

Supporting Information

Improving the Cycling and Air-Storage Stability of $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ through an Integrated Surface/Interface/Doping Engineering

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Table S1. Rietveld refinement results of lattice parameters based on XRD data and the I(003)/I(104) value for the pristine and Li₂ZrO₃ coated samples.

Samples	a/(Å)	c/(Å)	V/(Å ³)	Z _{ox} /(Å)	(003)/ (104)	R _p (%)
Pristine NCM	2.8688(1)	14.1793(1)	101.0619(10)	0.2419(3)	1.359	1.73
LZO@NCM	2.8702(1)	14.1869(1)	101.2128(9)	0.2430(2)	1.434	1.49

Table S2. Rietveld refinement results of lattice parameters from neutron diffraction for the pristine and Li₂ZrO₃ coated samples.

Samples	a/(Å)	c/(Å)	V/(Å ³)	R _{wp}	R _p
Pristine NCM	2.8704(2)	14.193(3)	101.269(12)	8.39	6.49
LZO@NCM	2.8725(1)	14.2003(8)	101.4713(10)	7.03	5.28

Table S3. Bond length for the pristine and Li₂ZrO₃-coated sample samples from Rietveld refinement results of neutron diffraction.

Samples	O-TM/(Å)	O-Li/(Å)	O-O/(Å)	Li-Li/(Å)	TM-Li/(Å)	R _{wp} (%)	R _p (%)
Pristine NCM	1.9660	2.1111	2.8704	2.8704	2.8882	8.39	6.49
LZO@NCM	1.9665	2.1134	2.8725	2.8725	2.8899	7.03	5.28

Table S4. The refined crystal sites and atom occupancies of the pristine sample from the neutron diffraction data.

Atom	site	x/a	y/b	z/c	Occ
Li	3a	0.0000	0.0000	0.0000	0.4875(19)
Ni	3a	0.0000	0.0000	0.0000	0.0121(19)
Ni	3b	0.0000	0.0000	0.5000	0.40(1)
Co	3b	0.0000	0.0000	0.5000	0.0488
Mn	3b	0.0000	0.0000	0.5000	0.0474
Li	3b	0.0000	0.0000	0.5000	0.01(7)
O	6c	0.0000	0.0000	0.24119(15)	1.00000

Table S5. The refined crystal sites and atom occupancies of the Li_2ZrO_3 -coated sample from the neutron diffraction data.

Atom	site	x/a	y/b	z/c	Occ
Li	3a	0.0000	0.0000	0.0000	0.491(2)
Ni	3a	0.0000	0.0000	0.0000	0.009(2)
Ni	3b	0.0000	0.0000	0.5000	0.405(4)
Co	3b	0.0000	0.0000	0.5000	0.04884
Mn	3b	0.0000	0.0000	0.5000	0.04754
Zr	3b	0.0000	0.0000	0.5000	0.00013
Li	3b	0.0000	0.0000	0.5000	0.0095(4)
O	6c	0.0000	0.0000	0.24108(12)	1.00000

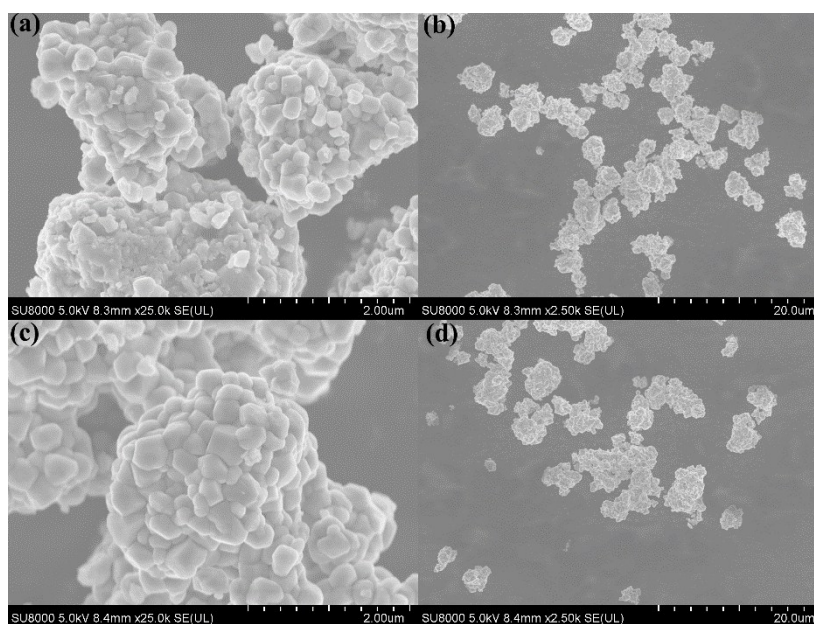


Fig S1 SEM image for pristine (a, b) and Li₂ZrO₃-coated NMC(c, d)

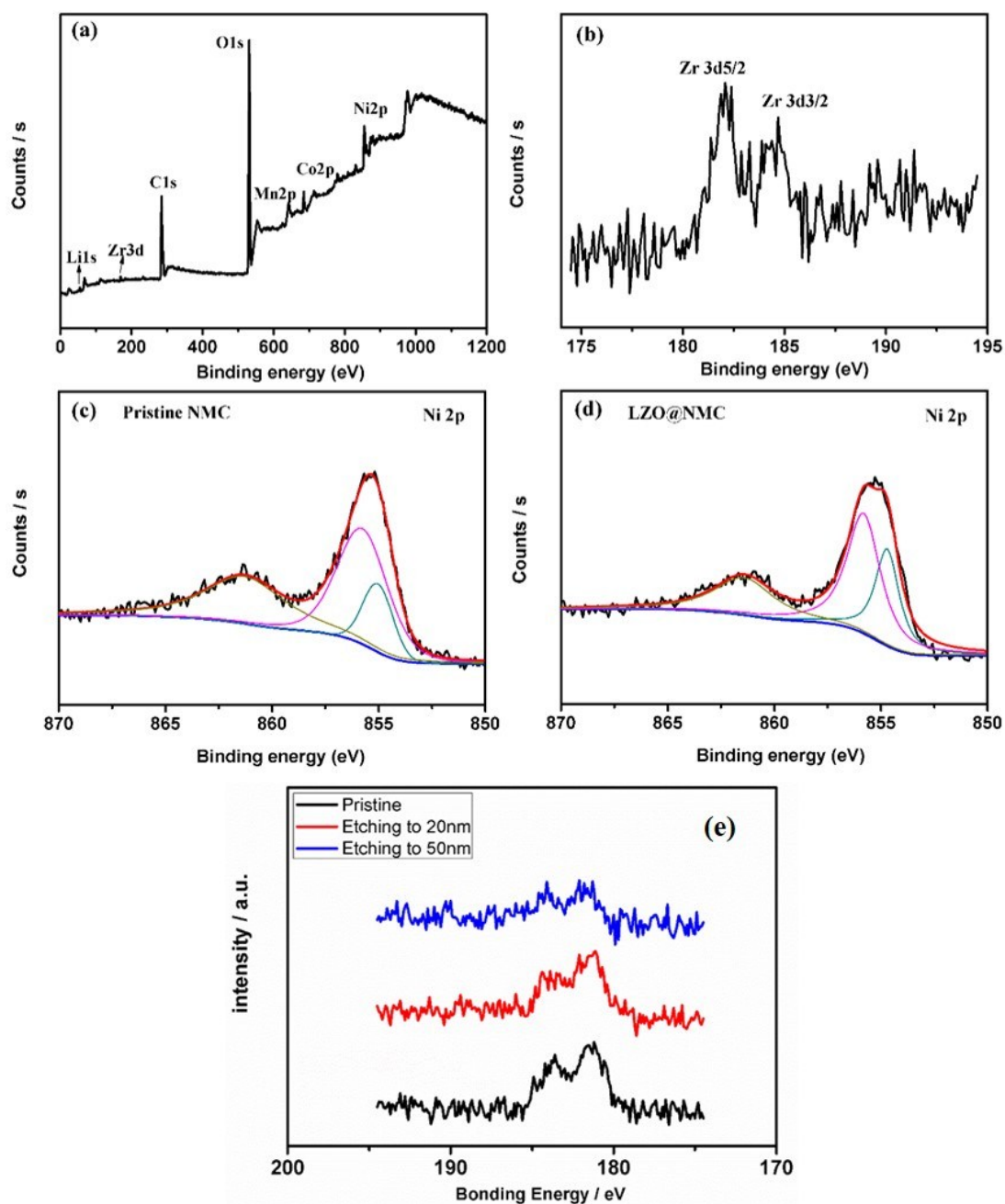


Figure S2. (a) XPS spectra of Li_2ZrO_3 coated sample; (b) XPS spectra for Zr 3d; XPS spectra for Ni 2p of the pristine sample (c) and Li_2ZrO_3 coated sample (d); XPS Zr 3d spectra collected after being etched to 0 nm, 20 nm and 50 nm for Li_2ZrO_3 -coated sample.

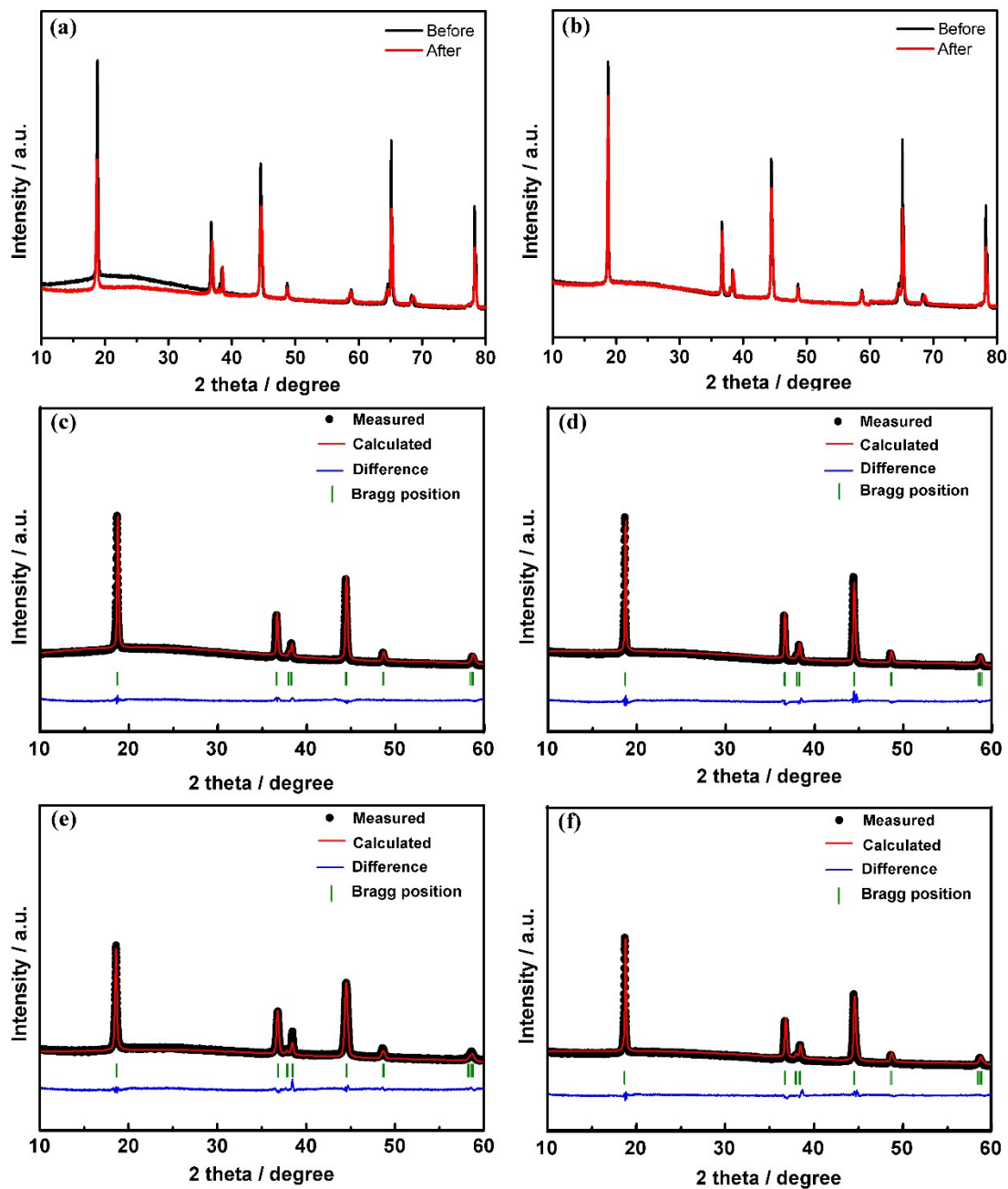


Figure S3. XRD patterns of the pristine sample (a) and Li₂ZrO₃-coated sample (b) before and after 500 cycles. Observed/calculated XRD patterns of the pristine sample (c, before cycling; e, after cycling) and Li₂ZrO₃ coated sample (d, before cycling; f, after cycling).

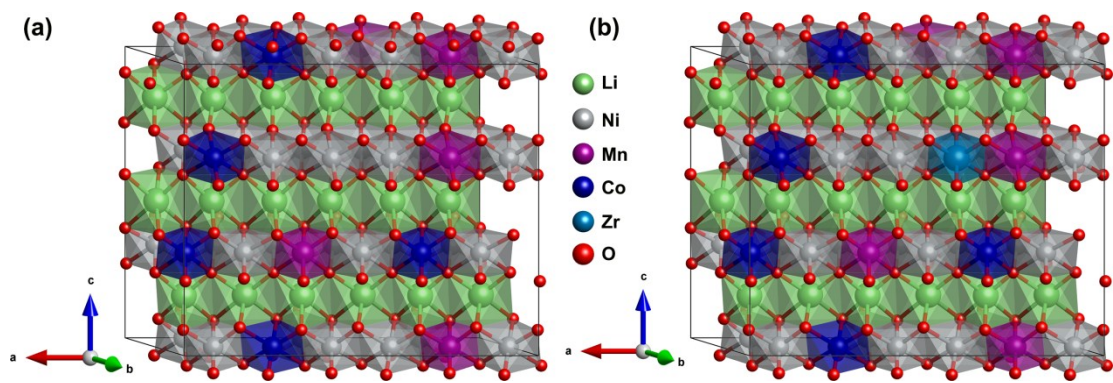


Figure.S4 The optimized structures of the pristine NMC(a) and Li_2ZrO_3 -coated NMC(b)