

Supplementary Information

## **The emergence of a robust lithium gallium oxide surface layer on gallium-doped LiNiO<sub>2</sub> cathodes enables extended cycling stability**

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## Literature survey of doped LiNiO<sub>2</sub> cycling

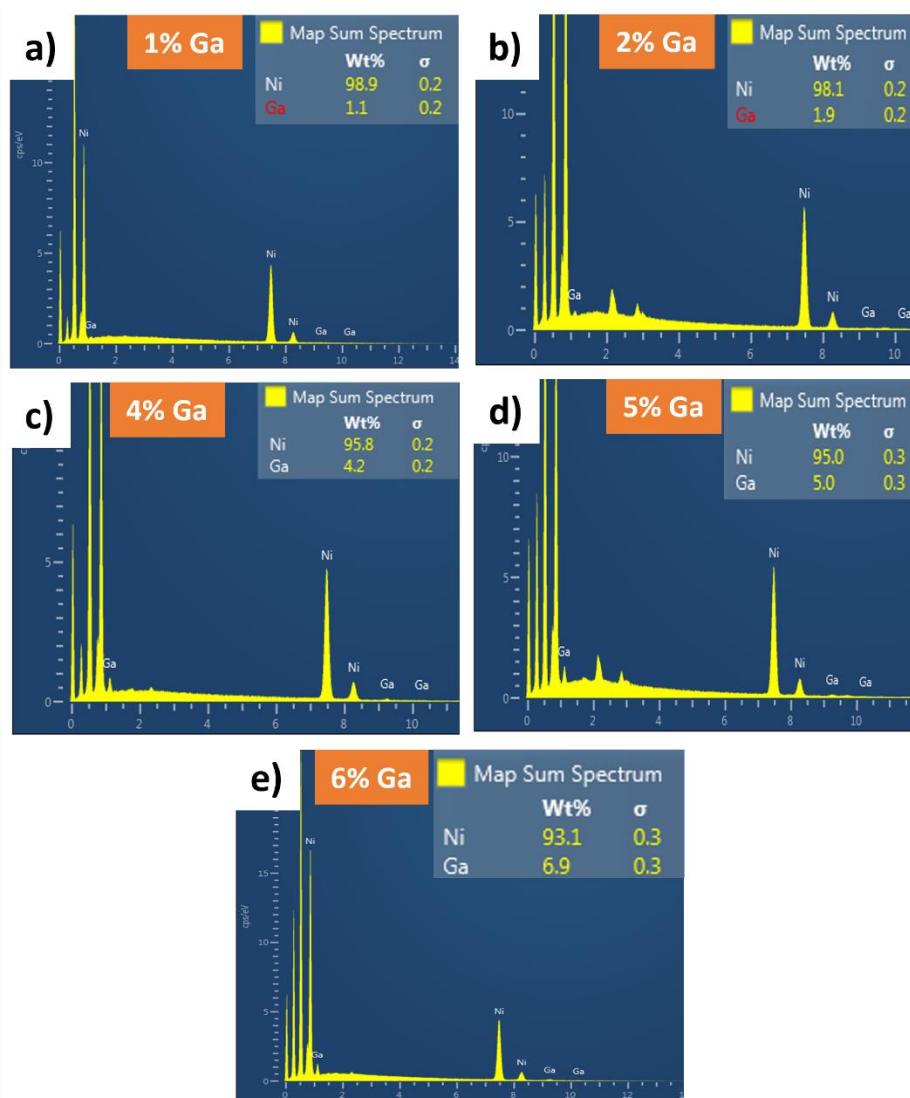
**Table S1.** Data table used for obtaining Fig.1 in the manuscript.

S.No.	Cathodes	% retention   Cycle No.	Discharge Capacity (mAh·g <sup>-1</sup> )	C-rate/Current density	Ref.
1	LiNiO <sub>2</sub>	83 50	247.5	C/10 1C = 180 mA·g <sup>-1</sup>	1
	1%W-LiNiO <sub>2</sub>	95 50	242.7		
	1.5%W-LiNiO <sub>2</sub>	96 50	236.1		
	2%W-LiNiO <sub>2</sub>	97 50	225.9		
2	LiNiO <sub>2</sub>	79 50	216	C/10 1C = 200 mA·g <sup>-1</sup>	2
	0.2%Cu-LiNiO <sub>2</sub>	90 50	218		
3	LiNiO <sub>2</sub>	85 50	250	C/10 1C = 180 mA·g <sup>-1</sup>	3
	1.4%Zr-LiNiO <sub>2</sub>	95 50	232.6		
4	LiNiO <sub>2</sub>	57 50	203.76	C/10 1C = -	4
	1%Nb-LiNiO <sub>2</sub>	81 50	203.27		
	1.5%Nb-LiNiO <sub>2</sub>	85 50	221.20		
	2%Nb-LiNiO <sub>2</sub>	70 50	201.50		
5	LiNiO <sub>2</sub>	85 50	247.5	C/10 1C = 180 mA·g <sup>-1</sup>	5
	0.5% Zr-LiNiO <sub>2</sub>	92 50	246.5		
6	LiNiO <sub>2</sub>	88 50	232.97	C/10 1C = 180 mA·g <sup>-1</sup>	6
	Mg-LiNiO <sub>2</sub>	89 50	235.45		
	MgCu-LiNiO <sub>2</sub>	91 50	229.49		
7	LiNiO <sub>2</sub>	71 50	215.9	C/10 1C = 270 mA·g <sup>-1</sup>	7
	1%Nb-LiNiO <sub>2</sub>	92 50	188.1		
8	LiNiO <sub>2</sub>	77 50	161.8	C/10 1C = -	8
	LiNi <sub>0.975</sub> Ga <sub>0.025</sub> O <sub>2</sub>	45 50	174.4		
	LiNi <sub>0.975</sub> Al <sub>0.025</sub> O <sub>2</sub>	46 50	170.5		
	LiNi <sub>0.995</sub> Ti <sub>0.005</sub> O <sub>2</sub>	41 50	172.9		
	LiNi <sub>0.990</sub> Al <sub>0.005</sub> Ti <sub>0.005</sub> O <sub>2</sub>	47 50	196.3		
9	LiNiO <sub>2</sub>	20 50	200	C/10 1C = 180 mA·g <sup>-1</sup>	9
	ZrO <sub>2</sub> -LiNiO <sub>2</sub>	92 50	190		
10	LiNiO <sub>2</sub>	76 50	210.3	C/10 1C = 180 mA·g <sup>-1</sup>	10
	C <sub>6</sub> H <sub>6</sub> CoO <sub>4</sub> -LiNiO <sub>2</sub>	87 50	214.7		
11	LiNiO <sub>2</sub>	51 50	210	36 mA·g <sup>-1</sup>	11
	2% Ga-LiNiO <sub>2</sub>	100 50	190		
	0.5% Ga-LiNiO <sub>2</sub>	83 50	180		
12	LiNiO <sub>2</sub>	57 50	230	C/10 1C = 225 mA·g <sup>-1</sup>	12
	1%Ga-LiNiO <sub>2</sub>	60 50	225		
	2%Ga-LiNiO <sub>2</sub>	80 50	225		
	3%Ga-LiNiO <sub>2</sub>	80 50	220		
	4%Ga-LiNiO <sub>2</sub>	84 50	205		
	5%Ga-LiNiO <sub>2</sub>	83 50	190		
13	LiNiO <sub>2</sub>	88 50	209	C/10 1C = 200 mA·g <sup>-1</sup>	13
	2% Al-LiNiO <sub>2</sub>	89 50	221		
	4% Al-LiNiO <sub>2</sub>	88 50	185		
	6% Al-LiNiO <sub>2</sub>	85 50	181		
14	LiNiO <sub>2</sub>	52 50	240	C/10 1C = 200 mA·g <sup>-1</sup>	14
15	LiNiO <sub>2</sub>	66 50	235.9	C/10 1C = 200 mA·g <sup>-1</sup>	15
	3%Al-LiNiO <sub>2</sub>	85 50	220.2		
	5%Al-LiNiO <sub>2</sub>	97 50	209.9		
16	LiNiO <sub>2</sub>	67 50	160	C/3 0.4 mA·cm <sup>-2</sup>	16
	1%Al-LiNiO <sub>2</sub>	90 50	149		
	3%Al-LiNiO <sub>2</sub>	100 50	136		
17	0% Ga-LiNiO <sub>2</sub>	45 50	197	C/10 1C = 180 mA·g <sup>-1</sup>	<b>This Work</b>
	2% Ga-LiNiO <sub>2</sub>	50 50	192		
	5% Ga-LiNiO <sub>2</sub>	84 50	174		

**Table S2.** Variance of the capacity retention value obtained from publications shown in **Fig. 1** in introduction.

Dopants in LiNiO <sub>2</sub>	Variance ( $\sigma^2$ )	Standard deviation ( $\sigma$ )
Undoped	387	19.67
Gallium	283	16.82
Tungsten	5	2.24
Zirconium	76	8.72
Niobium	85	9.22
Aluminium	277	16.64

### Energy Dispersive X-Ray Spectroscopy (EDS) measurements and analyses

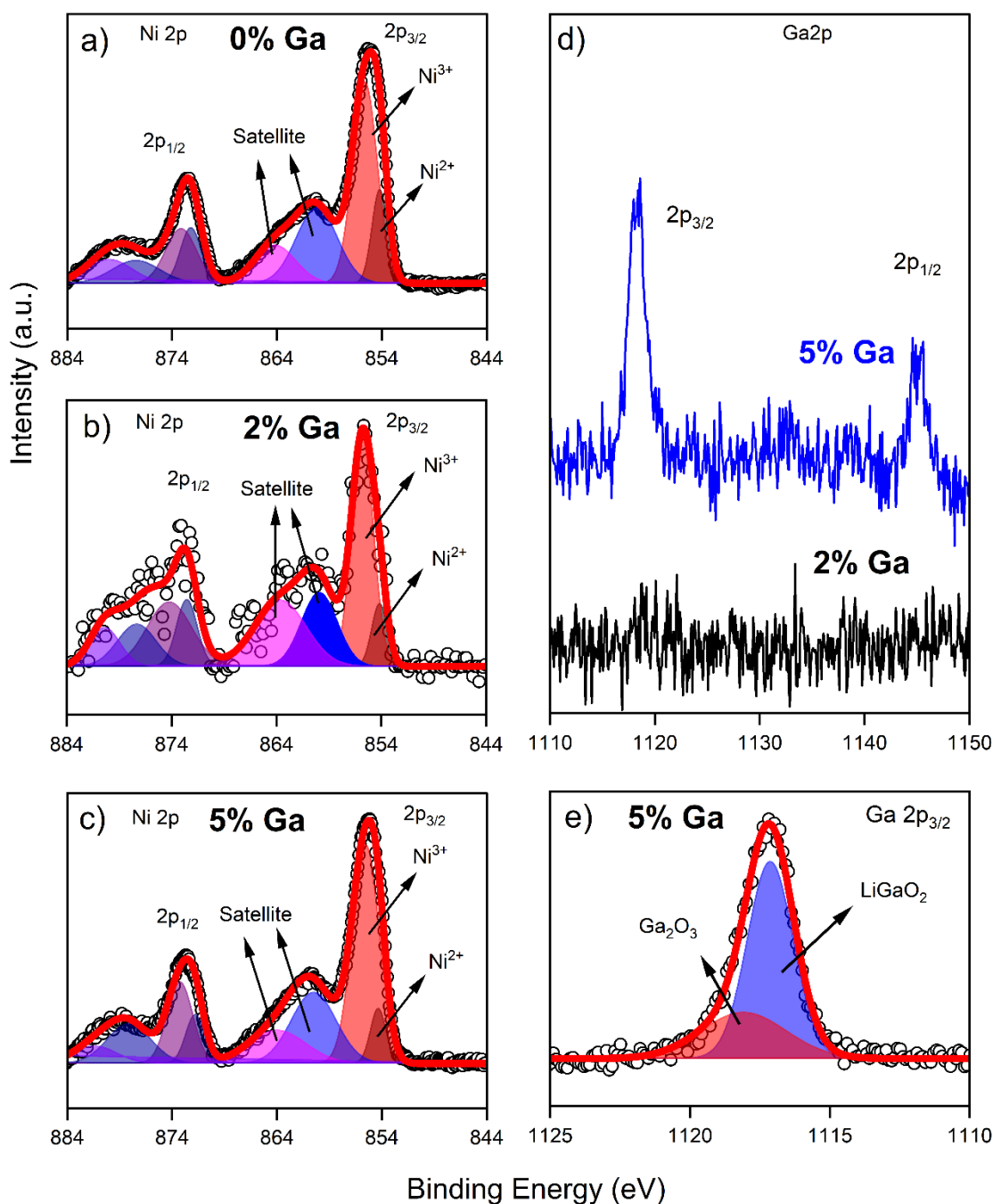


**Fig. S1.** (a-e) EDS spectrum of 0%-6% Ga-LiNiO<sub>2</sub> showing elemental composition obtained from one of the locations shown in **Table S3**.

**Table S3.** EDS data obtained from three distinct sites of 1% to 6% Ga-LiNiO<sub>2</sub>.

S.No.	Compounds	Wt(%) from EDS Ga : Ni	Mole(%) from EDS Ga : Ni	Targeted Mole (%) Ga : Ni
1	<b>1% Ga-LiNiO<sub>2</sub></b>			1 : 99
	Location 1	1.1 : 98.9	1.0 : 99.0	
	Location 2	1.3 : 98.7	1.1 : 98.9	
	Location 3	1.4 : 98.6	1.2 : 98.8	
	Average		1.1 : 98.9	
2	<b>2% Ga-LiNiO<sub>2</sub></b>			2 : 98
	Location 1	2.4 : 97.6	2.03 : 97.97	
	Location 2	2 : 98	1.69 : 98.31	
	Location 3	1.9 : 98.1	1.61 : 98.39	
	Average		1.77 : 98.23	
3	<b>4% Ga-LiNiO<sub>2</sub></b>			4 : 96
	Location 1	3.9 : 96.1	2.64 : 97.36	
	Location 2	4.2 : 95.8	3.60 : 96.40	
	Location 3	5 : 95	4.24 : 95.76	
	Average		3.50 : 96.50	
4	<b>5% Ga-LiNiO<sub>2</sub></b>			5 : 95
	Location 1	5.6 : 94.4	4.76 : 95.24	
	Location 2	5 : 95	4.24 : 95.76	
	Location 3	5.7 : 94.3	4.84 : 95.16	
	Average		4.61 : 95.39	
5	<b>6% Ga-LiNiO<sub>2</sub></b>			6 : 94
	Location 1	6.1 : 93.9	5.18 : 94.82	
	Location 2	6.9 : 93.1	5.80 : 94.20	
	Location 3	7.1 : 92.9	6.04 : 93.96	
	Average		5.67 : 94.33	

## X-ray Photoelectron Spectra (XPS) of 0%, 2%, and 5% Ga-LiNiO<sub>2</sub>



**Fig. S2.** Ni2p XPS of a) 0% Ga, b) 2% Ga, and c) 5% Ga-LiNiO<sub>2</sub>. d) Ga2p XPS of 2% and 5%Ga-LiNiO<sub>2</sub>. e) XPS spectra of Ga2p<sub>3/2</sub> of 5% Ga-LiNiO<sub>2</sub>.

XPS measurements were conducted on undoped and Ga-doped LiNiO<sub>2</sub> as shown in Fig. S2a-c. 2p orbital of Ni in 0%, 2%, and 5% Ga-LiNiO<sub>2</sub> yield a doublet (i.e., 2p<sub>3/2</sub> and 2p<sub>1/2</sub>) due to the spin-orbit coupling with the two possible states having different binding energies. Each energy state consists of Ni<sup>3+</sup> and Ni<sup>2+</sup> species along with their satellite peaks. The obtained XPS spectra were deconvoluted based on the previously reported XPS for nickel-rich oxide (NMC) cathodes.<sup>17,18</sup> The deconvoluted XPS spectra

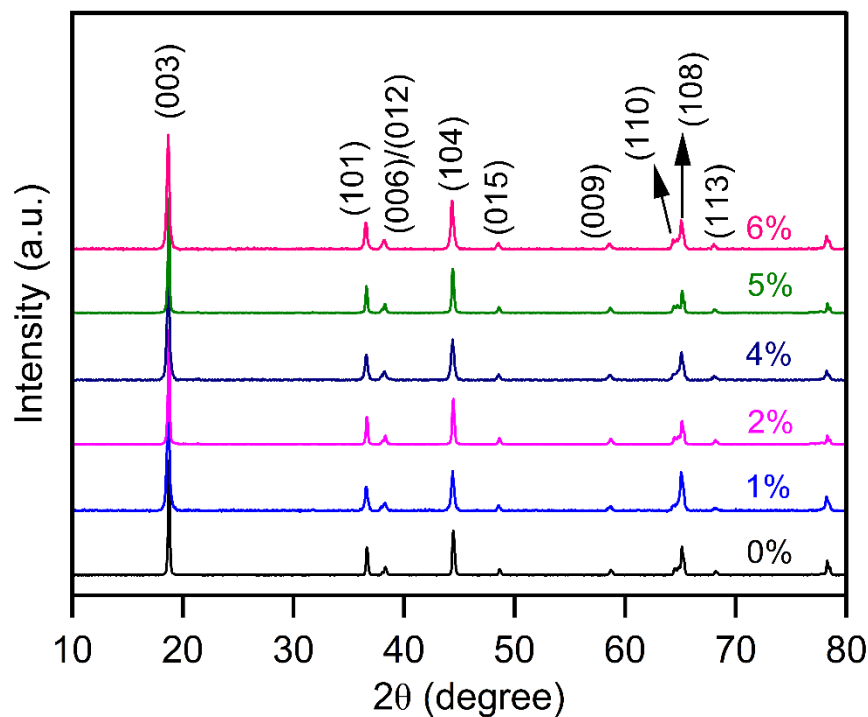
confirmed the presence of  $\text{Ni}^{3+}$  and  $\text{Ni}^{2+}$  in all three  $\text{LiNiO}_2$  cathodes and their peak positions and area are tabulated in **Table S4**. In agreement with the observations of Wu et al.<sup>19</sup> on  $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1-x}\text{Ga}_x\text{O}_2$ , a systematic increase in the  $\text{Ni}^{3+}/\text{Ni}^{2+}$  ratio upon higher Ga doping is found, pointing to decreasing cation mixing.

The Ga 2p XPS spectra shown in **Fig. S2d** were acquired to characterize the surface phases present on 2% and 5% Ga doped  $\text{LiNiO}_2$ . No Ga signals were observed on the surface of 2% Ga due to bulk doping, however, intense Ga 2p peaks were seen for 5% Ga. To confirm the emergence of the  $\text{LiGaO}_2$  phase on the surface of 5% Ga- $\text{LiNiO}_2$ , XPS spectra were deconvoluted and shown in **Fig. S2e**. Deconvolution of the XPS spectra revealed two discernible peaks centered at 1117.13 eV and 1118.09 eV, respectively. The predominant peak observed at a lower binding energy of 1117.13 eV is attributed to the  $\text{LiGaO}_2$  phase.<sup>20</sup> The minor peak appearing at a relatively higher binding energy of 1118.09 eV is associated with the  $\text{Ga}_2\text{O}_3$  phase.<sup>20,21</sup> This observation corroborates the dominance of the  $\text{LiGaO}_2$  phase as a prominent constituent at the surface of the 5% Ga- $\text{LiNiO}_2$  material, as confirmed by the XRD, EDS and HRTEM analysis.

**Table S4.** Peak position and area ratio from XPS spectra deconvolution of 0%, 2%, and 5% Ga- $\text{LiNiO}_2$ .

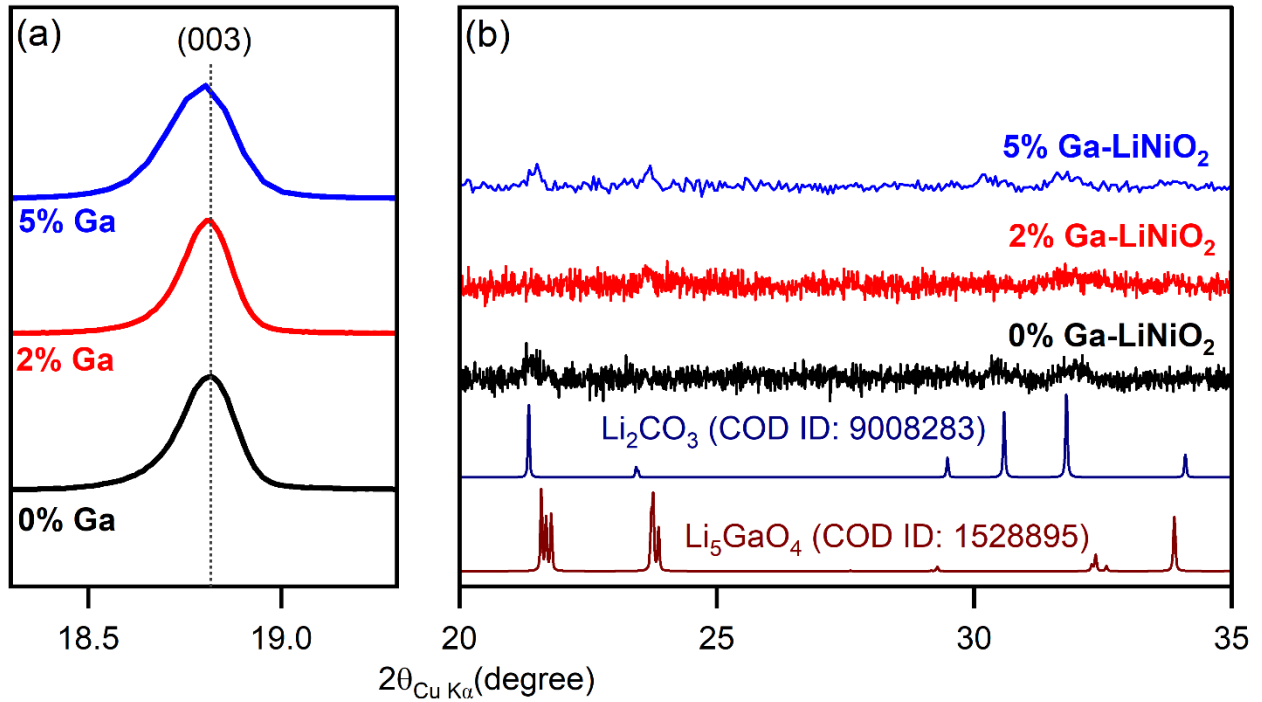
	$\text{Ni}^{2+}$		$\text{Ni}^{3+}$		Area Ratio ( $\text{Ni}^{3+}/\text{Ni}^{2+}$ )
	Peak Position (eV)	Area (%)	Peak Position (eV)	Area (%)	
0% Ga- $\text{LiNiO}_2$	854.20	22.80	855.61	77.20	3.38
2% Ga- $\text{LiNiO}_2$	854.17	19.36	855.79	80.64	4.16
5% Ga- $\text{LiNiO}_2$	854.35	12.57	855.54	87.43	6.95

### X-ray diffraction (XRD) patterns of as-synthesized 0%, 1%, 2%, 4%, 5% and 6% Ga doped $\text{LiNiO}_2$



**Fig. S3.** XRD pattern of 0%-6% Ga-doped  $\text{LiNiO}_2$  pristine powder electrodes.

**Close inspection of the X-ray diffraction (XRD) patterns of as-synthesized undoped and Ga doped LiNiO<sub>2</sub>**



**Fig. S4.** (a) Magnified XRD at the (003) plane peak of 0%, 2%, and 5% Ga-LiNiO<sub>2</sub> showing shift and broadening of the plane with increasing Ga content. (b) Magnification of the 20°-35° range for comparison against Li<sub>2</sub>CO<sub>3</sub> and Li<sub>5</sub>GaO<sub>4</sub> reference PDFs .

**Table S5.** 2θ and FWHM value of (003) reflection corresponding to 0%, 2%, and 5% Gallium doped LiNiO<sub>2</sub>.

	2θ of (003)	FWHM
0% Ga-LiNiO <sub>2</sub>	18.8060 ± 0.0016	0.16844 ± 0.00383
2% Ga-LiNiO <sub>2</sub>	18.8027 ± 0.0016	0.15270 ± 0.00359
5% Ga-LiNiO <sub>2</sub>	18.7888 ± 0.0043	0.20316 ± 0.01041

## Rietveld refinement analysis of 0%, 2% and 5% Ga-doped LiNiO<sub>2</sub>

In the structural model, we performed refinement on several key parameters, including the unit cell parameters, site occupancy, oxygen z-coordinate, and the isotropy  $U_{\text{iso}}$  parameters for oxygen (O), lithium (Li), gallium (Ga), and nickel (Ni) atoms. The following constraints were used:

- Similar  $U_{\text{iso}}$  parameters for atoms occupying the same Wyckoff site.
- The total occupancy of the 3a and 3b sites in a given  $R\bar{3}m$  phase adds to 1.
- The Ga content must be reasonably near the values targeted and measured by Energy dispersive X-ray spectroscopy (EDS).

It should be noted that Ga was investigated at several sites (i.e., 3a, 3a+3b, and 3b) and the best convergence was selected. At convergence, Ga appears to prefer the 3a sites within LiNiO<sub>2</sub>. Similar observations were made by Kitsche et al.<sup>12</sup> The possibility of Ga occupying Ni site has not been excluded, however.

Crystallographic coordinates corresponding to Wyckoff sites are as follows:

3a: (0, 0, 0), (1/3, 2/3, 2/3), (2/3, 1/3, 1/3)

3b: (0, 0, 1/2), (1/3, 2/3, 1/6), (2/3, 1/3, 5/6)

6c: (0, 0, ±z), (1/3, 2/3, 2/3±z), (2/3, 1/3, 1/3±z)



**Table S6.** Refined parameters of pristine LiNiO<sub>2</sub>.

<b>LiNiO<sub>2</sub></b>						
	x	y	z	Wyckoff site	Occupancy	U <sub>iso</sub>
Li	0.000	0.000	0.000	3a	0.964	0.07034
Ni	0.000	0.000	0.000	3a	0.036	0.07034
Li	0.000	0.000	0.500	3b	0.036	0.04030
Ni	0.000	0.000	0.500	3b	0.964	0.04030
O	0.000	0.000	0.242	6c	1	0.05273

R<sub>wp</sub> = 7.4%; R<sub>p</sub> = 5.32%; cation mixing = 3.6%

**Table S7.** Refined parameters of 2% Ga doped LiNiO<sub>2</sub>.

<b>2% Ga doped LiNiO<sub>2</sub></b>						
	x	y	z	Wyckoff site	Occupancy	U <sub>iso</sub>
Li	0.000	0.000	0.000	3a	0.983	0.00997
Ga	0.000	0.000	0.000	3a	0.017	0.00997
Ga	0.000	0.000	0.500	3b	0.001	0.01505
Ni	0.000	0.000	0.500	3b	0.999	0.01505
O	0.000	0.000	0.239	6c	1	0.01771

R<sub>wp</sub> = 7.12%; R<sub>p</sub> = 5.57%

**Table S8.** Refined parameters of 5% Ga doped LiNiO<sub>2</sub>.

<b>5% Ga doped LiNiO<sub>2</sub></b>						
<b>Phase 1: Ga-doped LiNiO<sub>2</sub></b>						
	x	y	z	Wyckoff site	Occupancy	U <sub>iso</sub>
Li	0.000	0.000	0.000	3a	0.984	0.03070
Ga	0.000	0.000	0.000	3a	0.016	0.03070
Ga	0.000	0.000	0.500	3b	0.004	0.03985
Ni	0.000	0.000	0.500	3b	0.989	0.03985
O	0.000	0.000	0.239	6c	1	0.04885
<b>Phase 2: LiGaO<sub>2</sub></b>						
Ga	0.000	0.000	0.500	3b	1	0.01689
Li	0.000	0.000	0.000	3a	1	0.04909
O	0.000	0.000	0.241	6c	1	0.21350

R<sub>wp</sub> = 8.47%; R<sub>p</sub> = 5.86%

## EDS line scan simulation assuming a core-shell particle configuration

The pseudocode for computing signal expectation based on a core-shell particle model is shown below. The beam penetration at position  $x$  in the Ga-rich and Ni-rich domains is a proxy for the signal strength from each element.

**Function** `EDS_signal_estimate( $R_o$ ,  $R_i$ ,  $NominalPenetration$ ,  $x$ )`:

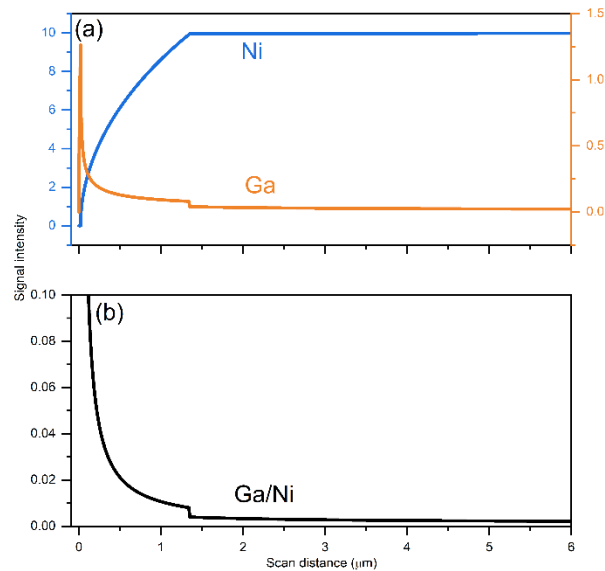
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# x is referenced from the particle center (0, 0)
if  $R_o < R_i$ : raise Exception

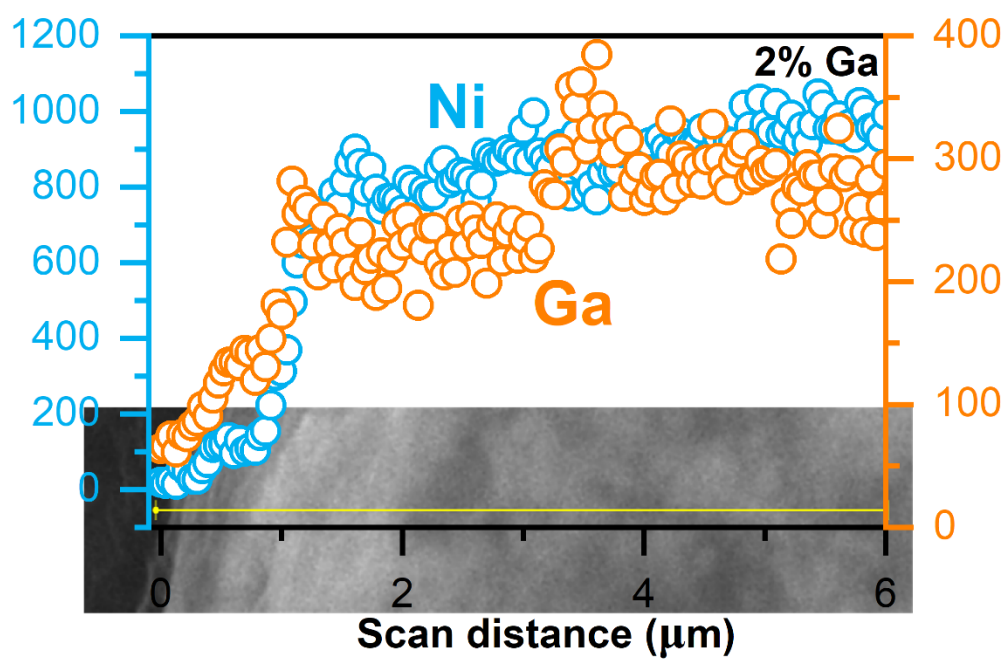
OuterSliceDepth =  $2 * (R_o^2 - x^2)^{1/2}$  if ( $R_o > |x|$ ) else 0
InnerSliceDepth =  $2 * (R_i^2 - x^2)^{1/2}$  if ( $R_i > |x|$ ) else 0
ProbeLength = min( $NominalPenetration$ ,  $OuterSliceDepth$ )
ShellLength = ( $OuterSliceDepth - InnerSliceDepth$ )/2
SurfaceToFarCoreLength =  $ShellLength + InnerSliceDepth$ 
# Signals calculation
if  $InnerSliceDepth \neq 0$ :
    if  $ProbeLength < SurfaceToFarCoreLength$ :
        Ga = min( $ProbeLength$ ,  $ShellLength$ )
        Ni = max[( $ProbeLength - Ga$ ), 0]
    else:
        Ga =  $ProbeLength - InnerSliceDepth$ 
        Ni =  $ProbeLength - Ga$ 
else:
    Ga =  $ProbeLength$ 
    Ni = 0

```

**Return** ( $Ga$ ,  $Ni$ )



**Fig. S5.** Simulation of EDS line scan signal intensity versus scan distance from the particle edge inward assuming a spherical particle: 20 μm particle outer diameter, 20 nm Ga shell, and a constant beam penetration depth of 10 μm. A Ga-rich shell and Ni-rich core are assumed for the simulation. Simulation data is presented over 6 μm starting from the particle left edge.



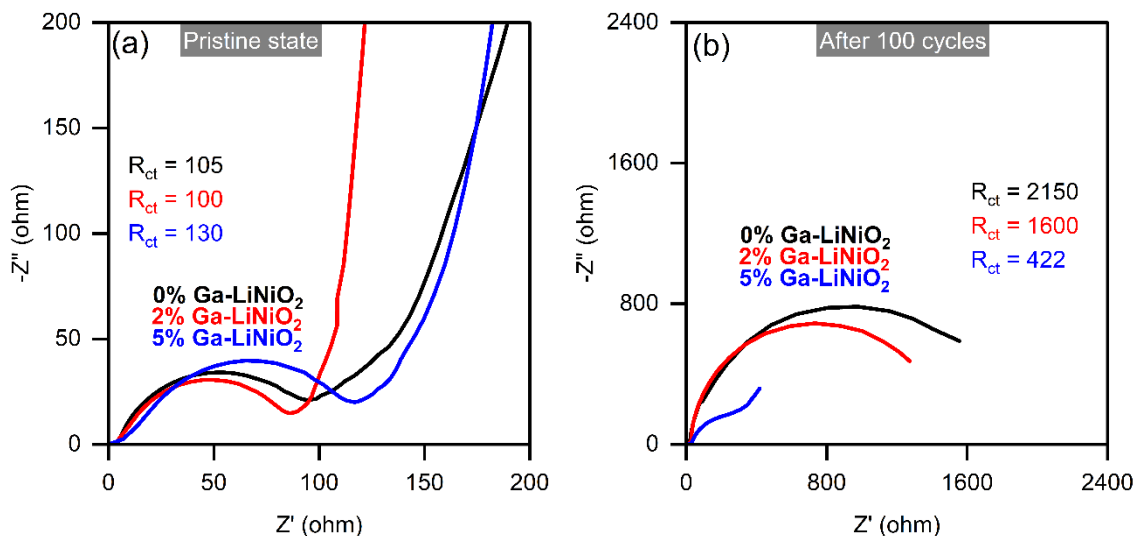
**Fig. S6.** Line scan EDS profile of 2% Ga-LiNiO<sub>2</sub>. The image inset between is the actual SEM image during the line scan.

## Estimation of theoretical specific capacities

**Table S9. Capacity calculation for 0%, 2%, and 5% Ga-LiNiO<sub>2</sub> electrodes.**

<b>Electrodes</b>	<b>Theoretical capacity (mAh·g<sup>-1</sup>)</b>	<b>Experimental initial charge capacity (mAh·g<sup>-1</sup>) (at 0.1C)</b>
0% Ga-LiNiO <sub>2</sub>	274.52 (1mol Li)	221.56 (0.81 mole Li)
2% Ga-LiNiO <sub>2</sub>	273.90 (1 mol Li)	213.33 (0.79 mole Li)
5% Ga-LiNiO <sub>2</sub>	268.16 (1 mole Li)	203.85 (0.77 mole Li)

## Electrochemical impedance spectroscopy (EIS) of electrodes in half-cells before and after cycling



**Fig. S7.** EIS Nyquist plot of (a) as-assembled and (b) cycled 0%, 2%, and 5% Ga-LiNiO<sub>2</sub> half-cells. The estimated charge transfer resistances  $R_{ct}$  are shown in the figures.

The impedance spectra (EIS) of as-assembled half-cells reveal a slightly higher charge transfer resistance ( $R_{ct}$ ) in the 5% Ga-doped cathode (**Fig. S7a**) attributable to the presence of surface  $\alpha$ -LiGaO<sub>2</sub>. However, after 100 cycles, the  $R_{ct}$  for the 0% (~ 2150  $\Omega$ ) and solution-doped 2% (~ 1600  $\Omega$ ) Ga-LiNiO<sub>2</sub> cells increased drastically compared to their 5% Ga-doped counterpart (**Fig. S7b**). This increased resistance is likely from surface reconstruction and the particle pulverization providing higher surface area for excessive growth of resistive cathode-electrolyte interphases (CEI). Conversely, the increase in  $R_{ct}$  for 5% Ga-LiNiO<sub>2</sub> at cycle 100 is markedly lower (~ 422  $\Omega$ ), underscoring the protective effect of the LiGaO<sub>2</sub> coating in mitigating surface degradation and particle breakage responsible for growing impedance.

### Differential capacity analysis (dQ/dV) at C/10

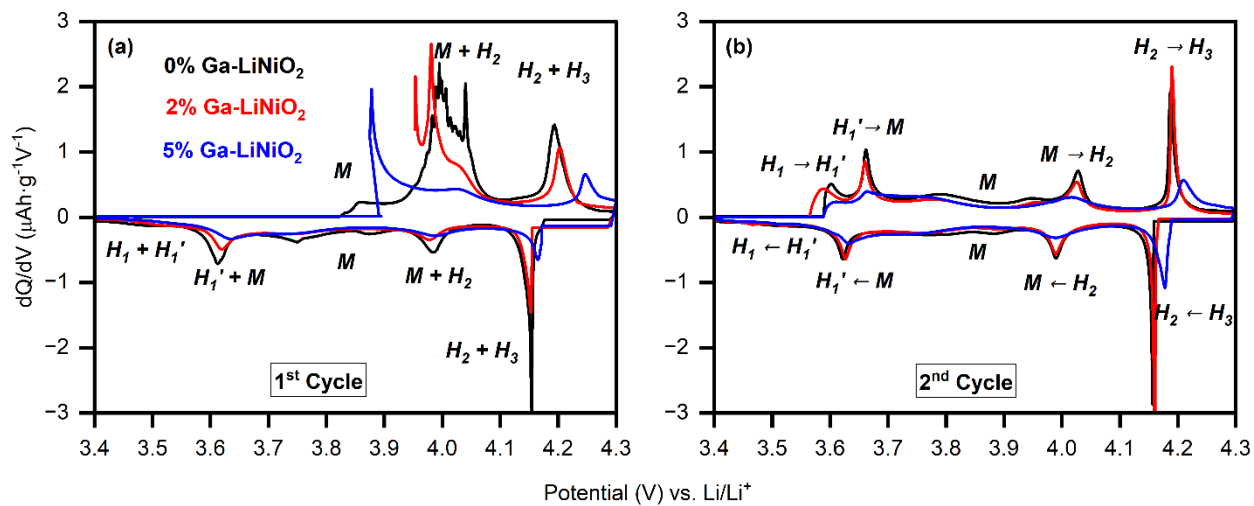


Fig. S8. dQ/dV at C/10 on the 1<sup>st</sup> (a) and 2<sup>nd</sup> (b) cycles of 0%, 2%, and 5% Ga-LiNiO<sub>2</sub>.

### Coulombic Efficiency (CE) profile

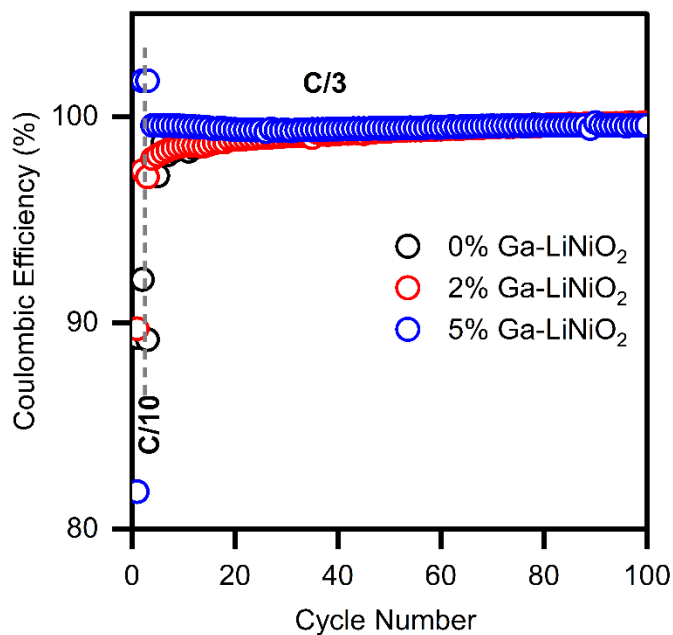
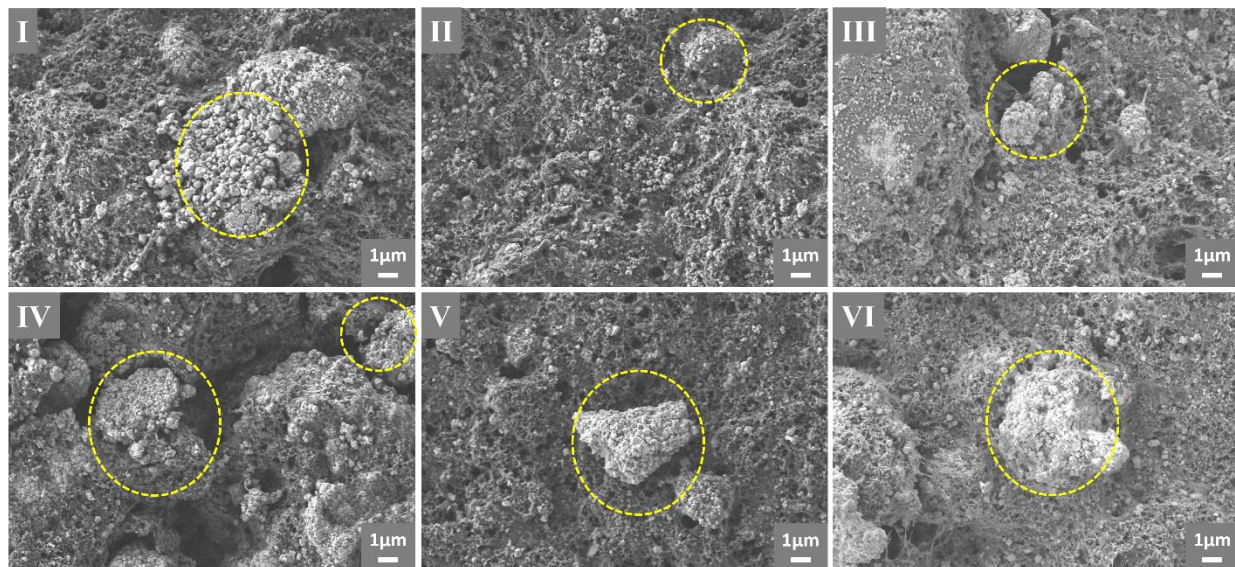
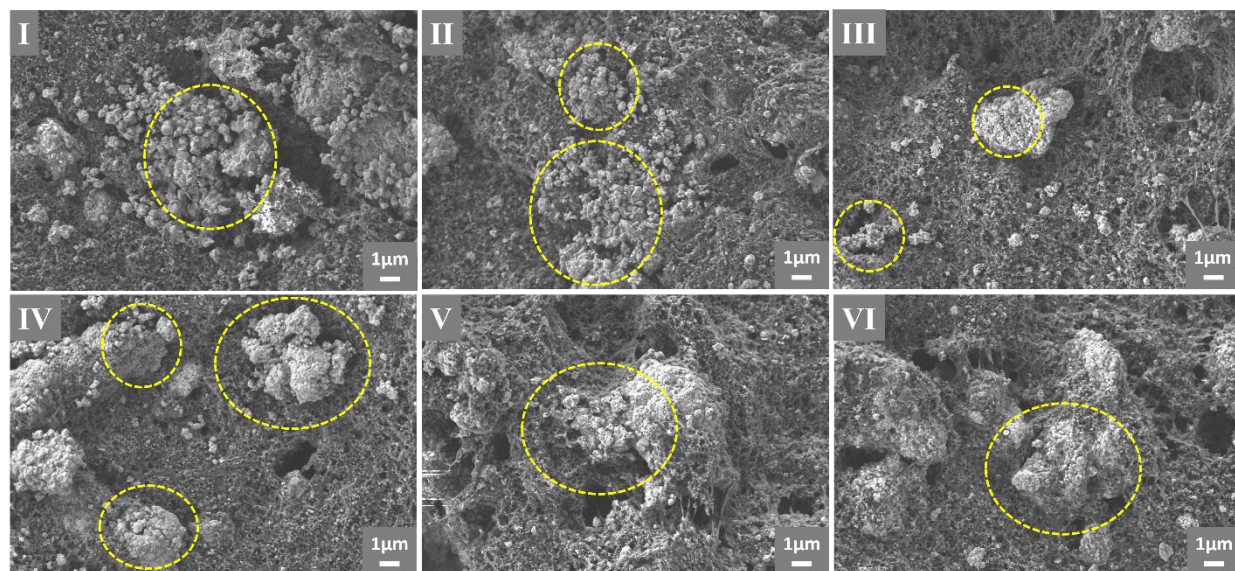


Fig. S9. Coulombic Efficiency profile of 0%, 2%, and 5% Ga-LiNiO<sub>2</sub>.

**Scanning electron microscopy (SEM) imaging of electrodes post 100 cycles**

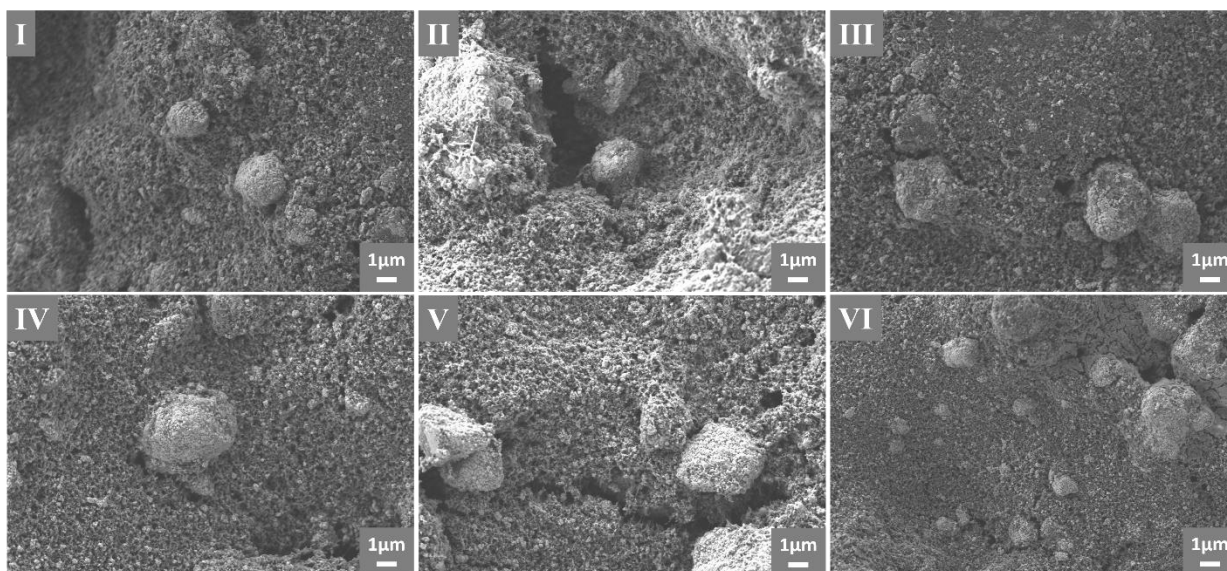


**Fig. S10.** SEM images of 0% Ga-LiNiO<sub>2</sub> electrodes obtained after 100 cycles at different locations showing numerous secondary particles are pulverized to primary nanoparticles.



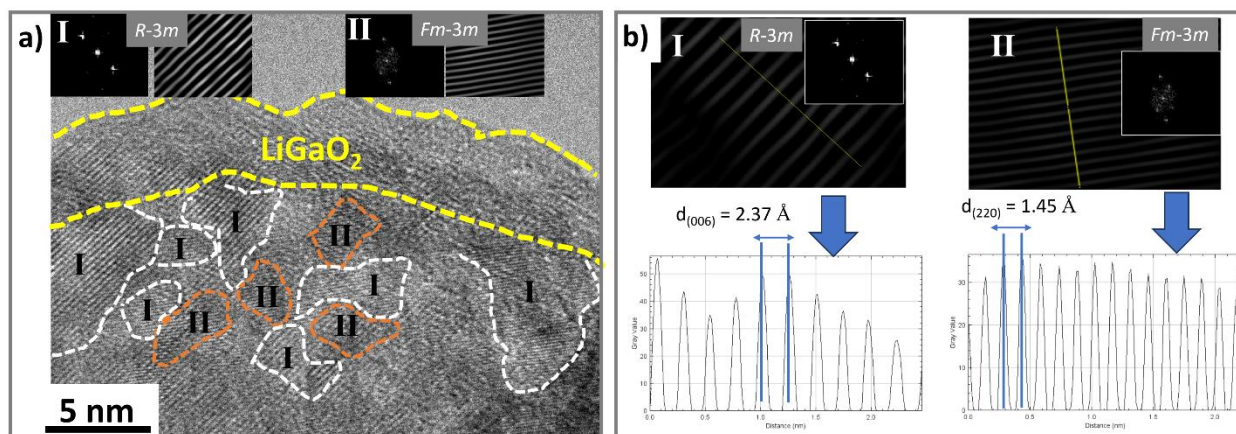
**Fig. S11.** SEM images of 2% Ga-LiNiO<sub>2</sub> electrodes obtained after 100 cycles at different locations also showing numerous secondary particles are pulverized to primary nanoparticles.





**Fig. S12.** SEM images of 5% Ga-LiNiO<sub>2</sub> electrodes obtained after 100 cycles at different locations showing minimal pulverization of secondary particles.

### HRTEM image of 5% Ga-LiNiO<sub>2</sub> electrodes after 100 cycles



**Fig. S13.** a) HRTEM of 5% Ga-LiNiO<sub>2</sub> obtained after 100 cycles demonstrating  $R\bar{3}m$  and  $Fm\bar{3}m$  distribution at nanoscale near the surface. Region I correspond to  $R\bar{3}m$  symmetry whereas Region II is the  $Fm\bar{3}m$  rock-salt phase from reconstruction. b) d-spacing calculations of region I and II. FFT and corresponding IFFT images of one of the spots are shown inset for clarity.



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Supplementary XRD refinement information clipped from the GSAS-II software. The tables below show improper refinement convergence under various conditions considered. These analyses exclude certain occupancy possibilities.

(a) Refining site occupancy and Uiso value of 2% Ga-LiNiO<sub>2</sub> when assuming Ga occupies only 3a site.

	Name	Type	refine	x	y	z	frac	site sym	mult	I/A	Uiso
0	Ni2	Ni+3	FU	0.00000	0.00000	0.50000	1.0119	-3m(100)	3	I	0.02267
1	Ga2	Ga+3	FU	0.00000	0.00000	0.00000	-0.0228	-3m(100)	3	I	-0.01034
2	Li2	Li+1	FU	0.00000	0.00000	0.00000	1.3487	-3m(100)	3	I	-0.01034
3	O1	O-2		0.00000	0.00000	0.23924	1.0000	3m(100)	6	I	0.02418

	Name	Type	refine	x	y	z	frac	site sym	mult	I/A	Uiso
0	Ni1	Ni+3	FU	0.00000	0.00000	0.50000	0.5824	-3m(100)	3	I	0.07930
1	Ga1	Ga+3	FU	0.00000	0.00000	0.00000	-0.1995	-3m(100)	3	I	0.09034
2	Li1	Li+1	FU	0.00000	0.00000	0.00000	1.1995	-3m(100)	3	I	0.09034
3	O1	O-2	XU	0.00000	0.00000	0.24329	1.0000	3m(100)	6	I	0.00343

(b) Refining site occupancy and Uiso value of 2% Ga-LiNiO<sub>2</sub> when assuming Ga occupies only 3b site.

	Name	Type	refine	x	y	z	frac	site sym	mult	I/A	Uiso
0	Ni1	Ni+3	U	0.00000	0.00000	0.50000	0.9800	-3m(100)	3	I	0.48393
1	Ga1	Ga+3	U	0.00000	0.00000	0.50000	0.0200	-3m(100)	3	I	0.51607
2	Li1	Li+1	U	0.00000	0.00000	0.00000	1.0000	-3m(100)	3	I	-2.89599
3	O1	O-2		0.00000	0.00000	0.23924	1.0000	3m(100)	6	I	0.02418

	Name	Type	refine	x	y	z	frac	site sym	mult	I/A	Uiso
0	Ni1	Ni+3	FU	0.00000	0.00000	0.50000	0.9524	-3m(100)	3	I	0.02330
1	Ga1	Ga+3	FU	0.00000	0.00000	0.50000	0.0476	-3m(100)	3	I	0.02330
2	Li1	Li+1	FU	0.00000	0.00000	0.00000	1.0460	-3m(100)	3	I	-3.66347
3	O1	O-2		0.00000	0.00000	0.23924	1.0000	3m(100)	6	I	0.02418