Supporting Information

1D-3D Mixed-Ligand Frameworks with an Unusual *dmp* Topology Tuned by Intersection Angles of Isomeric Benzenedicarboxylates: Magnetic Properties, Gas-Dependent Calcination-thermolysis and Energy Storage Performances

Zuo-Xi Li,*[a, b] Gan Ye,[a] Juan Han,[a] Ying Yang,[a] Kang-Yu Zou,[a] Xin Wang,[a] Xiao-Ling Wang[b] and Xiao-Feng Gou[a]

[a]*Key Laboratory of Synthetic and Natural Functional Molecule Chemistry (Ministry of Education), Shaanxi Key Laboratory of Physico-Inorganic Chemistry, College of Chemistry and Material Sciences, Northwest University, Xi'an 710069, P.R.China;*

[b]*Shannxi Key Laboratory of Phytochemistry, Baoji 721016, P.R.China.*

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*Corresponding author. *E-mail address:* Lizx@nwu.edu.cn.

Table S1. Selected Bond Lengths [Å] and Angles [º] for CPs **1**-**3**.

1

Co(1)-O(5)	1.937(4)	Co(1)-O(24)#1	1.953(4)
Co(1)-O(1)	1.975(3)	Co(1)-N(4)#2	2.001(4)
Co(2)-O(3)	2.059(3)	Co(2)-N(1)	2.074(4)
Co(2)-O(9)	2.104(4)	Co(2)-O(2)	2.124(3)
Co(2)-O(8)	2.134(3)	Co(2)-O(7)	2.181(4)
Co(3)-O(10)	1.935(3)	Co(3)-O(13)	1.961(4)
Co(3)-N(5)	2.000(4)	Co(4)-N(12)#3	2.076(4)
Co(4)-O(15)	2.086(3)	Co(4)-O(17)	2.096(3)
Co(4)-O(14)	2.114(3)	Co(4)-O(11)	2.186(4)
Co(4)-O(12)	2.188(4)	Co(5)-O(18)	1.933(4)
Co(5)-O(16)	1.965(3)	Co(5)-O(21)	1.982(4)
Co(5)-N(9)	2.009(4)	Co(6)-O(1W)	2.007(4)
Co(6)-O(23)	2.057(3)	Co(6)-O(22)	2.073(3) Co(6)-
N(8)#3	2.088(4)	Co(6)-O(20)	2.164(4)
Co(6)-O(19)	2.193(4)	O(5)-Co(1)-O(24)#1	126.02(16) O(5)-
Co(1)-O(1)	111.02(17)	O(24)#1-Co(1)-O(1)	94.64(16) O(5)-Co(1)-
N(4)#2	113.13(17)	O(24)#1-Co(1)-N(4)#2	100.34(17) O(1)-
Co(1)-N(4)#2	109.64(16)	O(3)-Co(2)-N(1)	109.77(16) O(3)-
Co(2)-O(9)	97.87(15)	N(1)-Co(2)-O(9)	91.78(17) O(3)-Co(2)-
O(2)	79.97(13)	N(1)-Co(2)-O(2)	88.34(15) O(9)-Co(2)-
O(2)	177.74(14)	O(3)-Co(2)-O(8)	153.46(13) N(1)-
Co(2)-O(8)	93.84(15)	O(9)-Co(2)-O(8)	93.20(14) O(2)-Co(2)-
O(8) 89.05(13)	O(3)-Co(2)-O(7)		96.00(13) N(1)-
Co(2)-O(7)	154.22(15)	O(9)-Co(2)-O(7)	85.22(16) O(2)-
Co(2)-O(7)	95.65(14)	O(8)-Co(2)-O(7)	60.88(12)
O(10)-Co(3)-O(13)	111.74(17)	O(10)-Co(3)-O(4)	130.10(16)

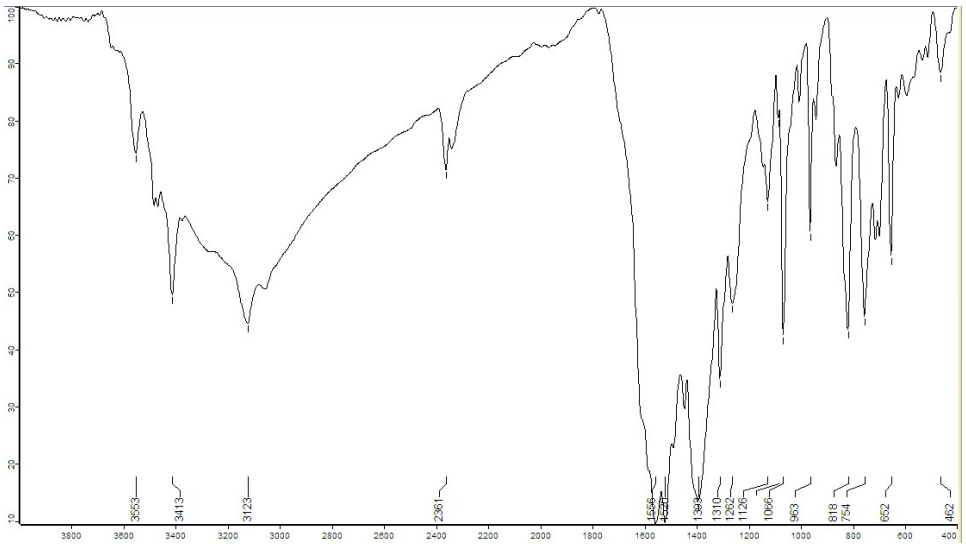
O(13)-Co(3)-O(4)	95.05(16)	O(10)-Co(3)-N(5)	106.05(17)
O(13)-Co(3)-N(5)	112.84(16)	O(4)-Co(3)-N(5)	100.46(17)
N(12)#3-Co(4)-O(15)	105.06(15)	N(12)#3-Co(4)-O(17)	93.28(16)
O(15)-Co(4)-O(17)	94.17(14)	N(12)#3-Co(4)-O(14)	88.31(15)
O(15)-Co(4)-O(14)	80.52(13)	O(17)-Co(4)-O(14)	174.69(14)
N(12)#3-Co(4)-O(11)	153.24(15)	O(15)-Co(4)-O(11)	101.56(13)
O(17)-Co(4)-O(11)	87.40(14)	O(14)-Co(4)-O(11)	93.46(14)
N(12)#3-Co(4)-O(12)	93.27(14)	O(15)-Co(4)-O(12)	159.83(13)
O(17)-Co(4)-O(12)	93.08(14)	O(14)-Co(4)-O(12)	91.88(13)
O(11)-Co(4)-O(12)	60.00(12)	O(18)-Co(5)-O(16)	126.90(15)
O(18)-Co(5)-O(21)	112.86(17)	O(16)-Co(5)-O(21)	6.22(16)
O(18)-Co(5)-N(9)	105.18(17)	O(16)-Co(5)-N(9)	102.02(16)
O(21)-Co(5)-N(9)	113.40(16)	O(1W)-Co(6)-O(23)	89.93(17)
O(1W)-Co(6)-O(22)	173.30(17)	O(23)-Co(6)-O(22)	83.78(13)
O(1W)-Co(6)-N(8)#3	90.77(19)	O(23)-Co(6)-N(8)#3	102.40(15)
O(22)-Co(6)-N(8)#3	88.36(16)	O(1W)-Co(6)-O(20)	89.18(18)
O(23)-Co(6)-O(20)	96.78(14)	O(22)-Co(6)-O(20)	93.82(15)
N(8)#3-Co(6)-O(20)	160.82(15)	O(1W)-Co(6)-O(19)	92.79(17)
O(23)-Co(6)-O(19)	156.95(13)	O(22)-Co(6)-O(19)	93.89(13)
N(8)#3-Co(6)-O(19)	100.45(15)	O(20)-Co(6)-O(19)	60.40(13)

2

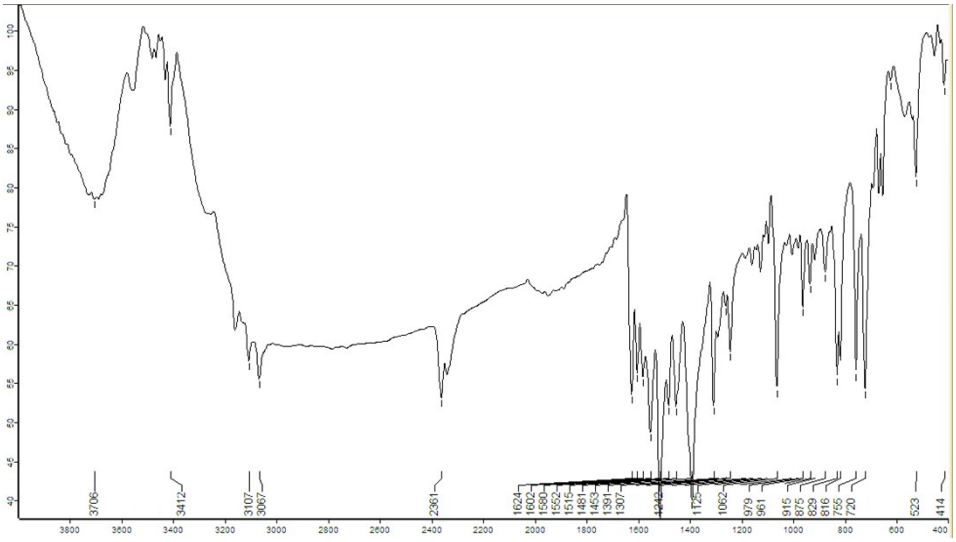
Co(1)-O(1)#1	2.0342(15)	Co(1)-O(2)	2.0581(14)
Co(1)-O(3)#3	2.1973(16)	Co(1)-O(4)#3	2.1936(15)
Co(1)-N(1)	2.1405(18)	Co(1)-N(4)#2	2.1462(17)
O(1)#1-Co(1)-O(2)	111.73(6)	O(1)#1-Co(1)-N(1)	85.36(7)
O(2)-Co(1)-N(1)	87.21(7)	O(1)#1-Co(1)-N(4)#2	91.84(7)
O(2)-Co(1)-N(4)#2	93.07(7)	N(1)-Co(1)-N(4)#2	177.08(6)

O(1)#1-Co(1)-O(4)#3	155.13(6)	O(2)-Co(1)-O(4)#3	92.49(6)
N(1)-Co(1)-O(4)#3	90.48(6)	N(4)#2-Co(1)-O(4)#3	92.41(7)
O(1)#1-Co(1)-O(3)#3	95.72(5)	O(2)-Co(1)-O(3)#3	152.51(6)
N(1)-Co(1)-O(3)#3	93.78(6)	N(4)#2-Co(1)-O(3)#3	87.31(6)
O(4)#3-Co(1)-O(3)#3	60.05(5)		
	3		
Co(1)-O(1)	1.9781(15)	Co(1)-O(1)#1	1.9781(15)
Co(1)-N(1)	2.0355(19)	Co(1)-N(1)#1	2.0355(19)
O(1)#1-Co(1)-O(1)	93.85(9)	O(1)#1-Co(1)-N(1)#1	112.90(7)
O(1)-Co(1)-N(1)#1	121.76(7)	O(1)#1-Co(1)-N(1)	121.76(7)
O(1)-Co(1)-N(1)	112.90(7)	N(1)#1-Co(1)-N(1)	95.82(11)

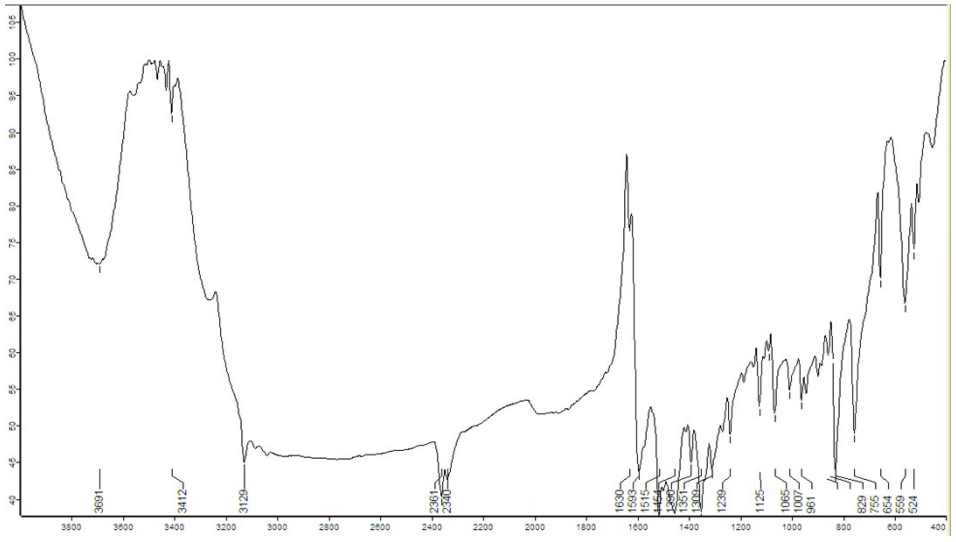
*Symmetry mode for **1**: #1 x+1, y, z+1; #2 -x+2, -y+2, -z+1; #3 -x+1,-y+2,-z. For **2**: #1 -x+1, -y+1, -z+1; #2 x-1, y-1, z+1; #3 x, y-1, z. For **3**: #1 x, -y+1/2, -z+1/2.



(a)



(b)



(c)

Figure **S1.** The IR figures: **(a) 1**; **(b) 2**; **(c) 3**.

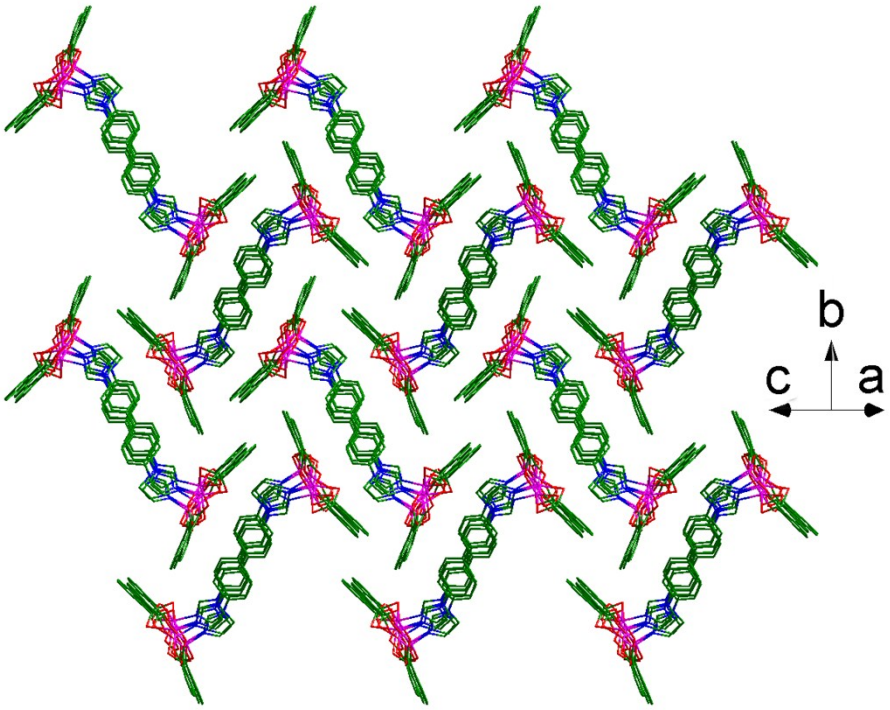


Figure **S2.** The 3D supermolecular structure in **1**.

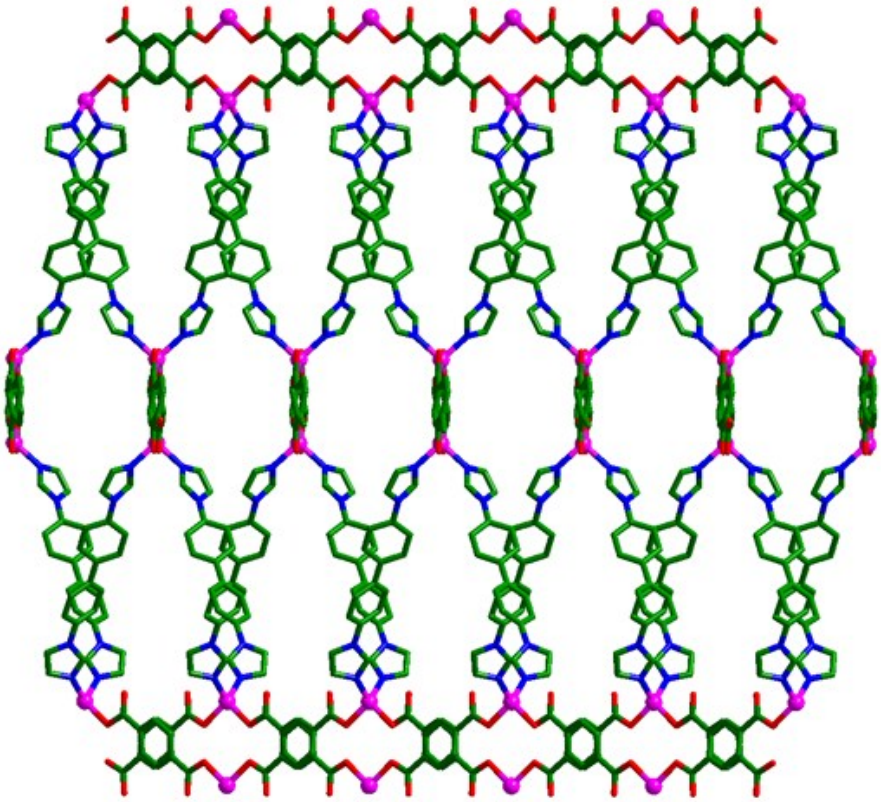


Figure **S3.** The 1D chain is connected by the **bibp** ligand in a criss-cross mode in **3**.

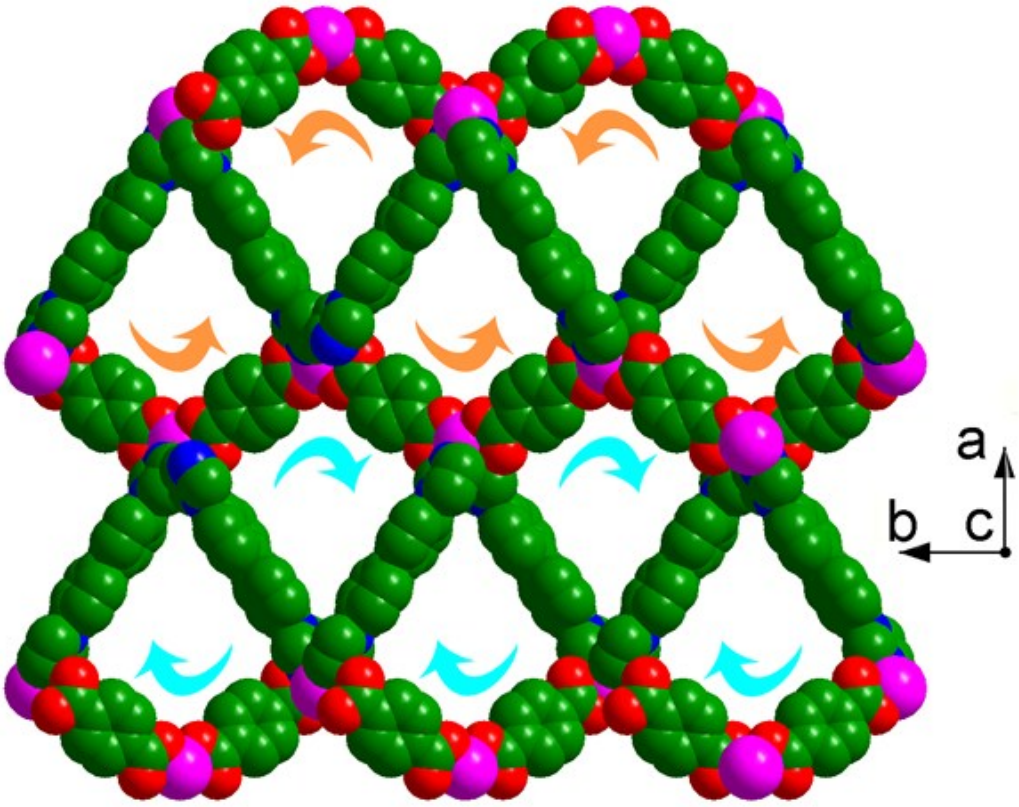
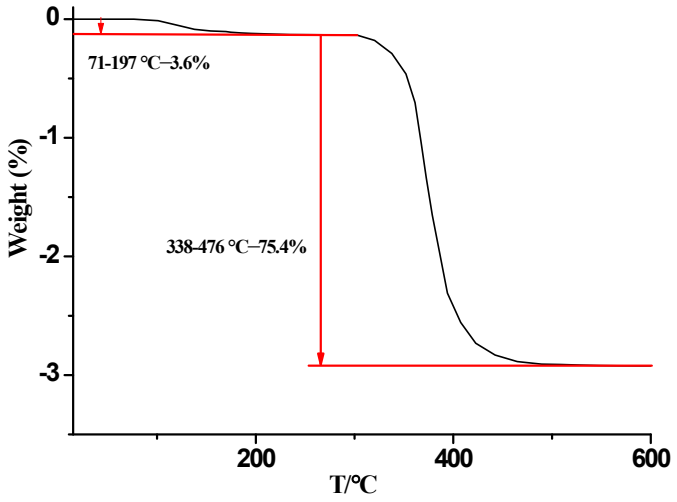
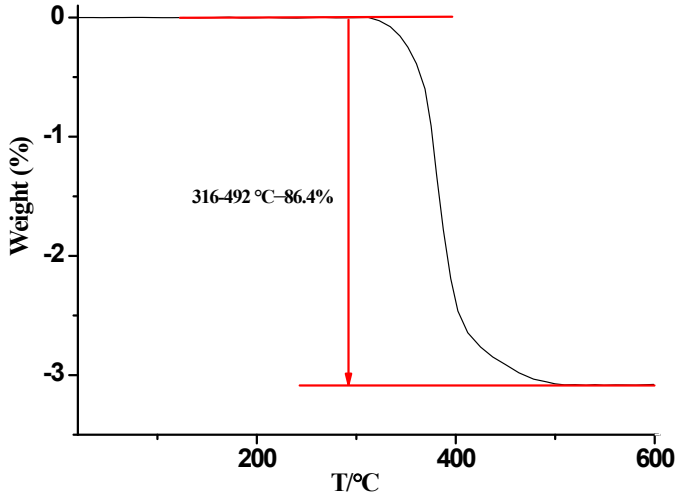


Figure **S4.** View of the quadrangular chiral channel along the *c* axis in **3**.



(a)



(b)

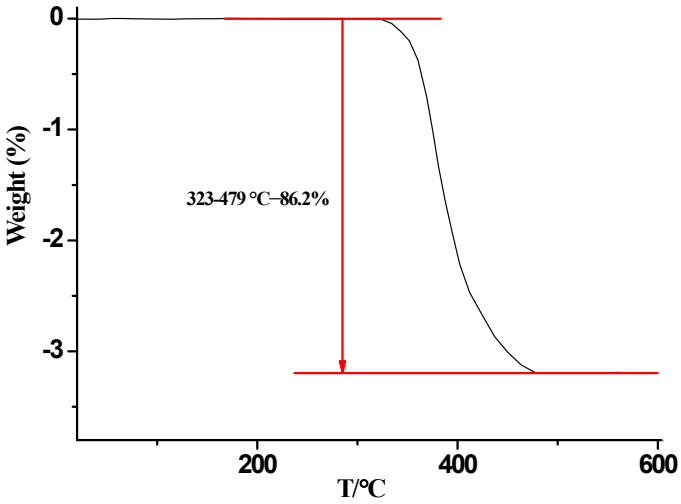
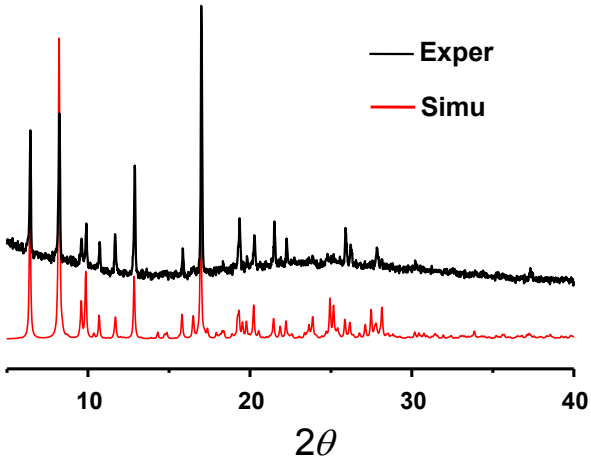
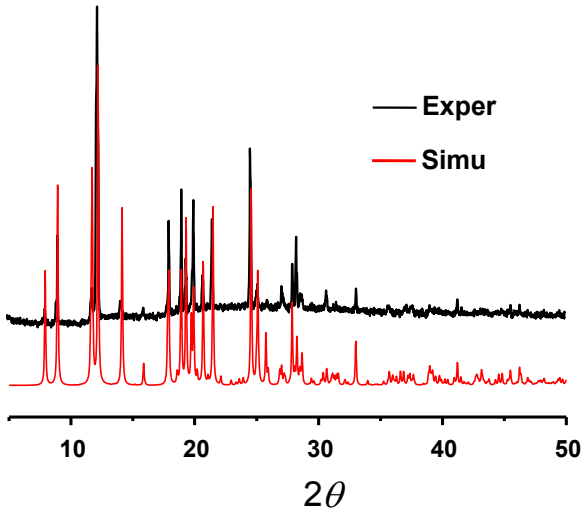


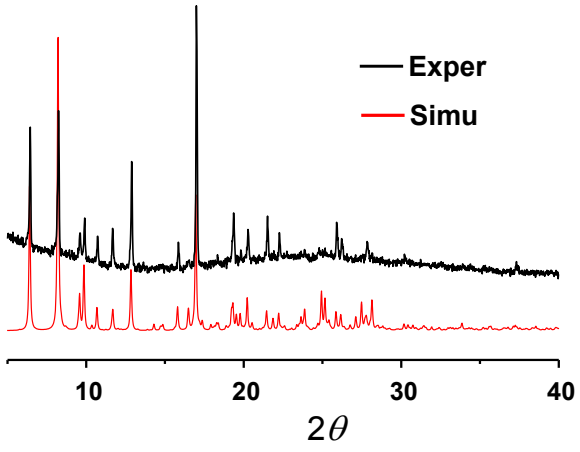
Figure S5. TG plots: **(a) 1**; **(b) 2**; **(c) 3**.



(a)

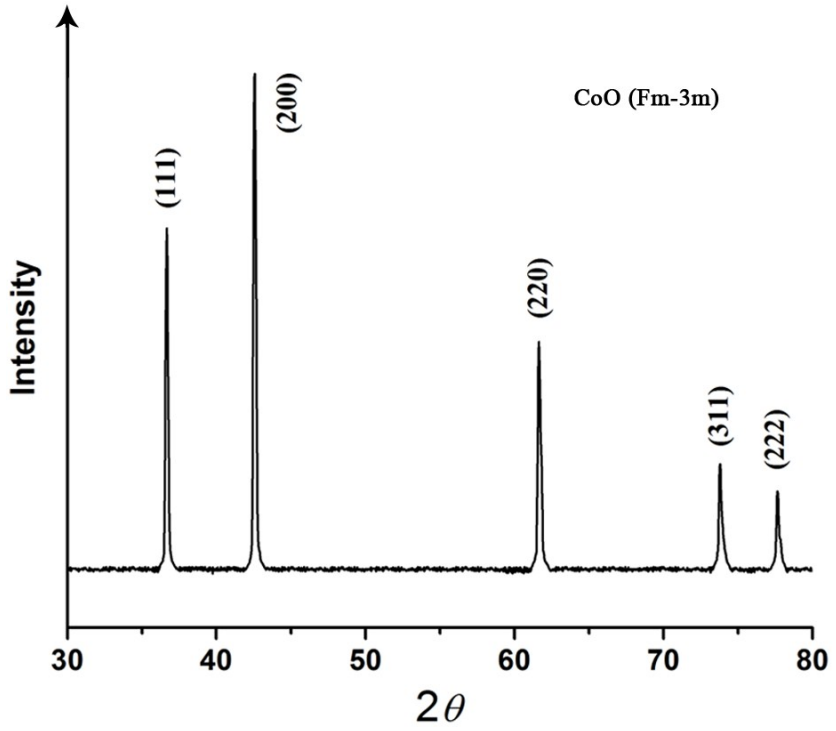


(b)

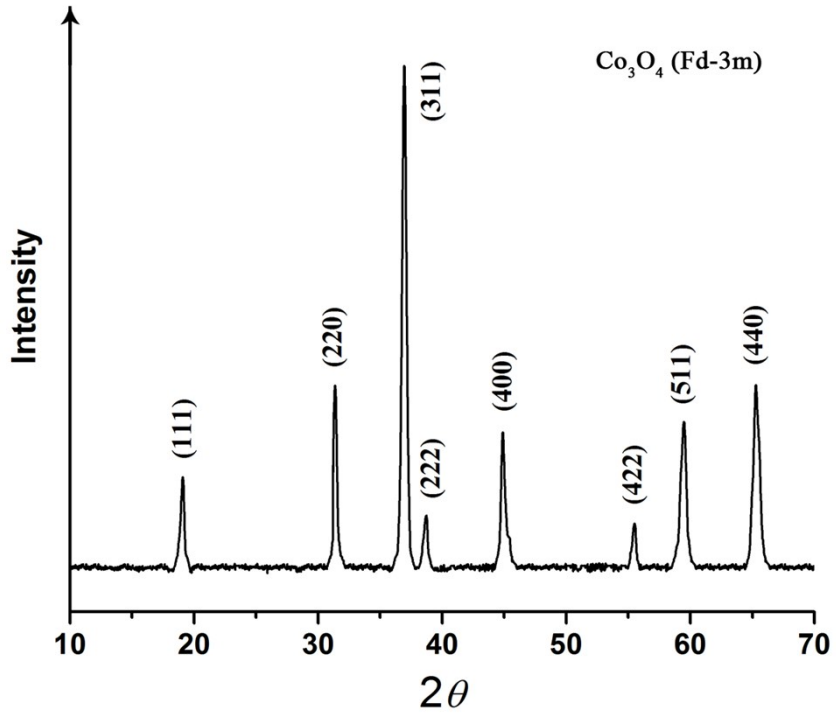


(c)

Figure **S6.** The experimental and simulated powder XRD patterns: **(a) 1**; **(b) 2**; **(c) 3**.

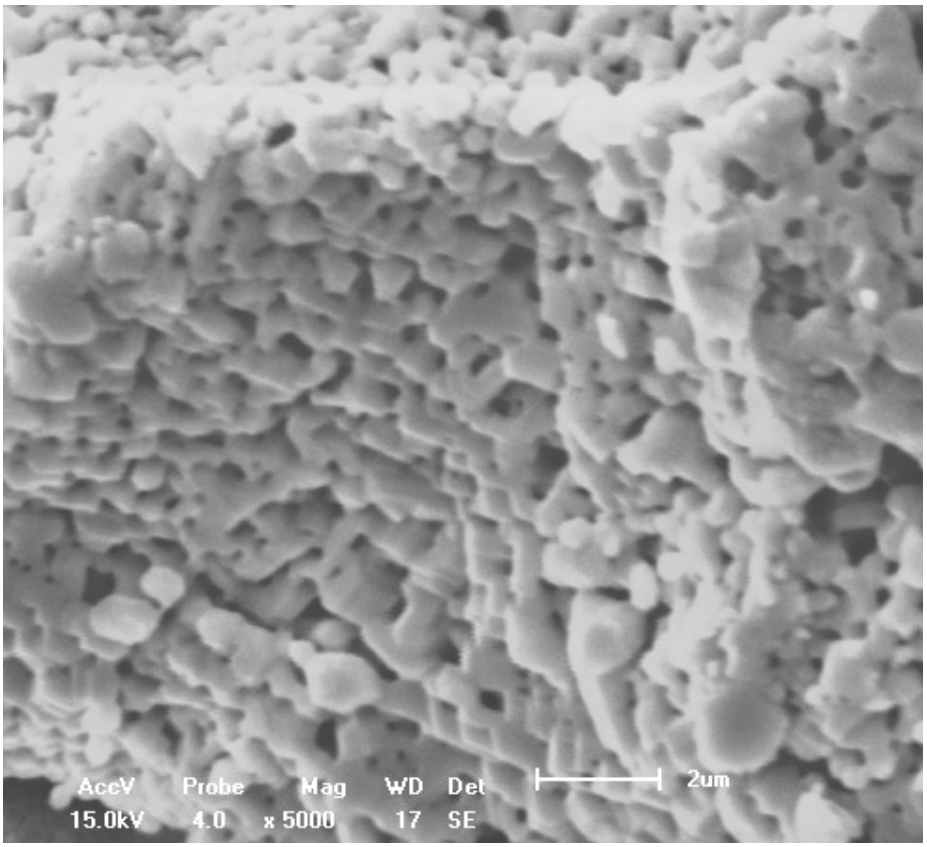


(a)

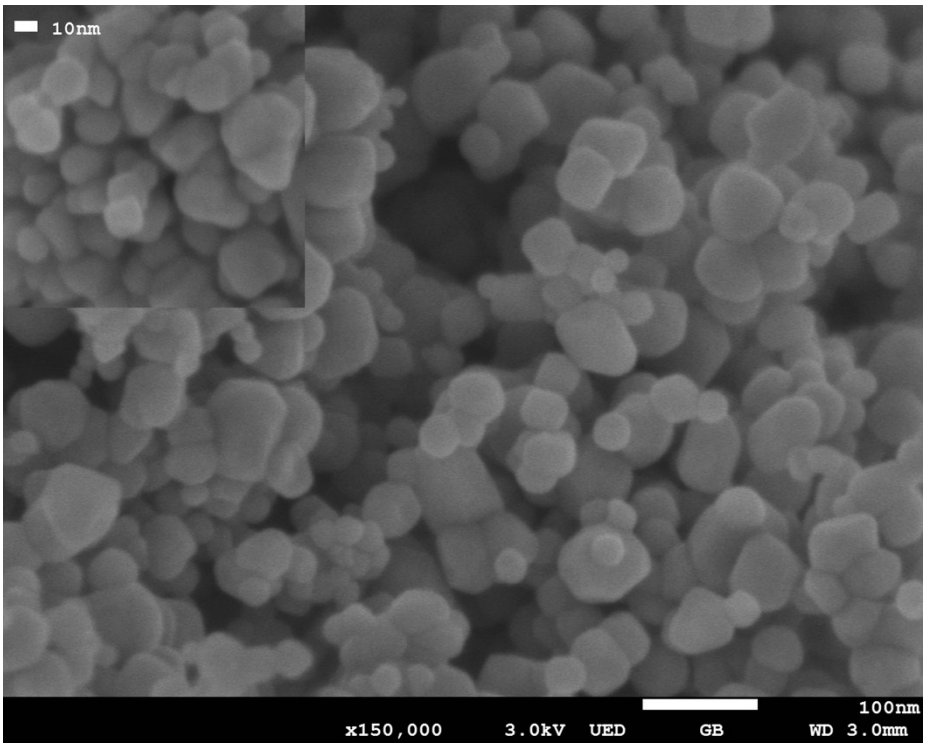


(b)

Figure **S7** Powder XRD patterns of CoO and Co_3O_4 nanoparticles.



(a)



(b)

Figure **S8** SEM images of (a) CoO and (b) Co_3O_4.

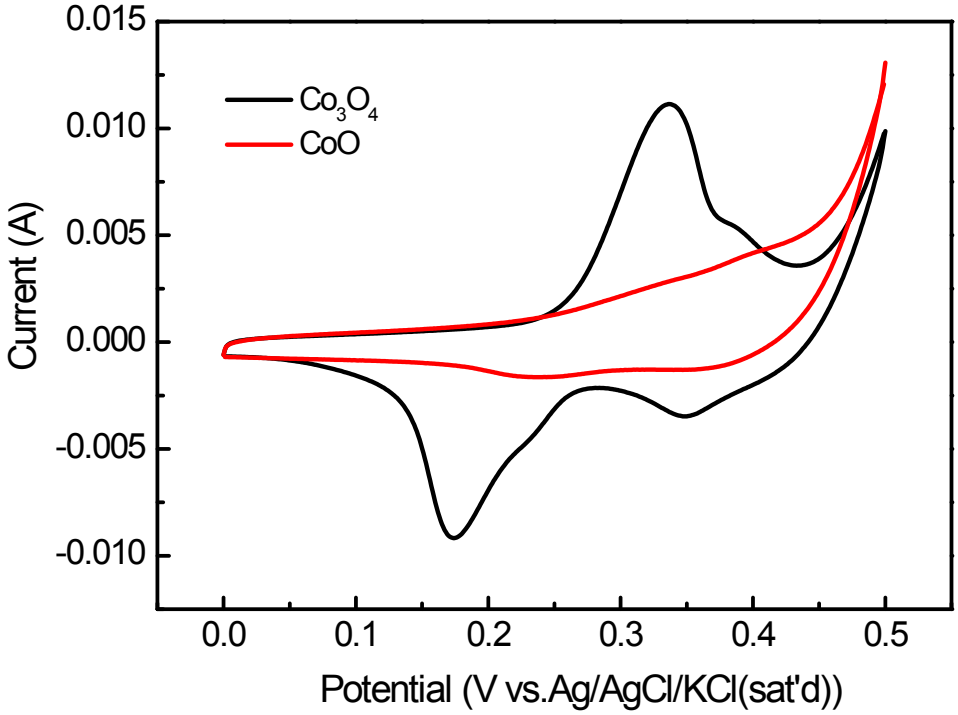


Figure **S9** CV curves of CoO and Co_3O_4 electrodes in 2 M KOH electrolyte at 5 $mV \cdot s^{-1}$.