Electronic Supplementary Material (ESI) for CrystEngComm.

Electrocatalytic hydrogen evolution of MOFs derived materials based on conjugated or unconjugated ligands

Chun-Pu Duan[a], Ya-Lu Ni[a], Xu-Dong Yang[a], Jing-Yu Huang[a], Yong-Hui Shen[b], Xun-Gang Gu[b], Gang Ni[a], Miao-Lian Ma[a], Juan Li[a], Ling Qin*[,a]

Single-crystal structure determination

Crystallographic data were collected on a Bruker Apex Smart CCD diffractometer with graphite-monochromated Mo-K_α radiation (λ = 0.71073 Å) at 293 K adopting the ω-scan technique. Using the SAINT program integrated the intensity data. An empirical absorption correction was applied using the SADABS program. The structure was solved by direct methods and refined anisotropically using full-matrix least-squares procedures based on F^2 values with the SHELXTL-97 package of crystallographic software. The hydrogen atoms were generated geometrically. Crystallographic data of complex **1** are presented in Reference, the selected bond lengths and angles are given in Table S1. The CCDC reference number is 2269367-2269368 for Co-PDS-TDC and Co-BPT-TDC.

Table S1. Crystallographic data and structure refinement details.

Crystal	Co-BPT-TDC	Co-PDS-TDC
Formula	$C_{36}H_{20}Co_2N_8O_8S_4$	$C_{32}H_{22}Co_2N_4O_9S_6$
Formula Weight	938.70	916.76
Crystal System	monoclinic	orthorhombic
Space group	$P2_{1/c}$	$C2_22_1$
a	15.156(3)	16.8320(14)
b	18.378(2)	14.5894(16)
c	15.9626(18)	23.725(3)
α	90	90
β	91.834(12)	90
γ	90	90
V	4443.9(11)	5826.1(11)
Z	4	4
D(calc) [g/cm^3]	1.403	1.045
Mu (MoKa) [/mm]	0.989	0.821
F(000)	1896	1856
Temperature (K)	293	293
Theta Min-Max	3.4, 25.0	3.4, 25.0
Tot., Uniq. Data,	7788, 7788	17266, 5117
R(int)	0.000	0.062
Observed Data	4039	4332
Nref, Npar	7788, 523	1198, 97
R	0.1141	0.0962
wR2	0.3041	0.2921
S	1.02	1.13
Max. and Av. Shift/Error	0.00, 0.00	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.83, 3.10	-0.74, 1.60

Table S2 Selected bond lengths (Å) and angles (deg.)

Crystal		Co-BPT-TDC	
Co1-O1	2.032(6)	O5-Co1-O8_c	149.3(2)
Co1-O5	2.094(6)	N1-Co1-N4_b	175.9(3)
Co1-N1	2.104(8)	O8_c-Co1-N1	87.4(2)
Co1-N4_b	2.127(9)	O5-Co1-N4_b	90.9(2)
Co1-O8_c	2.024(5)	O8_c-Co1-N4_b	88.5(2)
Co2-O2	2.005(6)	O2-Co2-N5	85.9(3)
Co2-N5	2.154(8)	O2-Co2-N8_a	89.4(3)
Co2-N8_a	2.088(8)	O2-Co2-O7_c	117.2(2)
Co2-O7_c	2.015(6)	O2-Co2-O4_d	148.4(2)
Co2-O4_d	2.092(6)	N5-Co2-N8_a	175.1(3)
O1-Co1-O5	93.6(2)	O7_c-Co2-N5	90.9(3)
O1-Co1-N1	91.7(3)	O4_d-Co2-N5	90.7(2)
O1-Co1-N4_b	90.6(3)	O7_c-Co2-N8_a	92.4(3)
O1-Co1-O8_c	117.1(2)	O4_d-Co2-N8_a	92.7(2)
O5-Co1-N1	92.3(2)	O4_d-Co2-O7_c	94.2(2)

Symmetry element: a = -1 + *x*, *y*, *z*; b = 1 + *x*, *y*, *z*; c = *x*, 1/2 - *y*, -1/2 + *z*; d = *x*, 3/2 - *y*, -1/2 + *z*.

Crystal		Co-PDS-TDC	
Co1-O1	2.084(6)	O1-Co1-O4_c	88.5(3)
Co1-O5	2.144(5)	O5-Co1-N1	90.7(3)
Co1-N1	2.167(9)	O3_a-Co1-O5	95.8(3)
Co1-O3_a	2.059(7)	O5-Co1-N2_b	174.7(2)
Co1-N2_b	2.151(9)	O4_c-Co1-O5	87.8(2)
Co1-O4_c	2.086(7)	O3_a-Co1-N1	89.3(3)
O4_c-Co1-N2_b	87.5(3)	N1-Co1-N2_b	94.0(3)
O1-Co1-O5	90.4(2)	O4_c-Co1-N1	177.9(3)
O1-Co1-N1	90.1(3)	O3_a-Co1-N2_b	86.8(3)
O1-Co1-O3_a	173.8(3)	O3_a-Co1-O4_c	92.3(3)
O1-Co1-N2_b	87.1(3)		

Symmetry element: a = -1/2 + *x*, 1/2 + *y*, *z*; b = 1/2 + *x*, 1/2 + *y*, *z*; c = 5/2 - *x*, 1/2 + *y*, 3/2 - *z*.

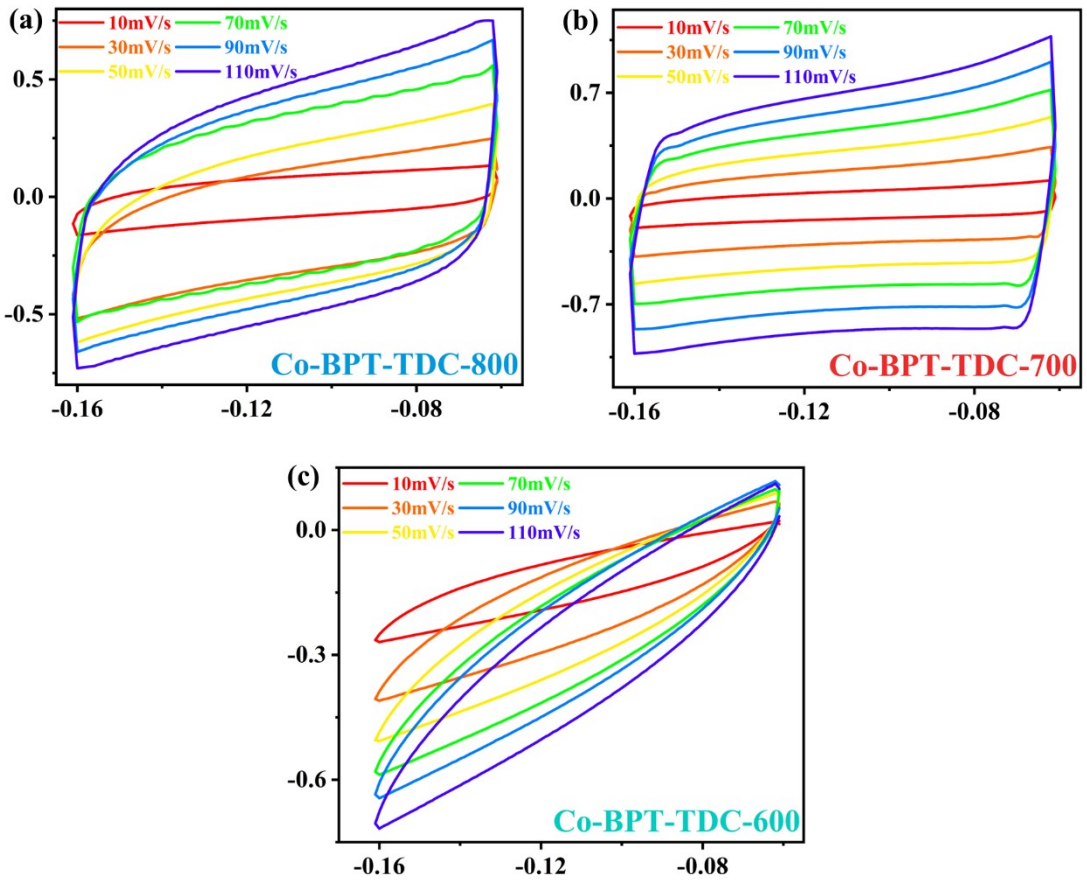

Figure S1 The CV of (a) Co-BPT-TDC-800, (b) Co-BPT-TDC-700 and (c) Co-BPT-TDC-600 with different sweep speed.

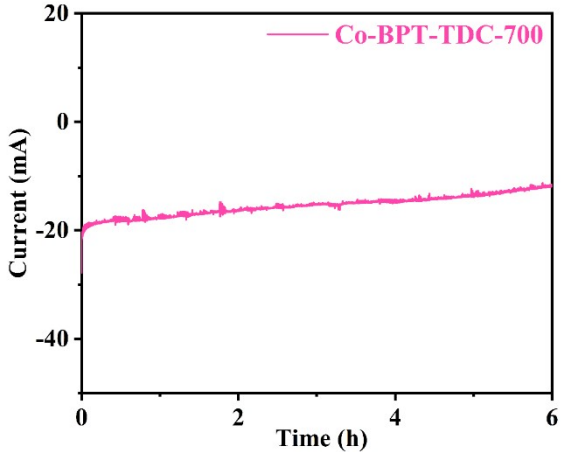

Figure S2 Co-BPT-TDC-700 sample stability test it curve.

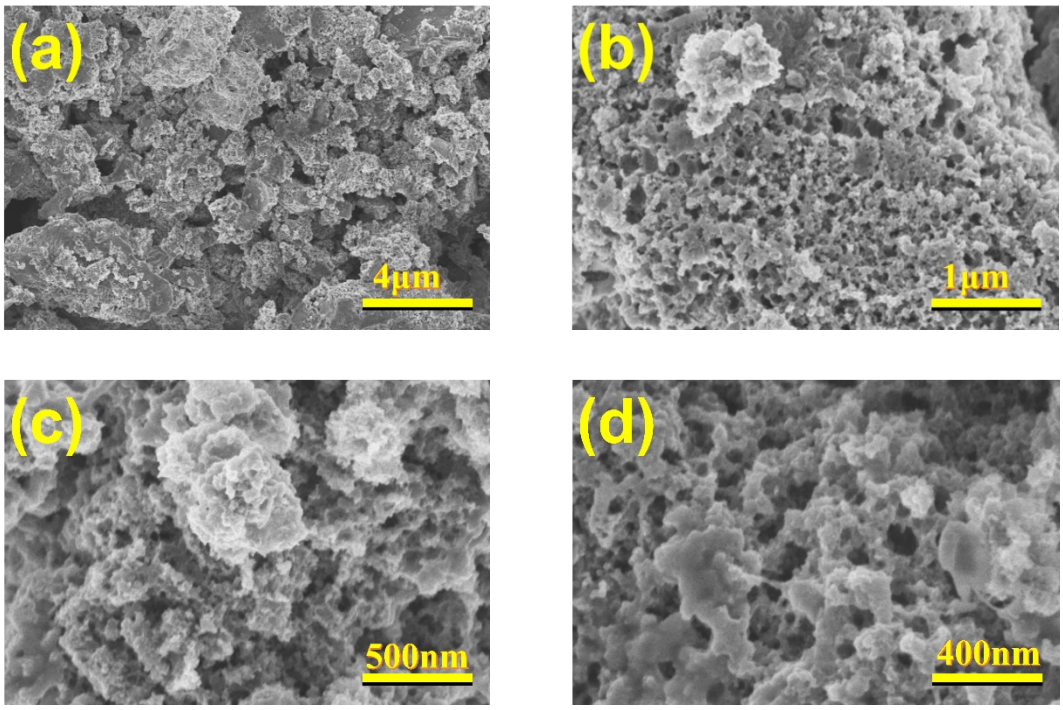

Figure S3 SEM patterns after Co-BPT-TDC-700 sample stability test.

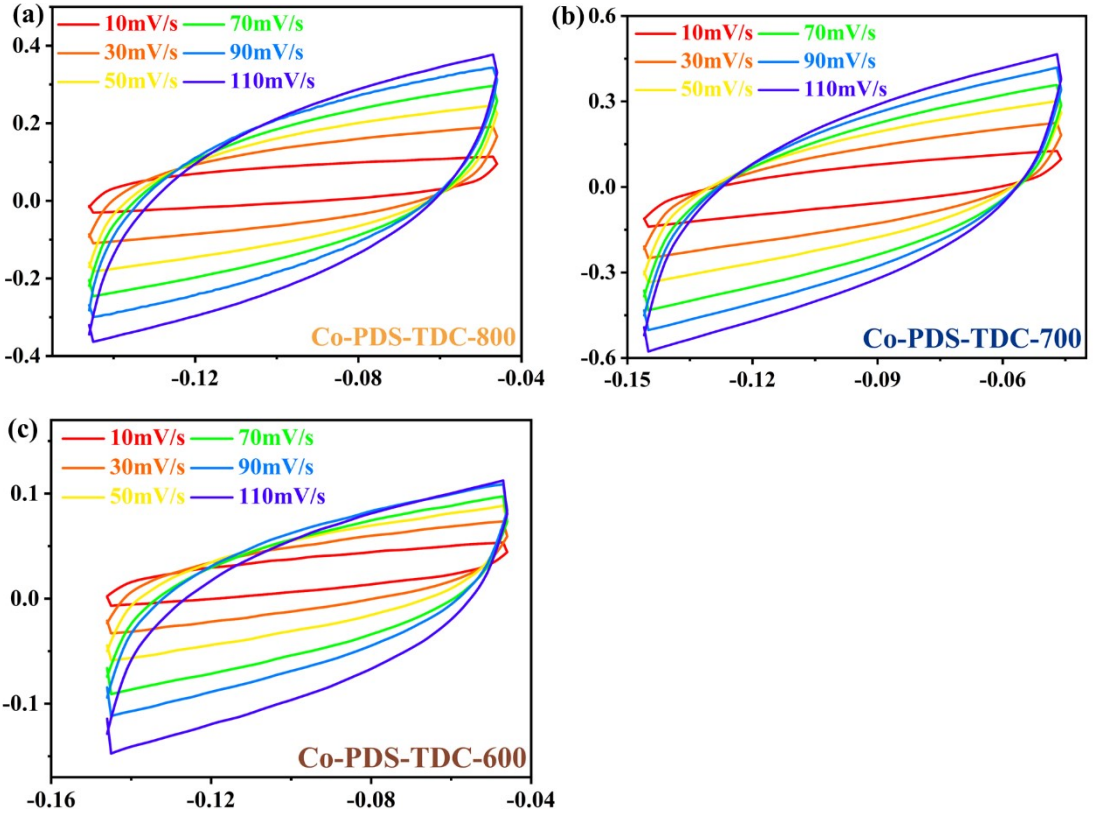

Figure S4 The CV of (a) Co-PDS-TDC-800, (b) Co-PDS-TDC-700 and (c) Co-PDS-TDC-600 with different sweep speed.