ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Sulfur-Containing Bimetallic Metal Organic Frameworks with Multi-Fold Helix as Anode of Lithium Ion Batteries

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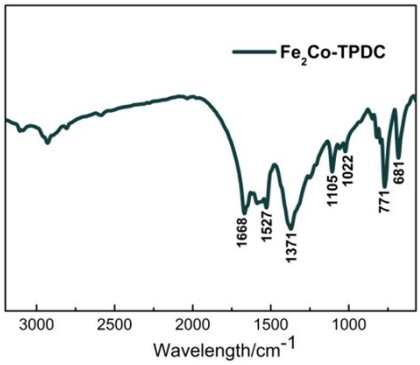

Fig. S1 FT-IR spectra of Fe_2Co-TPDC. IR (KBr, cm^{-1}): 1668s, 1527s, 1371s, 1105m, 1022w, 771s, 681m.

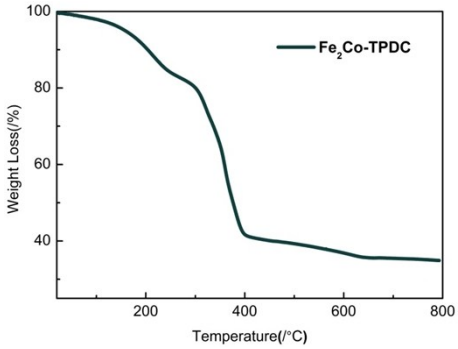

Fig. S2 The TGA curve of Fe_2Co-TPDC. The weight loss before 300°C was solvent molecules. The whole framework of Fe_2Co-TPDC completely collapsed after 400°C

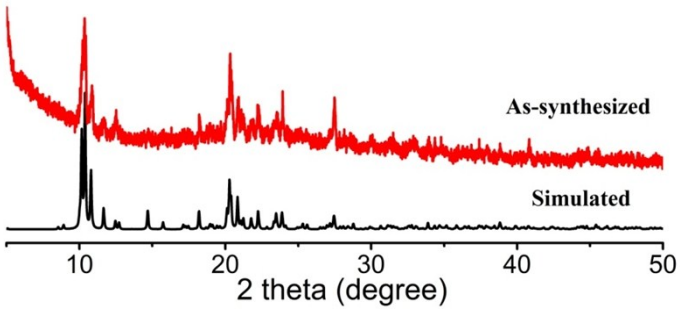

Fig.S3 The PXRD patterns and photos of Fe_2Co-TPDC.

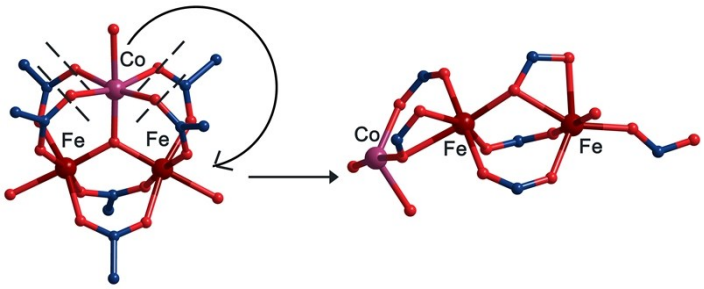

Fig. S4 Ball and stick diagrams of the $[Fe_2Co(\mu_3\text{-}O)(CH_3COO)_6]$ and the speculate fissile mechanism. Co^{2+} ion escaped from the original cluster, and recombined with two Fe^{3+} ions to form a lineal $[Fe_2Co(COO)_6]$ cluster. Color scheme: dark red (Fe), purple (Co), red (O), blue (C). All of the hydrogen atoms are omitted for clarity.

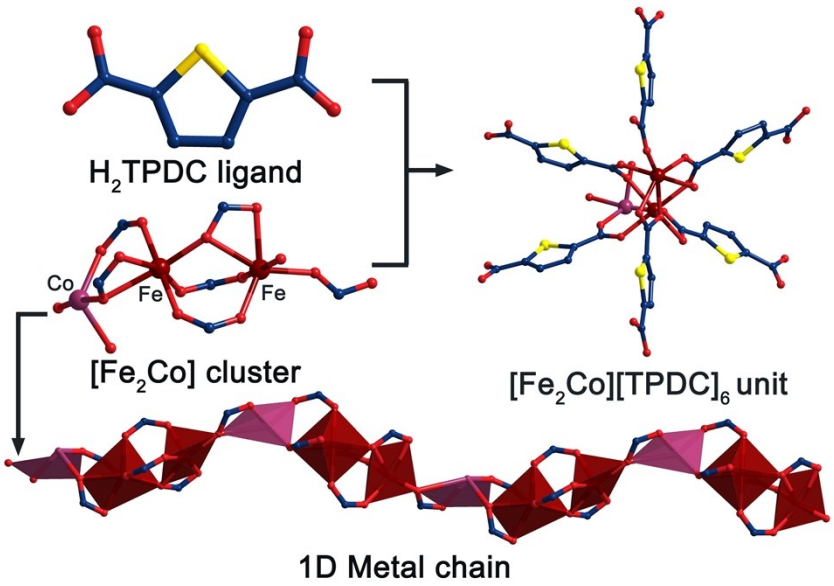

Fig. S5 Ball and stick diagrams of the H_2TPDC ligand, [Fe_2Co] cluster and [Fe_2Co][TPDC]$_6$ unit. Ball/stick/polyhedral diagrams of the 1D inorganic metal chain. Color scheme: yellow (S), dark red (Fe), purple (Co), red (O), blue (C). All of the hydrogen atoms are omitted for clarity.

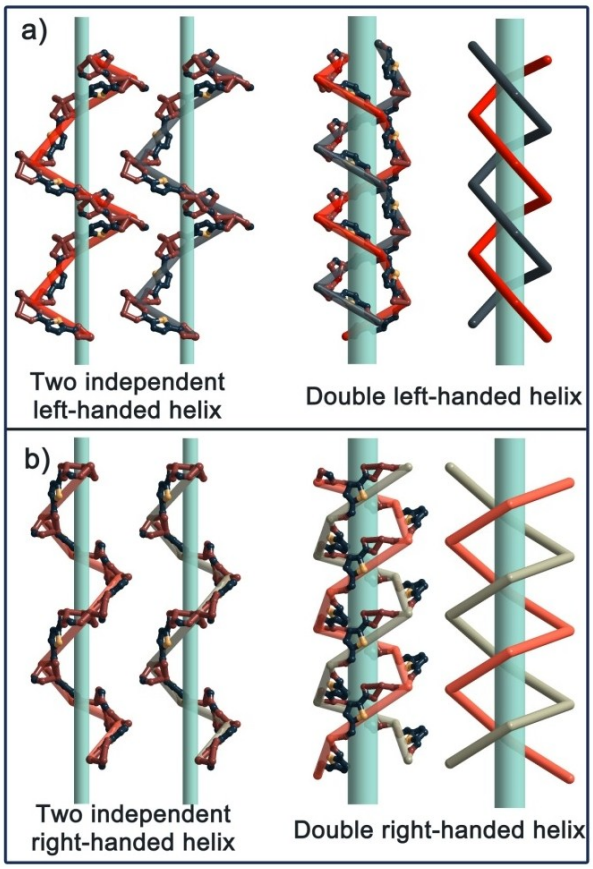

Fig. S6 Ball/stick diagrams of a) the single left-handed helix and double left-handed helix; b) single right-handed helix and double right-handed helix in Type-II 4-fold meso-helix of Fe_2Co-TPDC. All of the hydrogen atoms are omitted for clarity.

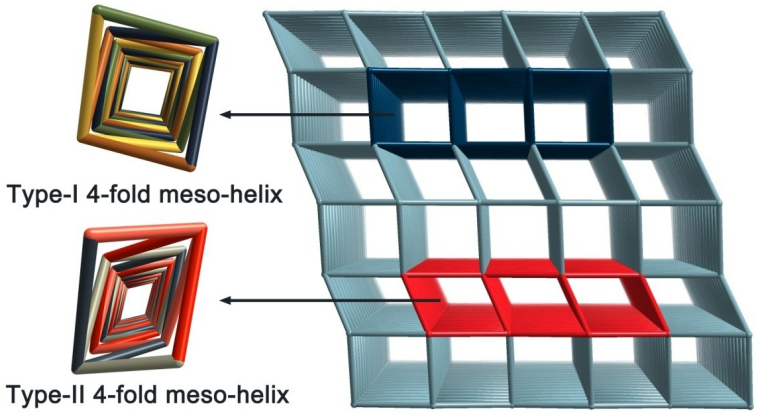

Fig. S7 Schematic illustration of the topology of Fe_2Co-TPDC, Type-I and Type-II 4-fold meso-helix.

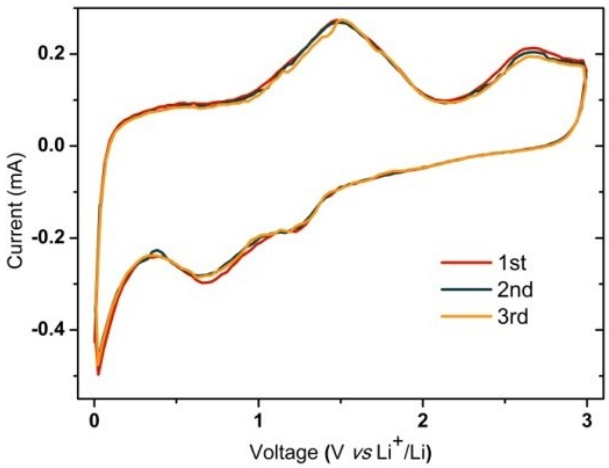

Fig.S8 Cyclic voltammograms for the Fe_2Co-TPDC anode at the range of 0.01-3 V (scan rate:0.1 mV s^{-1}).

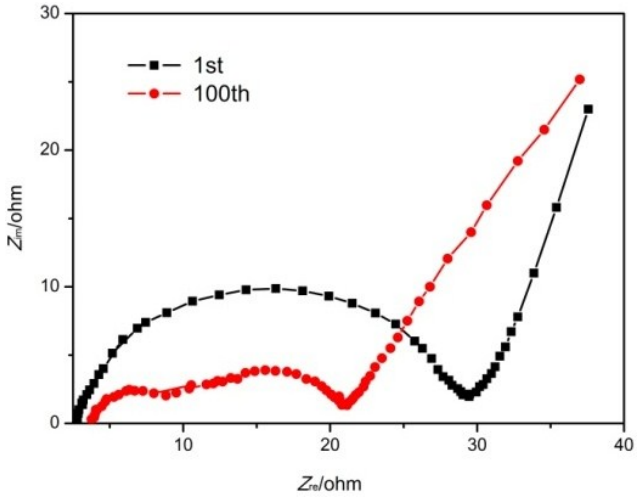

Fig.S9 Nyquist plots of Fe_2Co-TPDC anode after the first and 100th discharge-charge process.

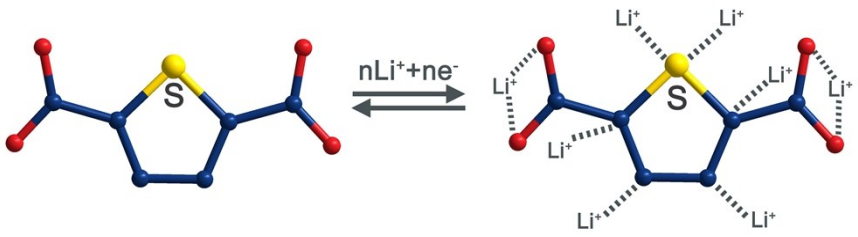

Fig.S10 Probable Li^+ binding sites provided by the sulfur-containing ligand of Fe_2Co-TPDC.

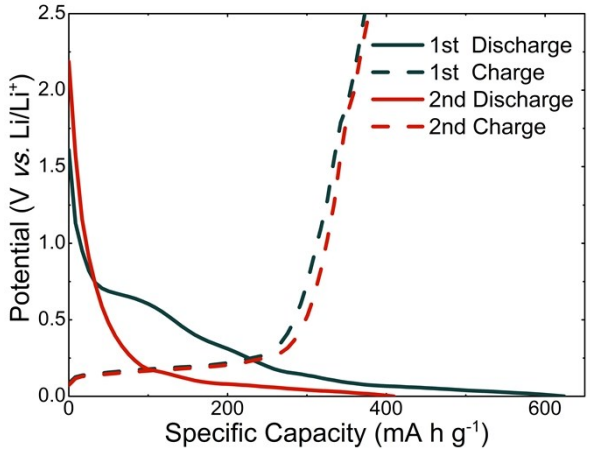

Fig.S11 The charge-discharge curves of graphite anode during the initial two cycles at a current density 0.1C (0.1C=100mA cm^{-2}).

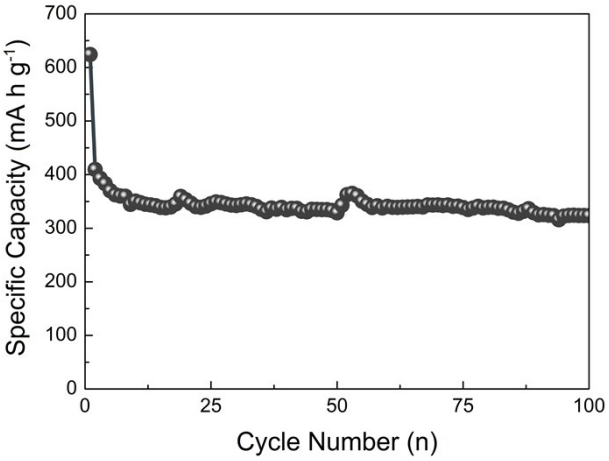

Fig.S12 The charge-discharge capacity and the coulombic efficiency of graphite anode during 100 cycles at a current density 0.1C (0.1C=100mA cm^{-2}).

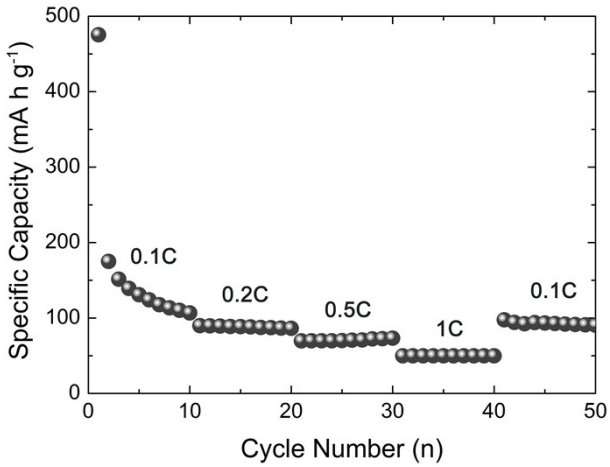

Fig.S13 Rate performance of graphite anode at current densities of 0.1C to 1C (0.1C=100mA cm^{-2}).

Table S1. Crystal data and structure refinement for Fe_2Co-TPDC.

Compound reference	Fe_2Co-TPDC
Chemical formula	$C_{27}H_{24}N_3O_{15}S_3Fe_2Co$
Formula Mass	897.31
Crystal system	Monoclinic
a/Å	17.8560
b/Å	9.7510
c/Å	21.2030
α/°	90
β/°	102.928
γ/°	90
Unit cell volume/Å3	3598(2)
Temperature/K	293(2)
Space group	$P2_1/c$
No. of formula units per unit cell, *Z*	4
No. of reflections measured	26760
Final R_1 values ($I > 2\sigma(I)$)	0.0404
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1100
Final R_1 values (all data)	0.0485
Final $wR(F^2)$ values (all data)	0.1139
Goodness of fit on F^2	1.169
CCDC no.	1814820

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

Table S2. Selected bonds lengths (Å) and angles (°) for Fe_2Co-TPDC.

Fe(1)-O(1)#1	2.038(3)	Fe(1)-O(9)#2	2.078(3)
Fe(1)-O(4)	2.078(3)	Fe(1)-O(6)#1	2.098(3)
Fe(1)-O(8)#3	2.178(3)	Fe(1)-O(7)#3	2.269(3)
Fe(2)-O(5)	2.020(3)	Fe(2)-O(11)	2.044(3)
Fe(2)-O(2)	2.081(3)	Fe(2)-O(13)	2.169(3)
Fe(2)-O(10)#4	2.181(3)	Fe(2)-O(9)#4	2.268(3)
Co(1)-O(3)	2.008(3)	Co(1)-O(12)#5	2.049(3)
Co(1)-O(14)	2.052(3)	Co(1)-O(15)	2.094(3)
Co(1)-O(7)#3	2.143(3)	O(6)-Fe(1)#2	2.098(3)
O(1)-Fe(1)#2	2.038(3)	O(12)-Co(1)#5	2.049(3)
O(7)-Co(1)#6	2.143(3)	O(7)-Fe(1)#6	2.269(3)
O(9)-Fe(1)#1	2.078(3)	O(9)-Fe(2)#7	2.268(3)
O(10)-Fe(2)#7	2.181(3)	O(8)-Fe(1)#6	2.178(3)
O(1)#1-Fe(1)-O(9)#2	100.80(11)	O(1)#1-Fe(1)-O(4)	87.87(13)

O(9)#2-Fe(1)-O(4)	90.34(11)	O(4)-Fe(1)-O(6)#1	179.22(13)
O(1)#1-Fe(1)-O(6)#1	92.79(13)	O(1)#1-Fe(1)-O(8)#3	158.35(12)
O(9)#2-Fe(1)-O(6)#1	89.12(11)	O(9)#2-Fe(1)-O(8)#3	100.77(11)
O(4)-Fe(1)-O(8)#3	93.88(13)	O(6)#1-Fe(1)-O(8)#3	85.66(11)
O(1)#1-Fe(1)-O(7)#3	99.31(11)	O(9)#2-Fe(1)-O(7)#3	158.71(10)
O(4)-Fe(1)-O(7)#3	97.31(11)	O(6)#1-Fe(1)-O(7)#3	82.99(11)
O(8)#3-Fe(1)-O(7)#3	59.05(10)	O(5)-Fe(2)-O(11)	112.97(12)
O(5)-Fe(2)-O(2)	98.91(13)	O(11)-Fe(2)-O(2)	89.94(12)
O(5)-Fe(2)-O(13)	83.98(14)	O(11)-Fe(2)-O(13)	87.70(13)
O(2)-Fe(2)-O(13)	176.82(14)	O(2)-Fe(2)-O(10)#4	92.63(13)
O(5)-Fe(2)-O(10)#4	149.33(11)	O(13)-Fe(2)-O(10)#4	85.46(14)
O(11)-Fe(2)-O(10)#4	95.25(11)	O(5)-Fe(2)-O(9)#4	92.58(11)
O(11)-Fe(2)-O(9)#4	153.61(10)	O(10)#4-Fe(2)-O(9)#4	58.41(10)
O(2)-Fe(2)-O(9)#4	92.59(11)	O(3)-Co(1)-O(12)#5	97.50(13)
O(13)-Fe(2)-O(9)#4	88.59(12)	O(3)-Co(1)-O(14)	117.62(14)
O(12)#5-Co(1)-O(14)	144.81(13)	O(14)-Co(1)-O(15)	86.88(14)
O(3)-Co(1)-O(15)	87.00(13)	O(3)-Co(1)-O(7)#3	97.65(12)
O(12)#5-Co(1)-O(15)	93.19(14)	O(12)#5-Co(1)-O(7)#3	91.30(12)
O(14)-Co(1)-O(7)#3	86.41(12)	O(15)-Co(1)-O(7)#3	173.06(13)

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