Electronic supplementary information (ESI)

Novel coordination polymer based on Co(II) hexanuclear clusters with azide and carboxylate bridges: structure, magnetism and its application as Li-ion battery anode

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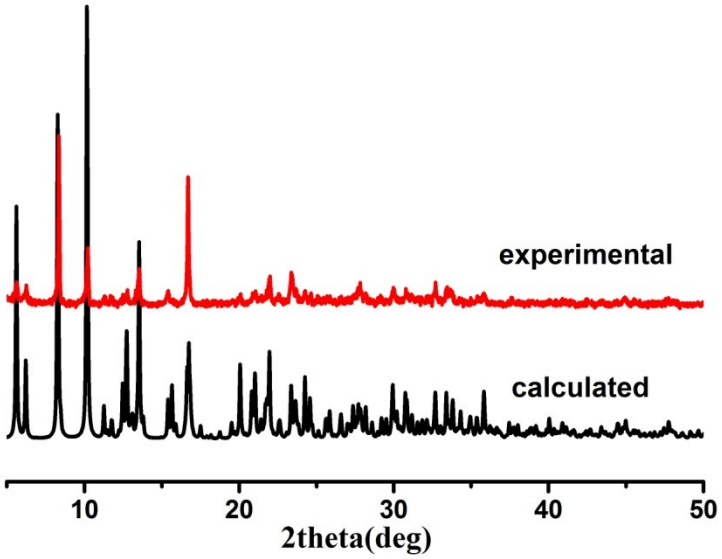

Fig. S1 PXRD patterns of **1.**

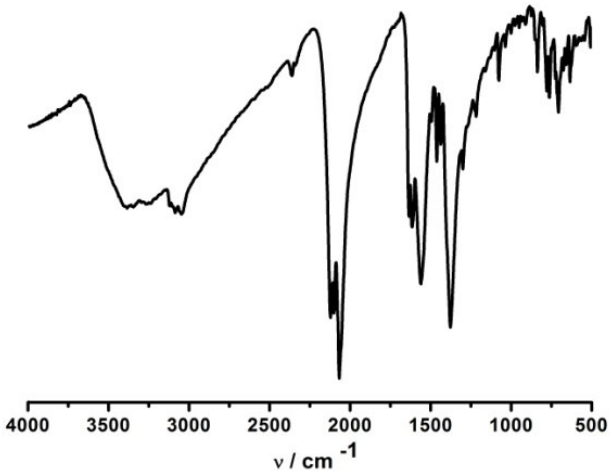

Fig. S2 IR spectrum of **1**.

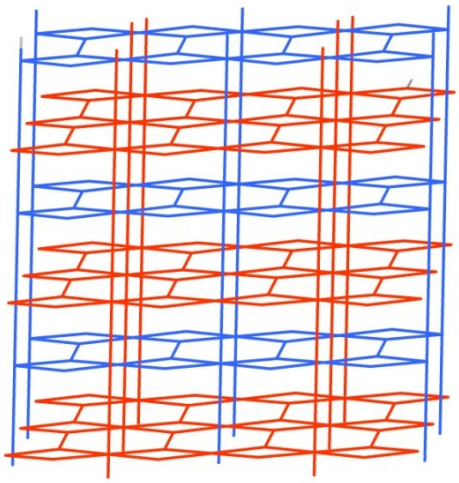

Fig. S3 Topological presentation of the two-fold interpentration in **1**.

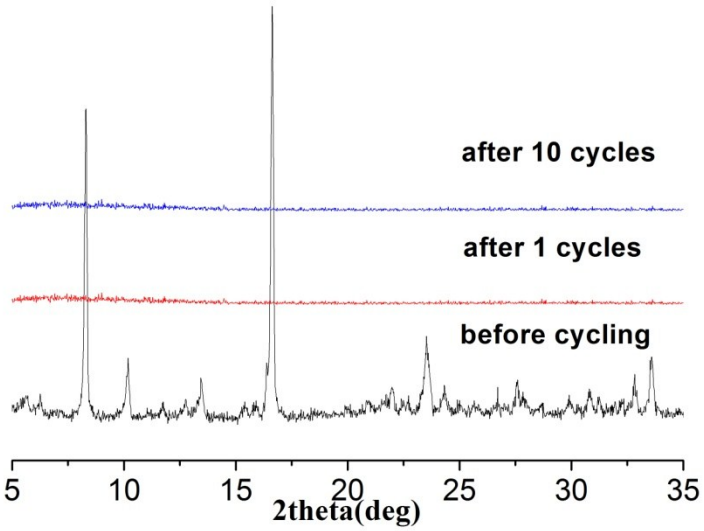

Fig. S4 PXRD patterns of the electrode before and after cycling.

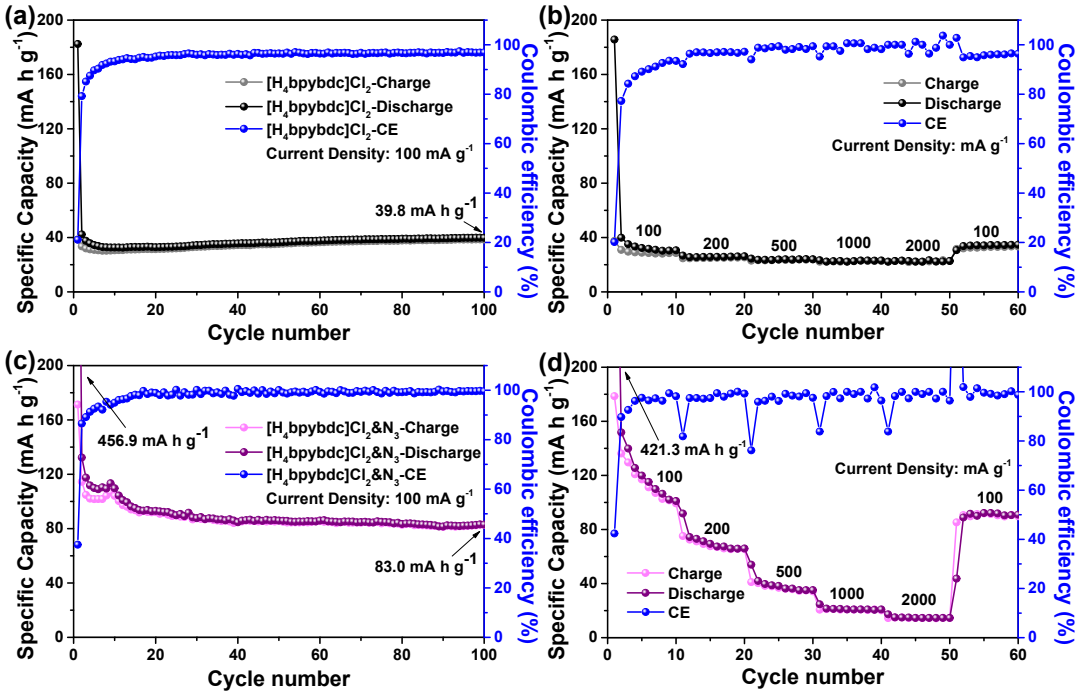

Fig. S5 Cyclic stability and Coulombic efficiency of $[H_4bpybdc]Cl_2$ (a) and $[H_4bpybdc]Cl_2$-NaN_3 (c) at 100 mA g^{-1}. Rate performance of $[H_4bpybdc]Cl_2$ (b) and $[H_4bpybdc]Cl_2$-NaN_3 (d) at different current densities.

Table S1 Hydrogen bond distances (Å) and angles (°) for compounds **1**.

D-H…A	dD-H)/Å	d(H…A)/ Å	d(D…A)/ Å	∠D-H…A/°
O9-H9B…O4A	0.86	1.91	2.72(6))	159(8)
O9-H9C…O5B	0.88	2.13	2.97(1)	158(5)
O10-H10B…O16	0.87	2.03	2.88(3)	168(7)
O10-H10B…O16'	0.87	1.92	2.76(3)	162(7)
O10-H10C…O6B	0.86	2.02	2.87(6)	169(7)
O11-H11B…O6C	0.87	1.78	2.63 (9)	167(10)
O11-H11B…O6'C	0.87	1.96	2.74(9)	151(9)
O11-H11C…O3D	0.87	1.95	2.76(0)	153(9)
O12-H12B…O4E	0.89	1.92	2.71(7)	148(5)
O12-H12C…O5C	0.87	1.95	2.80(4)	166(8)
O13-H13B…O3E	0.86	2.00	2.77(2)	148(4)
O13-H13C…O10F	0.87	2.11	2.90(8)	152(5)

Symmetry codes: (A) -x+1, -y, -z+2; (B) x+1, y, z+1; (C) x+1, y, z; (D) x, y+1, z-1; (E) 1-x, -y, 1-z; (F) x, y, z-1.

Table S2 Carboxylate-coordinated MOFs or CPs for LIBs anode for LIBs.

Organic ligands	MOFs or CPs	Voltage (V vs Li^+/Li)	Current Density (mA g^{-1})/C rate	Cycle Number	Reversible Capacity (mA h g^{-1})	Refs
H_3BTB	MOF-177	0.1–1.6	50	2	105	[1]
H_3TTPCA	Cd-MOF	0.1–3	100	100	302	[2]
Asp	Asp-Cu	0.01–3	50	200	233	[3]
HCOOH	$Zn_3(HCOO)_6$	0.005–3.0 V	60	60	560	[4]
	$Co_3(HCOO)_6$	0.005–3.0 V	60	60	410	
	$Zn_{1.5}Co_{1.5}(HCOO)_6$	0.005–3.0 V	60	60	510	
NTCDA	Ni-NTC	0.01–3	100	80	248	[5]
	Li-NTC	0.01–3	100	80	468	
	Li/Ni-NTC	0.01–3	100	80	482	
H_2BDC	$Co_2(OH)_2BDC$	0.02–3	50	100	650	[6]
	Ni-MOF	0.01–3	100	100	620	[7]
	$[Cu_2(C_8H_4O_4)_4]_n$	0.01–2.5	48	50	161	[8]
	Co–Zn-MOF	0.01–3	100	100	1211	[9]
H_3BTC	Mn-BTC	0.01–2	100	100	694	[10]
	CoBTC-EtOH	0.01–3	100	100	856	[11]
	$Cu_3(BTC)_2$	0.05–3	383	50	474	[12]
H_4BTC	MnCo-BTC	0.01–3	100	150	901	[13]
H_2TFBDC & 4,4'-bpy	Mn-LCP	0.1–3	50	50	390	[14]
terephthalate	$Li2C_8H_4O_4$	0.7-3.0	1C	80	125	[15]
trans–trans-muconate	$Li2C_6H_4O_4$	0.7-3.0	1C	50	234	
pda	$[Li_6(pda)_3]\cdot 2EtOH$	0.2-2.0	30	50	160	[16]

H_3BTB: 4,4',4''-benzene-1,3,5-triyl-tri-benzoic acid; H_3TTPCA: 1,1',1''-(1,3,5-triazine-2,4,6-triyl)tripiperidine-4-carboxylic acid; Asp: aspartic acid; HCOOH: methanoic acid; NTCDA: 1,4,5,8-Naphthalenetetracarboxylic dianhydride; H_2BDC: terephthalic acid; H_3BTC: trimesic acid; H_4BTC: 1,2,4,5-Benzenetetracarboxylic acid; H_2TFBDC: 2,3,5,6-tetrafluoroterephthalic acid; 4,4'-bpy: 4,4'-bipyridine; pda: 2,6-pyridinedicarboxylic acid.

Notes and references

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