

Supporting Information

Revealing the correlation between structural evolution and Li⁺ diffusion kinetics of Nickel-rich cathode materials in Li- ion batteries

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Table S1. The ratio of TM in NCM811 measured by ICP-OES

Sample	Measured Atomic Ratio		
	Ni	Co	Mn
NCM811	0.8	0.102	0.104

Table S2. Cell parameter of NCM811 and the deviation

	<i>a</i> (Å)	<i>c</i> (Å)	<i>V</i> (Å ³)	Li/Ni mixing	R _{wp}
NCM811	2.8724(9)	14.2001(2)	101.470(1)	1.53%	2.92%

Table S3. Specific capacity and CE of the first three cycles under different rates. 1 C=
200 mA·g⁻¹

(CC= Charge Capacity, DC= Discharge Capacity, CE= Coulombic Efficiency)

		0.05C	0.1C	0.5C	1C	5C	10C
1st	CC (mAh·g ⁻¹)	257	254	247	243	233	227
	DC (mAh·g ⁻¹)	230	226	213	208	190	177
	CE (%)	89.5	88.8	86.3	85.5	81.4	77.8
2nd	CC (mAh·g ⁻¹)	231	225	213	2208	188	179
	DC (mAh·g ⁻¹)	224	220	209	206	185	177
	CE (%)	97.2	98.0	97.9	98.7	98.5	99

	CC (mAh·g ⁻¹)	225	220	208	206	185	178
3rd	DC (mAh·g ⁻¹)	220	216	204	203	182	175
	CE (%)	97.5	98.4	98.3	98.9	98.6	98.1

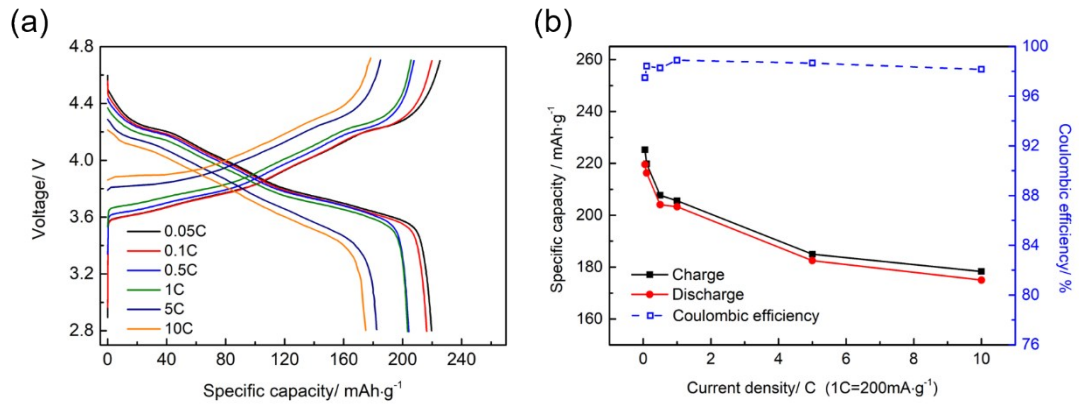


Figure S1. The third (a) Charge-discharge curves, and (b) corresponding capacity and CE at different rates.

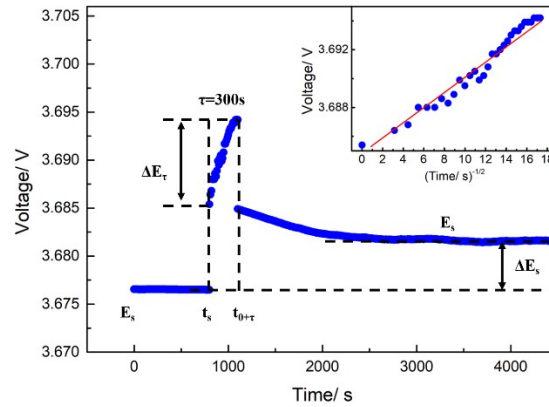


Figure S2. GITT schematic of single pulse. The embedded thumbnail is the relation curve between E and $\tau^{1/2}$.

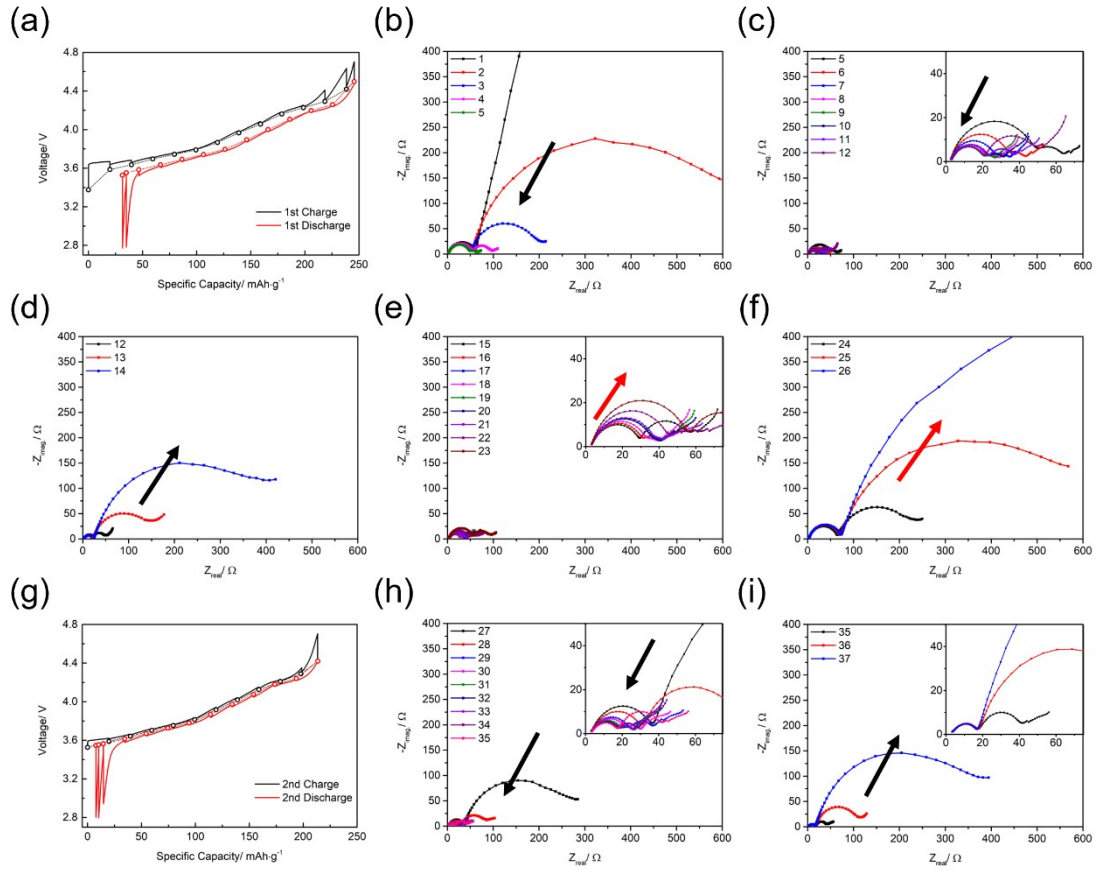


Figure S3. Nyquist diagram of charge/discharge process of NCM811, divided by the characteristic of the curves, C represents Charge, D represents discharge. (b)1C-I, (c) 1C-II, (d) 1C-III, (e) 1D-I and 1D-II, (f) 1D-III, (h) 2C-I and 2C-II, (i) 2C-III. The inserted picture is magnified image of the medium-frequency. The arrow represents the variation trend of the Nyquist semicircle; (a) and (g) are the electrochemical curves of the first two cycles. The hollow circles are collected points.

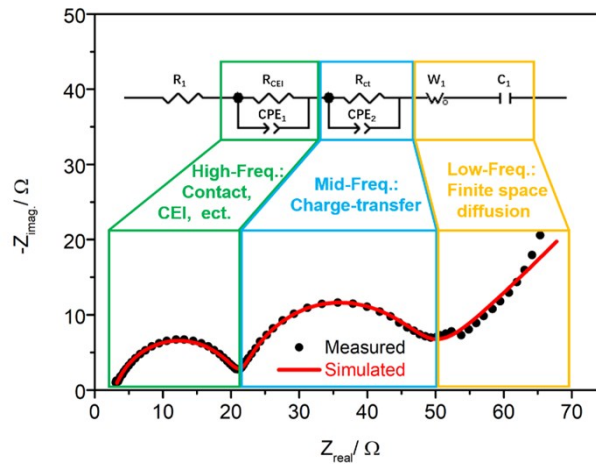


Figure S4. EIS result and the corresponding equivalent circuit.

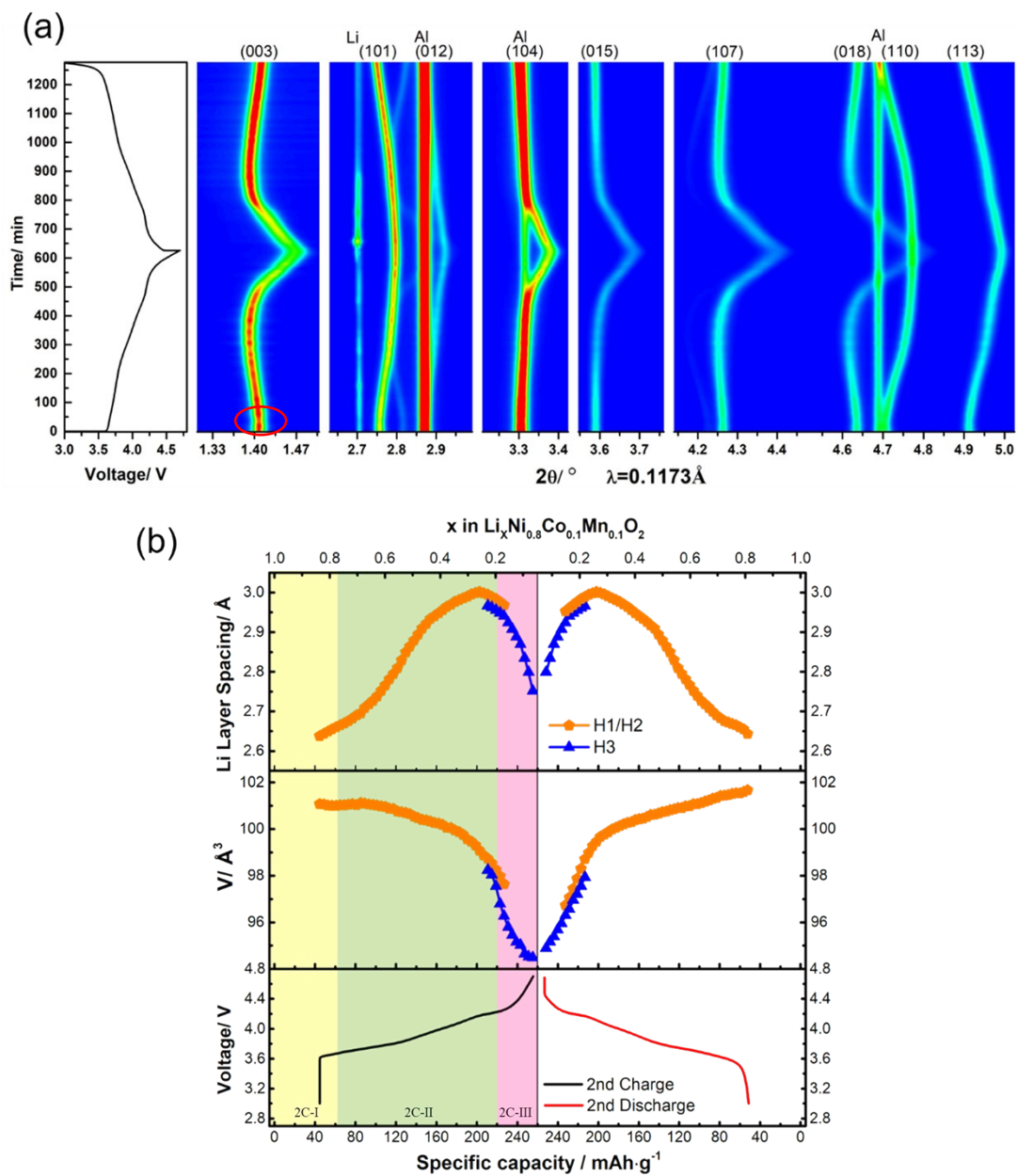


Figure S5. (a) In operando synchrotron XRD Contour plot and (b) thickness of the lithium layer and unit cell volume V obtained by Rietveld refinement for the second cycle of NCM811.

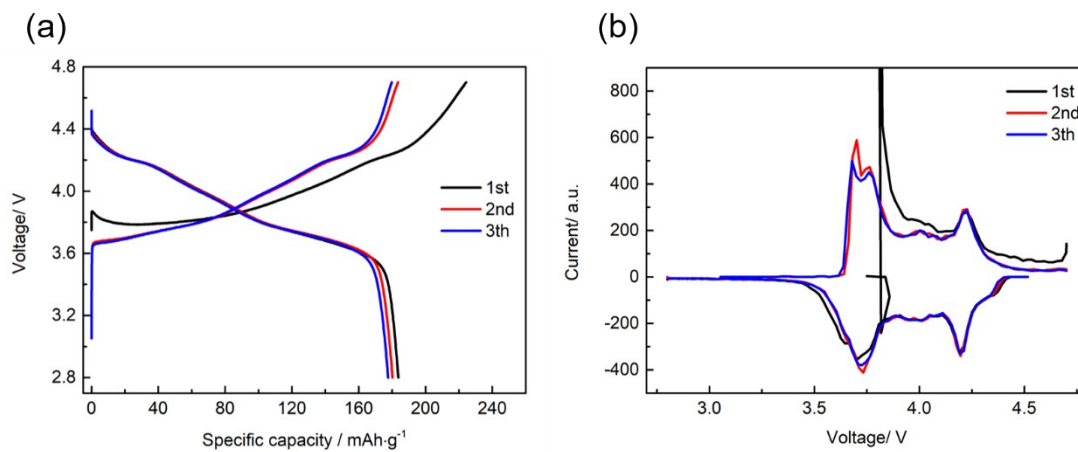


Figure S6. (a) Charge-discharge curves and (b) corresponding dQ/dV curves of NCM811 during the first three cycles at 0°C.