

Supplementary

Understanding the Effects of Surface Reconstruction on Electrochemical Cycling Performance of Spinel $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ Cathode Material at Elevated Temperatures†

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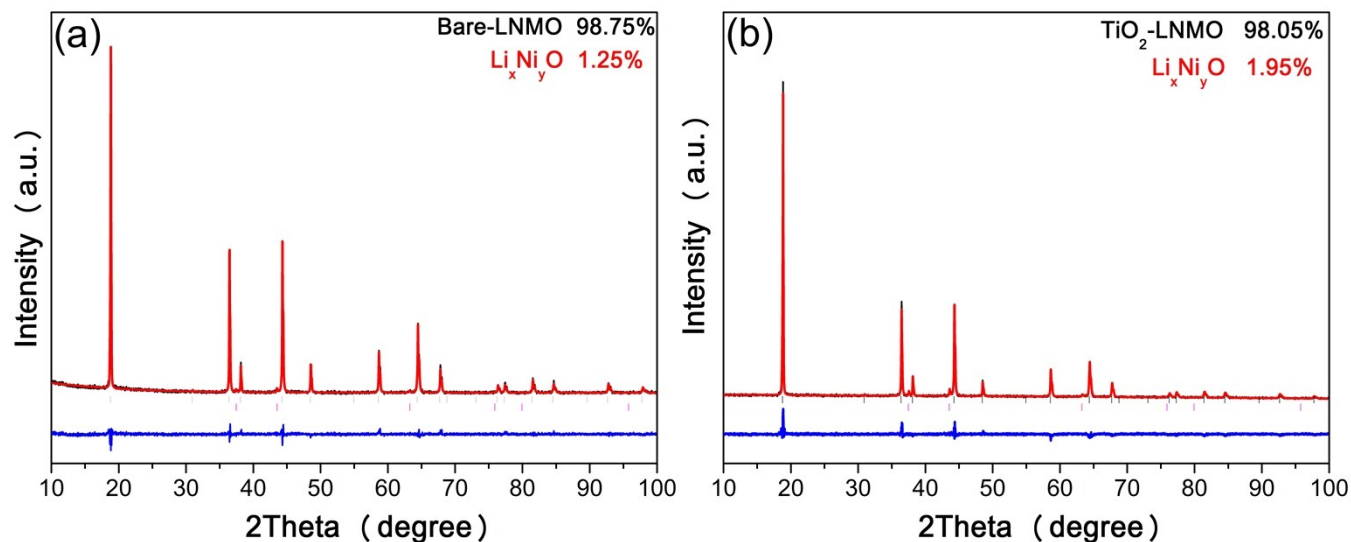


Figure S1. Rietveld refinement profiles using room-temperature XRD data for (a) Bare-LNMO sample refined in space group Fd-3m. $wRp = 6.156\%$, $Rp = 4.903\%$ and $Gof = 1.201$; (b) TiO_2 -LNMO refined in space group Fd-3m. $wRp = 8.949\%$, $Rp = 7.133\%$ and $Gof = 1.294$. Observed, calculated, and difference profiles shown in black, red, and blue, respectively; black and red tick marks show reflection positions for LNMO and Li_xNi_yO , respectively.

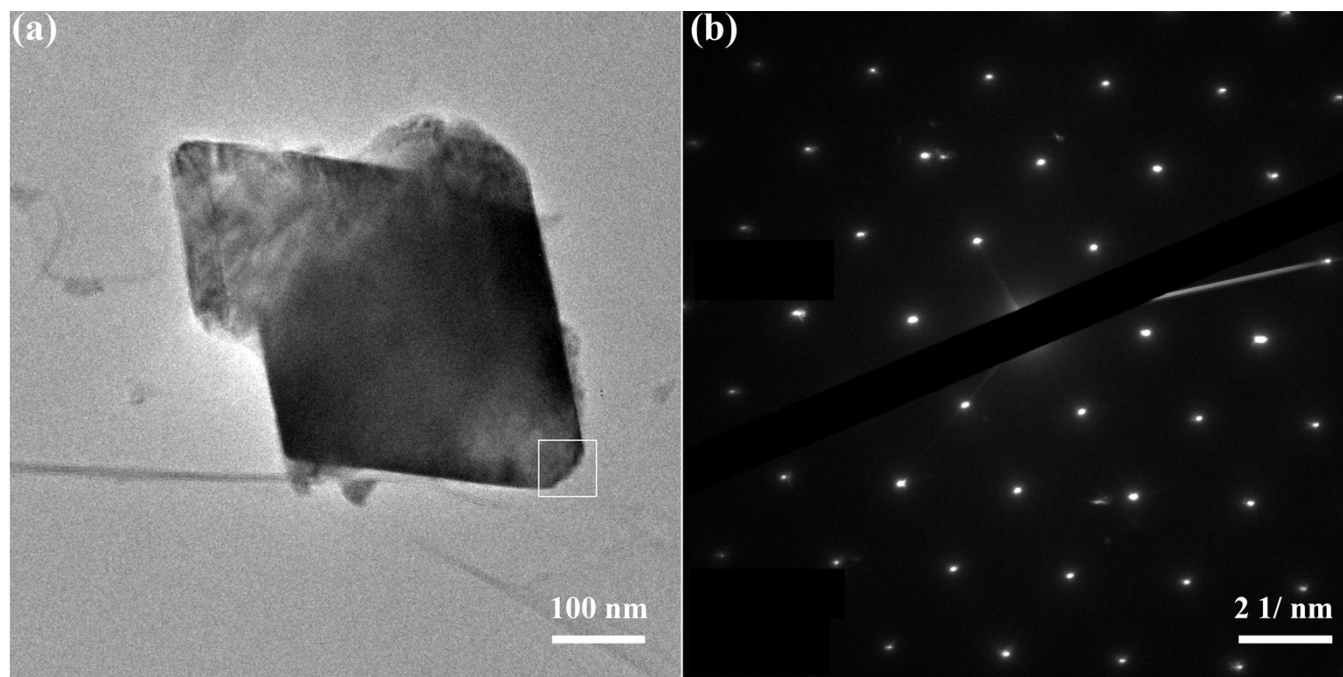


Figure S1b. (a) TEM bright-field image and (b) electron diffraction patterns in the [110] zone of TiO_2 -LNMO

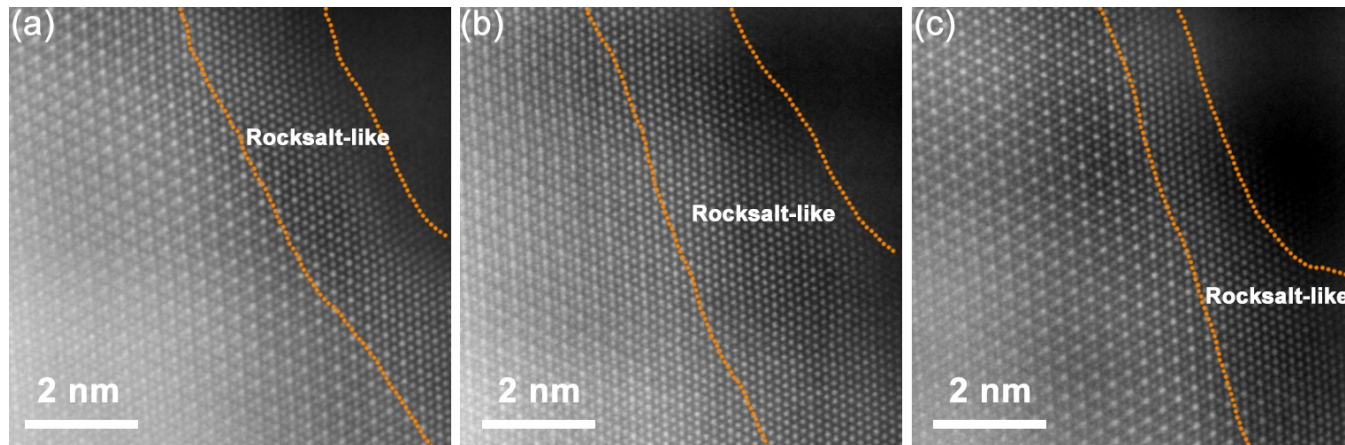


Figure S2. STEM HAADF images of TiO₂-LNMO showing various extent of surface reconstructed structure.

	Mn ⁴⁺					
Line Shape	GL(30)	GL(30)	GL(30)	GL(30)	GL(30)	GL(30)
Area	39352.7	51345.9	30171.7	16677.7	8618.2	3935.3
FWHM	1.09768	1.20648	1.14777	0.995472	1.09119	1.3
Position	642.053	642.882	643.565	644.333	645.381	646.376
%Concentration	19.53	25.48	14.97	8.28	4.28	1.92
	Mn ³⁺					
Line Shape	GL(30)	GL(30)	GL(30)	GL(30)	GL(30)	
Area	12345	12345	14299.6	9002	3446.7	
FWHM	1.13254	1.3	0.846851	1.17995	0.7	
Position	640.94	641.866	642.286	643.66	644.926	
%Concentration	6.13	6.13	7.1	4.47	1.71	

Table S1a. Mn(2p_{3/2}) peak parameters for Mn in the Bare- LNMO.

	Mn ⁴⁺					
Line Shape	GL(30)	GL(30)	GL(30)	GL(30)	GL(30)	GL(30)
Area	7855.7	10249.9	6023.0	3329.3	1720.4	1071.2
FWHM	0.911326	1.3	1.15676	0.960127	0.987678	1.3
Position	642.074	642.919	643.468	644.28	645.434	646.4
%Concentration	16.43	21.44	12.60	6.96	3.60	2.24
	Mn ³⁺					
Line Shape	GL(30)	GL(30)	GL(30)	GL(30)	GL(30)	
Area	4213.7	4213.7	4880.9	3072.6	1176.5	
FWHM	1.3	1.19923	1.05842	1.29507	0.747367	
Position	640.927	641.739	642.45	643.663	644.876	
%Concentration	8.81	8.81	10.21	6.43	2.46	

Table S1b. Mn($2p_{3/2}$) peak parameters for Mn in TiO₂-LNMO.

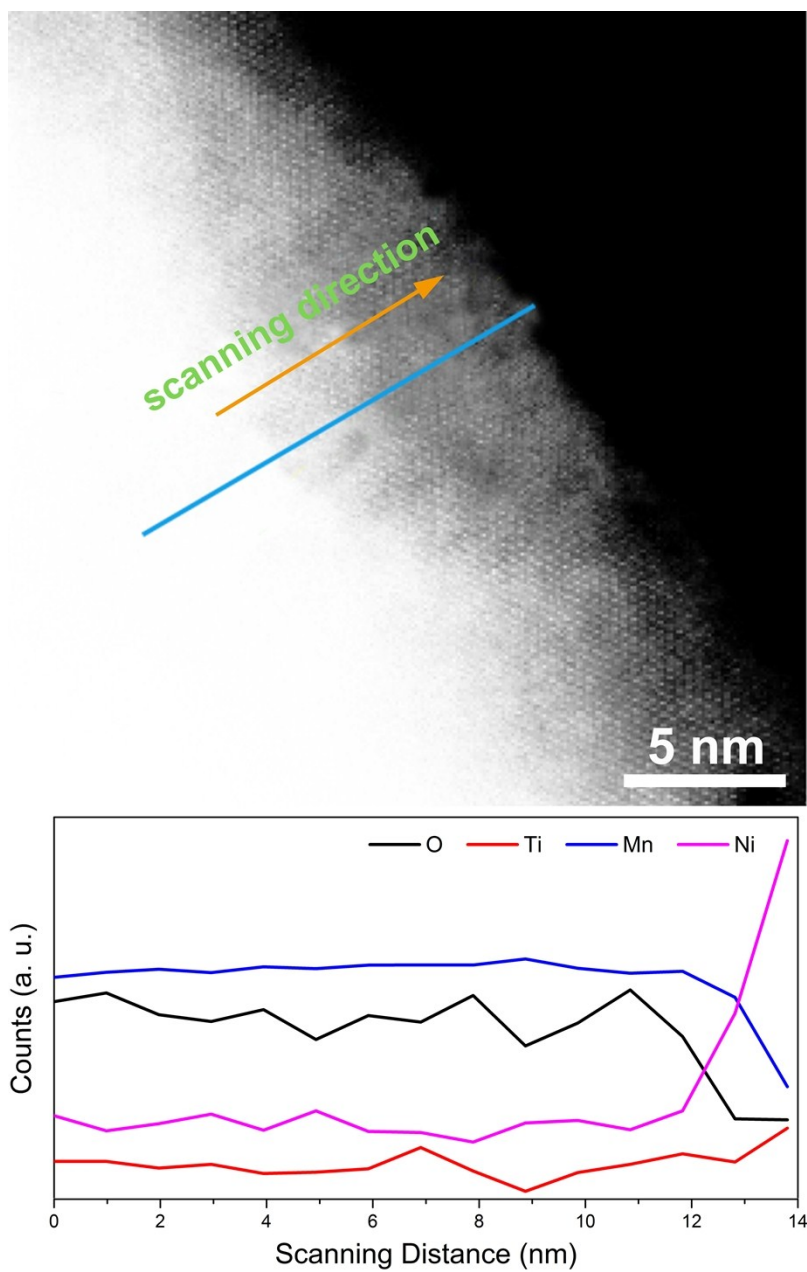


Figure S3. STEM-EDS of TiO₂-LNMO showing concentraton profile of O, Ti, Mn and Ni.

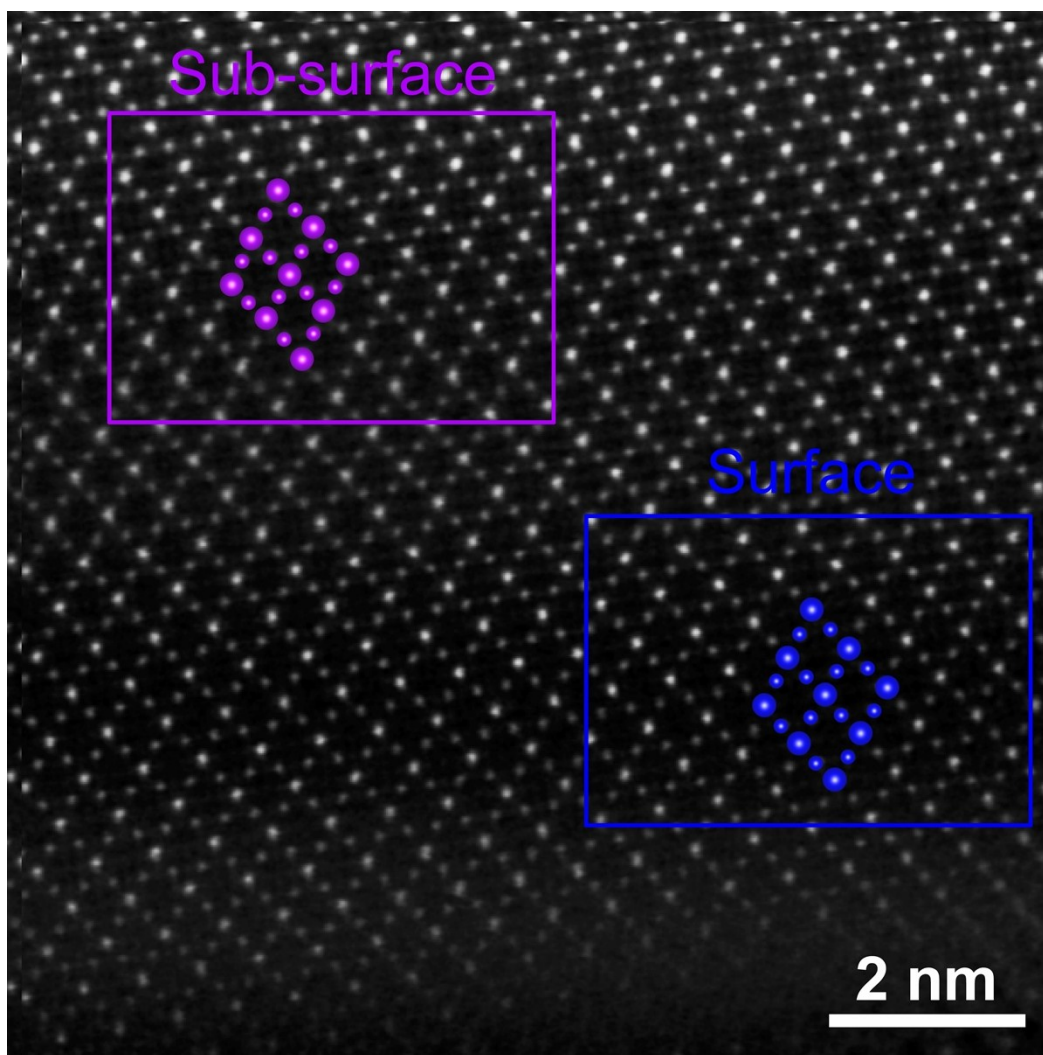


Figure S4. STEM HAADF images of TiO₂-LNMO processed at 500 °C showing no surface structural reconstruction.

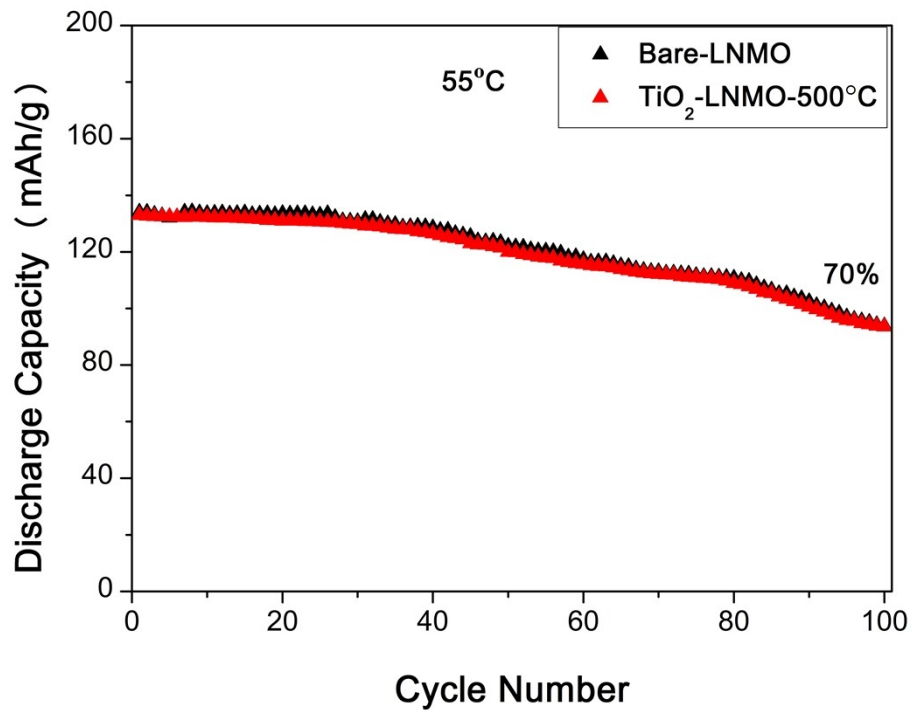


Figure S5. Electrochemical cycling performance of Bare-LNMO and TiO₂-modified LNMO (processed at 500 °C) at 55 °C.

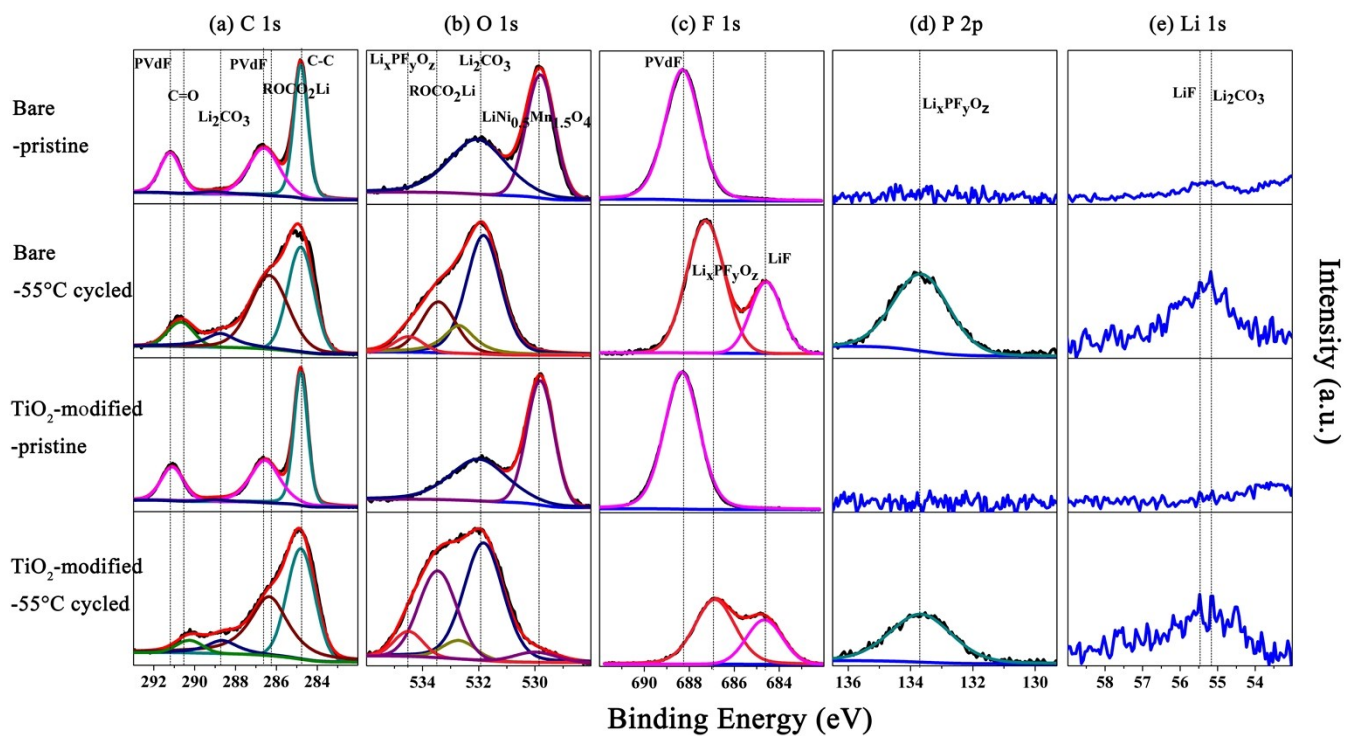


Figure S6. Ex-situ XPS results of bare and TiO₂-coated LNMO electrodes before and after cycling at 55 °C for 100 cycles. The signals for C 1s, O 1s, F 1s, P 2p and Li 1s are shown in (a), (b), (c), (d) and (e), respectively.