

## Supporting Information

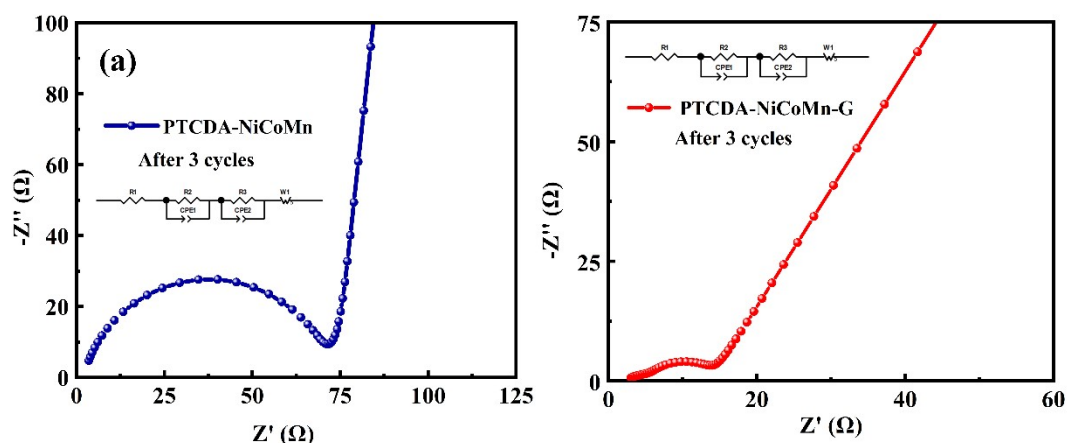
### Ni-Co-Mn complexed 3,4,9,10-perylene tetracarboxylic acid complexes as novel organic electrode material for lithium-ion batteries

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**Fig. S1** (a) AC impedance curve of PTCDA-NiCoMn after 3 turns of polarization; (b) AC impedance curve of PTCDA-NiCoMn-G after 3 turns of polarization

**Table S1** Impedance fitting data for materials

Samples	$R_1$ (Ω)	$R_2$ (Ω)	$R_3$ (Ω)
3 Cycles PTCDA-NiCoMn	4.257	3.501	42.86
3 Cycles PTCDA-NiCoMn-G	2.376	3.889	7.545

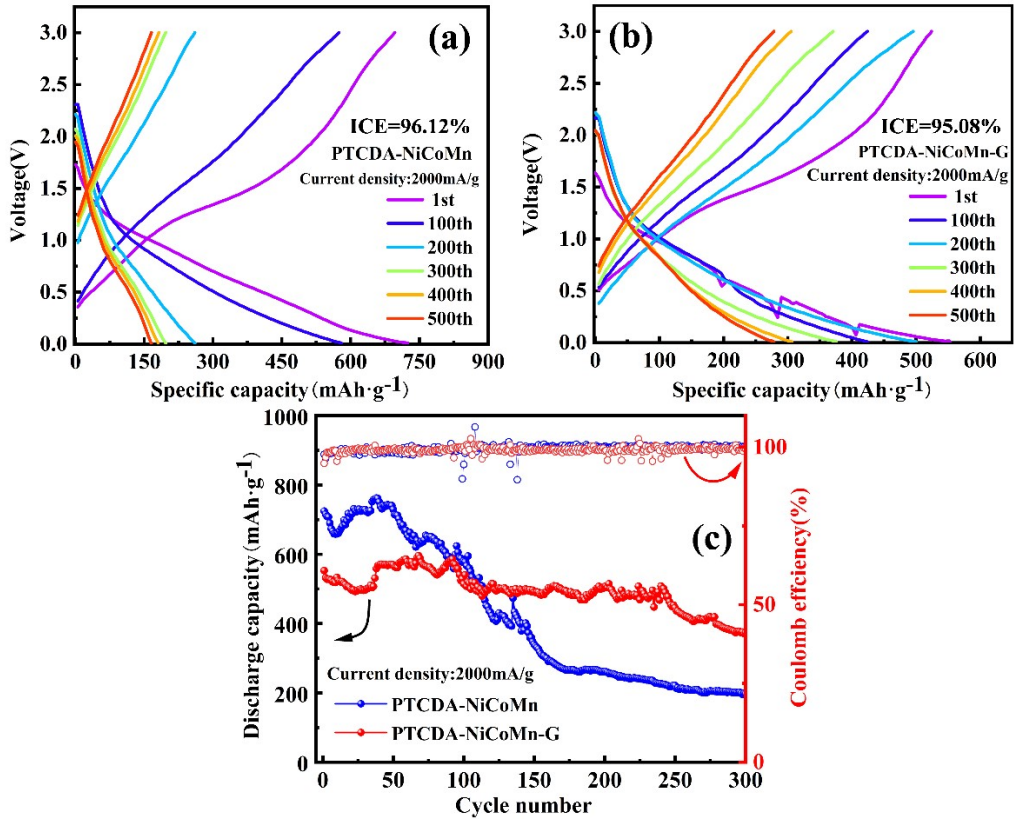


Fig. S2 (a) charge/discharge curves of PTCDA-NiCoMn electrode at 2000 mA g<sup>-1</sup> current density; (b) charge/discharge curves of PTCDA-NiCoMn-G electrode at 2000 mA g<sup>-1</sup> current density; (c) cycling performance of PTCDA-NiCoMn and PTCDA-NiCoMn-G electrodes at 2000 mA g<sup>-1</sup> current density

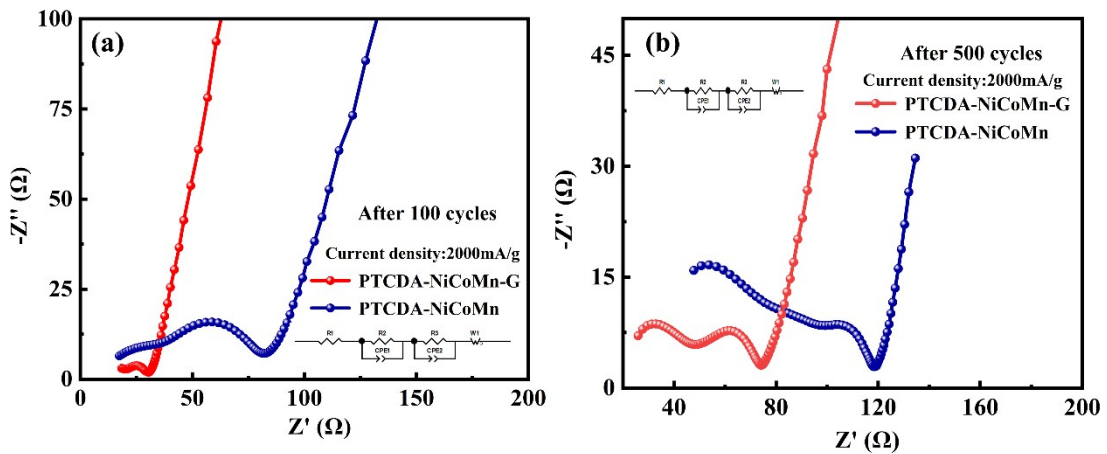


Fig. S3 (a) AC impedance curves of PTCDA-NiCoMn and PTCDA-NiCoMn-G electrodes after 100 cycles; (b)

AC impedance curves of both electrodes after 500 cycles

**Table S2** Impedance fitting data for PTCDA-NiCoMn and PTCDA-NiCoMn-G electrodes

	Samples	$R_1$ ( $\Omega$ )	$R_2$ ( $\Omega$ )	$R_3$ ( $\Omega$ )
100 Cycles	PTCDA-NiCoMn	15.98	19.68	46.06
	PTCDA-NiCoMn-G	16.89	3.67	9.60
500 Cycles	PTCDA-NiCoMn	47.10	53.01	18.27
	PTCDA-NiCoMn-G	25.83	22.28	25.66

**Table S3** Discharge capacity contributed from PTCDA-NiCoMn at different potentials (The voltage window is 0.01-3 V at 0.1 V intervals, C: discharge capacity, mAh·g<sup>-1</sup>, V: voltage, V)

PTCDA-NiCoMn							
4 <sup>th</sup> cycle		50 <sup>th</sup> cycle		125 <sup>th</sup> cycle		200 <sup>th</sup> cycle	
C	V	C	V	C	V	C	V
0	3.0	0	3.0	0	3.0	0	3.0
0	2.9	0	2.9	0	2.9	0	2.9
0	2.8	0	2.8	0	2.8	0	2.8
0	2.7	1.9	2.7	0	2.7	0	2.7
1.1	2.6	5.5	2.6	0.3	2.6	0.3	2.6
2.5	2.5	10.8	2.5	2.2	2.5	2.5	2.5
4.2	2.4	17.2	2.4	5.8	2.4	6.2	2.4
6.7	2.3	23.3	2.3	10.5	2.3	11.3	2.3
10	2.2	29.1	2.2	15.8	2.2	16.4	2.2
15	2.1	34.6	2.1	21.1	2.1	22.1	2.1
21.6	2.0	40.2	2.0	26.6	2.0	27.8	2.0
29.9	1.9	45.7	1.9	32.1	1.9	33.7	1.9
39.3	1.8	51.8	1.8	38.5	1.8	40.3	1.8
48.8	1.7	58.4	1.7	46	1.7	47.4	1.7
58.5	1.6	66.2	1.6	54	1.6	55.9	1.6
70.4	1.5	75.9	1.5	63.1	1.5	65.5	1.5
87.8	1.4	88.3	1.4	74.5	1.4	77.4	1.4
113.3	1.3	105.8	1.3	89.5	1.3	91.6	1.3
151	1.2	129.9	1.2	109.4	1.2	109.7	1.2
196.4	1.1	164.3	1.1	132.1	1.1	131	1.1
250.2	1.0	209.7	1.0	161.4	1.0	156.8	1.0
314.2	0.9	260.6	0.9	196.1	0.9	185.1	0.9
382	0.8	314.9	0.8	231.2	0.8	216.3	0.8
445.8	0.70	0.7	0.7	264.2	0.7	249	0.7
509.5	0.6	442.9	0.6	316.8	0.6	285.8	0.6
572.6	0.5	513.5	0.5	367.8	0.5	326.1	0.5
642.2	0.4	585.2	0.4	422.3	0.4	371.2	0.4
723.1	0.3	658.6	0.3	486.8	0.3	420.2	0.3

828.4	0.2	755.2	0.2	558.6	0.2	475.9	0.2
976.3	0.1	874.6	0.1	645.8	0.1	541.2	0.1
1218.8	0.01	1051.20	0.01	761	0.01	622.6	0.01

**Table S4** Total capacity attenuation over different cyclic ranges and the attenuation ratio of C=O, C=C, benzene ring correspondence

<b>Cycle range</b>	<b>Total capacity attenuation, mAh·g<sup>-1</sup></b>	<b>Capacity attenuation (C=O), mAh·g<sup>-1</sup></b>	<b>Percentage</b>	<b>Capacity attenuation (C=C), mAh·g<sup>-1</sup></b>	<b>Percentage</b>	<b>Capacity attenuation (benzene ring), mAh·g<sup>-1</sup></b>	<b>Percentage</b>
20-50	167.6	51.52	30.74%	38.64	23.05%	77.3	46.21 %
50-125	290.2	89.28	30.76%	67.32	23.19%	133.92	46.14%
125-200	138.4	42.57	30.76%	31.59	22,82%	63.89	46.16%