Electronic Supplementary Information

Porous Co_3O_4 Materials Prepared by Solid-State Thermolysis of Novel Co-MOF Crystal and Their Superior Storage-Energy Performances for Supercapacitors

Fanli Meng[1+], Zhiguo Fang[1+], Zuoxi Li[1], Weiwei Xu[1], Mengjiao Wang[1], Yanping Liu[1], Ji Zhang[1], Wanren Wang[1], Dongyuan Zhao[2], Xiaohui Guo[1*]

Crystallographic data for the structure reported in this article have been deposited with the Cambridge Crystallographic Data Centre, CCDC No. 928997.

These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table. S1 Crystal data and structure refinement for Co-MOF

Complex	**Co-MOF**
Formula	$C_{60}\ H_{42}\ Co_3\ N_9\ O_{23}$
FW/g mol^{-1}	1433.82
System	Triclinic
Space group	*P*-1
a/ Å	11.4215(12)
b/ Å	13.8731(15)
c/ Å	20.777(2)
α/ ^{o}	98.208(2)
β/ ^{o}	99.762(2)
γ/ ^{o}	108.660(2)
V/ Å^3	3004.7(5)
Z	2
Dc/g cm^{-3}	1.585
μ/mm^{-1}	0.910
F[000]	1460
R_1 I>2θ	0.0570
wR_2 I>2θ	0.1493
R_1 all	0.0893
*wR*2 all	0.1796
GOF	0.978

$R_1=\sum||F_0|-|F_c||/\sum|F_0|$, $wR_2=\{\sum[w(F_0^2-F_c^2)^2]/\sum(F_0^2)^2\}^{1/2}$

Table 2. Selected bond distances [Å] and angles [°] for complex Co-MOF

Co(1)-O(13)#1	2.063(3)	Co(1)-O(21)#2	2.065(3)
Co(1)-O(1)	2.095(3)	Co(1)-O(2)	2.129(3)
Co(1)-O(3)	2.248(3)	Co(2)-O(14)#2	2.074(3)
Co(2)-O(19)#3	2.105(3)	Co(2)-O(4)	2.138(3)
Co(2)-O(6)	2.138(3)	Co(2)-O(5)	2.183(3)
Co(3)-O(10)	2.071(3)	Co(3)-O(16)	2.071(3)
Co(3)-O(9)	2.092(4)	Co(3)-O(7)	2.129(3)
Co(3)-O(8)	2.220(3)	Co(1)-N(1)	2.157(4)
Co(2)-N(5)#4	2.144(4)	Co(3)-N(4)	2.142(4)

O(13)#1-Co(1)-O(21)#2	113.09(13)	O(13)#1-Co(1)-O(1)	92.14(12)
O(21)#2-Co(1)-O(1)	91.78(14)	O(13)#1-Co(1)-O(2)	93.40(12)
O(21)#2-Co(1)-O(2)	152.96(12)	O(1)-Co(1)-O(2)	92.55(13)
O(13)#1-Co(1)-O(3)	153.57(12)	O(21)#2-Co(1)-O(3)	93.16(12)
O(1)-Co(1)-O(3)	89.96(12)	O(2)-Co(1)-O(3)	60.18(10)
O(14)#2-Co(2)-O(19)#3	115.36(13)	O(14)#2-Co(2)-O(4)	89.14(12)
O(19)#3-Co(2)-O(4)	155.43(12)	O(14)#2-Co(2)-O(6)	89.87(15)
O(19)#3-Co(2)-O(6)	86.83(13)	O(4)-Co(2)-O(6)	91.74(13)
O(14)#2-Co(2)-O(5)	149.84(12)	O(19)#3-Co(2)-O(5)	94.79(12)
O(4)-Co(2)-O(5)	60.76(11)	O(6)-Co(2)-O(5)	92.72(13)
O(10)-Co(3)-O(16)	116.34(12)	O(10)-Co(3)-O(9)	86.78(15)
O(16)-Co(3)-O(9)	84.34(14)	O(10)-Co(3)-O(7)	147.14(13)
O(16)-Co(3)-O(7)	96.15(12)	O(9)-Co(3)-O(7)	91.98(17)
O(10)-Co(3)-O(8)	87.50(12)	O(16)-Co(3)-O(8)	156.11(12)
O(9)-Co(3)-O(8)	96.09(15)	O(7)-Co(3)-O(8)	59.96(12)
O(13)#1-Co(1)-N(1)	90.39(13)	O(21)#2-Co(1)-N(1)	88.18(14)
O(1)-Co(1)-N(1)	177.27(13)	O(2)-Co(1)-N(1)	86.26(13)
O(14)#2-Co(2)-N(5)#4	94.39(14)	O(19)#3-Co(2)-N(5)#4	84.43(13)
N(1)-Co(1)-O(3)	87.31(12)	O(4)-Co(2)-N(5)#4	95.96(13)
O(6)-Co(2)-N(5)#4	171.25(13)	O(10)-Co(3)-N(4)	87.52(14)
O(16)-Co(3)-N(4)	91.44(13)	O(9)-Co(3)-N(4)	170.54(17)
O(7)-Co(3)-N(4)	96.90(15)	N(5)#4-Co(2)-O(5)	87.44(13)
N(4)-Co(3)-O(8)	91.19(13)		

Symmetry transformations used to generate equivalent atoms: #1 x+1,y-1,z; #2 x+1,y-1,z+1; #3 x,y,z+1; #4 -x+1,-y+1,-z+1; #5 x-1,y+1,z; #6 x-1,y+1,z-1; #7 x,y,z-1;#8 -x+2,-y,-z+1

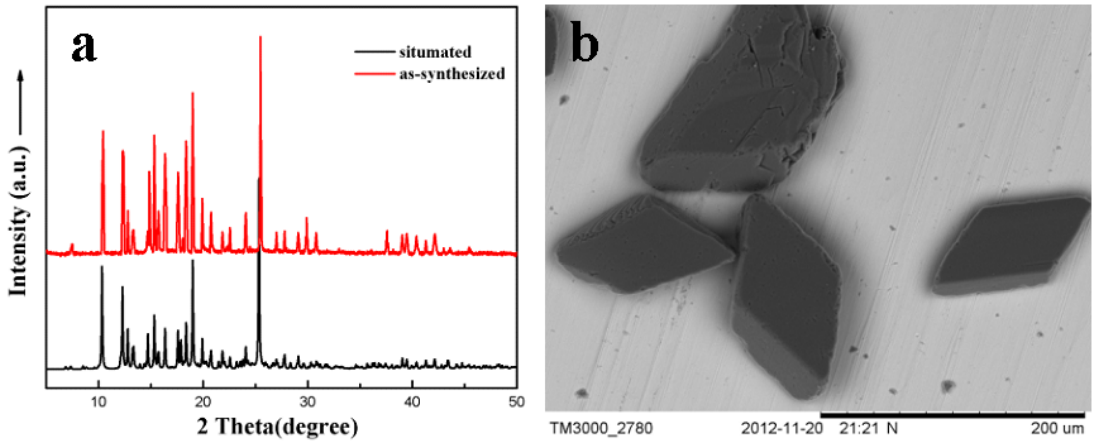

Figure S1. (a) XRD patterns of Co-MOF ({[$Co_3(ABTC)_3(byp)_{1.5}\cdot(H_2O)_3]\cdot(H_2O)_2\}_n$); (b) Low-magnification SEM image of Co-MOF.

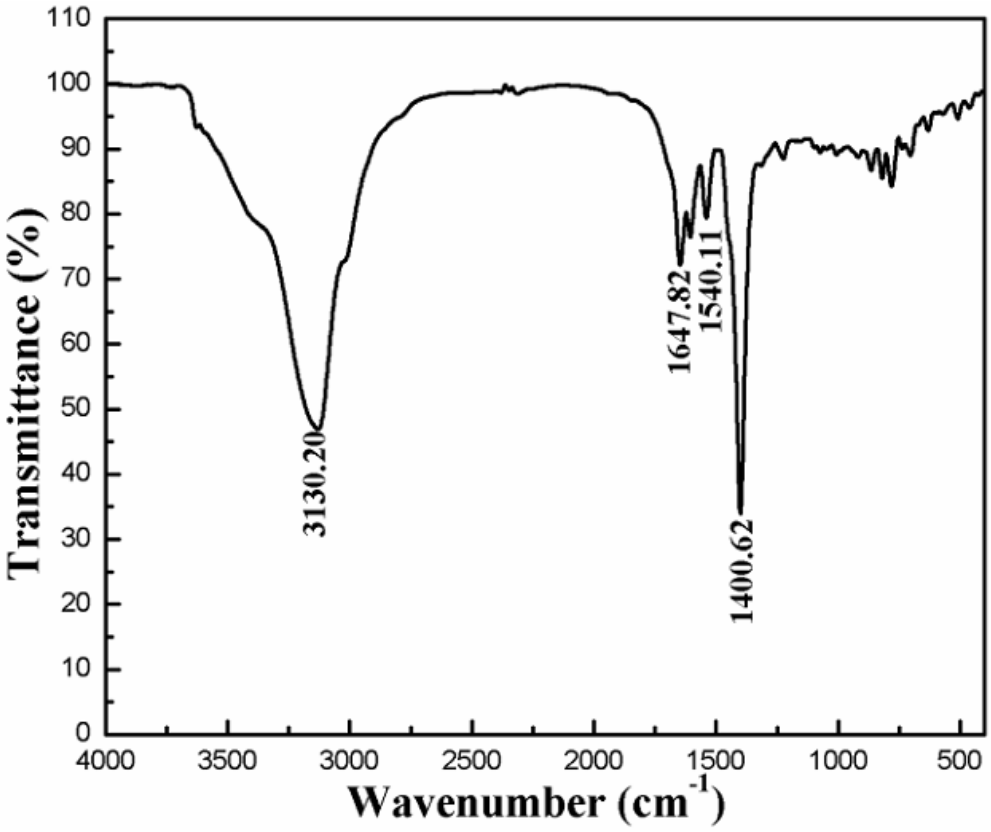

Figure. S2. FTIR spectrum of Co-MOF ({[$Co_3(ABTC)_3(byp)_{1.5}\cdot(H_2O)_3]\cdot(H_2O)_2\}_n$).

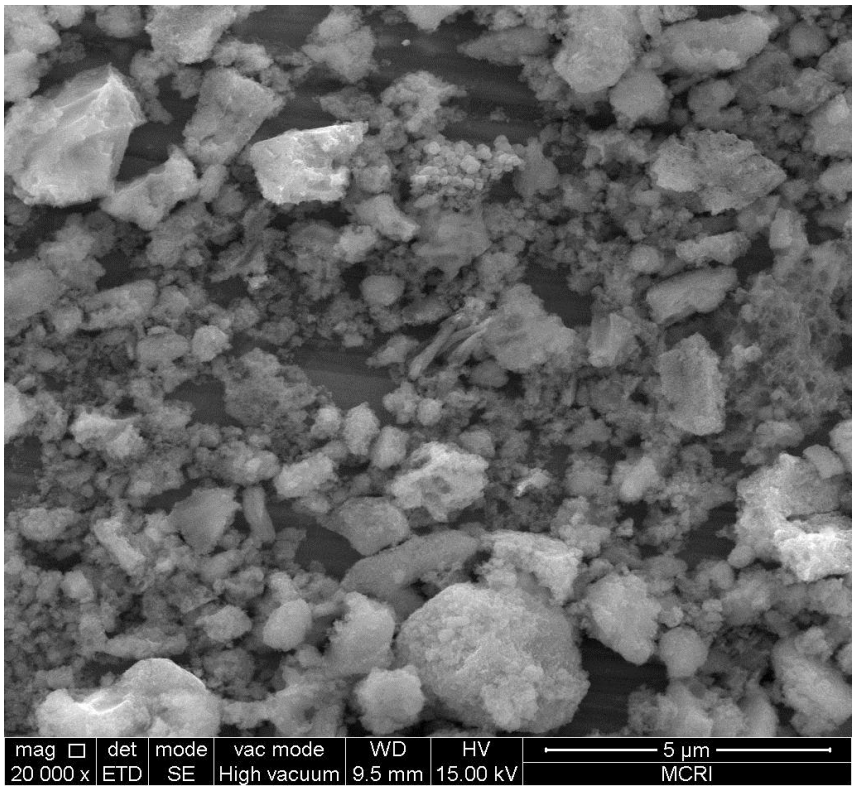

Figure. S3. SEM image of the porous Co_3O_4 material prepared from the thermolysis of the as-made Co-MOF crystal.