

## SUPPLEMENTARY INFORMATION

### The role of supramolecular interactions and pyridine groups in the (photo)electrocatalytic properties of a non-precious Co-based MOF

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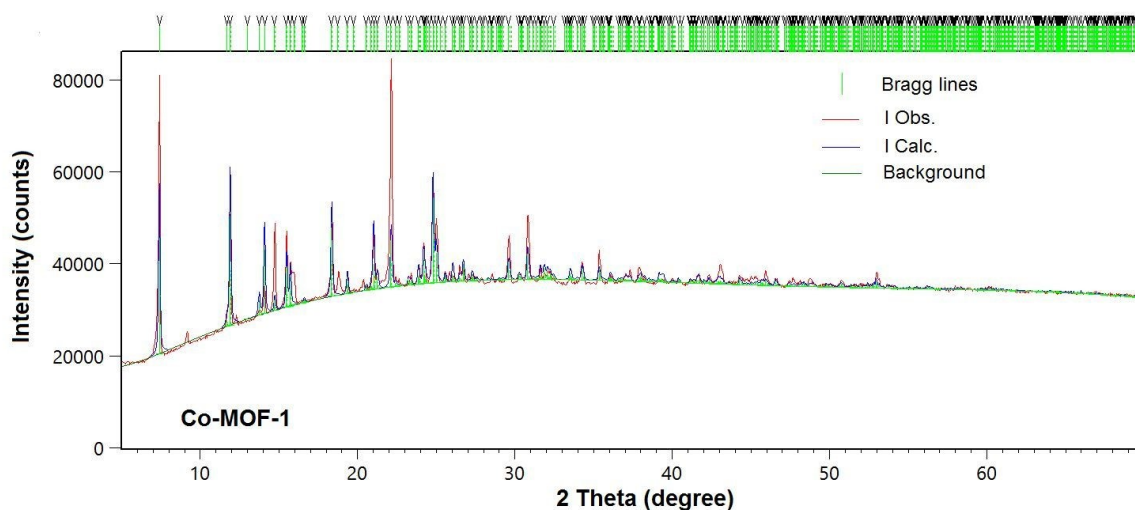
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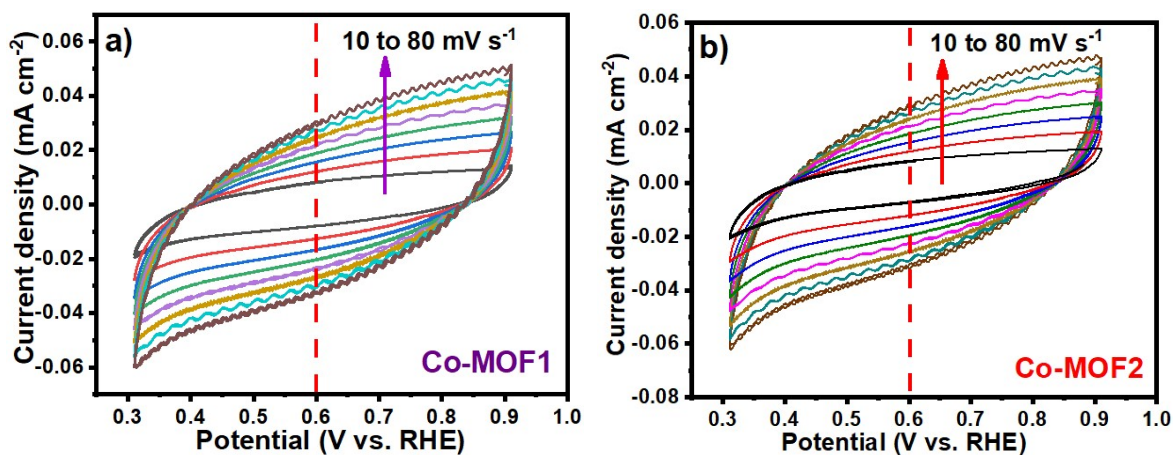
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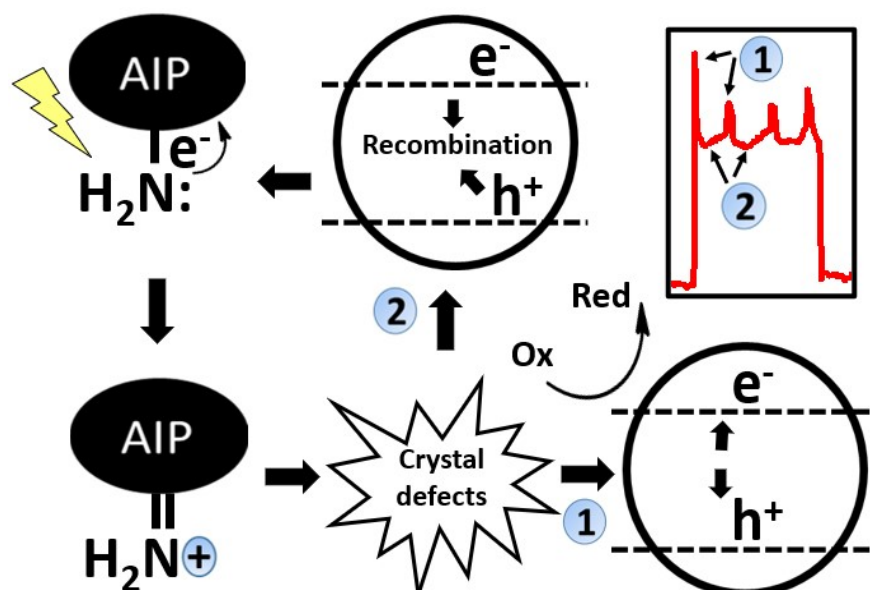
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**Figure S1.** Rietveld refinement of the XRD pattern from sample Co-MOF-1 employing the HighScore Plus software



**Figure S2.** Cyclic voltammety tests in the capacitive region for Co-MOF1 and Co-MOF2 at different scan rates.



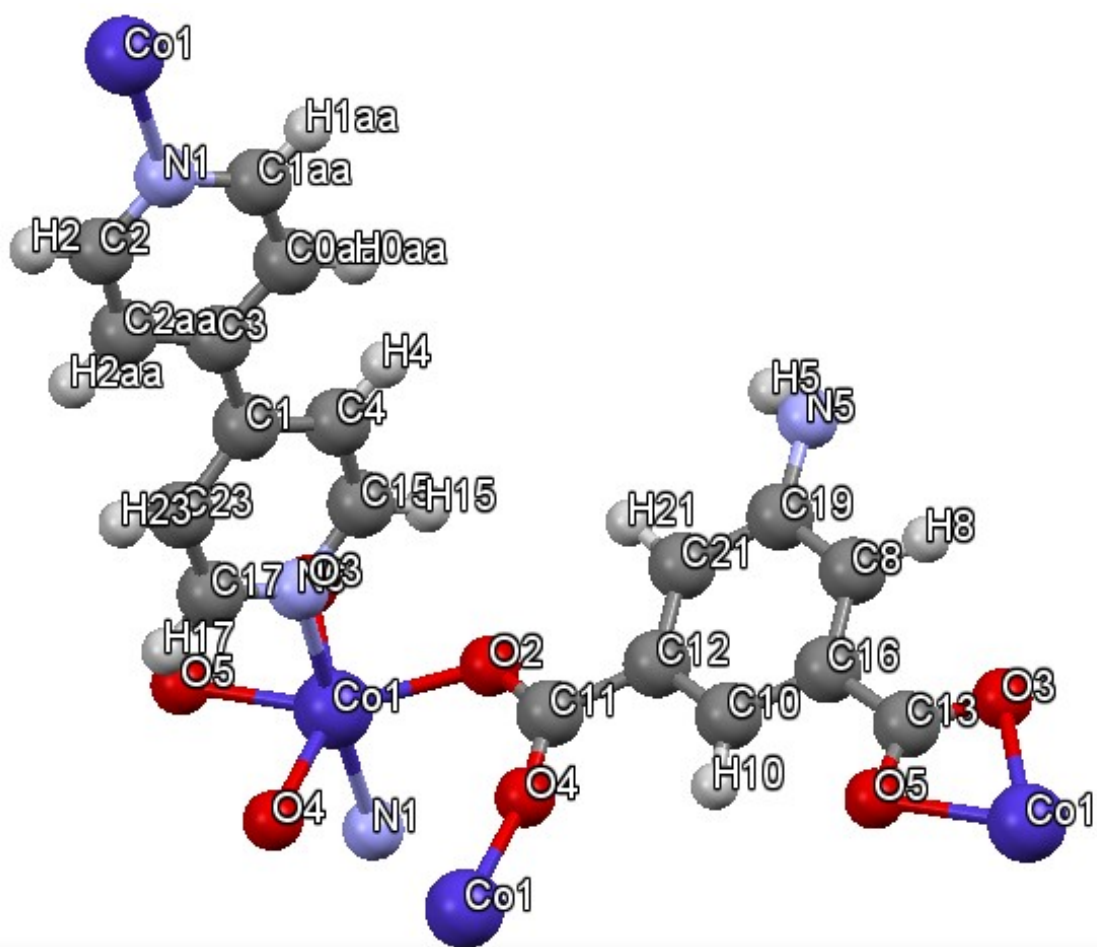
**Figure S3.** Charge carriers transport and recombination mechanism for Co-MOF2

## Co-MOF2 crystal information

### Crystatolographic data

Compound	Co-MOF2
Chemical formula	C <sub>18</sub> H <sub>12</sub> Co N <sub>3</sub> O <sub>4</sub>
Formula weight	393.24
Space group	Triclinic
Crystal system	P -1
Crystal color and shape	Red needles
a(Å)	10.0194(2)
b(Å)	10.0233(10)
c(Å)	10.1363(10)
α(°)	78.030
β(°)	68.659
γ(°)	78.785
Volume (Å <sup>3</sup> )	919.60
Formula units per cell, Z	2
δ <sub>calc</sub> (g cm <sup>-3</sup> )	1.420
μ (mm <sup>-1</sup> )	0.960
R-Factor (%)	5.98
F(000)	400
Temperature of measurement (K)	297

### Atoms labels



Bond distances list

Atom1	Atom2	Type	Polymeric	Cyclicity	Length (Å)
Co1	O2	Coordination	no	acyclic	2.035(2)
Co1	N6	Coordination	no	acyclic	2.145(2)
Co1	O3	Coordination	yes	acyclic	2.243(4)
Co1	O4	Coordination	yes	acyclic	2.020(4)
Co1	O5	Coordination	yes	acyclic	2.113(2)
Co1	N1	Coordination	yes	acyclic	2.150(2)
O2	C11	covalent	no	acyclic	1.261(5)
O3	C13	covalent	no	cyclic	1.241(4)
O3	Co1	Coordination	yes	cyclic	2.243(4)
O4	C11	covalent	no	acyclic	1.237(6)
O4	Co1	Coordination	yes	acyclic	2.020(4)
O5	C13	covalent	no	cyclic	1.257(6)
O5	Co1	Coordination	yes	cyclic	2.113(2)
N6	C15	covalent	no	cyclic	1.338(5)
N6	C17	covalent	no	cyclic	1.329(5)
C8	C16	covalent	no	cyclic	1.387(7)
C8	C19	covalent	no	cyclic	1.384(7)
C8	H8	covalent	no	acyclic	1.02(4)
C10	C12	covalent	no	cyclic	1.383(6)
C10	C16	covalent	no	cyclic	1.395(4)
C10	H10	covalent	no	acyclic	0.99(5)
C11	C12	covalent	no	acyclic	1.501(4)
C12	C21	covalent	no	cyclic	1.379(7)
C13	C16	covalent	no	acyclic	1.487(6)
C15	C4	covalent	no	cyclic	1.372(5)
C15	H15	covalent	no	acyclic	0.96(4)
C17	C23	covalent	no	cyclic	1.379(5)
C17	H17	covalent	no	acyclic	0.94(5)
C19	C21	covalent	no	cyclic	1.401(5)
C19	N5	covalent	no	acyclic	1.381(9)
C21	H21	covalent	no	acyclic	1.01(6)
C23	C1	covalent	no	cyclic	1.375(5)
C23	H23	covalent	no	acyclic	0.89(5)
C1	C3	covalent	no	acyclic	1.484(5)
C1	C4	covalent	no	cyclic	1.378(5)
C3	C0aa	covalent	no	cyclic	1.343(6)
C3	C2aa	covalent	no	cyclic	1.329(7)
C4	H4	covalent	no	acyclic	0.930(5)
N5	H5	covalent	no	acyclic	0.60(5)
N1	C1aa	covalent	no	cyclic	1.296(6)
N1	C2	covalent	no	cyclic	1.274(7)

N1	Co1	covalent	yes	acyclic	2.150(2)
C0aa	C1aa	covalent	no	cyclic	1.379(6)
C0aa	H0aa	covalent	no	acyclic	0.929(7)
C1aa	H1aa	covalent	no	acyclic	0.930(7)
C2aa	C2	covalent	no	cyclic	1.373(7)
C2aa	H2aa	covalent	no	acyclic	0.930(9)
C2	H2	covalent	no	acyclic	0.930(8)

### Angle bond list

Atom1	Atom2	Atom3	Angle
O2	Co1	N6	87.5(1)
O2	Co1	O3	90.3(1)
O2	Co1	O4	119.6(1)
O2	Co1	O5	149.7(1)
O2	Co1	N1	90.9(1)
N6	Co1	O3	88.7(1)
N6	Co1	O4	88.8(1)
N6	Co1	O5	89.7(1)
N6	Co1	N1	178.1(1)
O3	Co1	O4	149.9(1)
O3	Co1	O5	59.5(1)
O3	Co1	N1	92.3(1)
O4	Co1	O5	90.5(1)
O4	Co1	N1	91.1(1)
O5	Co1	N1	92.2(1)
Co1	O2	C11	120.1(2)
C13	O3	Co1	87.5(2)
C11	O4	Co1	165.4(3)
C13	O5	Co1	93.0(2)
Co1	N6	C15	122.0(3)
Co1	N6	C17	121.7(3)
C15	N6	C17	116.2(4)
C16	C8	C19	121.4(4)
C16	C8	H8	118(2)
C19	C8	H8	120(2)
C12	C10	C16	119.1(3)
C12	C10	H10	124(2)
C16	C10	H10	117(2)
O2	C11	O4	123.4(4)
O2	C11	C12	117.4(3)
O4	C11	C12	119.2(3)

C10	C12	C11	119.7(3)
C10	C12	C21	120.5(4)
C11	C12	C21	119.8(3)
O3	C13	O5	120.0(3)
O3	C13	C16	121.4(3)
O5	C13	C16	118.6(3)
N6	C15	C4	123.9(4)
N6	C15	H15	113(3)
C4	C15	H15	123(3)
C8	C16	C10	120.0(4)
C8	C16	C13	120.0(3)
C10	C16	C13	120.0(3)
N6	C17	C23	123.4(4)
N6	C17	H17	115(3)
C23	C17	H17	121(3)
C8	C19	C21	117.8(4)
C8	C19	N5	119.6(4)
C21	C19	N5	122.6(4)
C12	C21	C19	121.2(4)
C12	C21	H21	123(3)
C19	C21	H21	116(3)
C17	C23	C1	120.0(4)
C17	C23	H23	118(3)
C1	C23	H23	122(3)
C23	C1	C3	122.1(4)
C23	C1	C4	117.1(4)
C3	C1	C4	120.8(4)
C1	C3	C0aa	123.0(4)
C1	C3	C2aa	122.8(4)
C0aa	C3	C2aa	114.3(5)
C15	C4	C1	119.4(4)
C15	C4	H4	120.3(5)
C1	C4	H4	120.3(5)
C19	N5	H5	117(5)
C1aa	N1	C2	114.6(4)
C1aa	N1	Co1	122.9(3)
C2	N1	Co1	122.4(4)
C3	C0aa	C1aa	121.0(5)
C3	C0aa	H0aa	119.5(6)
C1aa	C0aa	H0aa	119.5(7)
N1	C1aa	C0aa	123.9(5)
N1	C1aa	H1aa	118.1(6)
C0aa	C1aa	H1aa	118.0(6)

C3	C2aa	C2	121.3(6)
C3	C2aa	H2aa	119.3(8)
C2	C2aa	H2aa	119.4(8)
N1	C2	C2aa	125.0(6)
N1	C2	H2	117.5(8)
C2aa	C2	H2	117.5(8)
O3	Co1	O5	59.5(1)