Electronic Supplementary Material (ESI) for CrystEngComm.

Design and Synthesis of Nanoporous carbon materials Using Cd-based Homochiral Metal-Organic Framework as Precursors for Supercapacitor Application

(Supplementary Information)

Synthesis of compound L-1： A mixture of $Cd(OAc)_2 \cdot 4H_2O$ (0.4 mmol), L-DBTA (0.3 mmol), 4,4'-bpy (0.4 mmol), HCl aqueous solution (0.3 mL, 1 M), ethylalcohol (2 mL) and water (8 mL) was placed in an 18 mL Teflon-lined stainless steel vessel and stirred about 15 min in air. The vessel was sealed and heated at 120 ºC for 5 d under autogenous pressure, and then cooled to room temperature naturally. Colorless block crystals of **L-1** were obtained (70% yield based on Cd). Elemental analyses. Calcd. for $C_8H_8O_{12}Cd_2$ (520.94): C 17.12, H 8.62, O 34.21; found: C 17.01, H 8.43, O 34.07. FT-IR (KBr): v = 3587(w), 3066(w), 2954(w), 2864(w), 2358(w), 1616(s), 1388(s), 1313(w), 1230(m), 1118(s), 1056(s), 1010(m), 923(w), 810(m), 711(m), 607(w), 517(w).

Synthesis of compound D-1： A mixture of $Cd(OAc)_2 \cdot 4H_2O$ (0.4 mmol), D-DBTA (0.3 mmol), 4,4'-bpy (0.4 mmol), HCl aqueous solution (0.3 mL, 1 M), ethylalcohol (2 mL) and water (8 mL) was placed in an 18 mL Teflon-lined stainless steel vessel and stirred about 15 min in air. The vessel was sealed and heated at 120 ºC for 5 d under autogenous pressure, and then cooled to room temperature naturally. Colorless block crystals of **D-1** were obtained (70% yield based on Cd). Elemental analyses. Calcd. for $C_8H_8O_{12}Cd_2$ (520.94): C 17.12, H 8.62, O 34.21; found: C 17.01, H 8.43, O 34.07. FT-IR (KBr): v = 3587(w), 3066(w), 2954(w), 2864(w), 2358(w), 1616(s), 1388(s), 1313(w), 1230(m), 1118(s), 1056(s), 1010(m), 923(w), 810(m), 711(m), 607(w), 517(w).

Preparation of NPC800 and NPC900 material

Prior to the electrochemical examination, the sample was activated by the following procedure: the obtained cadmium based coordination polymer was placed under vacuum at 150 ℃ for 4 h to remove all water molecules. The nanoporous carbon materials were designed by the heat treatment at 800 and 900℃ in a argon atmosphere, respectively.

FT-IR spectra analysis

The FT-IR spectra of NPC800 and NPC900 are shown in Fig. S3. The absorptions at 3400 cm^{-1} could be ascribed to -OH groups stretching vibration. The strong and abroad absorptions at around 1720 cm^{-1} could be attributed to -COOH groups. The absorptions at 1408 cm^{-1} could be ascribed to C-O stretching vibration.

X-ray crystallography

Suitable single crystals with dimensions of 0.19 × 0.18 × 0.17 mm for compound **L-1** and 0.19 × 0.18 × 0.17 mm for compound **D-1** were glued on a glass fiber. Diffraction intensity data were collected on a Bruker Smart Apex-II CCD diffractometer with Mo Ka mono-chromated radiation (λ= 0.71073 Å) at 296 K. Absorption corrections were applied using the multiscan technique. The structures were solved by the direct method and refined by the full-matrix least-squares method on F^2 using the *SHELXL*-97 and olex 2 software [1]. All of the non-hydrogen atoms were refined anisotropically. The organic hydrogen atoms were generated geometrically. The aqua hydrogen atoms were located from difference Fourier maps.

Reference

[1] (a) Sheldrick, G. M. *SHELXS*-97, Program for Crystal Structure Solution. University of Göttingen, Germany, **1997**; (b) Sheldrick, G. M. *SHELXL*-97, Program for Crystal Structure Refinement. University of Göttingen,Germany, **1997**. (c) O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: A complete structure solution, refinement and analysis program, J. Appl. Crystallogr., **2009**, 42, 339.

Electrochemical measurements.

The electrochemical behaviour of the nanoporous carbon materials was performed using button cell. The working electrode consisted of the active material, carbonblack, and a PTFE binder in a weight ratio of 8:1:1 onto a piece of nickel foam, which was dried at 70℃ for 18 h. The galvanostatic charge and discharge performance, cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) were performed with a CHI660e electrochemical instrument (Chenhua Inc.,China).

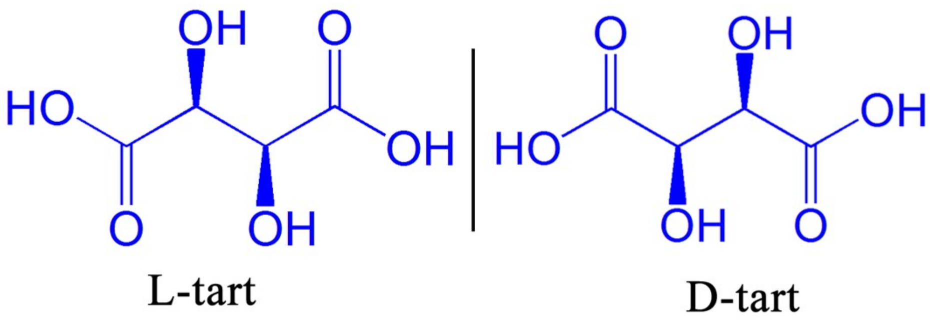
Materials and General Methods

All chemicals were commercially purchased and used as supplied. Elemental analyses of C, H, O and N were performed using an EA1110 elemental analyzer. The IR spectrum was recorded in the range 4000-400 cm^{-1} on a Nicolet 360 spectrometer with a pressed KBr pellet.

X-ray Powder diffraction for L-1

In order to check the phase purity of these compounds, the X-ray powder diffraction (XRPD) of **L-1** was checked at room temperature, as shown in Figure S1. The peak positions of simulated and experimental XRPD patterns are in agreement with each other, indicating the good phase purity of **L-1**. The differences in intensity may be due to the preferred orientation of the crystalline powder sample.

Supporting Figures



Scheme S1. The structure of L-tart and D-tart.

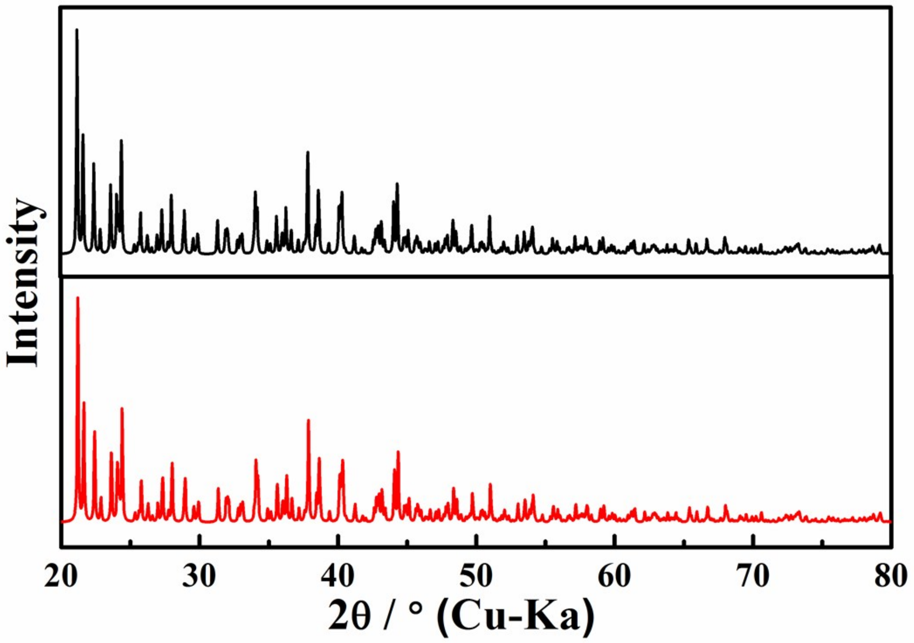


Fig. S1. The XRPD patterns based on the single-crystal structure of **L-1**: as-synthesized sample (black) and simulated one (red).

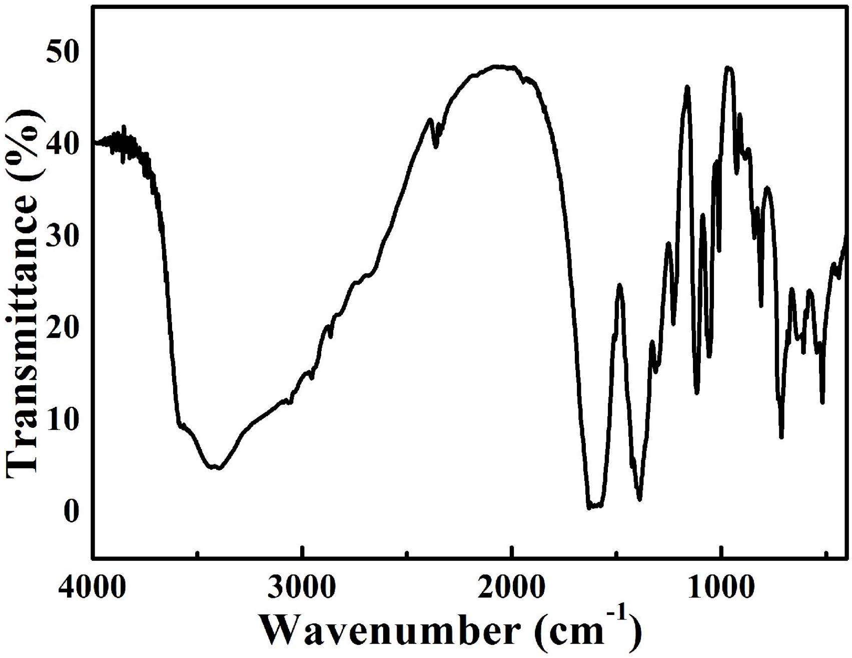


Fig. S2. IR spectrum of **L-1**.

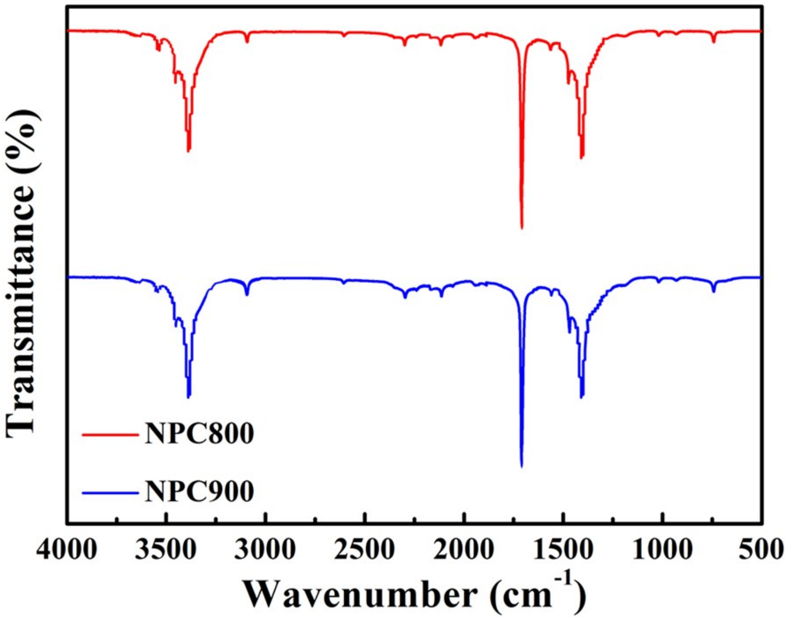


Fig. S3. IR spectrum of NPC800 andNPC900.

Table S1. Crystal data and structure refinements for **L-1 and D-1**.

compound	**L-1**	**D-1**
formula	$C_8H_8O_{12}Cd_2$	$C_8H_8O_{12}Cd_2$
fw	520.94	520.94
T (K)	293(2)	296.15
λ (Å)	0.71073	0.71073
crystal system	Orthorhombic	Orthorhombic
space group	$P2_12_12_1$	$P2_12_12_1$
a (Å)	7.5242(3)	7.5194(3)

b (Å)	7.9258(3)	7.9248(3)
c (Å)	19.5829(8)	19.5768(8)
V (Å^3)	1167.83(8)	1166.58(8)
Z	4	4
*D*c (g/cm^3)	2.963	2.966
μ (mm^{-1})	3.715	3.719
R_1[a] [$I > 2\sigma(I)$]	0.0291	0.0169
wR_2[b] (all data)	0.0699	0.0356

[a] $R_1 = \sum||F_0|-|F_C||/\sum|F_0|$; [b] $wR_2 = \sum[w(F_0^2-F_C^2)^2]/\sum[w(F_0^2)^2]^{1/2}$

Table S2. Selected bond lengths [Å] and angles [°] for **L-1** and **D-1**.

L-1							
02	Cd2	09	86.81(17)	01	Cd1	C1	27.02(19)
02	Cd2	07	146.19(18)	Cd2	02	Cd1	152.0(2)
02	Cd2	03	70.51(17)	C1	02	Cd2	120.7(4)
05^1	Cd2	02	84.6(2)	C1	02	Cd1	87.2(4)
05^1	Cd2	012^2	116.5(2)	C4	05	Cd2^5	135.3(5)
05^1	Cd2	09	81.92(18)	C8	010	Cd1^6	111.0(4)
05^1	Cd2	07	111.1(2)	C5	012	Cd2^7	117.8(4)
05^1	Cd2	03	150.9(2)	C7	09	Cd2	115.7(4)
012^2	Cd2	02	121.30(19)	C4	06	Cd1^6	122.2(4)
012^2	Cd2	09	146.14(17)	C6	07	Cd2	125.7(4)
012^2	Cd2	07	79.46(17)	C3	04	Cd1^6	112.8(3)
012^2	Cd2	03	90.00(18)	C5	011	Cd1^6	116.8(4)
07	Cd2	09	67.11(16)	C6	08	Cd1^8	118.6(4)
07	Cd2	03	84.23(16)	C2	03	Cd2	114.4(3)
03	Cd2	09	81.76(16)	02	Cd1	C1	28.17(19)
02	Cd1	010^3	156.54(17)	010^3	Cd1	C1	165.98(19)
06^3	Cd1	02	99.80(18)	06^3	Cd1	010^3	80.60(17)
06^3	Cd1	01	78.93(19)	06^3	Cd1	04^3	70.64(16)
06^3	Cd1	C1	85.4(2)	06^3	Cd1	08^4	116.28(17)
04^3	Cd1	02	83.46(16)	02	C1	Cd1	64.6(3)
04^3	Cd1	010^3	74.50(15)	02	C1	C2	119.7(6)
04^3	Cd1	C1	101.32(19)	01	C1	Cd1	58.9(4)
011^3	Cd1	02	98.44(17)	C2	C1	Cd1	160.0(5)
011^3	Cd1	010^3	71.11(16)	08^4	Cd1	010^3	81.70(16)
011^3	Cd1	06^3	145.22(18)	08^4	Cd1	04^3	153.87(17)
011^3	Cd1	04^3	82.39(17)	08^4	Cd1	C1	104.31(19)
011^3	Cd1	08^4	79.78(18)	01	Cd1	02	54.64(17)

O11^3	Cd1	O1	135.34(19)	O1	Cd1	O10^3	146.24(17)
O11^3	Cd1	C1	122.1(2)	O1	Cd1	O4^3	122.29(18)
O8^4	Cd1	O2	117.92(17)	O1	Cd1	O8^4	83.68(18)

Cd2	O2	2.257(5)	O6	Cd1^6	2.273(5)
Cd2	O5^1	2.198(5)	O4	Cd1^6	2.448(5)
Cd2	O12^2	2.200(5)	O11	Cd1^6	2.262(5)
Cd2	O9	2.523(5)	O8	Cd1^8	2.327(5)
Cd2	O7	2.311(5)	O10	Cd1^6	2.457(5)
Cd2	O3	2.430(5)	O12	Cd2^7	2.200(5)
Cd1	O2	2.451(5)	Cd1	O8^4	2.327(5)
Cd1	O10^3	2.457(5)	Cd1	O1	2.327(5)
Cd1	O6^3	2.273(5)	Cd1	C1	2.709(7)
Cd1	O4^3	2.448(5)	O5	Cd2^5	2.198(5)
Cd1	O11^3	2.262(5)			

D-1

O2	Cd2	O9	86.77(9)	O1	Cd1	C1	27.01(10)
O2	Cd2	O7	146.12(9)	Cd2	O2	Cd1	151.99(13)
O2	Cd2	O3	70.43(9)	C1	O2	Cd2	120.5(2)
O5^1	Cd2	O2	84.74(11)	C1	O2	Cd1	87.3(2)
O5^1	Cd2	O9	82.25(9)	C4	O5	Cd2^5	134.9(2)
O5^1	Cd2	O7	111.15(11)	C8	O10	Cd1^6	111.32(19)
O5^1	Cd2	O3	151.07(11)	C5	O12	Cd2^7	118.0(2)
O12^2	Cd2	O2	121.44(10)	C7	O9	Cd2	115.98(19)
O12^2	Cd2	O5^1	116.34(11)	C4	O6	Cd1^6	122.1(2)
O12^2	Cd2	O9	145.94(9)	C6	O7	Cd2	125.3(2)
O12^2	Cd2	O7	79.31(9)	C3	O4	Cd1^6	112.98(19)
O12^2	Cd2	O3	89.90(10)	C5	O11	Cd1^6	116.9(2)
O7	Cd2	O9	67.07(9)	C6	O8	Cd1^8	118.9(2)
O7	Cd2	O3	84.28(9)	C2	O3	Cd2	114.5(2)
O3	Cd2	O9	81.75(8)	C1	O1	Cd1	94.1(2)
O2	Cd1	C1	28.11(10)	O9	C7	C6	110.4(3)
O10^3	Cd1	O2	156.45(9)	O9	C7	C8	108.4(3)
O10^3	Cd1	C1	166.06(10)	O8^4	Cd1	O10^3	81.76(9)
O6^3	Cd1	O2	99.92(10)	O8^4	Cd1	O4^3	153.90(9)
O6^3	Cd1	O10^3	80.41(9)	O8^4	Cd1	C1	104.29(10)
O6^3	Cd1	O4^3	70.46(9)	O1	Cd1	O2	54.59(9)
O6^3	Cd1	O8^4	116.34(9)	O1	Cd1	O10^3	146.38(9)
O6^3	Cd1	O1	79.23(10)	O1	Cd1	O4^3	122.26(10)
O6^3	Cd1	C1	85.66(11)	O1	Cd1	O8^4	83.68(10)
O4^3	Cd1	O2	83.41(9)	O11^3	Cd1	O1	135.22(10)

O4^{3}	Cd1	O10^{3}	74.46(9)	O11^{3}	Cd1	C1	121.98(11)
O4^{3}	Cd1	C1	101.30(11)	O8^{4}	Cd1	O2	117.94(9)
O11^{3}	Cd1	O2	98.40(9)	O11^{3}	Cd1	O8^{4}	79.79(10)
O11^{3}	Cd1	O10^{3}	71.13(9)	O2	C1	Cd1	64.6(2)
O11^{3}	Cd1	O6^{3}	145.03(9)	O1	C1	Cd1	58.9(2)
O11^{3}	Cd1	O4^{3}	82.43(9)	C2	C1	Cd1	159.8(3)

Cd2	O2	2.256(3)	O6	Cd1^{6}	2.281(3)
Cd2	O5^{1}	2.200(3)	O4	Cd1^{6}	2.439(2)
Cd2	O12^{2}	2.194(2)	O11	Cd1^{6}	2.256(2)
Cd2	O9	2.526(2)	O8	Cd1^{8}	2.328(3)
Cd2	O7	2.309(3)	O5	Cd2^{5}	2.200(3)
Cd2	O3	2.431(3)	O10	Cd1^{6}	2.447(3)
Cd1	O2	2.451(3)	O12	Cd2^{7}	2.194(2)
Cd1	O10^{3}	2.447(3)	Cd1	O8^{4}	2.328(3)
Cd1	O6^{3}	2.281(3)	Cd1	O1	2.327(3)
Cd1	O4^{3}	2.439(2)	Cd1	C1	2.711(4)
Cd1	O11^{3}	2.256(2)			

Symmetry transformations used to generate equivalent atoms: for L-1: #1 -x+3/2,-y+1,z-1/2, #2 -x+2,y+1/2,-z-1/2, #3 -x+1,y-1/2,-z-1/2, #4 -x+1,y+1/2,-z-1/2, #5 -x+2,y-1/2,-z-1/2, #6 -x+3/2,-y+1,z+1/2; for D-1: 11+x,+y,+z; 2+x,1+y,+z; 31/2+x,-1/2-y,-1-z; 41/2-x,-y,1/2+z; 5-1+x,+y,+z; 6-1/2+x,-1/2-y,-1-z; 7+x,-1+y,+z; 81/2-x,-y,-1/2+z