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Supporting Information

Dual-ligand engineering of Ti-Based MOFs for efficient piezo-photocatalytic overall water splitting

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Supplemental Figures and Supplemental Tables

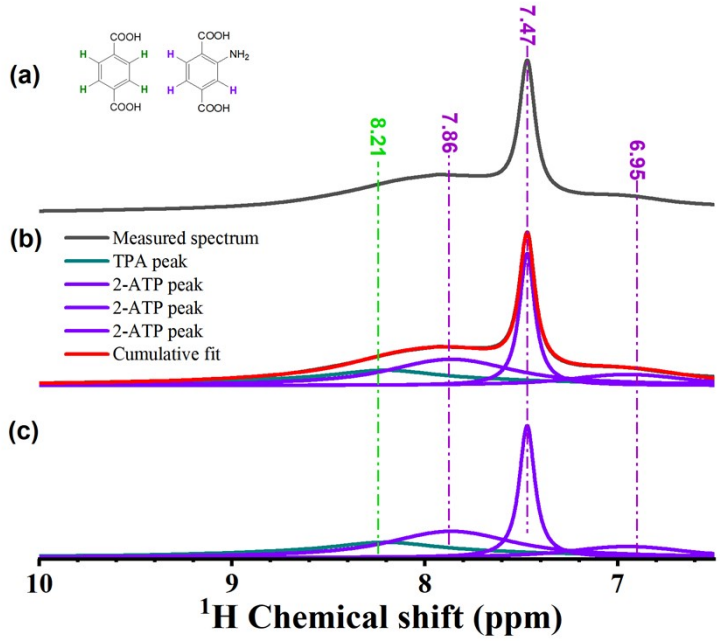

Figure S1. (a) ^{1}H MAS NMR spectra of MOF measured, (b) fitted TPA, 2-ATP peaks and (c) comulative fit, fitted TPA, 2-ATP peaks.

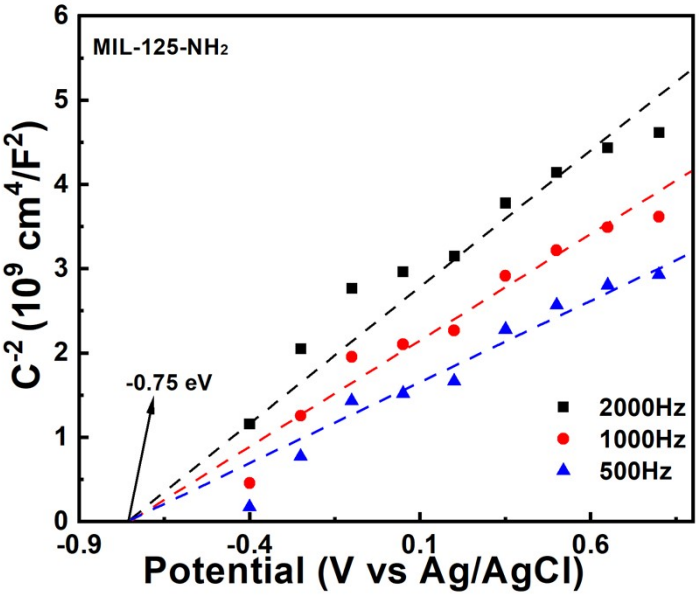

Figure S2. Mott-Schottky curves of MIL-125-NH_2.

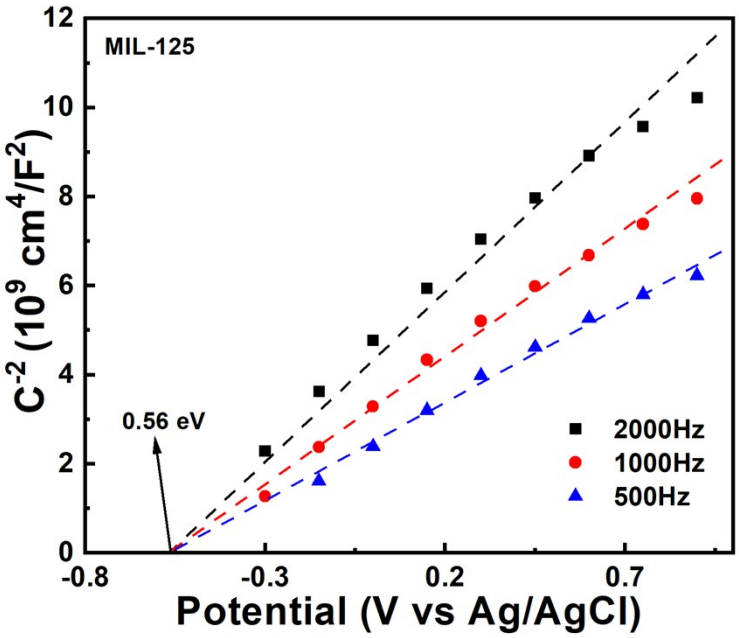

Figure S3. Mott-Schottky curves of MIL-125-NH_2.

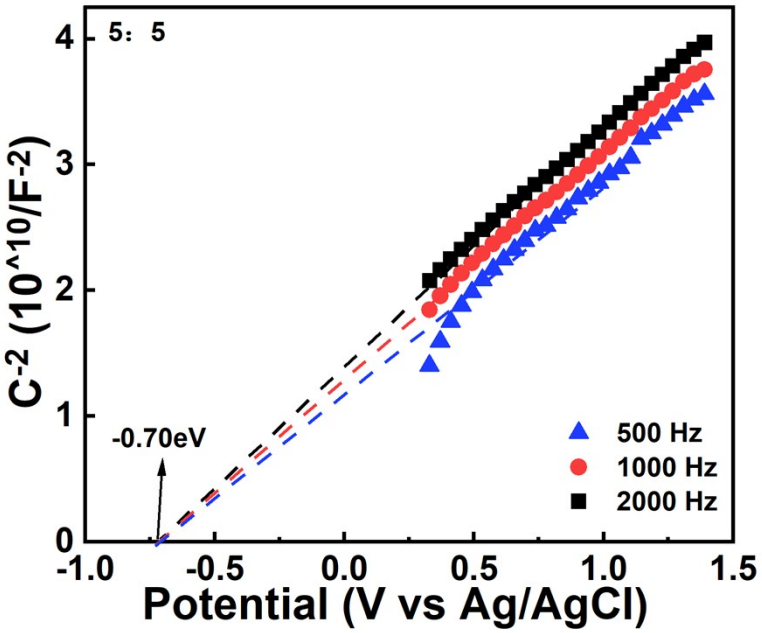

Figure S4. Mott-Schottky curves of MTV-MIL-125 (5:5).

Table S1 Comparison of MOF catalytic overall water splitting rate.

Photocatalyst	Light source	Ultrasonic	Cocatalyst	HER ($\mu mol\ g^{-1}\ h^{-1}$)	OER ($\mu mol\ g^{-1}\ h^{-1}$)	References
MTV-MIL-125 (5:5)	**300 W Xe lamp (λ>420 nm)**	**300 W, 45 KHz**	**N/A**	**358.2**	**178.4**	**This work**
MIL-173(Zr/Ti)-40	Xe-Hg lamp 150 W, 1.5 AM filter	N/A	N/A	381 in 22 h	145 in 22 h	*J. Mater. Chem. A, 2022, 10,24938-24950*
UiO-66(Zr)−NH_2 @MIL-88B(Fe)	150 W Hg-Xe lamp through an AM 1.5G filter (320 mW/cm^2)	N/A	N/A	690 in 3 h	279 in 3 h	*ACS Nano 2024, 18, 20201-20212*
Ti-MOF: IEF-11	150 W Xe-Hg lamp, 1.5 AM filter	N/A	N/A	672 in 22 h	322 in 22 h	*Adv.Mater. 2021, 33 (52), 2106627*
UiO-66(Zr)-NH_2	150 W Hg-Xe lamp through an AM 1.5G filter, 220 mW/cm^2	N/A	N/A	450 in 5 h	160 in 5 h	*Nano Res. 17, 4134-4150 (2024)*
UiO-66(Zr)−NH_2 @UiO-66(Ce)	150 W Hg-Xe lamp through an AM 1.5G filter	N/A	N/A	708 in 22 h	320 in 22 h	*Energy Fuels 2023, 37, 5457-5468*
$MgIn_2S_4$/UiO-66-NH_2	300 W Xe lamp (λ>420 nm)	N/A	N/A	24.69	12.93	*Langmuir 2023, 39, 7294-7306*
RuOx-MIL-125(Ti)-NH_2	300 W Xe lamp (UV/Vis light)	N/A	0.23 wt% RuO_x	3.33	1.67	*Appl. Catal. B: Environ.* 2019, 254, 677-68.
UiO-66(Zr/Ce/Ti)	300 W Xe lamp (UV light)	N/A	N/A	9.58	4.58	*Appl. Catal. B: Environ.* 2020, 278, 11934.
Pt@NH_2-UiO-66@MnO_x	300 W Xe lamp (λ>400 nm)	N/A	3.2 wt% Pt 0.1 wt% MnO_x	19.6	10.1	*Adv. Mater.* 2020, 32, 2004747.