Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Fabrication of heterostructured Pd-porphyrin MOFs/$ZnIn_2S_4$ composites to boost photocatalytic hydrogen evolution under visible light irradiation

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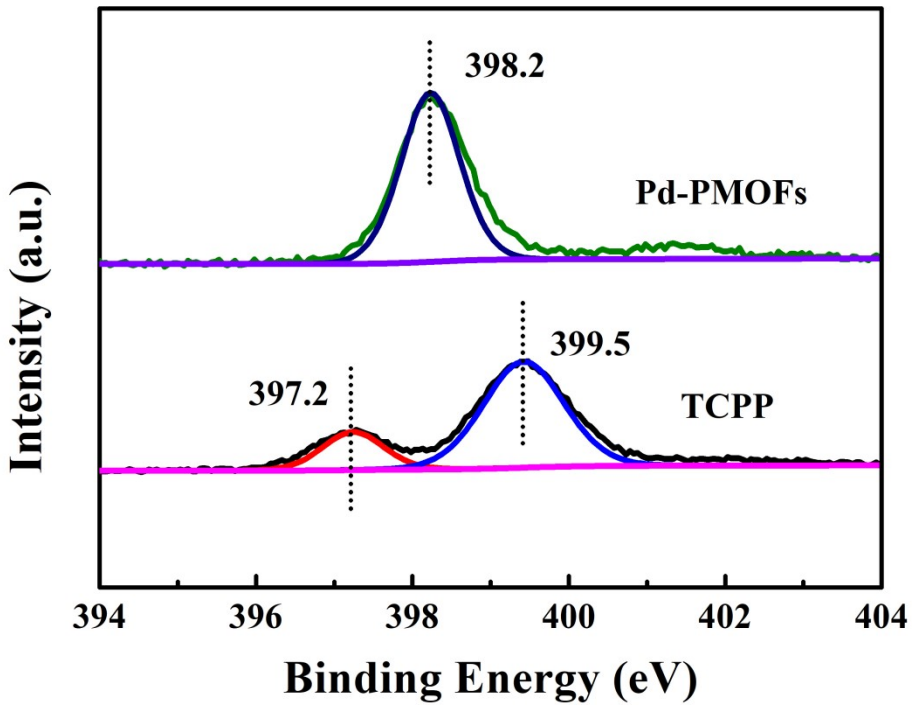
1. Fig. S1 high resolution XPS spectra (N 1s) of pure TCPP and Pd-PMOFs.



2. Description of Density Functional Theory (DFT) calculations

In Density Functional Theory calculation, we constructed $ZnIn_2S_4$(102) slab model. The Pd-PMOF molecule was built in a 30 × 30 × 30 $Å^3$ box. The Pd-PMOF was put on the surface of $ZnIn_2S_4$(102) 1 × 3 × 1 supercell to form the heterostructure. Structural optimization were performed by Vienna *Ab-initio* Simulation Package(VASP) with the projector augmented wave (PAW) method [1, 2]. The exchange-functional was treated using the Perdew-Burke-Ernzerhof (PBE) functional [3]. DFT-D3 correction was introduced to describe the weak interactions between atoms [4]. The cut-off energy of the plane-wave basis was set at 450 eV in structural optimization. For the optimization of both geometry and lattice size, the Brillouin zone integration was performed with 1× 1 × 1 Gamma[4] *k*-point sampling. The self-consistent calculations applied a convergence energy threshold of 10^{-5} eV. The equilibrium geometries and lattice constants were optimized with maximum stress on each atom within 0.02 eV $Å^{-1}$.

Fig. S2 The HOMO/LUMO orbitals of pure TCPP and Pd-PMOFs from DFT.

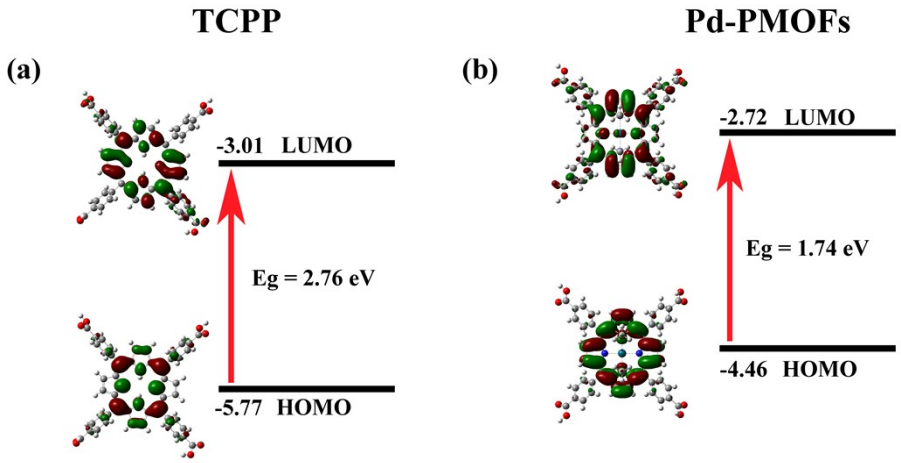
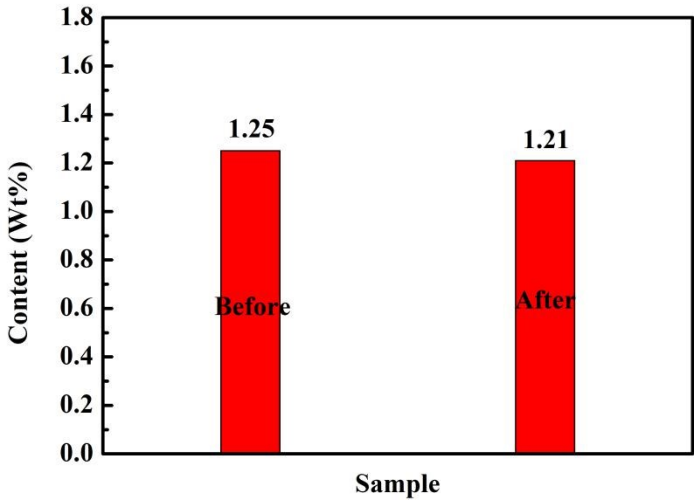


Fig. S3 The actual Pd content in Pd-PMOFs@ZIS-2 before and after experiments.



Reference

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