Supporting Information

A one-dimensional cobalt-based coordination polymer as a cathode material of lithium-ion batteries

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1. Figures and Tables

Table S1 Crystallographic data of Co-DTBPT

Compound	Co-DTBPT
Empirical formula	$C_{52}H_{38}CoN_{18}O_{20}$
Formula weight	1293.93
T(K)	296(2)
Crystal system	triclinic
space group	*P-1*
a (Å)	9.1717(13)
b (Å)	10.5650(13)

c(Å)	18.044(2)
a (°)	74.318(4)
β (°)	86.913(4)
γ (°)	73.682(4)
V(Å^3)	1615.1(4)
Z, $D_{calculated}$ (g·cm^{-3})	1, 1.330
Mu (Mo K_α) (mm^{-1})	0.349
F (000)	663
Crystal size(mm)	0.05×0.04×0.02
θ range for data collection (°)	2.31 to 23.99
Index ranges	-11/11, -13/13,-23/23
no. of total reflns	25601
Unique reflns	7474(R_{int}=0.0690)
Data / restraints / parameters	7474/409/0
Goodness- of-fit on F^2	1.004
R_1, wR_2 [$I>2\sigma(I)$]	0.0627,0.1509
R_1, wR_2 (all data)	0.1295,0.1509
Largest diff. peak and hole/e·Å^{-3}	0.433and-0.369

Table S2 Main bond length (Å) and bond angle (°) in Co-DTBPT

Co-DTBPT			
Co1-O6	2.024 (2)	Co1-O5^i	2.126 (2)
Co1-O6^i	2.024 (2)	Co1-N1	2.165 (2)
Co1-O5	2.126 (2)	Co1-N1^i	2.165 (2)
O6^i -Co1-O6	180.00 (11)	O6- Co1- O5^i	88.87(9)
O6-Co1-O5	91.13(9)	O6^i -Co1- O5^i	91.13(9)
O6^i -Co1-O5	88.87(9)	O5^i -Co1-O5	180.0
O6^i -Co1-N1	90.98(9)	O6-Co1-N1	89.02(9)
O5^i -Co1-N1^i	97.40(9)	O5^i -Co1-N1	82.60(9)
O6^i -Co1- N1^i	89.02(9)	O6-Co1-N1	90.98(9)
O5^i -Co1- N1^i	82.60(9)	O5-Co1-N1	97.40(9)
N1^i -Co1-N1	180.00(13)		

Symmetry codes:(i) 1 - x,1 - y, 1 - z.

Table S3 Bond length (Å) and bond angle (°) of hydrogen bond in Co-DTBPT

D–H···A	D–H	H···A	D···A	∠D–H···A
O(6)–H(6A) ···N (6)	0.99	1.88	2.813 (4)	155
O(6)–H(6B) ···N (6)	0.85	2.2	2.813 (4)	129
C (2)–H (2) ···O (9) [iii]	0.93	2.35	3.117 (5)	140
C (10)–H (10) ···O (10) [iv]	0.93	2.58	3.407 (5)	149
C (18)–H (18) ···O (3)[v]	0.93	2.39	2.223 (4)	149
C(20)–H(20C) ···O (5)	0.96	2.39	2.767 (6)	103
C (23)–H (23) ···O (7)	0.93	2.36	2.732 (5)	103
C (23)–H (23) ···O (9)	0.93	2.32	2.690 (5)	103

Symmetry codes: (iii) *x*, *y*, -1 + z; (iv) 1 + *x*, *y*, -1 + z; (v) 1 + *x*, *y*, *z*.

Table S4 The capacity comparison of some CP/MOF based cathode materials for LIBs.

Cathode materials	Content of active materials	Specific Capacity (mAh g^{-1})	Current Density (mA g^{-1})/C rate	Cycle number/cycels	Voltage (V *vs.* Li/Li^+)	Ref.
Co (HAT-CN)	60%	136	40	200	1.2-3.9	S1
CuFe-PBA	70%	25	10	50	2.5-4.3	S2
MIL-53(Fe)	85%	70	50	50	1.5-3.5	S3
MIL-68	70%	32	C/10	12	1.5-3.5	S4
MIL-136(Co)	70%	20	10 C	50	2.0-4.0	S5
SNNU-73	60%	67.5	50	50	0.3-3.0	S6
SNNU-74	60%	41.5	50	50	0.3-3.0	S6
$Cu_3(HHTP)_2$	80%	95	1 C	100	1.7-3.5	S7
Cu-THQ	70%	340	50	100	1.2-4.0	S8
Zinc(II) Complex 5	10%	57	1 C	1000	1.4-4.0	S9
$(H_2NMe_2)_2Fe_2(Cl_2dhbq)_3$	80%	150	40	50	1.8-4.2	S10

1D-DS-Co-MOF	30%	72	200	100	2.5-3.2	S11
2D-DS-Cu-MOF	30%	84	50	100	2.4-4.1	S11
3D-DS-Mn-MOF	30%	109	200	100	1.7-4.2	S11
Cu-TCA	80%	39.9	0.5 C	200	1.4-4.3	S12
Cd(II)MOF 1	45%	32.5	100	50	1.8-3.4	S13
Cd(II)MOF 2	45%	36.7	100	50	1.8-3.4	S13
Co(II)MOF 3	45%	~3	100	50	1.8-3.4	S13
Co(II)MOF 4	45%	~6	100	50	1.8-3.4	S13
NiDI	70%	~46	250	300	2.0-4.5	S14
$Fe_2(DFc)_3$	60%	70	2000	10000	2.0-4.2	S15
Co-DTBPT	30%	55	50	100	1.5-4.0	This work

Table S5 electrochemical Impedance Spectroscopy fitting values of Co-DTBPT electrode in different cycle stages

Sample	R_1	R_{ct}	R_s	CPE_1-T	CPE1-P	CPE_2-T	CPE_2-P	W_1-R	W_1-T	W_1-P
After 1 cycle	8.14	13.55	70.6	1.80×10^{-5}	0.833	2.92×10^{-6}	1.00	33.29	5.09	0.435
After 50 cycles	12.69	96.68	67.8	5.42×10^{-3}	0.474	3.03×10^{-5}	0.73	0.010	1.33×10^{-4}	0.428

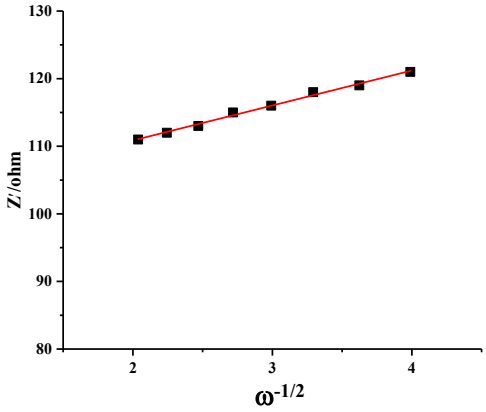

Figure S1. The linear fitting of the Z′ *vs* square root of frequency ($\omega^{-1/2}$) relationship, where ω is the angle frequency and Z′ is the real part of Nyquist impedance of the Co-DTBPT electrode after 1 cycle.

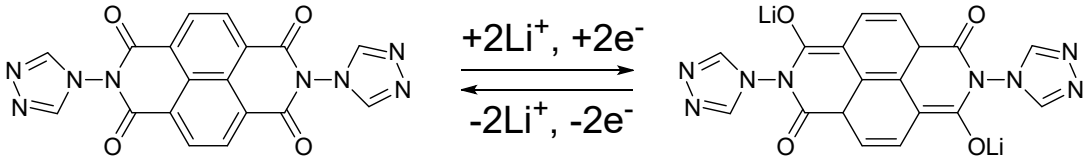

Figure S2. The possible mechanism of lithium ions intercalation/deintercalation for 4-DTBPT

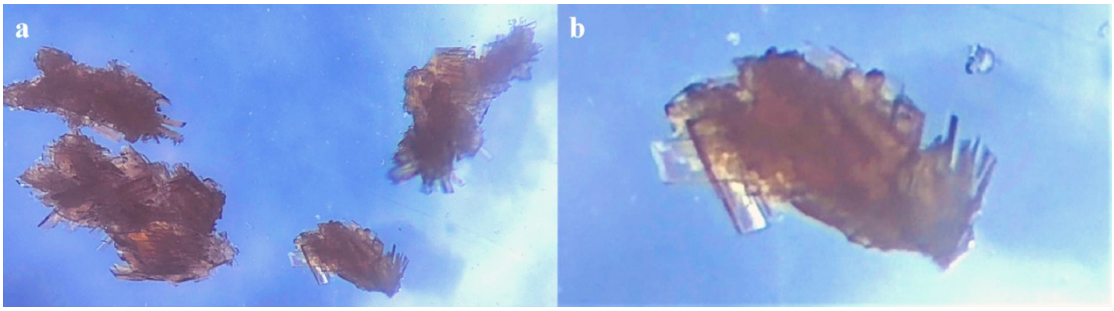

Figure S3. The crystal optical photos of Co-DTBPT (a) Low and (b) high magnification.

Figure S4. Photographs of Co-DTBPT soaked in the electrolyte for different time durations.

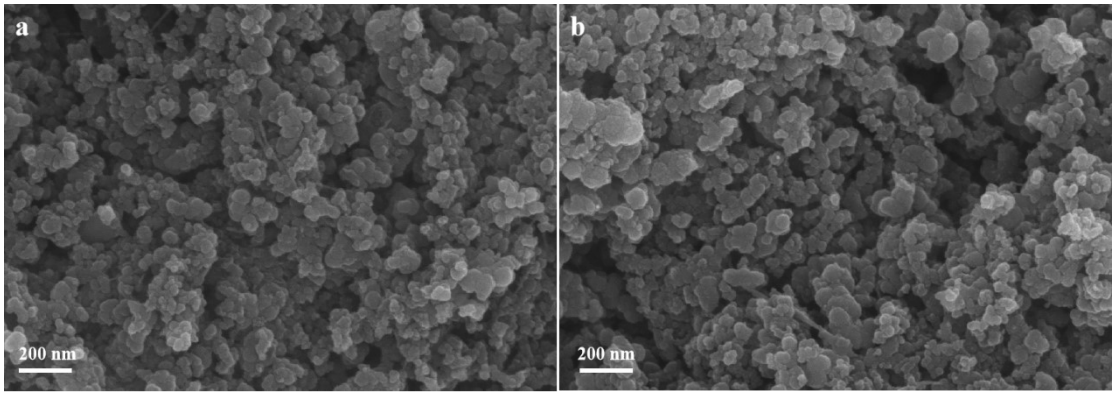

Figure S5. The SEM images of the Co-DTBPT electrode: (a) pristine; (b) after 20 cycles

The theoretical capacity of Co-DTBPT and 4-DTBPT can be calculated based on following formula:

$$C = 26.8\frac{n}{M}$$

Co-DTBPT: $C = 26.8\frac{n}{M} = 26.8 \times \frac{5}{1293.93} = 0.1036\ Ah\ g^{-1} = 103.6\ mAh\ g^{-1}$

4-DTBPT： $C = 26.8\frac{n}{M} = 26.8 \times \frac{2}{400} = 0.1340\ Ah\ g^{-1} = 134.0\ mAh\ g^{-1}$

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