

Supplementary information

High structural stability and Li-conduction of $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ cathode coated by Al_2O_3 and LiNbO_3 for high performance lithium-ion battery

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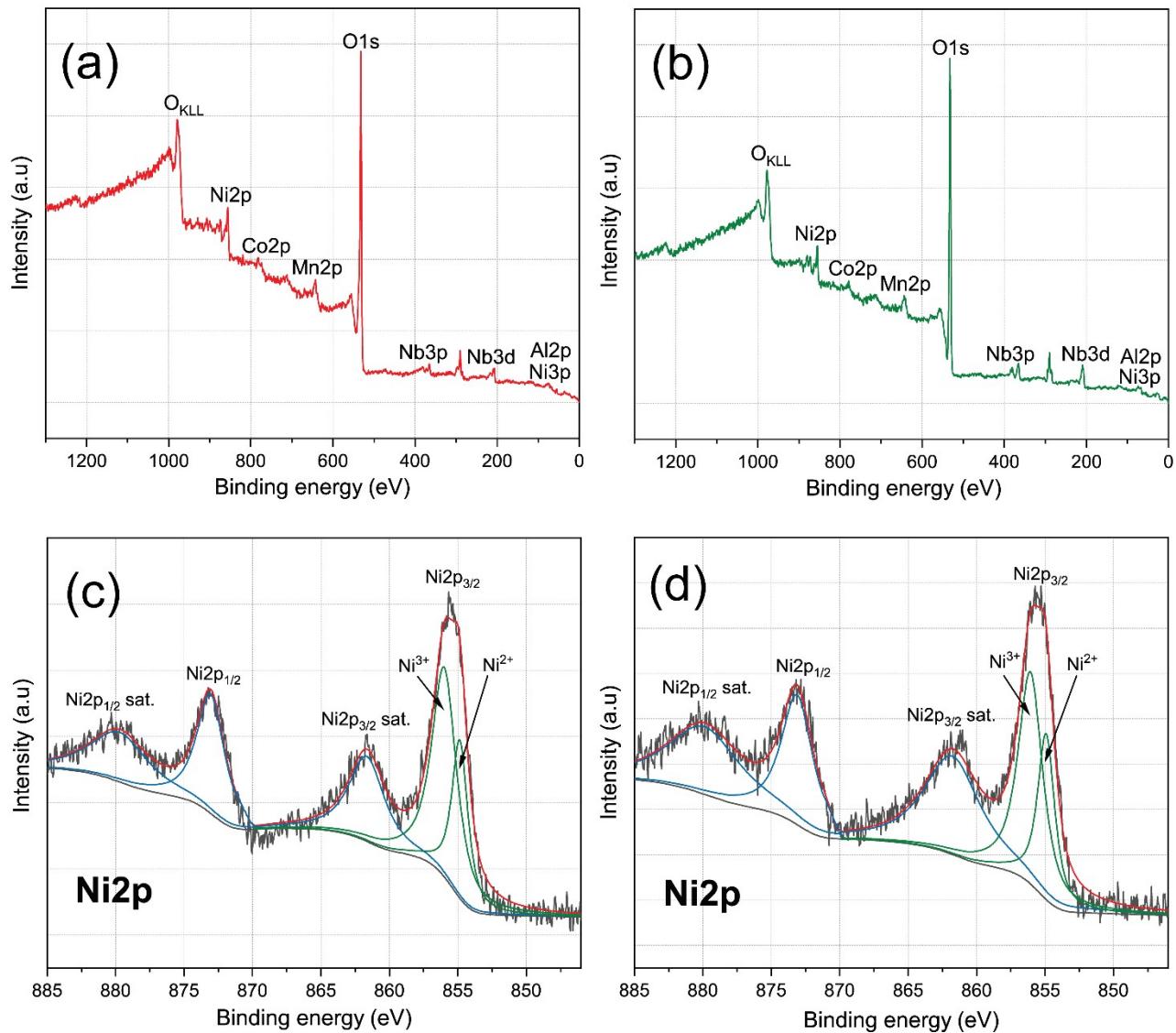


Figure S1. (a) Full-scan and (c) Ni2p XPS spectra of NCM-AlNb-0.25; (b) full-scan and (d) Ni2p XPS spectra of NCM-AlNb-1.

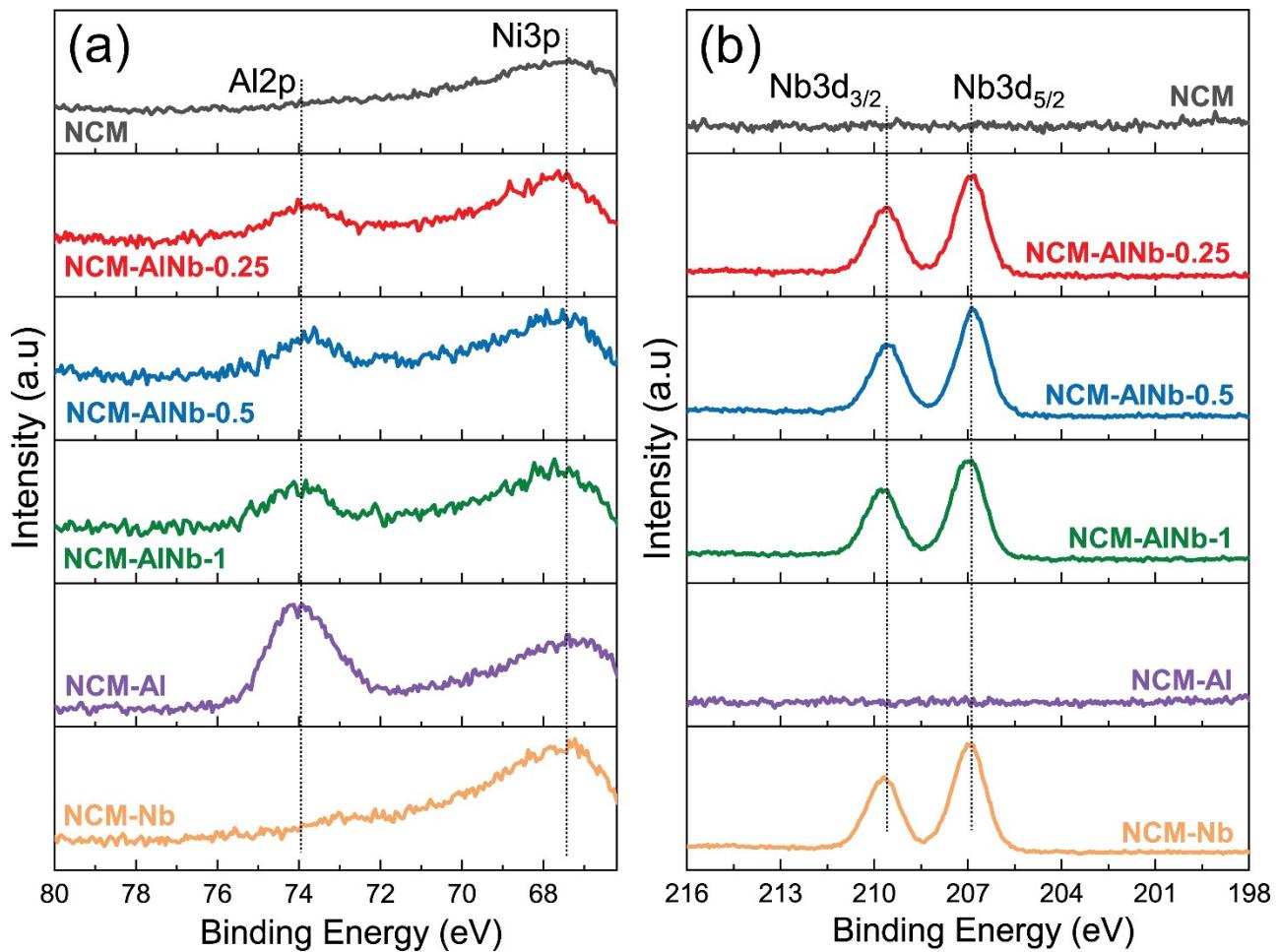


Figure S2. (a) Al2p XPS spectra and (b) Nb3d XPS spectra of uncoated and coated NCMs.

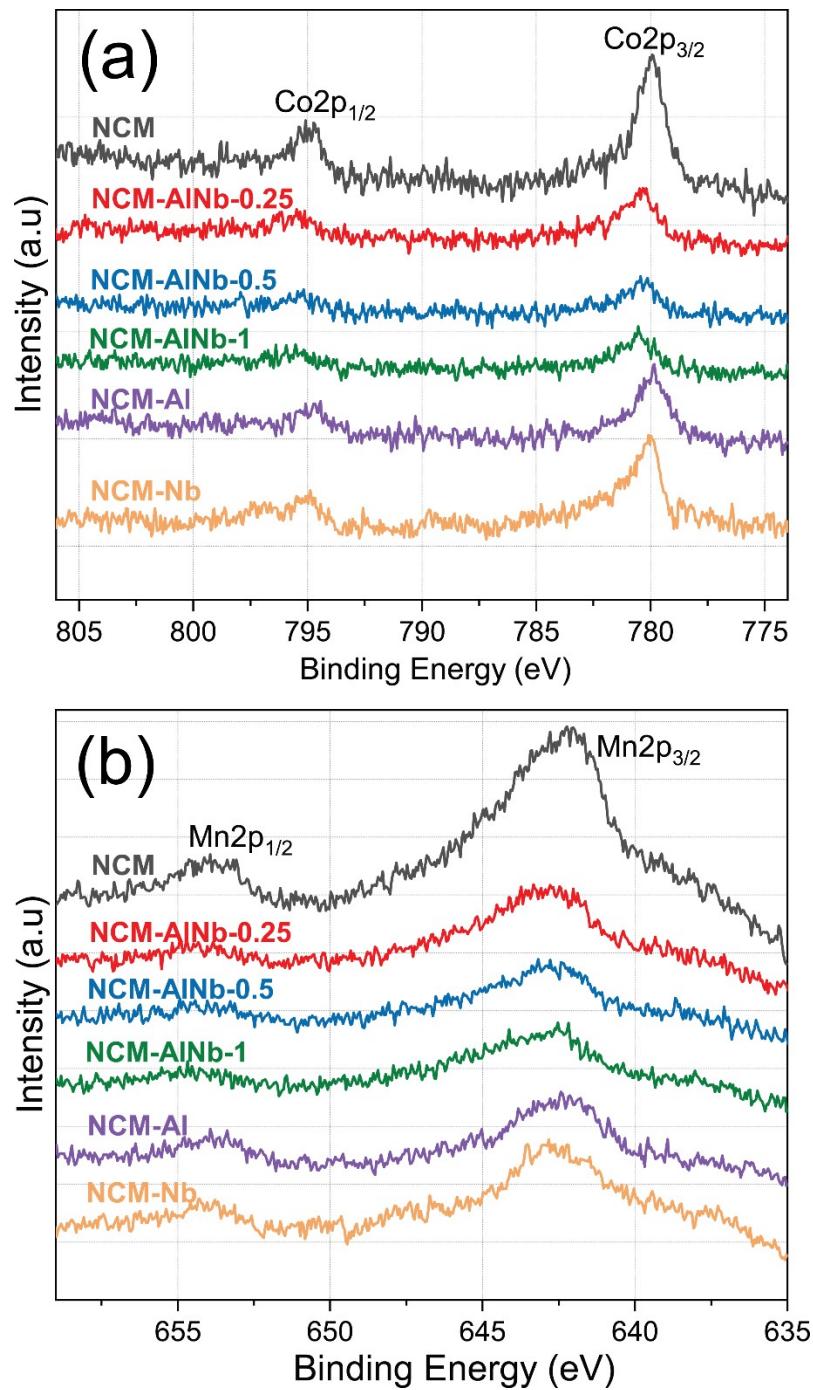
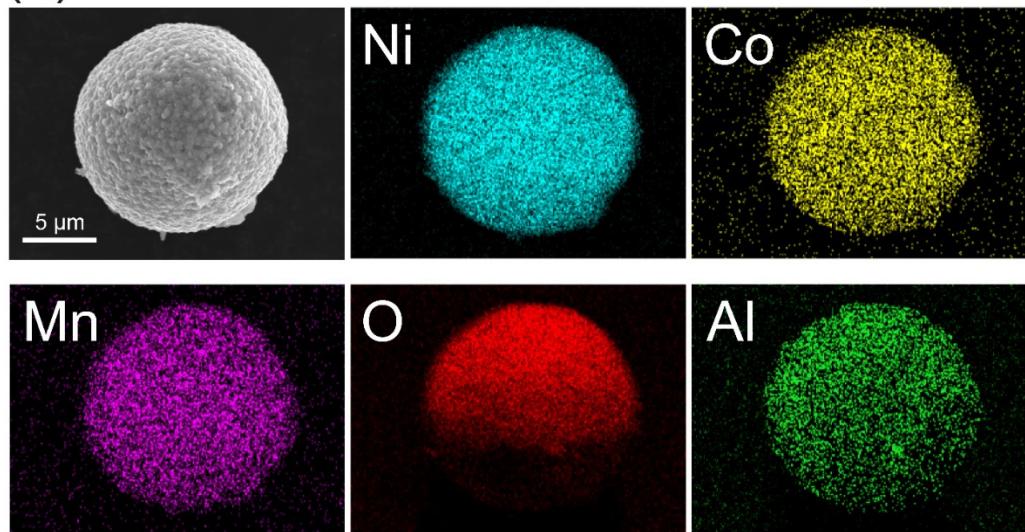


Figure S3. (a) Co $2p$ XPS spectra and (b) Mn $2p$ XPS spectra of uncoated and coated NCMs.

(a) NCM-Al



(b) NCM-Nb

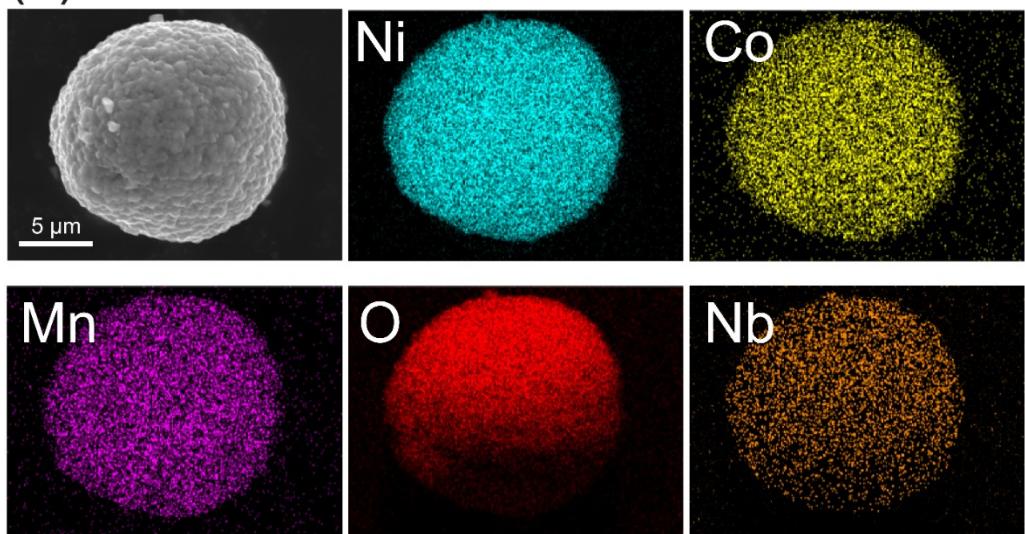
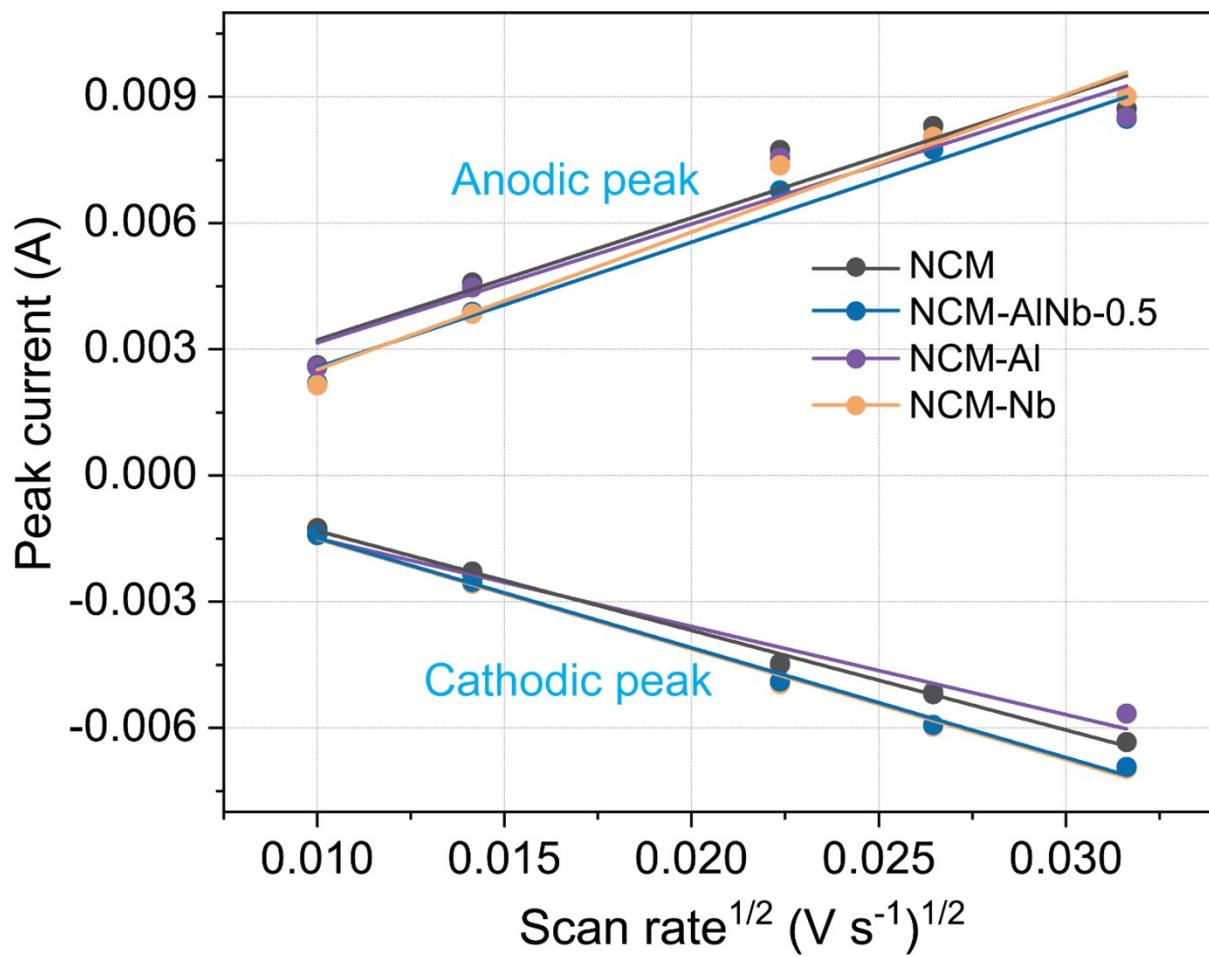


Figure S4. SEM images and EDS mapping of (a) NCM-Al, and (b) NCM-Nb.

Table S1. Comparison of electrochemical performances of Al_2O_3 - LiNbO_3 co-coated NCM811 with those in other recently published papers that use either Al or Nb-based materials for coating.

Active material	Coating material	Specific capacity (mAh g ⁻¹)	Retention	Ref.
$\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$	Al_2O_3 - LiNbO_3 (wet process)	180.85 (0.5C, 2.75-4.3V)	92.08% (0.5C, 100 cycles)	This work
$\text{LiNi}_{0.7}\text{Co}_{0.15}\text{Mn}_{0.15}\text{O}_2$	Al_2O_3 (wet process)	160 (0.5C, 3.0-4.3V)	~90% (0.5C, 130 cycles)	¹
LiCoO_2	Al_2O_3 (wet process)	174 (0.1C, 2.75-4.4V)	~97% (0.5C, 50 cycles)	²
$\text{Li}[\text{Ni}_{0.8}\text{Co}_{0.2}]_{0.7}[\text{Ni}_{0.2}\text{Mn}_{0.8}]_{0.3}\text{O}_2$	Al_2O_3 (wet process)	197 (0.2C, 2.7-4.5V)	88.83% (0.2C, 100 cycles)	³
$\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$	Al_2O_3 (wet process)	171.4 (0.1C, 2.5-4.2V)	83.4% (0.1C, 100 cycles)	⁴
$\text{LiNi}_{0.6}\text{Co}_{0.2}\text{Mn}_{0.2}\text{O}_2$	PVA/ Al_2O_3 (sol-gel)	203.95 (0.5C, 3.0-4.55V)	90% (0.5C, 100 cycles)	⁵
Mg-doped $\text{LiNi}_{0.6}\text{Co}_{0.2}\text{Mn}_{0.2}\text{O}_2$	LiNbO_3 (wet process)	155 (1C, 2.8-4.3V)	90.82% (1C, 100 cycles)	⁶
$\text{LiNb}_{0.83}\text{Co}_{0.11}\text{Mn}_{0.06}\text{O}_2$	$\text{C}_4\text{H}_4\text{NNbO}_9$	211.8 (0.2C, 2.7-4.4V)	86.6% (1C, 100 cycles)	⁷
$\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$	Nb_2O_5	200.2 (0.1C, 3.0-4.3V)	90.6 % (0.1C, 100 cycles)	⁸
$\text{LiNb}_{0.83}\text{Co}_{0.11}\text{Mn}_{0.06}\text{O}_2$	Nb_2O_5	195 (0.1C)	86.6% (1C, 200 cycles)	⁹
$\text{LiNi}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$	LiNbO_3	207.2 (0.2C, 3.0-4.5V)	~83% (1C, 100 cycles)	¹⁰



Anodic peak

Sample	NCM	NCM-AlNb-0.5	NCM-AI	NCM-Nb
Intercept	3.15876E-4	-4.02915E-4	3.33203E-4	-7.53677E-4
Slope	0.29041 ± 0.045	0.29733 ± 0.028	0.2821 ± 0.043	0.32685 ± 0.034

Cathodic peak

Sample	NCM	NCM-AlNb-0.5	NCM-AI	NCM-Nb
Intercept	0.00105	0.00112	5.98284E-4	0.00111
Slope	-0.2367 ± 0.008	-0.26092 ± 0.010	-0.20949 ± 0.020	-0.26221 ± 0.011

Figure S5. Relationship between the peak current (I_p) and the square root of the scan rate ($v^{1/2}$).

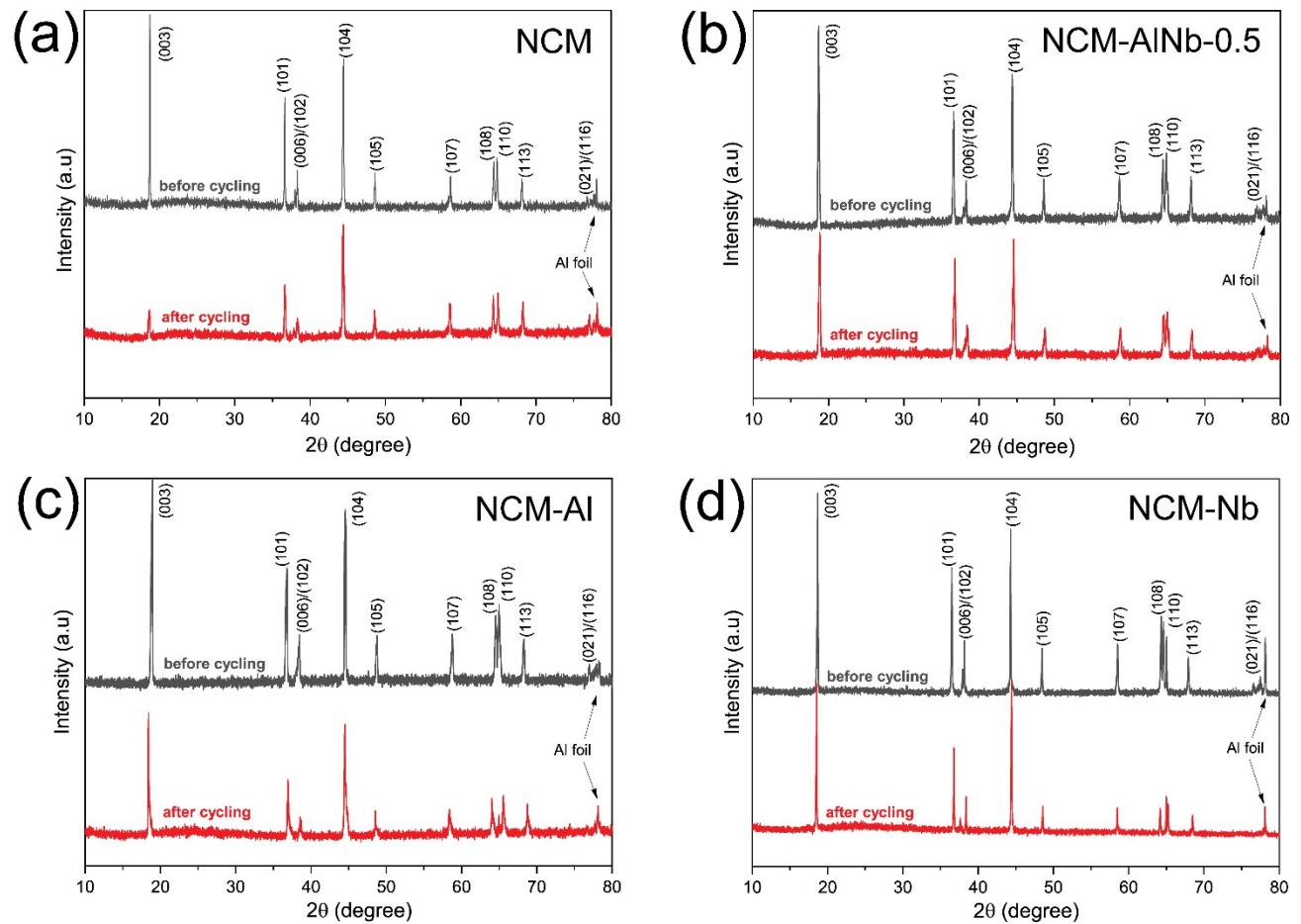


Figure S6. XRD spectra of (a) uncoated NCM, (b) NCM-AlNb-0.5, (c) NCM-Al and (d) NCM-Nb electrode before and after 100 charge-discharge cycles.

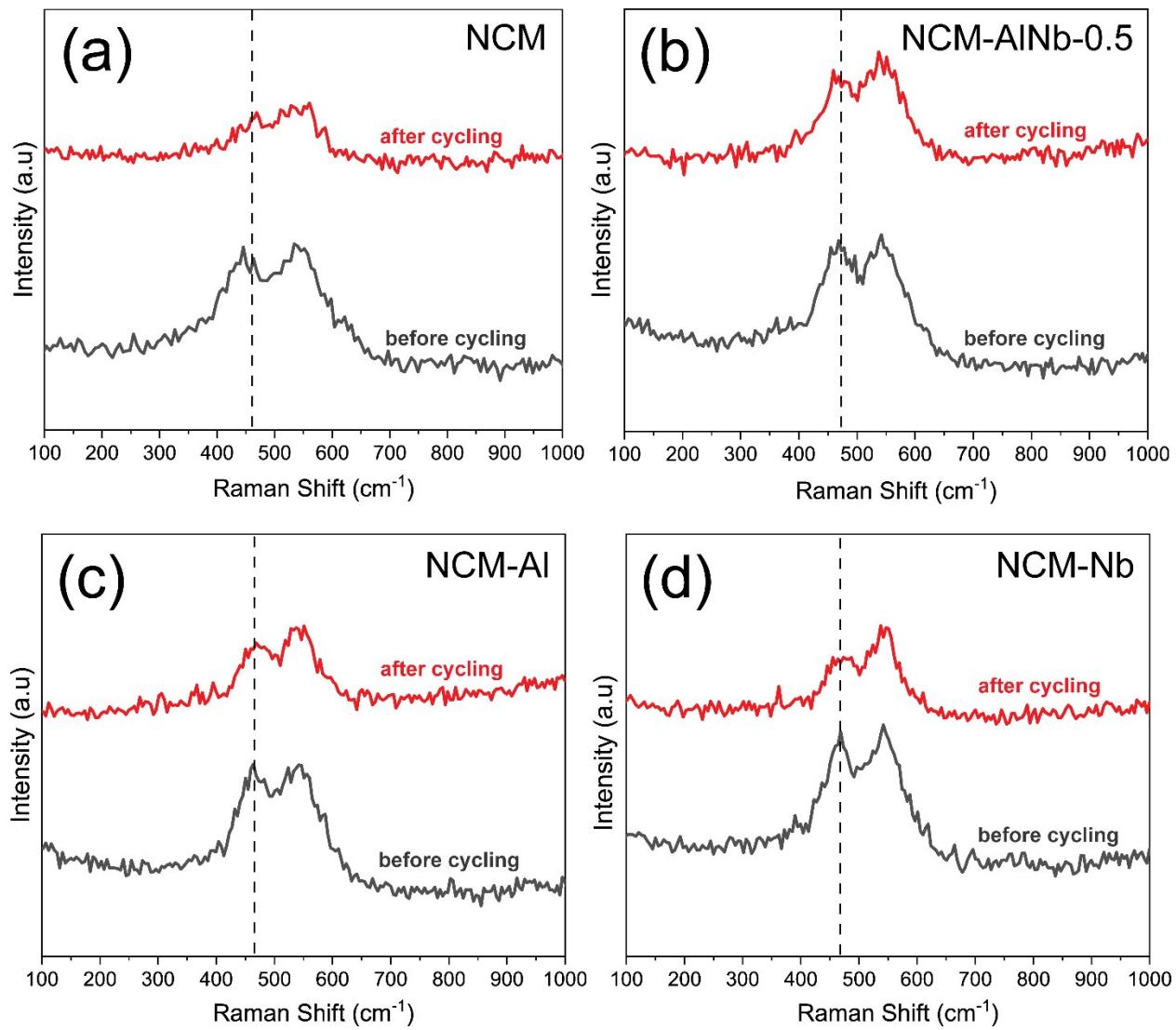


Figure S7. Raman spectra of (a) uncoated NCM, (b) NCM-AlNb-0.5, (c) NCM-Al and (d) NCM-Nb electrode before and after 100 charge-discharge cycles.

References

- 1 R. S. Negi, S. P. Culver, A. Mazilkin, T. Brezesinski and M. T. Elm, *ACS Appl. Mater. Interfaces*, 2020, **12**, 31392–31400.
- 2 J. Cho, Y. J. Kim and B. Park, *Chem. Mater.*, 2000, **12**, 3788–3791.
- 3 J.-Y. Liao and A. Manthiram, *Journal of Power Sources*, 2015, **282**, 429–436.
- 4 S. Hildebrand, C. Vollmer, M. Winter and F. M. Schappacher, *Journal of The Electrochemical Society*, 2017, **164**, A2190.
- 5 Y. Wu, M. Li, W. Wahyudi, G. Sheng, X. Miao, T. D. Anthopoulos, K.-W. Huang, Y. Li and Z. Lai, *ACS Omega*, 2019, **4**, 13972–13980.
- 6 P. Venkatachalam, K. K. Duru, M. Rangarajan, S. Sangaraju, P. S. Maram and S. Kalluri, *Journal of Solid State Electrochemistry*, , DOI:10.1007/s10008-024-05863-0.
- 7 T. Li, X. Chang, Y. Xin, Y. Liu and H. Tian, *J. Phys. Chem. C*, 2023, **127**, 8448–8461.
- 8 Y.-R. Kim, Y.-W. Yoo, D.-Y. Hwang, T.-Y. Shim, C.-Y. Kang, H.-J. Park, H.-S. Kim and S.-H. Lee, *Solid State Ionics*, 2023, **389**, 116108.
- 9 J. Wang, Z. Yi, C. Liu, M. He, C. Miao, J. Li, G. Xu and W. Xiao, *Journal of Colloid and Interface Science*, 2023, **635**, 295–304.
- 10 H. Yu, S. Wang, Y. Hu, G. He, L. Q. Bao, I. P. Parkin and H. Jiang, *Green Energy & Environment*, 2022, **7**, 266–274.