Supporting Information

Stabilizing the (003) facet of single-crystal $LiNi_{0.6}Co_{0.2}Mn_{0.2}O_2$ cathode material using tungsten oxide as an exemplar

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Table S1. Lattice constants and atom positions for the bare and WO_3-coated NCM cathode materials from the Rietveld refinement of the XRD patterns. The space group used for the refinement was R-3m.

Bare NCM					
a = 2.8666(3) Å, c = 14.2066(1) Å, V = 101.107(2) Å^3,					
R_{wp} = 4.63%, R_p = 3.57%, gof = 1.48					
Atoms	Wyckoff positions	x	y	z	Site occupancy
Li	3b	0	0	1/2	1
Ni	3a	0	0	0	0.6
Co	3a	0	0	0	0.2
Mn	3a	0	0	0	0.2
O	6c	0	0	0.2592(2)	1
WO_3-coated NCM					
a = 2.8701(1) Å, c = 14.2133(2) Å, V = 101.396(2) Å^3					
R_{wp} = 4.84%, R_p = 3.70%, gof = 1.54					
Atoms	Wyckoff positions	x	y	z	Site occupancy
Li	3b	0	0	1/2	1
Ni	3a	0	0	0	0.6
Co	3a	0	0	0	0.2
Mn	3a	0	0	0	0.2
O	6c	0	0	0.2599(4)	1

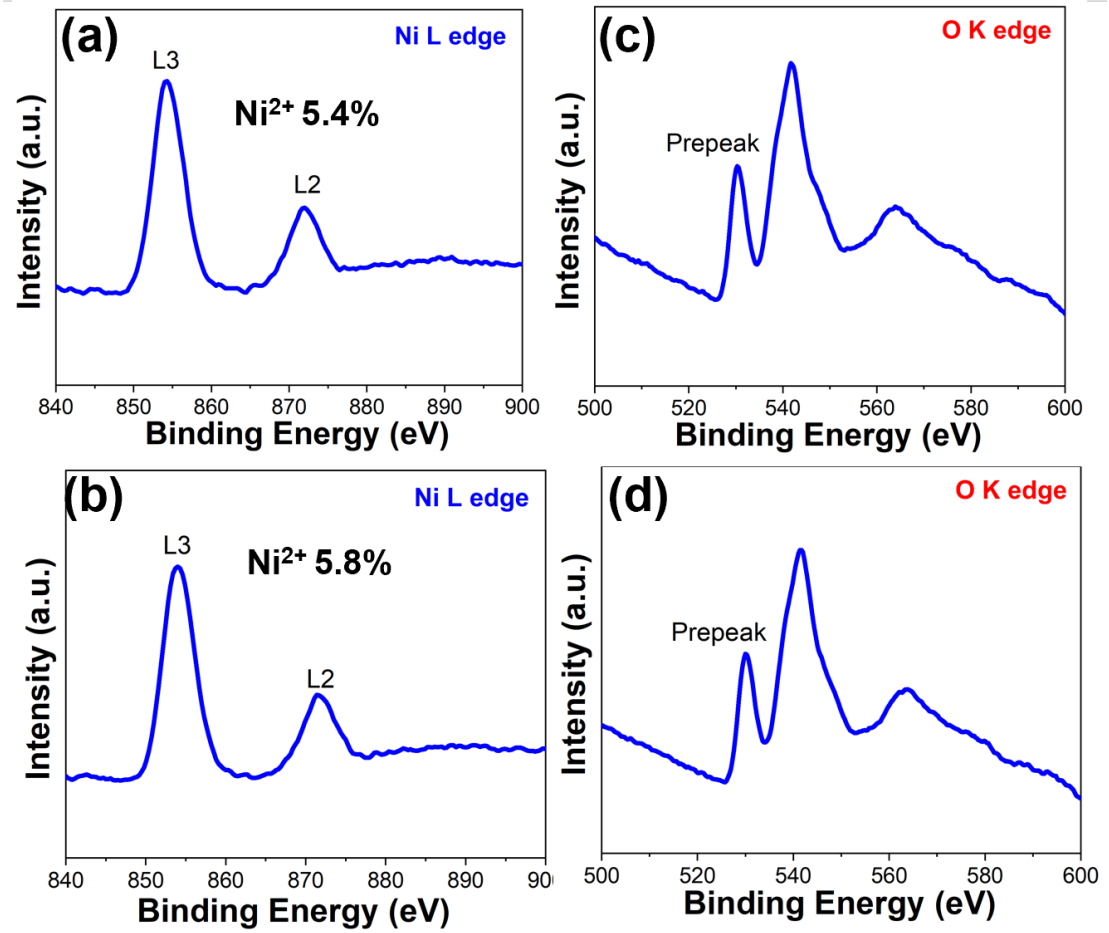

Figure S1. EELS Ni L edge and O K edge spectra for uncycled bare NCM from (a, c) ROI-A and (b, d) ROI-B.

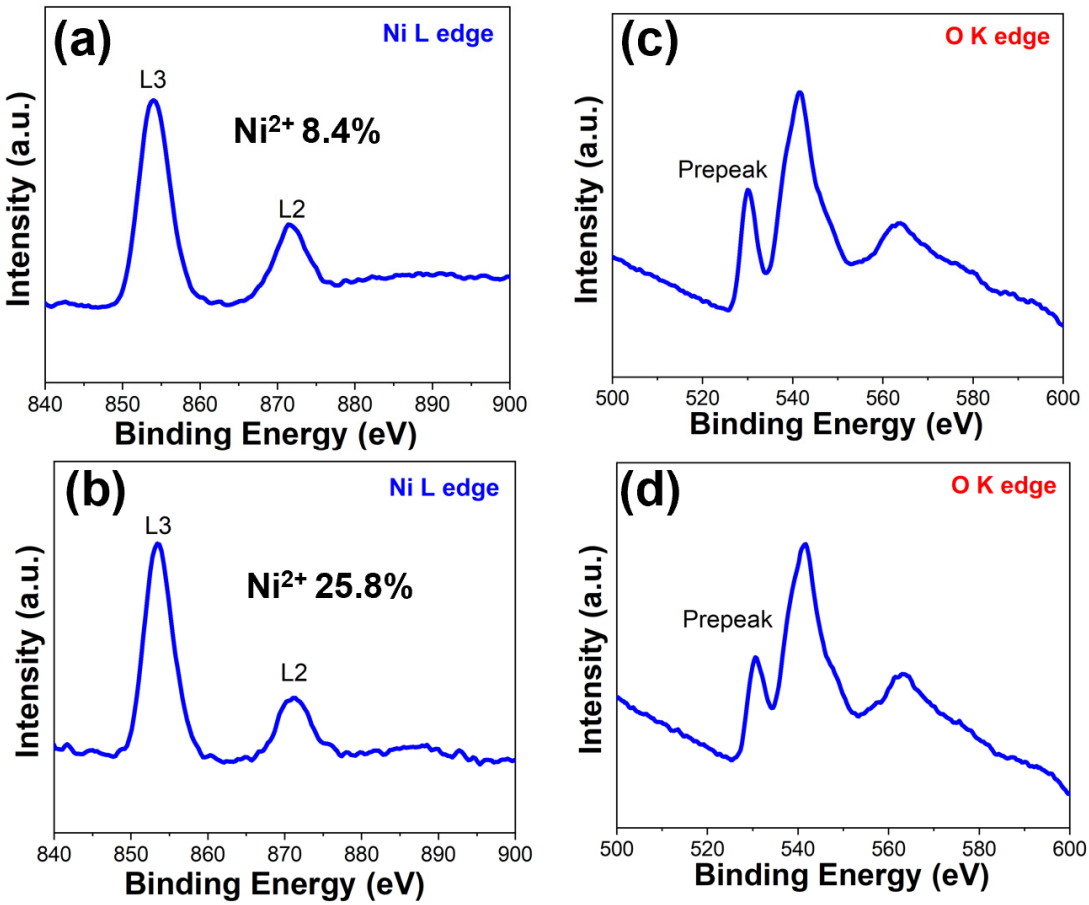

Figure S2. EELS Ni L edge and O K edge spectra for uncycled WO_3-coated NCM from (a, c) ROI-C and (b, d) ROI-D.

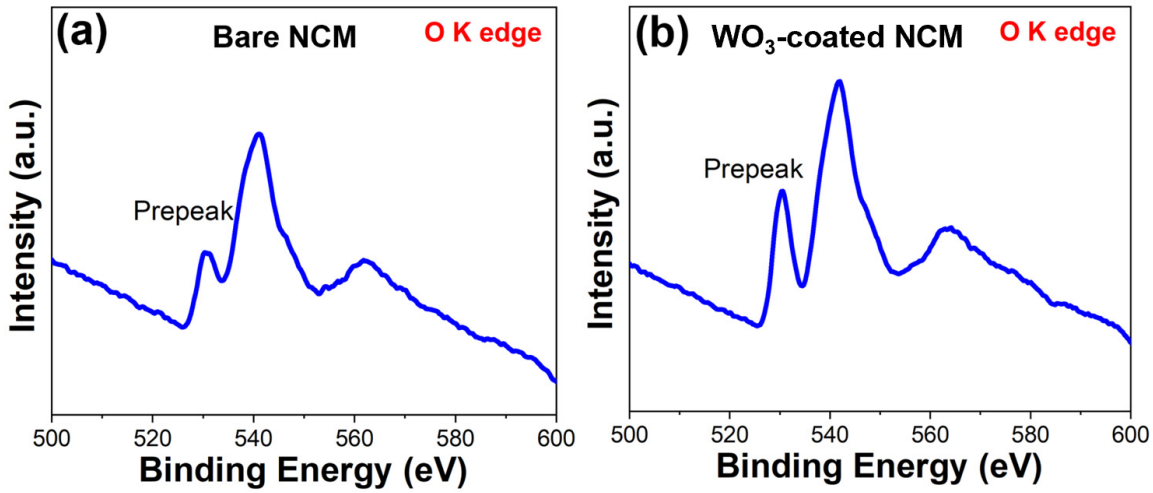

Figure S3. EELS oxygen K edge spectra from bulk region of cycled (a) bare and (b) WO_3-coated NCM.

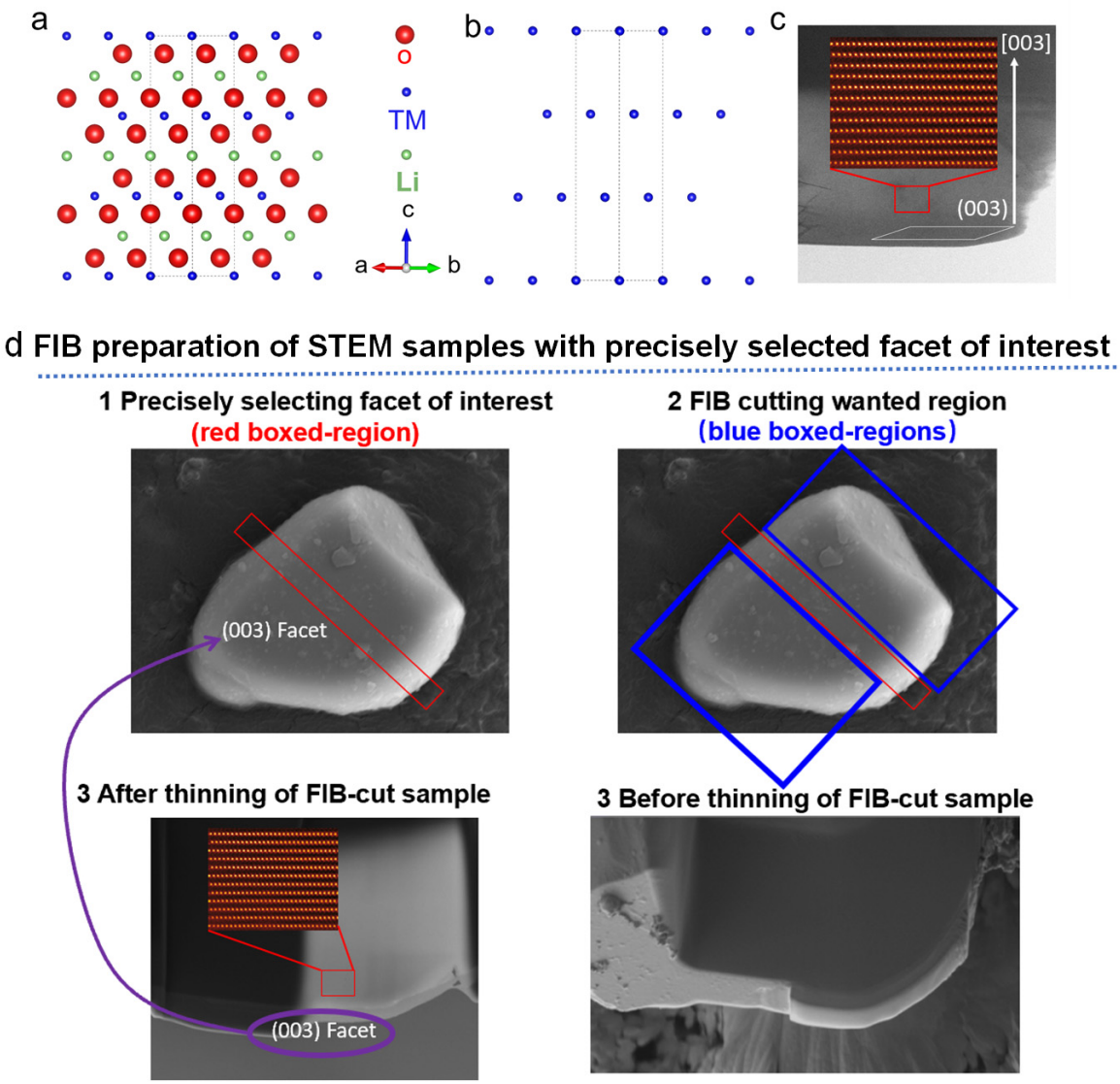

Figure S4. (a) Crystal structure and (b) arrangement of TM ions of NCM layered cathode material viewed along the [010] zone axis. (c) A STEM HAADF image showing arrangement of TM atoms with respect to the FIB-cut single crystal. (d) FIB preparation of STEM samples with precisely selected facet of interest. Based on the arrangement of TM atoms, the crystallographic [003] direction and (003) plane are indexed.

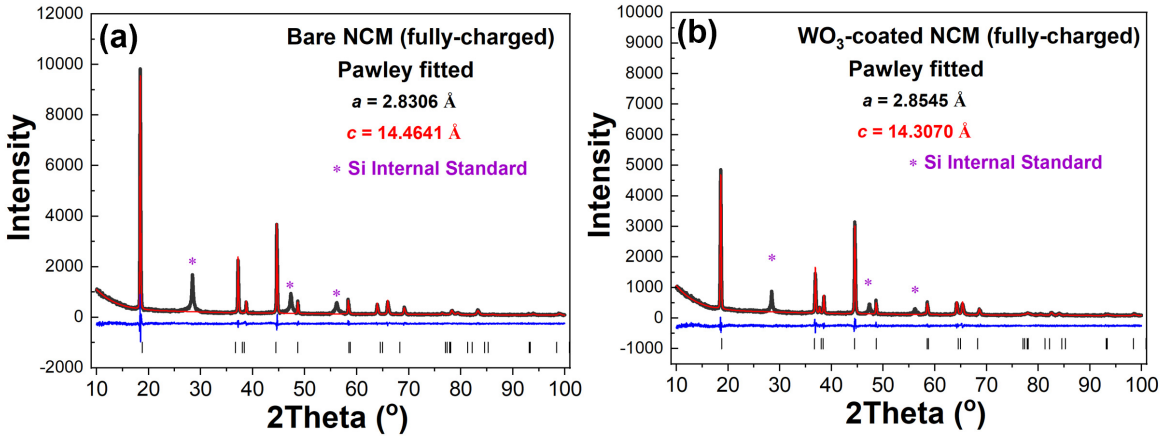

Figure S5. Pawley fitting of XRD patterns for 1st cycle fully-charged (a) bare and (b) WO_3-coated NCM cathode powders scraped from electrodes. Silicon internal standard is marked with *. The Pawley fitting started with fitting XRD patterns related to silicon internal standard (a = 5.4313 Å) to obtain a specimen displacement value; then, the value was fixed for fitting of XRD patterns related to cycled bare NCM and WO_3-coated NCM samples.