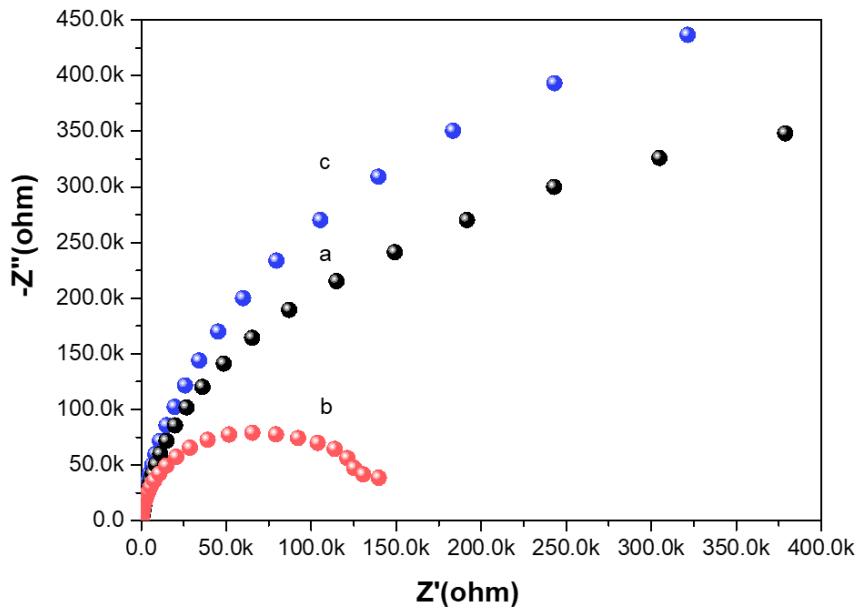


Fig. S7 EIS Nyquist plots of P-COF-1/CTF samples. (a) CTF, (b) 5% P-COF-1/CTF, (c) P-COF-1.

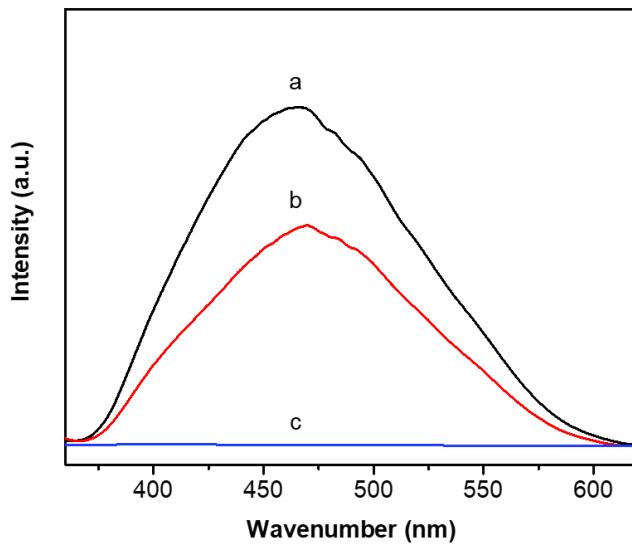


Fig. S8 Photoluminescence spectra of P-COF-1/CTF samples. (a) CTF, (b) 5% P-COF-1/CTF, (c) P-COF-1.

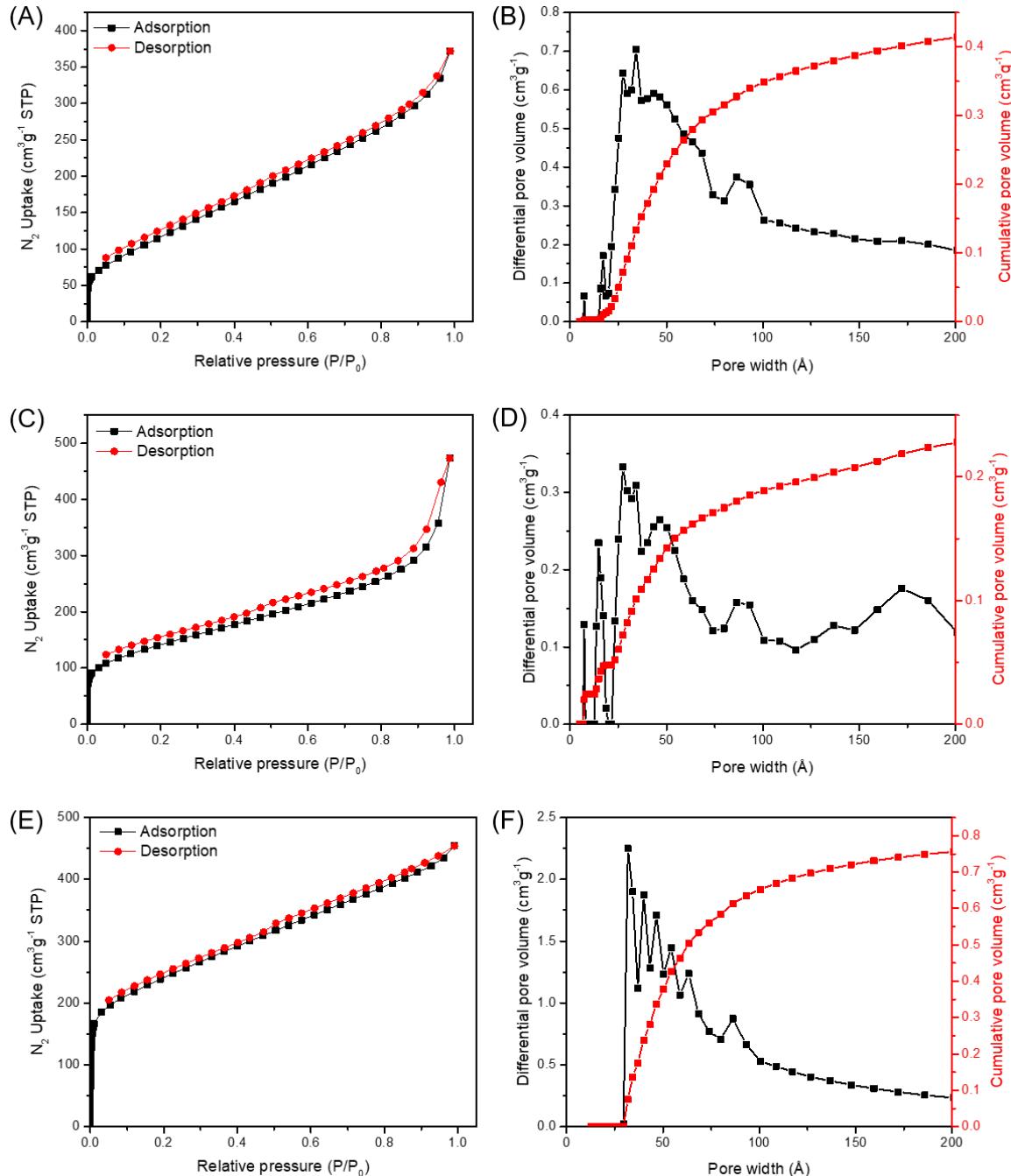


Fig. S9 Nitrogen adsorption/desorption isotherms (A, C, E) and pore size distribution curves (B, D, F) of P-COF-1/CTF samples. (A, B) CTF, (C, D) 5% P-COF-1/CTF, (E, F) P-COF-1.

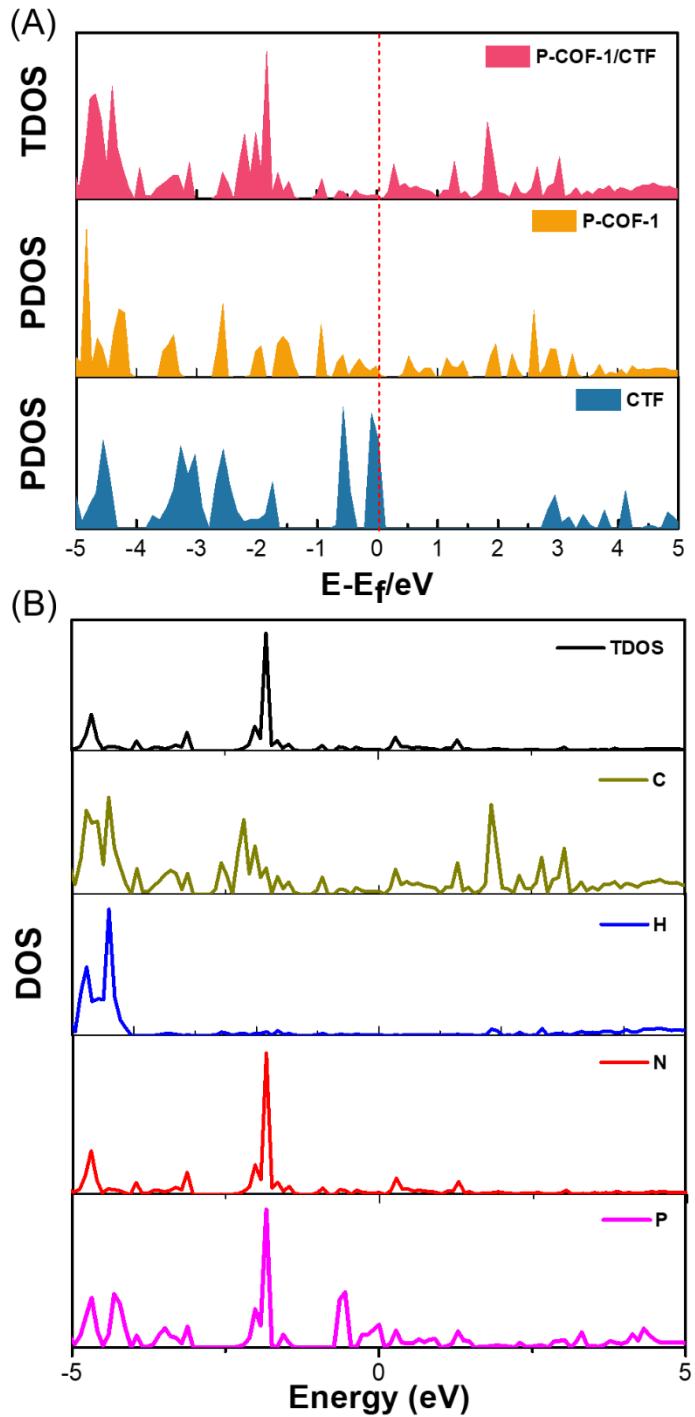


Fig. S10 (A) The total and partial density of states (DOS) of CTF, P-COF-1 and P-COF-1/CTF,
(B) The total and atomic-orbital projected DOS of P-COF-1/CTF heterojunctions.

Supporting references

- (1) Liu, Y.; Dikhtiarenko, A.; Xu, N.; Sun, J.; Tang, J.; Wang, K.; Xu, B.; Tong, Q.; Heeres, H. J.; He, S.; Gascon, J.; Fan, Y., Triphenylphosphine-Based Covalent Organic Frameworks and Heterogeneous Rh-P-COFs Catalysts. *Chem. -Eur. J.* **2020**, 26 (53), 12134-12139.
- (2) Wang, K.; Yang, L.-M.; Wang, X.; Guo, L.; Cheng, G.; Zhang, C.; Jin, S.; Tan, B.; Cooper, A., Covalent Triazine Frameworks via a Low-Temperature Polycondensation Approach. *Angew Chem. Int. Ed.* **2017**, 56 (45), 14149-14153.