Supporting Information

Twin Boundary Induced by High Temperature Shock Boosts Li-rich Layered-oxide Structural Stability

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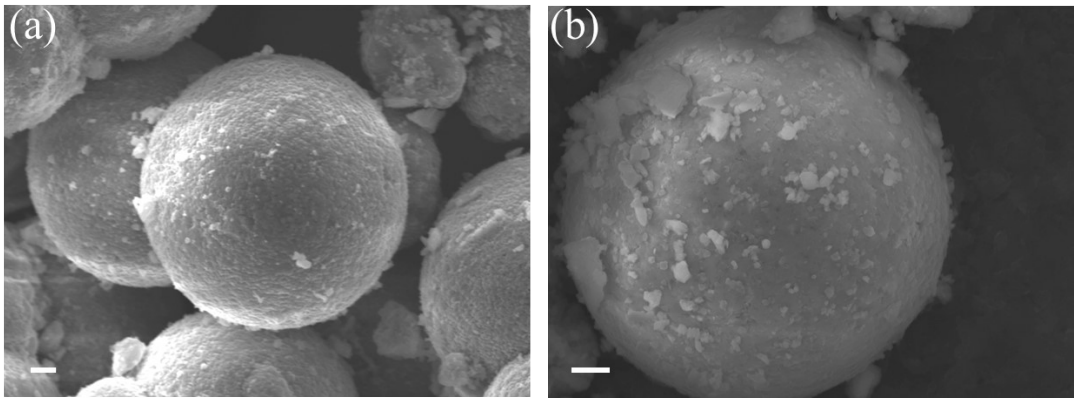

Figure S1. SEM images. a) LRO-TB. b) LRO, scale bar, 1 μm.

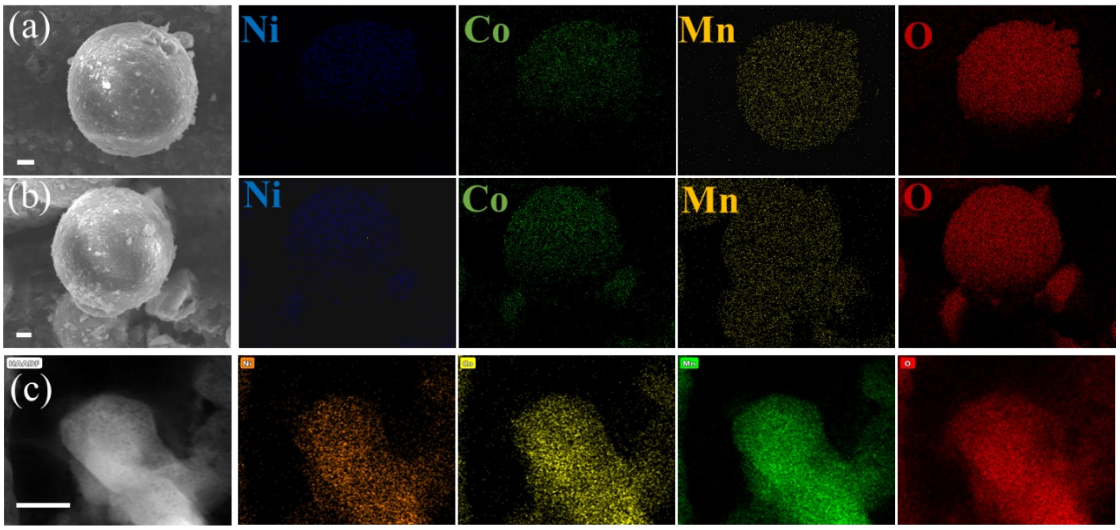

Figure S2. Elemental mappings. a) LRO-TB. b) LRO, scale bar, 1 μm. c) primary particle of LRO-TB after FIB, scale bar, 50 nm.

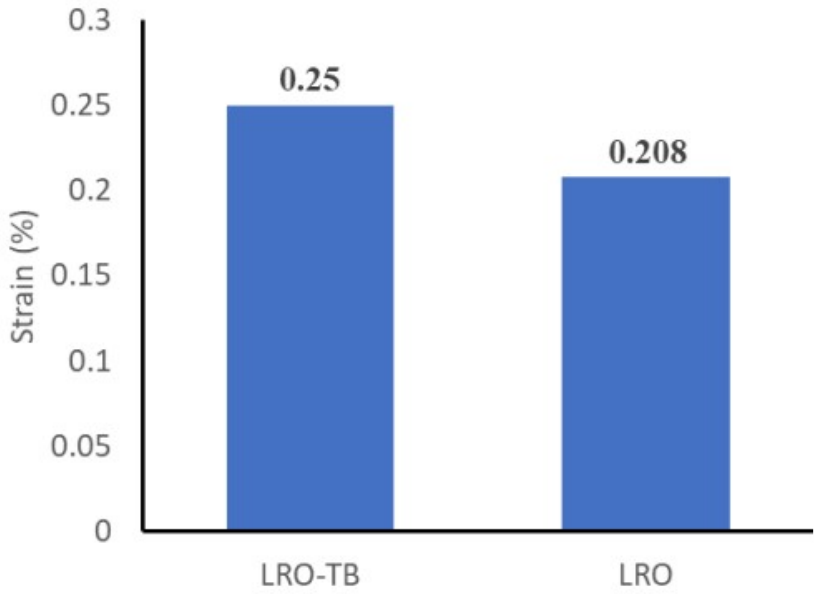

Figure S3. Strains exhibited in forms of histograms of LRO-TB and LRO.

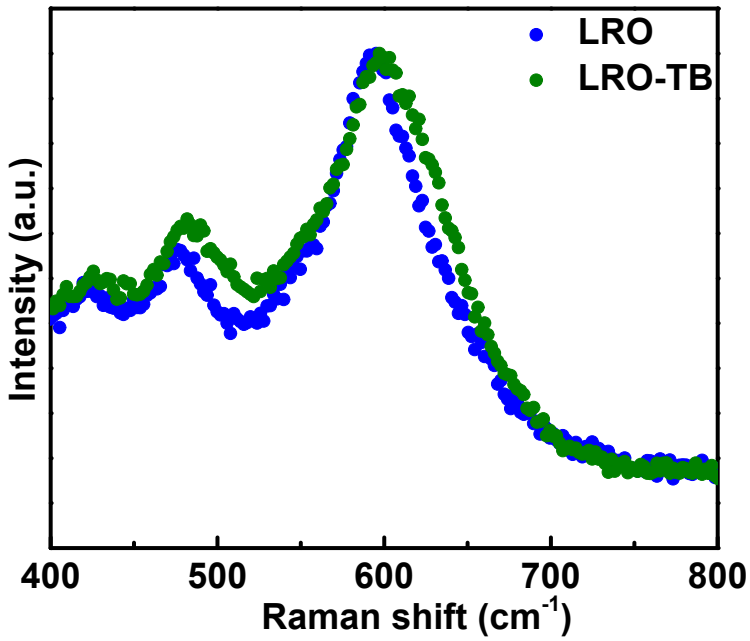

Figure S4. Raman spectrum of LRO-TB and LRO.

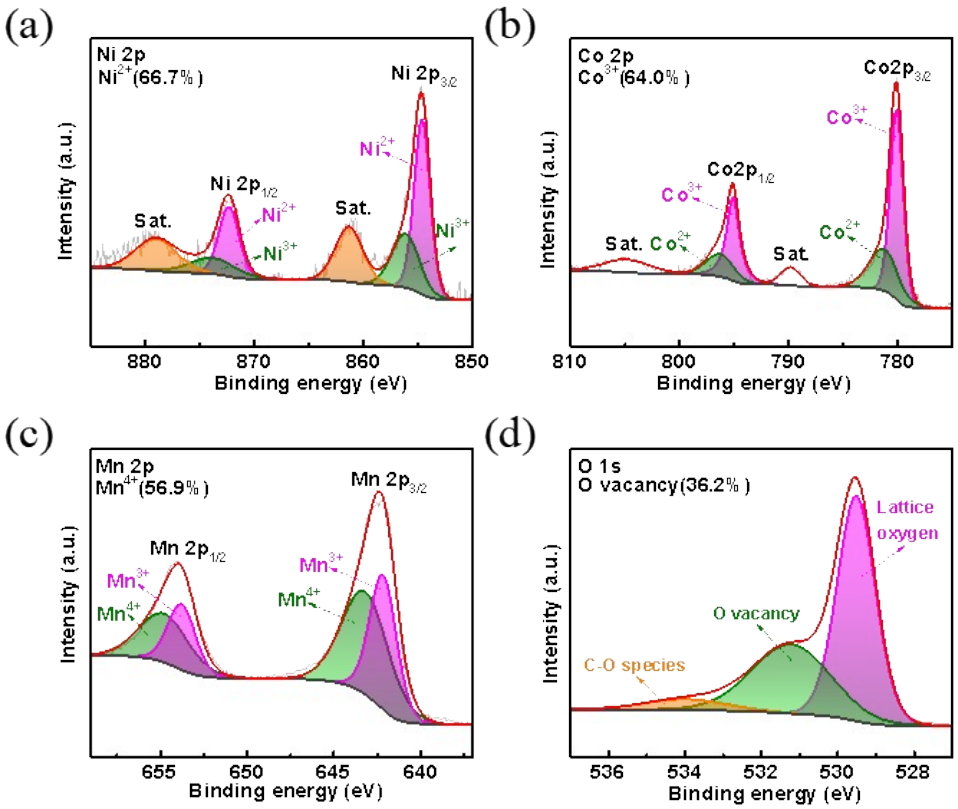

Figure S5. XPS spectra of Ni 2p, Co 2p, Mn 2p and O 1s of LRO.

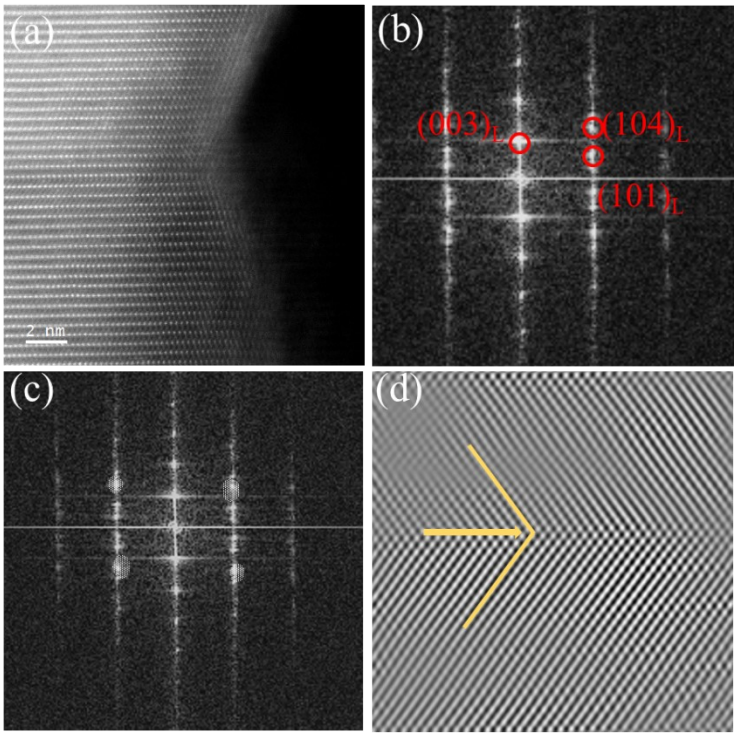

Figure S6. Structural characterizations of LRO-TB. a) HAADF STEM. b-c) FFT patterns. d) IFFT pattern corresponding to the two groups of white points in c).

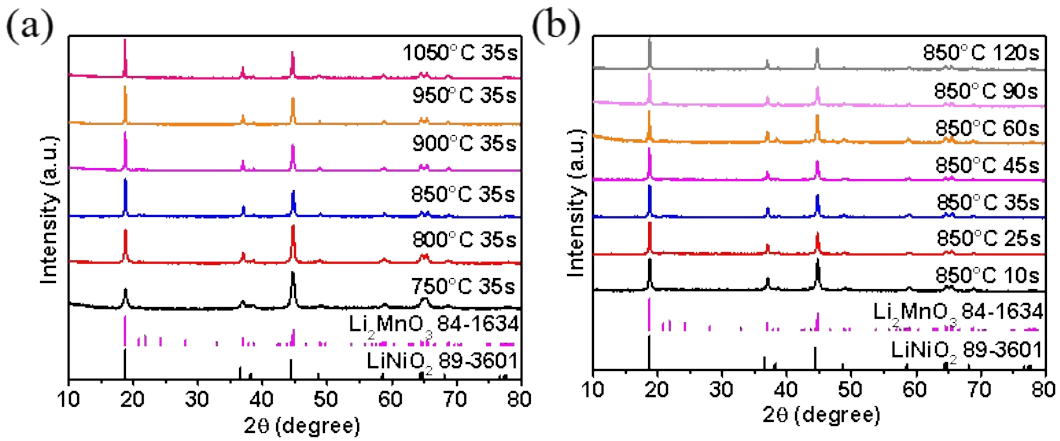

Figure S7. XRD patterns of samples obtained by changing calcination temperature and time using HTS. a) Calcination at different temperatures for 35 s. b) Calcination for different times at 850°C.

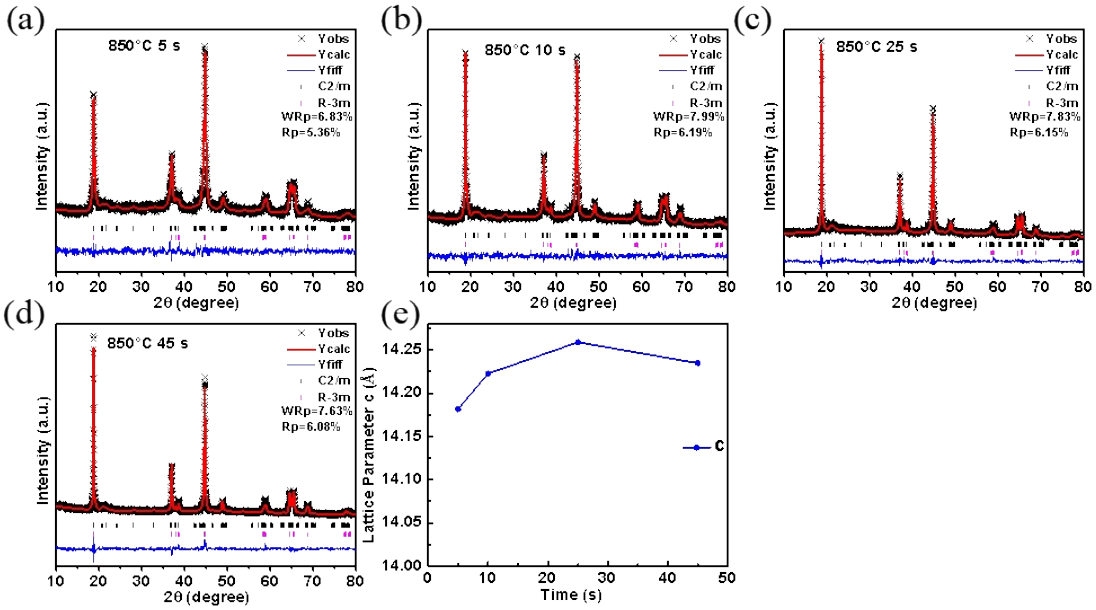

Figure S8. XRD refinement patterns calcinated for different times at 850°C. a) 5 s. b) 10 s. c) 25 s. d) 45 s. e) Chang curve of lattice parameters with calcination time.

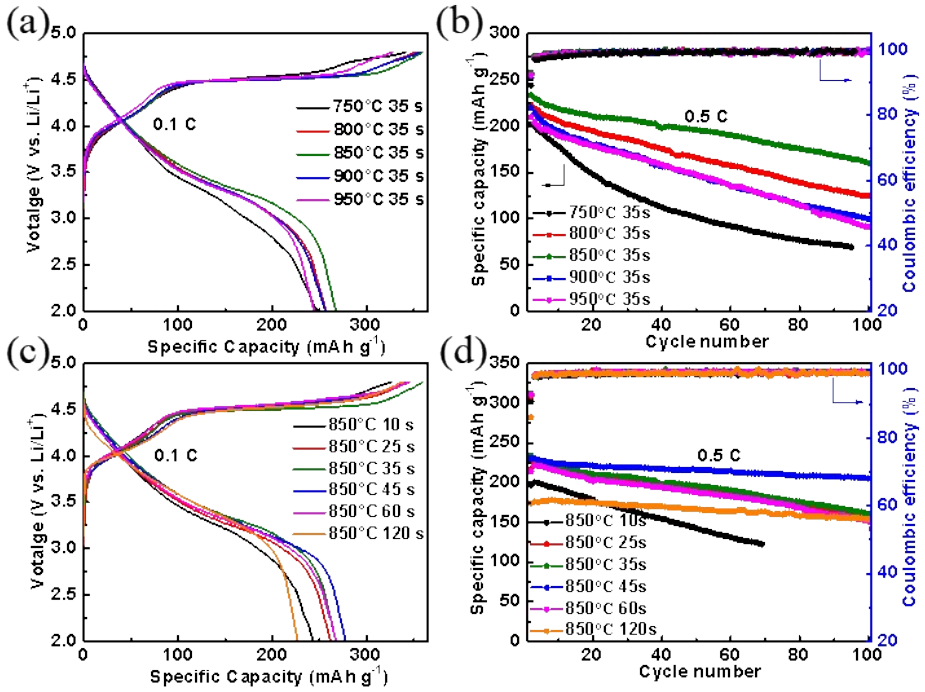

Figure S9. Electrochemical performances of HTS samples. a) Initial charge-discharge profiles of samples calcinated at different temperatures for 35 s at 0.1 C. b) Cycling performance of samples calcinated at different temperatures for 35 s at 0.5 C. c) Initial charge-discharge profiles of samples calcinated at 850 °C for different times at 0.1 C. d) Cycling performance of samples calcinated at 850 °C for different times at 0.5 C.

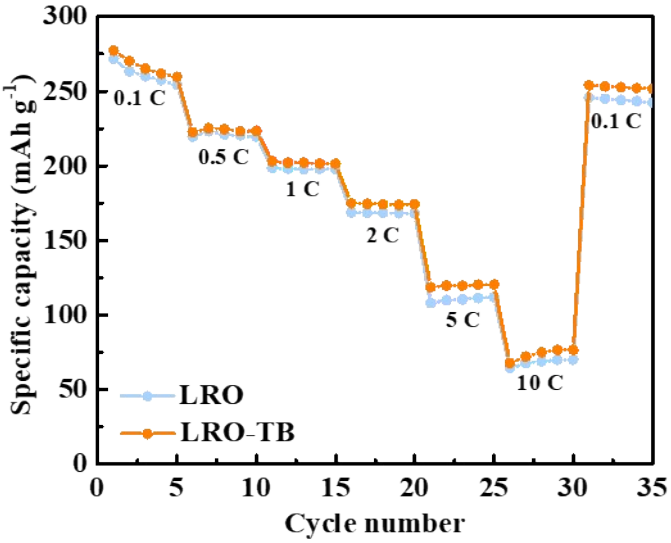

Figure S10. Rate capability of LRO-TB and LRO

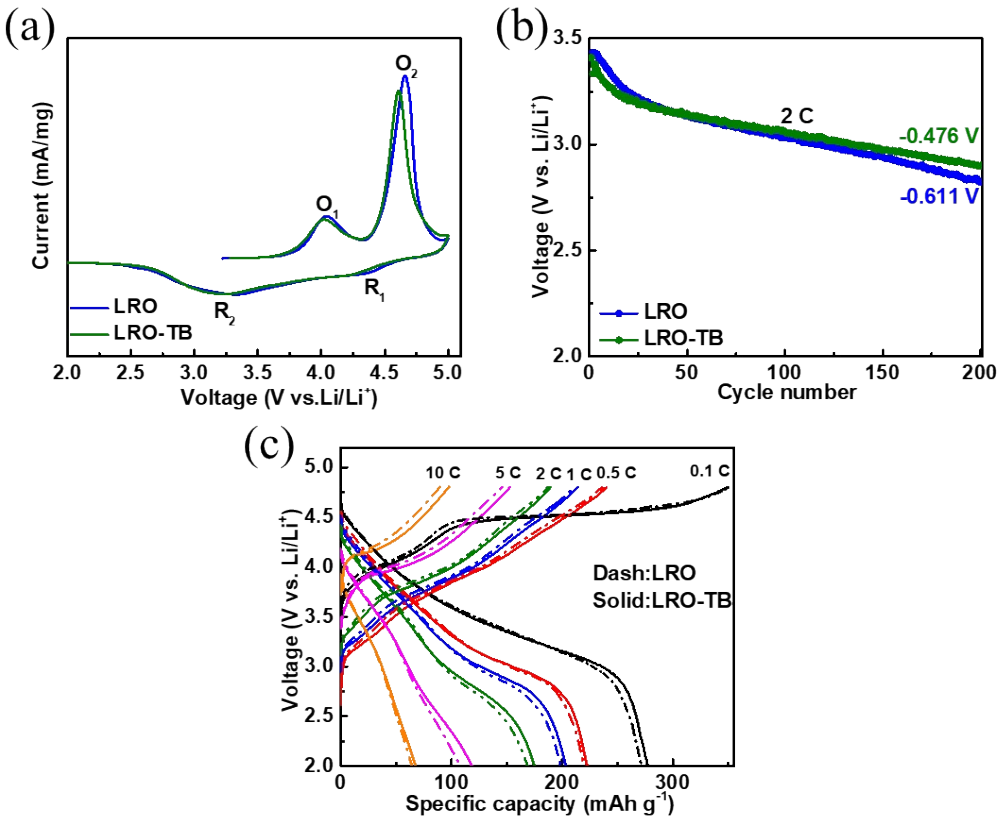

Figure S11. Electrochemical performances. a) Initial CV profiles obtained at 0.1 mV s-1. b) Voltage decay curves at 2 C. c) The corrospending charge-discharge profiles at different rates from 0.1 C to 10 C.

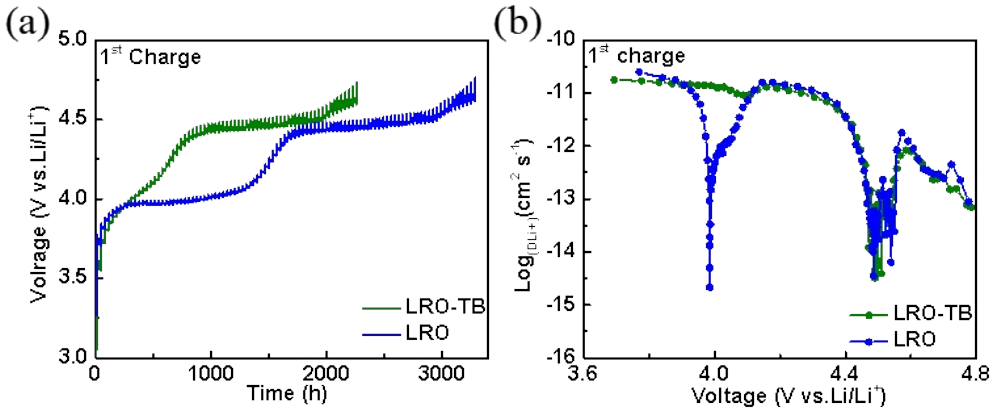

Figure S12. Li ion diffusion kinetics of LRO-TB and LRO. a) GITT curves of first charging process. b) Li-ion diffusion coefficient.

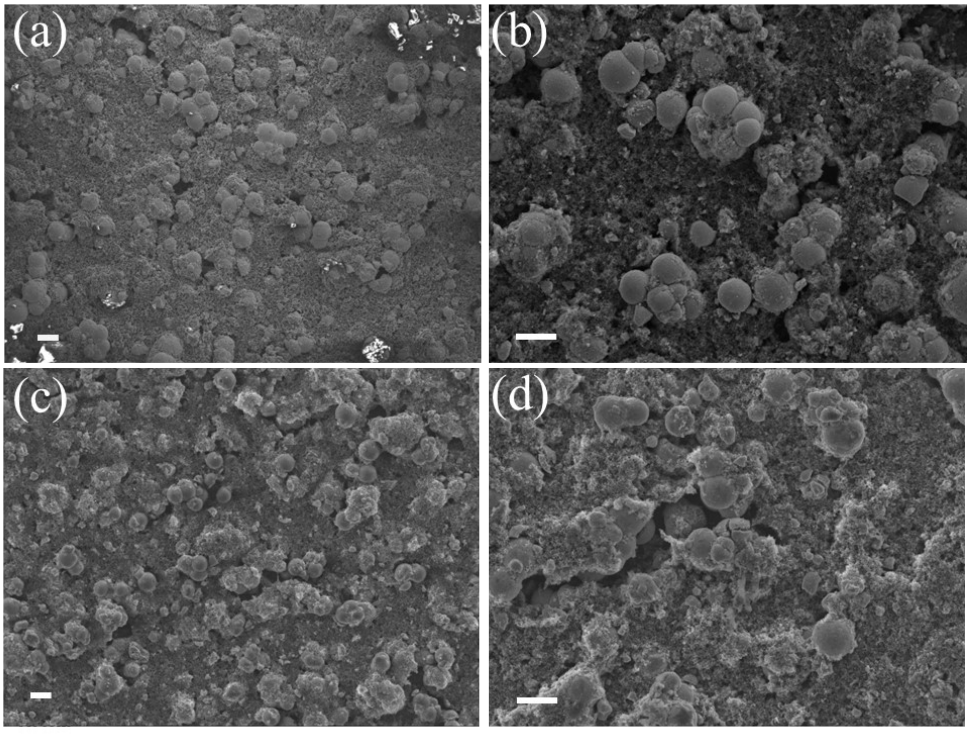

Figure S13. SEM images. Before cycling a) LRO-TB, c) LRO, scale bar, 10 μm. After 100 cycles at 0.5 C b) LRO-TB, d) LRO, scale bar, 10 μm.

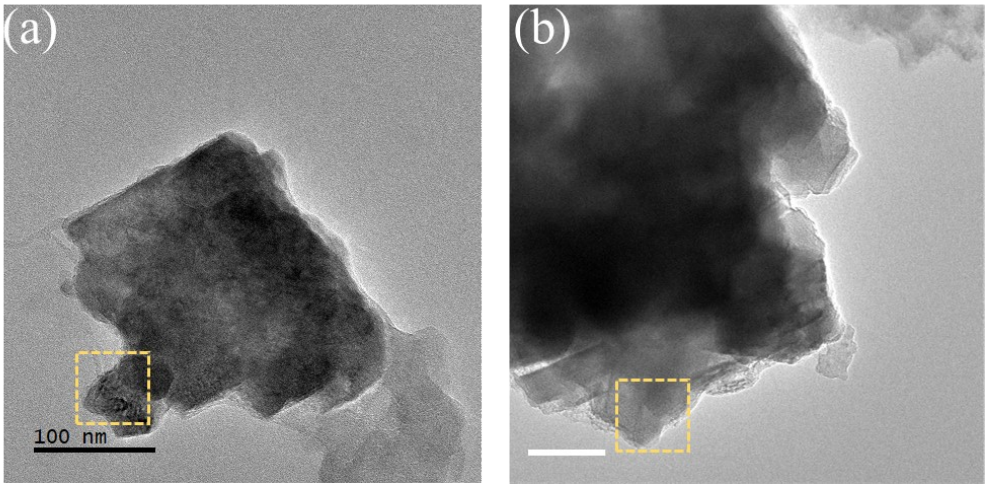

Figure S14. Ex-situ TEM imagines after 200 cycles at 2 C. a) LRO-TB. b) LRO, scale bar, 100 nm.

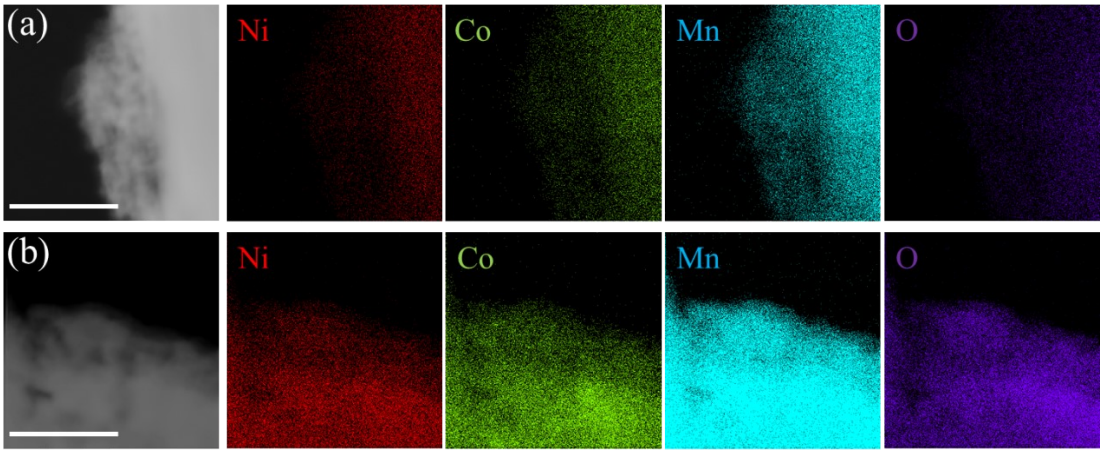

Figure S15. Elemental mapping after 200 cycles at 2 C. a) LRO-TB. b) LRO, scale bar, 500 nm.

Table S1. Crystal structure parameters obtained by XRD refinement.

Material	$I_{(003)}/I_{(104)}$	R-3m				Li^+/Ni^{2+} (%)
		a (Å)	c (Å)	c/a	V (Å^3)	
LRO-TB	1.297	2.8525(0)	14.2346(0)	4.990	100.307	1.89
LRO	1.346	2.8490(8)	14.2202(2)	4.991	99.965	0.88

Table S2. Rietveld Refinement Results of atoms occupancy of LRO-TB.

	Atom	Site	x	y	z	Occ
R-3m	Mn	4g	0.0000	0.1665	0.0000	1.0000
	Li1	2b	0.0000	0.5000	0.0000	1.0000
	Li2	2c	0.0000	0.0000	0.5000	1.0000
	Li3	4h	0.0000	0.7361	0.5000	1.0000
	O1	4i	0.2275	0.0000	0.2154	1.0000
	O2	8j	0.2157	0.3224	0.2162	1.0000
C/2m	O	6c	0.0000	0.0000	0.2572	1.0000
	Li1	3a	0.0000	0.0000	0.0000	0.9811
	Li2	3b	0.0000	0.0000	0.5000	0.0189
	Ni1	3b	0.0000	0.0000	0.5000	0.9811
	Ni2	3a	0.0000	0.0000	0.0000	0.0189

Table S3. Rietveld Refinement Results of atoms occupancy of LRO.

	Atom	Site	x	y	z	Occ
R-3m	Mn	4g	0.0000	0.1618	0.0000	1.0000
	Li1	2b	0.0000	0.5000	0.0000	1.0000
	Li2	2c	0.0000	0.0000	0.5000	1.0000
	Li3	4h	0.0000	0.7385	0.5000	1.0000
	O1	4i	0.2071	0.0000	0.2113	1.0000
	O2	8j	0.2327	0.3174	0.1971	1.0000
C/2m	O	6c	0.0000	0.0000	0.2552	1.0000
	Li1	3a	0.0000	0.0000	0.0000	0.9912
	Li2	3b	0.0000	0.0000	0.5000	0.0088
	Ni1	3b	0.0000	0.0000	0.5000	0.9912
	Ni2	3a	0.0000	0.0000	0.0000	0.0088

Table S4. Crystal parameters obtained by Rietveld refinement of HTS materials.

Time (s)	Content (%)		R-3m				Li^+/Ni^{2+} (%)
			a (Å)	c (Å)	c/a	V (Å^3)	
	C/2m	R-3m					
5	64.8	35.2	2.8465(0)	14.1815(0)	4.991	99.965	4.89
10	59.4	40.6	2.8483(5)	14.2225(1)	4.993	99.930	3.45
25	57.6	42.4	2.8542(7)	14.2589(3)	4.996	100.602	2.53
45	52.2	47.8	2.8525(0)	14.2346(0)	4.990	100.307	1.89