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Aminopyridine Derivatives Controlled Assembly and Various Properties of Cu–BTC Metal–Organic Frameworks

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Table S1 Selected bond distances (Å) and angles (°) for complexes **1**–**3**.

Complex **1**			
Cu(1)-O(1)	1.950(2)	O(3W)-Cu(2)	1.981(2)
Cu(1)-O(4)	1.952(2)	O(3W)-Cu(1)#1	2.002(2)
Cu(1)-O(3W)	1.982(2)	Cu(2)-O(2)	1.942(2)
Cu(1)-O(3W)#1	2.002(2)	Cu(2)-O(3)#1	1.956(2)
Cu(1)-O(1W)	2.391(3)	Cu(2)-O(2W)	2.331(3)
N(1)-Cu(2)	2.052(3)	O(3)-Cu(2)#1	1.956(2)
O(1)-Cu(1)-O(4)	87.35(10)	O(2)-Cu(2)-O(3)#1	173.30(10)
O(1)-Cu(1)-O(3W)	94.88(10)	O(2)-Cu(2)-O(3W)	94.65(10)
O(4)-Cu(1)-O(3W)	175.24(10)	O(3)#1-Cu(2)-O(3W)	92.05(10)
O(1)-Cu(1)-O(3W)#1	174.48(10)	O(2)-Cu(2)-N(1)	86.83(11)
O(4)-Cu(1)-O(3W)#1	97.75(10)	O(3)#1-Cu(2)-N(1)	86.50(11)
O(3W)-Cu(1)-O(3W)#1	80.19(10)	O(3W)-Cu(2)-N(1)	177.23(11)
O(1)-Cu(1)-O(1W)	88.31(11)	O(2)-Cu(2)-O(2W)	91.47(12)
O(4)-Cu(1)-O(1W)	86.99(11)	O(3)#1-Cu(2)-O(2W)	89.29(12)
O(3W)-Cu(1)-O(1W)	97.26(10)	O(3W)-Cu(2)-O(2W)	85.39(13)
O(3W)#1-Cu(1)-O(1W)	89.85(10)	N(1)-Cu(2)-O(2W)	92.23(14)
O(1)-Cu(1)-Cu(1)#1	135.17(8)	O(2)-Cu(2)-H(3WA)	100.2
O(4)-Cu(1)-Cu(1)#1	137.45(8)	O(3)#1-Cu(2)-H(3WA)	86
O(3W)-Cu(1)-Cu(1)#1	40.33(7)	O(3W)-Cu(2)-H(3WA)	24.1
O(3W)#1-Cu(1)-Cu(1)#1	39.85(7)	N(1)-Cu(2)-H(3WA)	153.2
O(1W)-Cu(1)-Cu(1)#1	94.61(8)	O(2W)-Cu(2)-H(3WA)	62
Symmetry code for **1**: #1 $-x + 1, -y + 1, -z$			
Complex **2**			
Cu(1)-O(1)	1.9288(17)	Cu(2)-O(5)	1.9372(18)
Cu(1)-O(3)	1.9406(17)	Cu(2)-N(2)	1.983(2)
Cu(1)-N(1)	2.010(2)	Cu(2)-O(3W)	1.9945(18)
Cu(1)-O(1W)	2.020(2)	Cu(2)-N(3)	1.998(2)
Cu(1)-O(2W)	2.298(2)	Cu(2)-N(4)#1	2.312(2)
O(1)-Cu(1)-O(3)	153.25(8)	O(5)-Cu(2)-N(2)	93.54(8)

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O(1)-Cu(1)-N(1)	90.60(8)	O(5)-Cu(2)-O(3W)	94.31(7)
O(3)-Cu(1)-N(1)	94.91(8)	N(2)-Cu(2)-O(3W)	160.57(8)
O(1)-Cu(1)-O(1W)	85.43(8)	O(5)-Cu(2)-N(3)	173.37(8)
O(3)-Cu(1)-O(1W)	86.65(8)	N(2)-Cu(2)-N(3)	81.30(8)
N(1)-Cu(1)-O(1W)	173.91(9)	O(3W)-Cu(2)-N(3)	89.37(8)
O(1)-Cu(1)-O(2W)	97.34(8)	O(5)-Cu(2)-N(4)#1	97.91(8)
O(3)-Cu(1)-O(2W)	107.68(8)	N(2)-Cu(2)-N(4)#1	104.83(8)
N(1)-Cu(1)-O(2W)	98.28(8)	O(3W)-Cu(2)-N(4)#1	91.65(8)
O(1W)-Cu(1)-O(2W)	86.82(8)	N(3)-Cu(2)-N(4)#1	87.49(8)
Symmetry code for **2**: #1 *x*, *–y* + 1/2, *z* + 1/2			
Complex **3**			
Cu(1)-O(1W)#1	1.9274(19)	Cu(2)-O(1W)	1.9454(19)
Cu(1)-N(1)	1.980(3)	Cu(2)-O(2)	1.932(2)
Cu(1)-O(1)	1.987(2)	Cu(2)-O(3)	1.986(2)
Cu(1)-O(4)#1	2.069(2)	Cu(2)-O(1W)#1	2.0031(19)
Cu(1)-O(5)#2	2.136(2)	Cu(2)-O(6)#2	2.239(2)
O(1W)#1-Cu(1)-N(1)	171.49(10)	O(2)-Cu(2)-O(1W)	172.05(9)
O(1W)#1-Cu(1)-O(1)	93.70(8)	O(2)-Cu(2)-O(3)	86.59(9)
N(1)-Cu(1)-O(1)	92.37(10)	O(1W)-Cu(2)-O(3)	98.75(8)
O(1W)#1-Cu(1)-O(4)#1	89.23(8)	O(2)-Cu(2)-O(1W)#1	93.07(9)
N(1)-Cu(1)-O(4)#1	82.27(10)	O(1W)-Cu(2)-O(1W)#1	79.83(8)
O(1)-Cu(1)-O(4)#1	132.73(10)	O(3)-Cu(2)-O(1W)#1	159.12(9)
O(1W)#1-Cu(1)-O(5)#2	91.64(8)	O(2)-Cu(2)-O(6)#2	92.42(9)
N(1)-Cu(1)-O(5)#2	90.56(10)	O(1W)-Cu(2)-O(6)#2	92.25(8)
O(1)-Cu(1)-O(5)#2	119.51(10)	O(3)-Cu(2)-O(6)#2	101.68(9)
O(4)#1-Cu(1)-O(5)#2	107.52(8)	O(1W)#1-Cu(2)-O(6)#2	99.19(8)
Symmetry code for **3**: #1 *–x* + 1, *–y*, *–z*; #2 *x* + 1/2, *–y* + 1/2, *z* + 1/2			

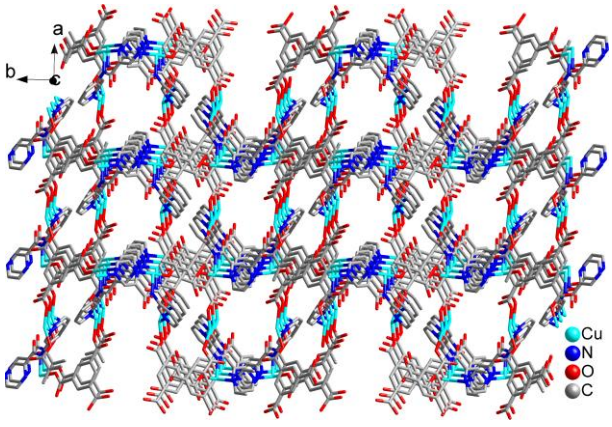


Fig. S1 View of the 3D network in complex **2**.

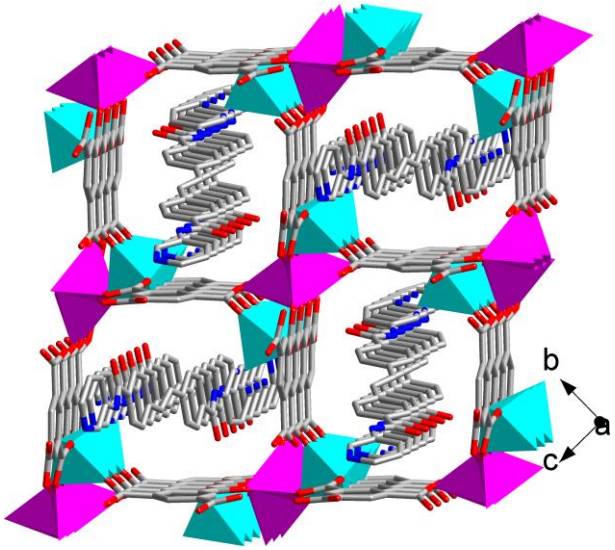


Fig. S2 View of the 3D network in complex **3**.

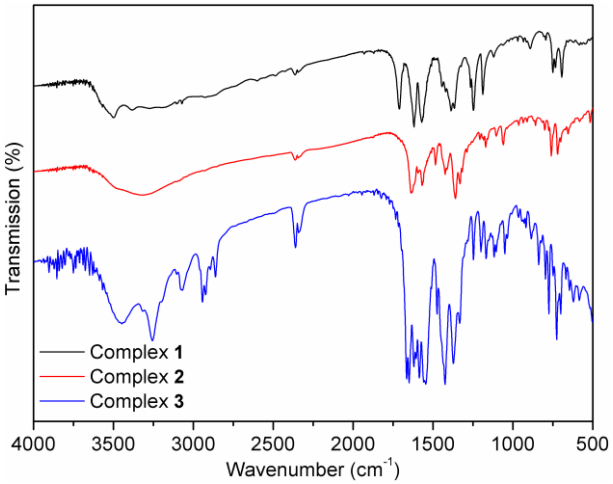
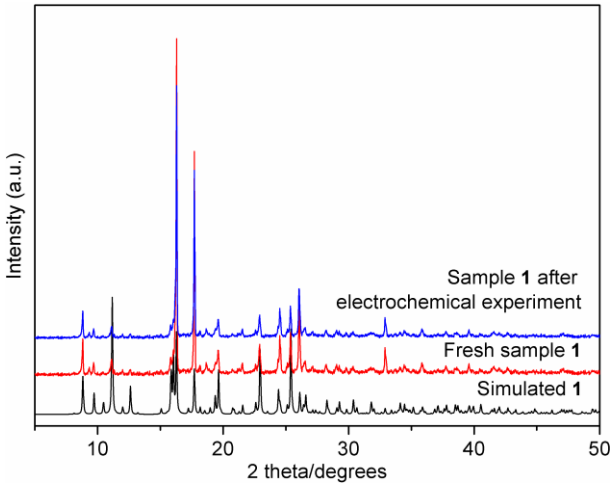


Fig.S3 The IR spectra of complexes **1**–**3**.



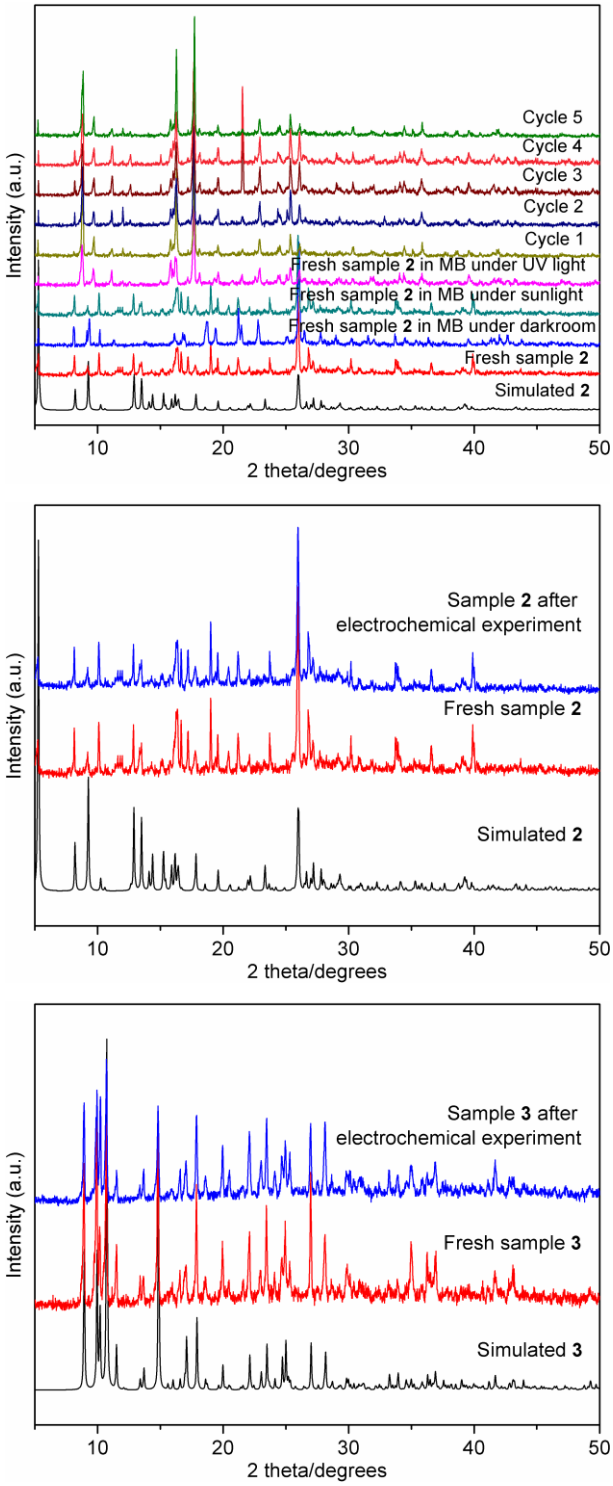


Fig. S4 The simulated, fresh samples, and samples after electrochemical experiments and/or photocatalytic experiments powder X-ray diffraction patterns for complexes **1**–**3**.

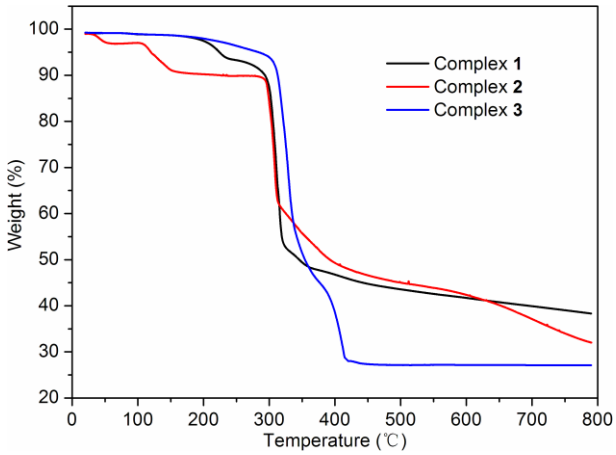
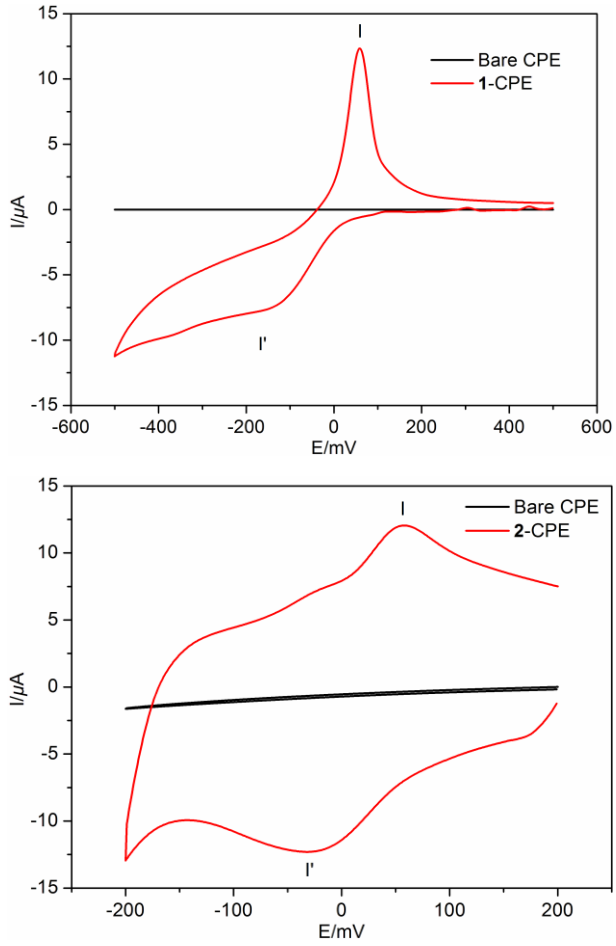


Fig. S5 The TG curves of complexes **1**–**3**.



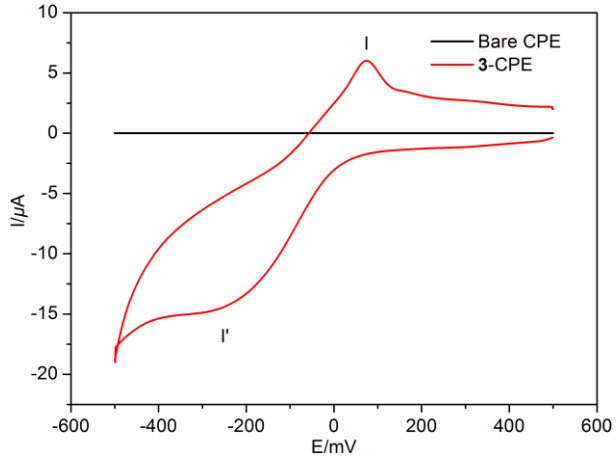


Fig. S6 The Cyclic voltammograms of **1**-CPE (–500 to +500 mV), **2**-CPE (–200 to +200 mV), and **3**-CPE (–500 to +500 mV) in 0.01 M H_2SO_4 + 0.5 M Na_2SO_4 aqueous solution. Scan rate: 50 mV s^{-1}, respectively.

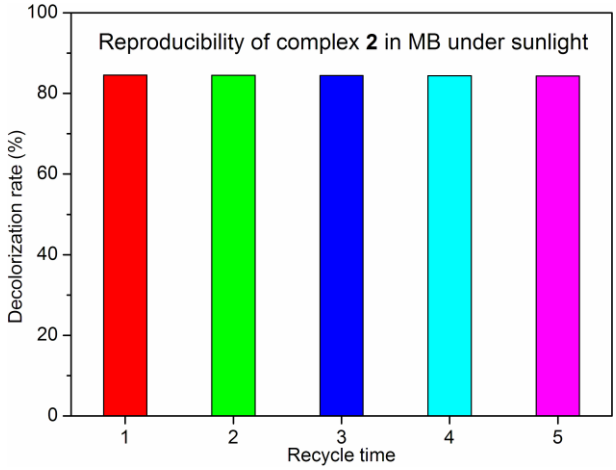


Fig. S7 Cycling runs of **2** in the degradation of MB solution under sunlight.