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## Supplementary Materials for

## High-Ni Cathode Material improved by Zr for Stable Cycling of Li-Ion Rechargeable Batteries

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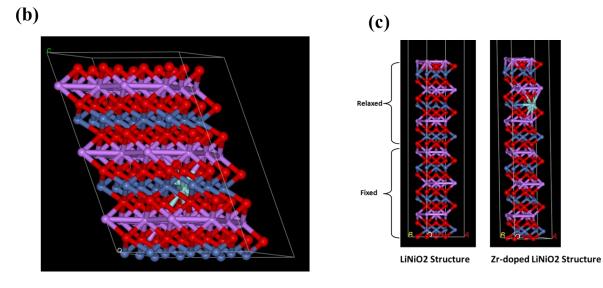
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Sample	a (Å)	c (Å)	Intensity ratio (003)/(104)
Pristine NCM	2.8729	14.1976	1.50
S-NCM	2.8735	14.2028	1.62
L-NCM	2.8745	14.2079	1.63

## Table S1.

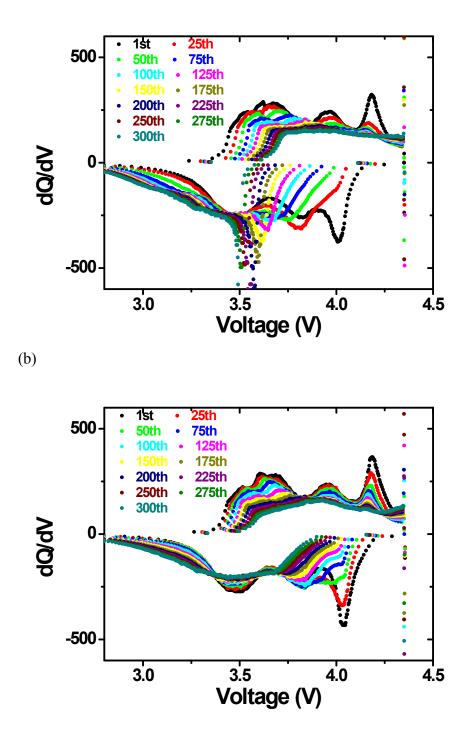
Lattice parameters of pristine NCM, Zr solid NCM, and Zr solution NCM.

<b>(a)</b>		
	2nd phase@ Bulk	
	2nd phase@ Bulk $Li_{36}Ni_{36-x}Zr_xO_{72} + x\left(Li + \frac{1}{2}O_2\right) \leftrightarrow (36-x)LiNiO_2 + xLi_2ZrO_3$	$\Delta H_1$
	$Li_{36}Ni_{36-x}Zr_{x}O_{72} + x\left(2Li + \frac{3}{4}O_{2}\right) \leftrightarrow (36-x)LiNiO_{2} + \frac{x}{2}Li_{6}Zr_{2}O_{7}$	$\Delta H_2$
	2nd phase@ surface	
	$(Li_{24}Ni_{23}ZrO_{48}) + LiNiO_2 + Li + \frac{1}{2}O_2 \leftrightarrow (Li_{24}Ni_{24}O_{48}) + Li_2ZrO_3$	$\Delta H_1$
	$(Li_{24}Ni_{23}ZrO_{48}) + LiNiO_2 + 2Li + \frac{3}{4}O_2 \leftrightarrow (Li_{24}Ni_{24}O_{48}) + \frac{1}{2}Li_6Zr_2O_7$	$\Delta H_2$

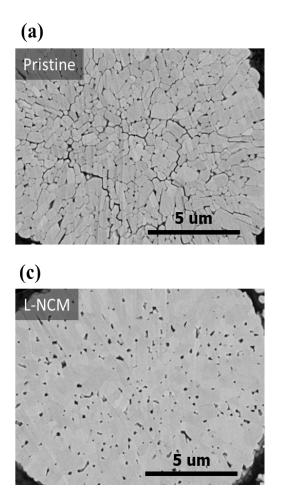


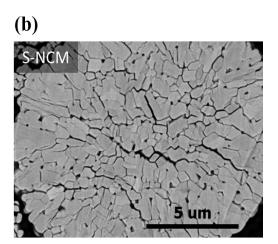


(a) Reactions of the bulk and surface(b) Atomic model of LiNiO<sub>2</sub> slabs from the surface to the bulk



**Fig. S2**. dQ/dV at intervals of 25 cycles for (a) S-NCM (b) L-NCM





## Fig. S3.

Cross-sectional SEM images of the powder after the 1<sup>st</sup> cycle for (a) pristine NCM (b) S-NCM and (c) L-NCM.