Electronic Supporting Information

Trinuclear Ni(II) Oriented Highly Dense Packing and π-Conjugation Degree of Metal-Organic Framework for Efficient Water Oxidation

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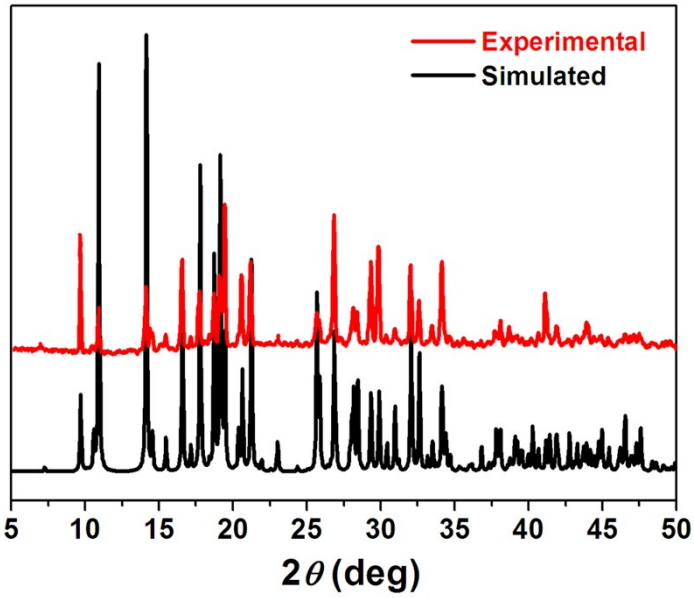


Figure S1. PXRD patterns of Ni-BTC crystal samples.

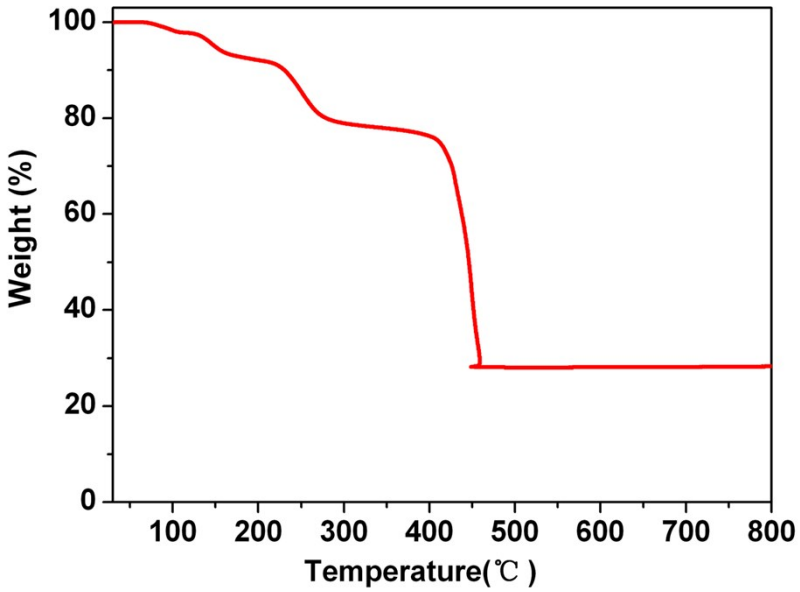


Figure S2. Thermogravimetric analysis (TGA) of Ni-BTC.

The first weight loss in the range of 80-100 °C was attributed to the release of water molecules occupied in the pores, the following weight loss observed from 100 °C to 220 °C correspond to the loss of other coordinated water molecules, the third weight loss in the range of 220-280 °C is due to the loss of μ_2-H_2O (connect two Ni(II) ions). The host framework starts to decompose when heating above 280 °C. In all, the total weight loss of 19.9% up to about 280 °C correspond to the loss of coordinated water molecules (calcd 19.6%).

Figure S3. Photograph of Ni-BTC crystals under daylight.

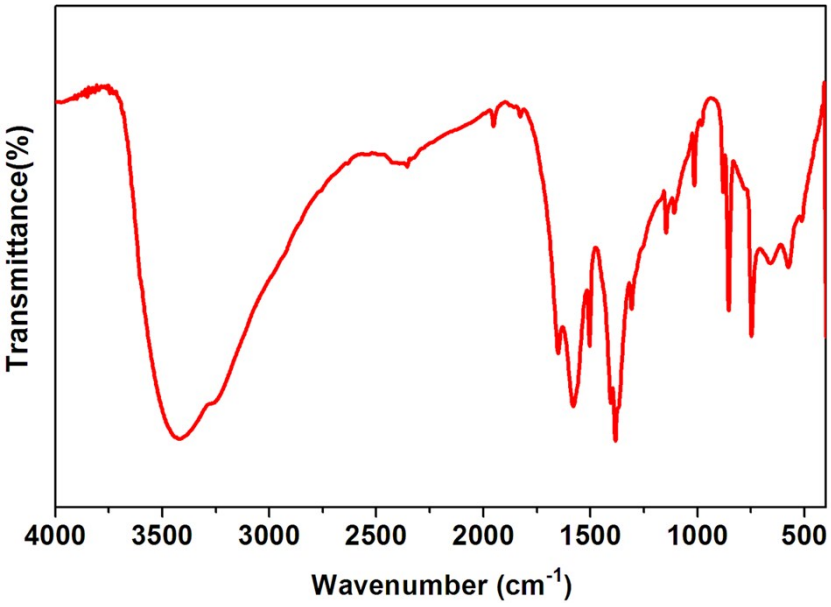


Figure S4. FT-IR spectrum of Ni-BTC.

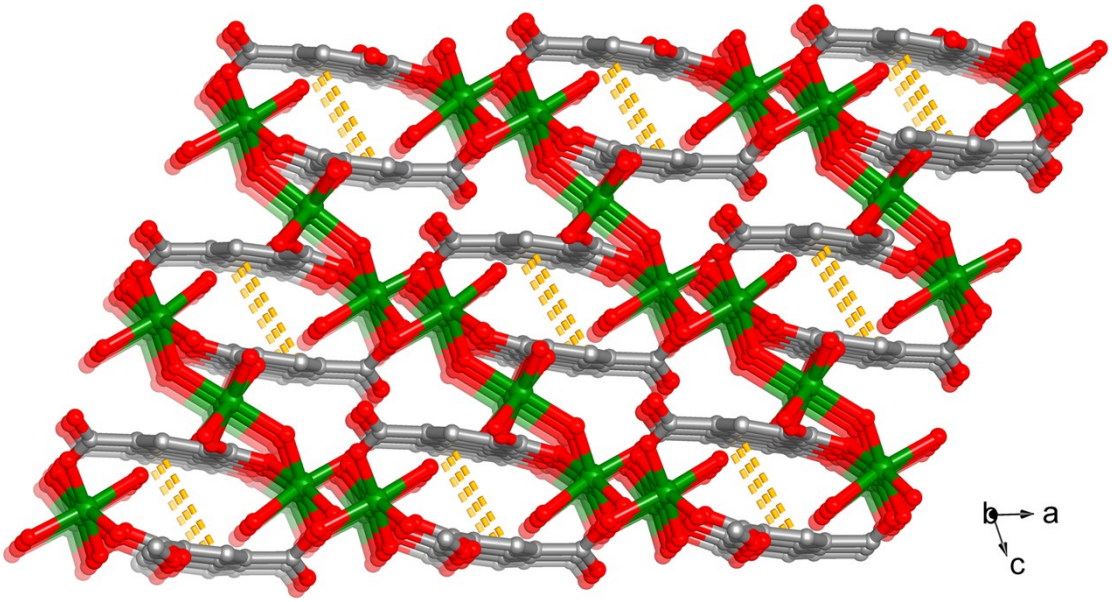


Figure S5. Ball-and-stick view of 3D network of Ni-BTC along [010] direction. Broken lines represent π···π stacking between the centroid of benzene rings.

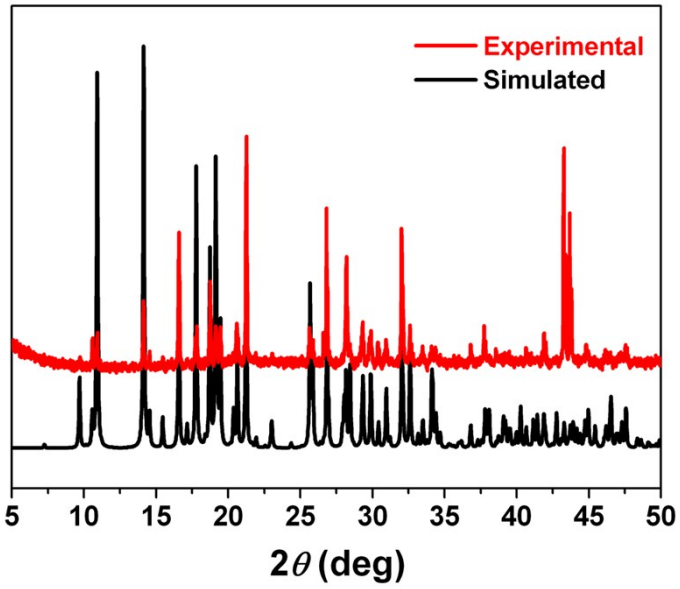


Figure S6. PXRD patterns of Ni-BTC powder sample after soaked in 0.1 M KOH aqueous solution for 48 h.

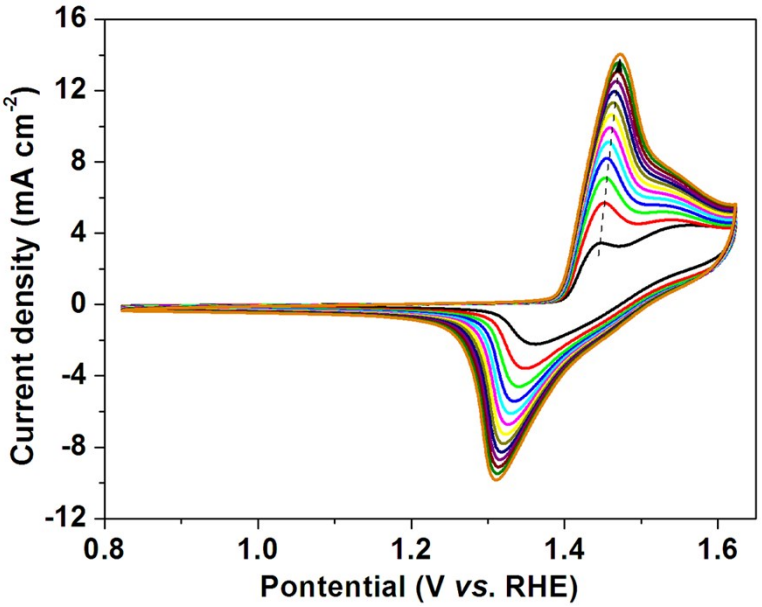
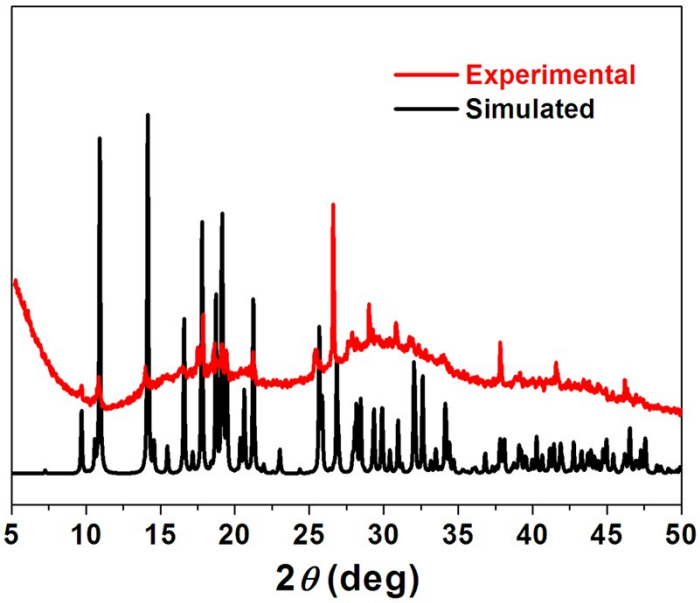
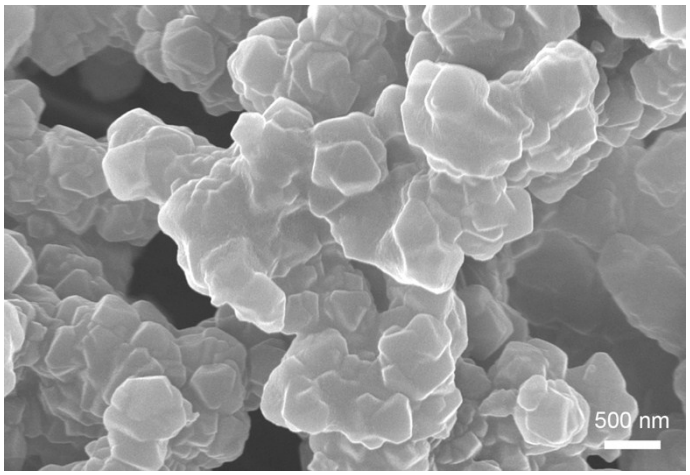


Figure S7. Cyclic voltammetry (CV) curves of Ni-BTC after 50 cycles.



(a)



(b)

Figure S8. PXRD patterns (a) and SEM image (b) of Ni-BTC after long-term oxygen evolution reaction (OER).

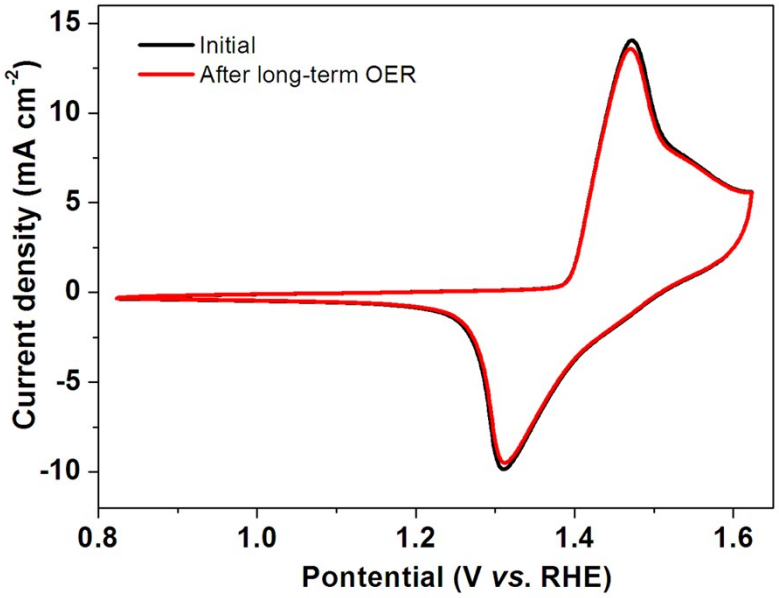


Figure S9. Cyclic voltammetry (CV) curves of Ni-BTC before and after long-term oxygen evolution reaction (OER).

Table S1. Crystallographic data for Ni-BTC.

Samples	Ni-BTC
Empirical formula	$C_{18}H_{22}Ni_3O_{20}$
Formula weight	734.44
CCDC	1933076
Temperature/K	290
Crystal system	triclinic
Space group	$P\bar{1}$
a/ Å	10.0281(6)
b/ Å	10.0845(5)
c/ Å	13.1425(7)
α/ °	75.763(5)
β/ °	68.657(5)
γ/ °	65.460(5)
V/Å^3	1119.04(12)
Z	2
D (g cm^{-3})	2.1795
μ (mm^{-1})	2.605
R_{int}	0.0348
Goof	1.049
R_1 ($I>2\sigma(I)$)[a]	0.0507
wR_2 ($I>2\sigma(I)$)[a]	0.1367

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2. Partial bond length and bond Angle of Ni-BTC.

Atoms	Length/Å	Atoms	Length/Å
Ni(1)–O(2)	2.032(2)	Ni(3)–O(8)#5	2.044(2)
Ni(1)–O(2)#1	2.032(2)	Ni(3)–O(8)	2.044(2)
Ni(1)–O(3)#2	2.138(3)	Ni(3)–O(11)#6	2.105(3)
Ni(1)–O(3)#3	2.138(3)	Ni(3)–O(11)#7	2.105(3)
Ni(1)–O(13)	2.045(3)	Ni(3)–O(17)#5	2.073(3)
Ni(1)–O(13)#1	2.045(3)	Ni(3)–O(17)	2.073(3)
Ni(2)–O(1)	2.039(3)	Ni(4)–O(7)	2.035(3)
Ni(2)–O(5)#4	2.084(3)	Ni(4)–O(10)#8	2.071(3)
Ni(2)–O(13)	2.039(3)	Ni(4)–O(17)#5	2.067(3)
Ni(2)–O(14)	2.055(2)	Ni(4)–O(18)	2.066(3)
Ni(2)–O(15)	2.082(3)	Ni(4)–O(19)	2.061(3)
Ni(2)–O(16)	2.067(3)	Ni(4)–O(20)	2.066(3)
Atoms	Angle/°	Atoms	Angle/°
O(2)#1–Ni(1)–O(2)	180.0	O(11)#6–Ni(3)–O(8)	92.37(10)
O(3)#2–Ni(1)–O(2)	87.20(10)	O(11)#7–Ni(3)–O(8)	87.63(10)
O(3)#3–Ni(1)–O(2)	92.80(10)	O(11)#7–Ni(3)–O(8)#5	92.37(10)
O(3)#3–Ni(1)–O(2)#1	87.20(10)	O(11)#6–Ni(3)–O(8)#5	87.63(10)
O(3)#2–Ni(1)–O(2)#1	92.80(10)	O(11)#6–Ni(3)–O(11)#7	180.0
O(3)#2–Ni(1)–O(3)#3	180.0	O(17)#5–Ni(3)–O(8)	89.49(10)
O(13)#1–Ni(1)–O(2)#1	91.57(10)	O(17)#5–Ni(3)–O(8)#5	90.51(10)
O(13)–Ni(1)–O(2)#1	88.43(10)	O(17)–Ni(3)–O(8)	90.51(10)
O(13)#1–Ni(1)–O(2)	88.43(10)	O(17)–Ni(3)–O(8)#5	89.49(10)
O(13)–Ni(1)–O(2)	91.57(10)	O(17)#5–Ni(3)–O(11)#7	91.84(11)
O(13)–Ni(1)–O(3)#3	88.16(11)	O(17)–Ni(3)–O(11)#7	88.16(11)
O(13)#1–Ni(1)–O(3)#3	91.84(11)	O(17)#5–Ni(3)–O(11)#6	88.16(11)
O(13)–Ni(1)–O(3)#2	91.84(11)	O(17)–Ni(3)–O(11)#6	91.84(11)
O(13)#1–Ni(1)–O(3)#2	88.16(11)	O(17)–Ni(3)–O(17)#5	180.0
O(13)#1–Ni(1)–O(13)	180.0	O(10)#8–Ni(4)–O(7)	96.93(11)
O(5)#4–Ni(2)–O(1)	96.46(11)	O(17)#5–Ni(4)–O(7)	94.32(10)

O(13)–Ni(2)–O(1)	95.76(10)	O(17)#5–Ni(4)–O(10)#8	88.33(11)
O(13)–Ni(2)–O(5)#4	88.66(11)	O(18)–Ni(4)–O(7)	172.69(12)
O(14)–Ni(2)–O(1)	88.04(11)	O(18)–Ni(4)–O(10)#8	87.90(12)
O(14)–Ni(2)–O(5)#4	88.21(10)	O(18)–Ni(4)–O(17)#5	91.29(12)
O(14)–Ni(2)–O(13)	175.33(11)	O(19)–Ni(4)–O(7)	93.33(11)
O(15)–Ni(2)–O(1)	170.94(11)	O(19)–Ni(4)–O(10)#8	169.37(12)
O(15)–Ni(2)–O(5)#4	90.41(11)	O(19)–Ni(4)–O(17)#5	93.65(11)
O(15)–Ni(2)–O(13)	90.29(11)	O(19)–Ni(4)–O(18)	81.62(13)
O(15)–Ni(2)–O(14)	86.27(11)	O(20)–Ni(4)–O(7)	87.35(11)
O(16)–Ni(2)–O(1)	89.76(11)	O(20)–Ni(4)–O(10)#8	87.61(11)
O(16)–Ni(2)–O(5)#4	173.78(11)	O(20)–Ni(4)–O(17)#5	175.76(11)
O(16)–Ni(2)–O(13)	90.86(12)	O(20)–Ni(4)–O(18)	87.38(12)
O(16)–Ni(2)–O(14)	91.88(11)	O(20)–Ni(4)–O(19)	90.13(12)
O(16)–Ni(2)–O(15)	83.39(11)		

Symmetry codes: #1: 2-x, 2-y, -z; #2: 2-x, 1-y, -z; #3: +x, 1+y, +z; #4: 1+x, +y, +z; #5: 1-x, -y, 1-z; #6: 1-x, 1-y, 1-z; #7:+x, -1+y, +z; #8:-1+x, +y, +z.