Supplemental information

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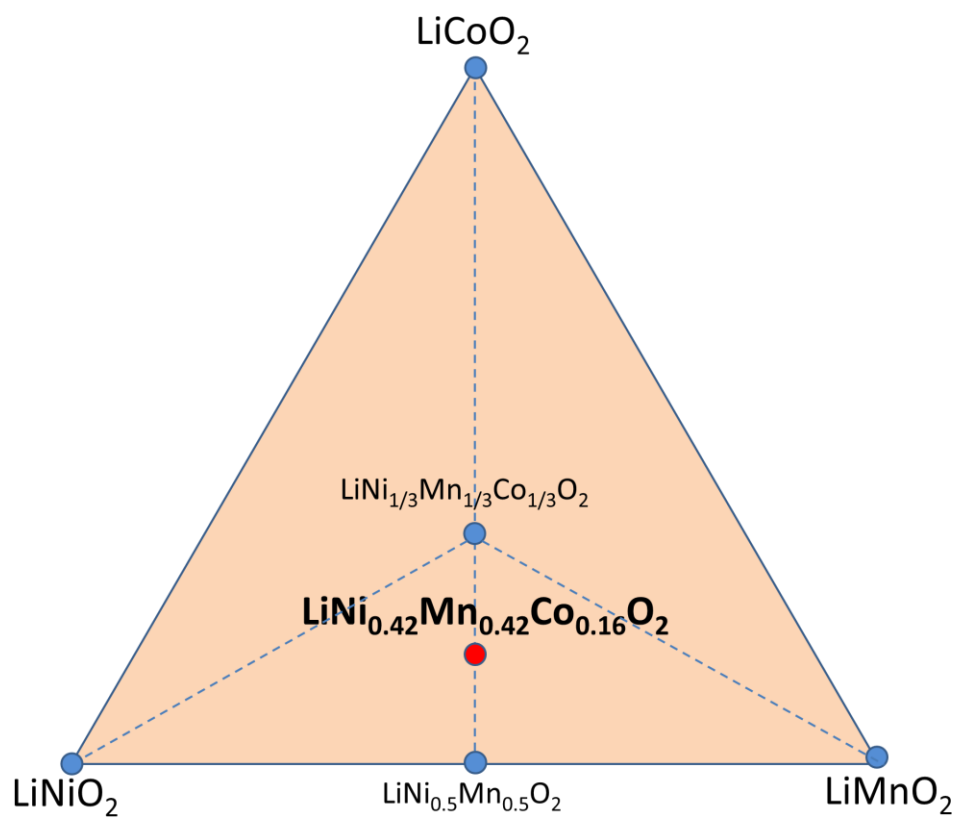
Figure S1 The composition of $LiMn_{0.42}Ni_{0.42}Co_{0.16}O_2$ electrode material in this study
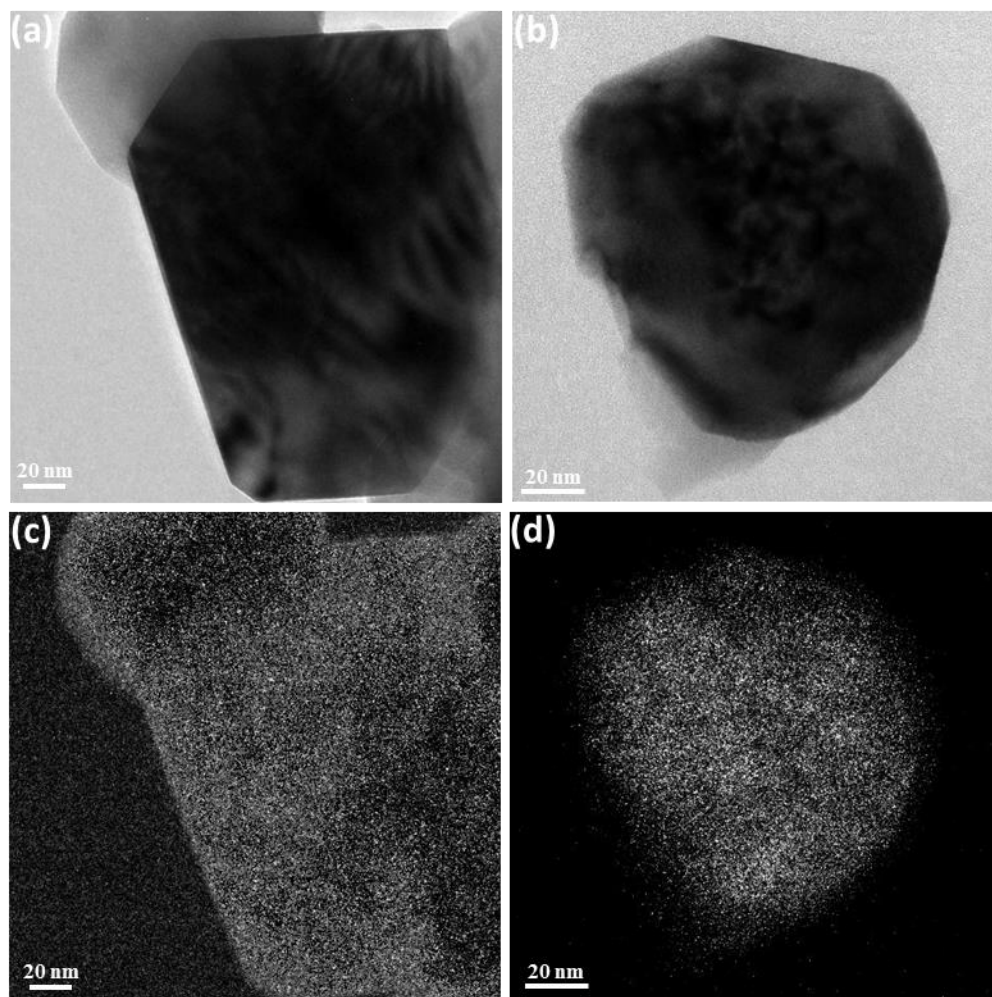
Figure S2 (a) and (b) High-resolution transmission electron microscopy image of Sample A and Sample B, respectively; (c) and (d) Ni EELS maps on the single particle of Sample A and Sample B, respectively.
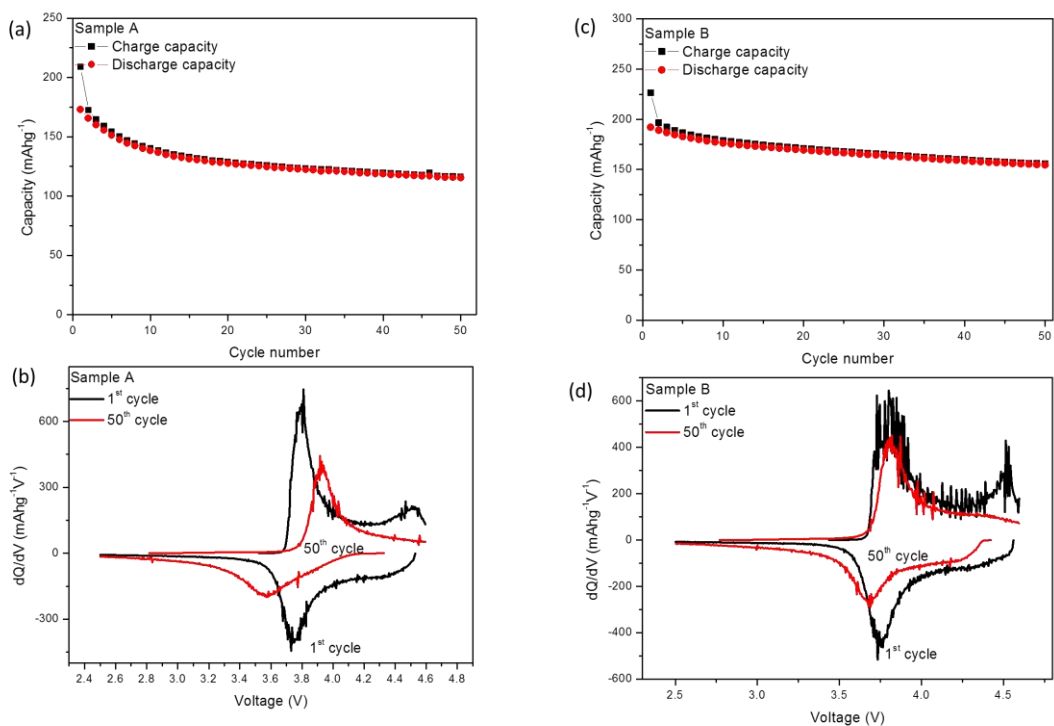
Figure S3 Electrochemical performance of Sample A and Sample B with 4.6 *V* cut-off voltage and 20 mA/g current density: (a) and (b), cycle life and dQ/dV curves of Sample A; (c) and (d), cycle life and dQ/dV curves of Sample B.   The discharge capacity of the 1st cycle for Sample A and Sample B are 173 mAh/g and 191 mAh/g, respectively.   The cycle life of Sample A and Sample B after 50 times charge and discharge processes are 66% and 81%, respectively.
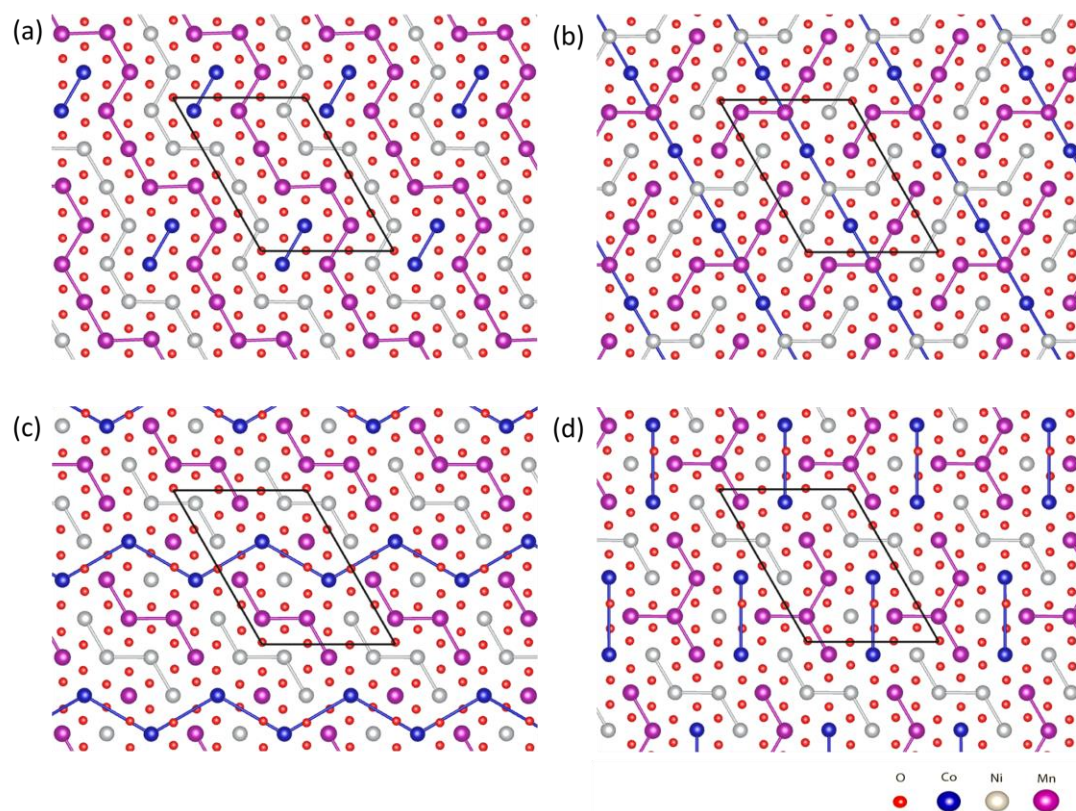
Figure S4 Different models for the cation ordering of transitional metal layer adopted in the calculation: (a) Co ions ordering with ordering parameter of 1; (b) Co ions ordering with ordering parameter of 2; (c) Co ions ordering with ordering parameter of $\sqrt{3}$; (d) Co ions ordering with the same ordering parameter of $\sqrt{3}$ as (c), but different pattern.
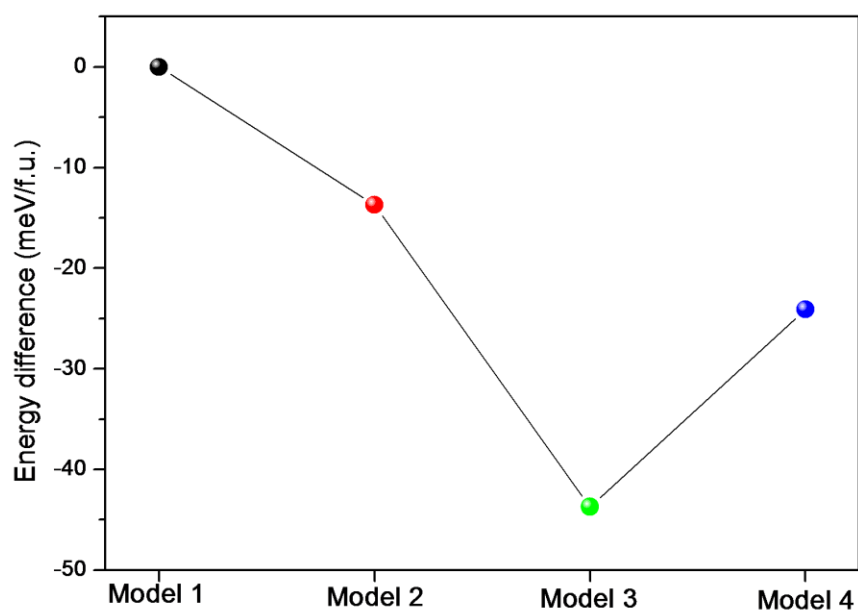
Figure S5 The calculated total energy per formula unit based on the different cation ordering in Figure S3a, b, c and d (0meV, -13.7meV, -43.7meV and -24.1meV per formula unit (f.u.)).

Table S1 Rietveld refinement atomic coordinates for Sample A prepared by the solid-state reaction method based on the X-ray powder diffraction data.

Atom	Wyck position	x	y	z	Biso*	Occupancy
Mn	3a	0.000	0.000	0.000	0.11	0.42
Co	3a	0.000	0.000	0.000	0.11	0.16
Ni	3a	0.000	0.000	0.000	0.11	0.357(4)
Li	3a	0.000	0.000	0.000	0.11	0.062(4)
Ni	3b	0.000	0.000	0.500	0.14	0.062(4)
Li	3b	0.000	0.000	0.500	0.14	0.947(4)
O	6c	0.000	0.000	0.2582(1)	0.33	1.0

* Fixed

Table S2 Rietveld refinement atomic coordinates for Sample B prepared by the co-precipitation method based on the X-ray powder diffraction data.

Atom	Wyck position	x	y	z	Biso*	Occupancy
Mn	3a	0.000	0.000	0.000	0.11	0.45
Co	3a	0.000	0.000	0.000	0.11	0.15
Ni	3a	0.000	0.000	0.000	0.11	0.352(3)
Li	3a	0.000	0.000	0.000	0.11	0.037(3)
Ni	3b	0.000	0.000	0.500	0.14	0.037(3)
Li	3b	0.000	0.000	0.500	0.14	1.082(3)
O	6c	0.000	0.000	0.2599(1)	0.33	1.0

* Fixed