

Supporting Information

Insights into Boron-based Polyanion-tuned High-nickel Cathodes for High-energy-density Lithium-ion Batteries

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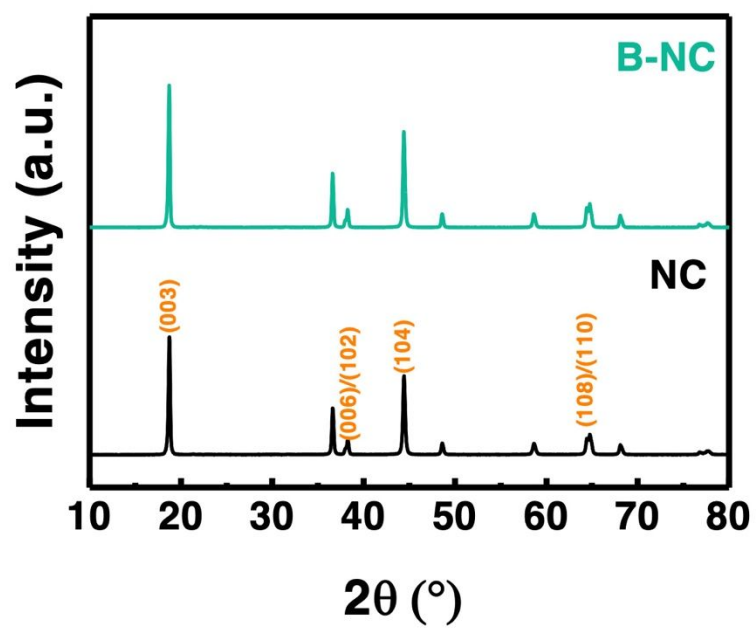


Figure S1. XRD patterns of the fresh NC and B-NC samples.

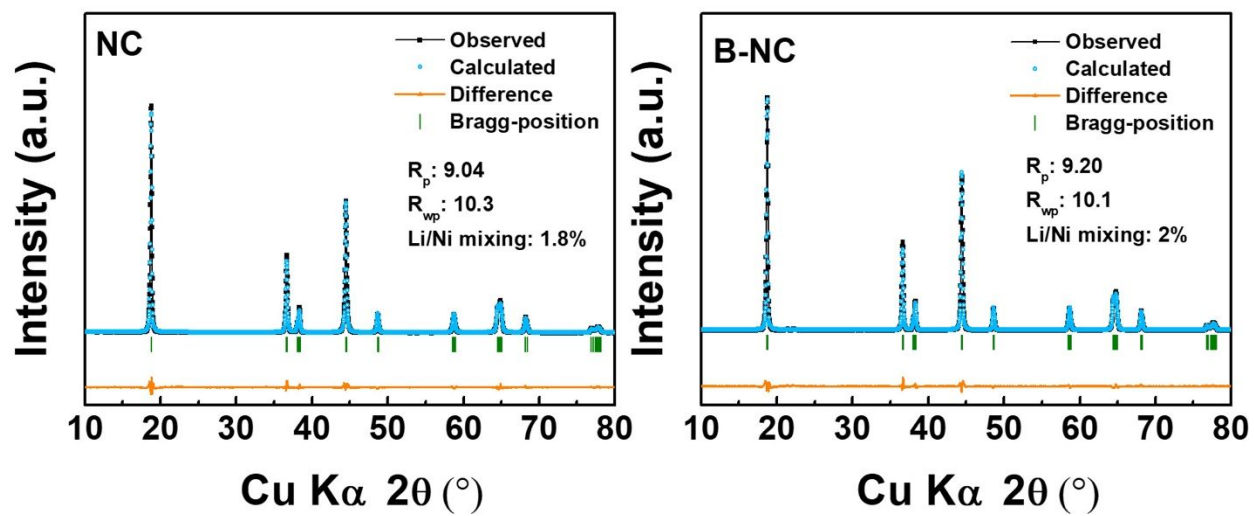


Figure S2. XRD refinement results of the fresh NC and B-NC samples. $\chi^2 = 3.88$ for NC, and $\chi^2 = 4.97$ for B-NC.

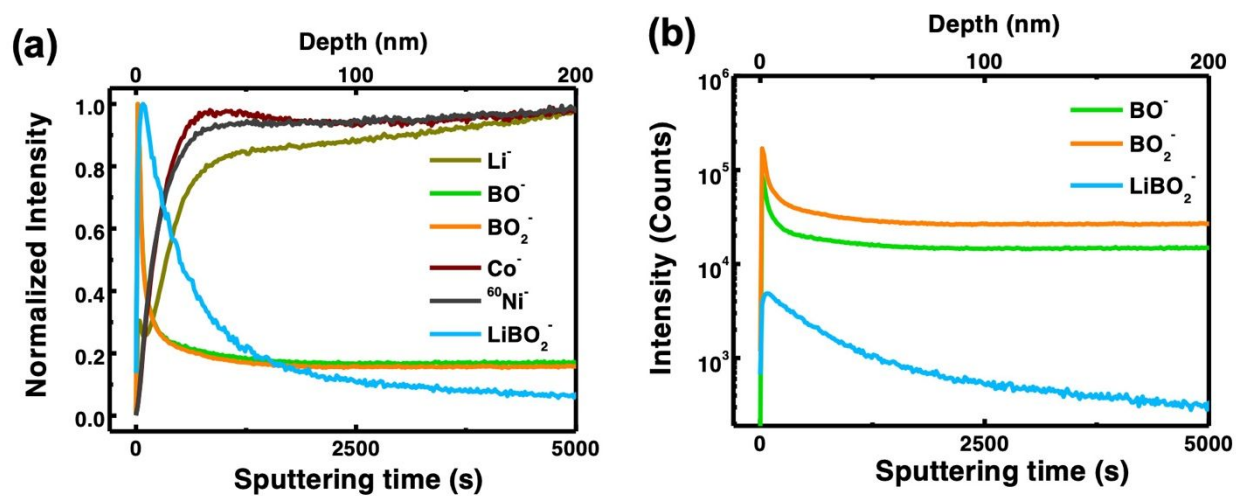


Figure S3. TOF-SIMS depth profiling of the representative boron-bearing and bulk-material species in the fresh pristine B-NC sample.

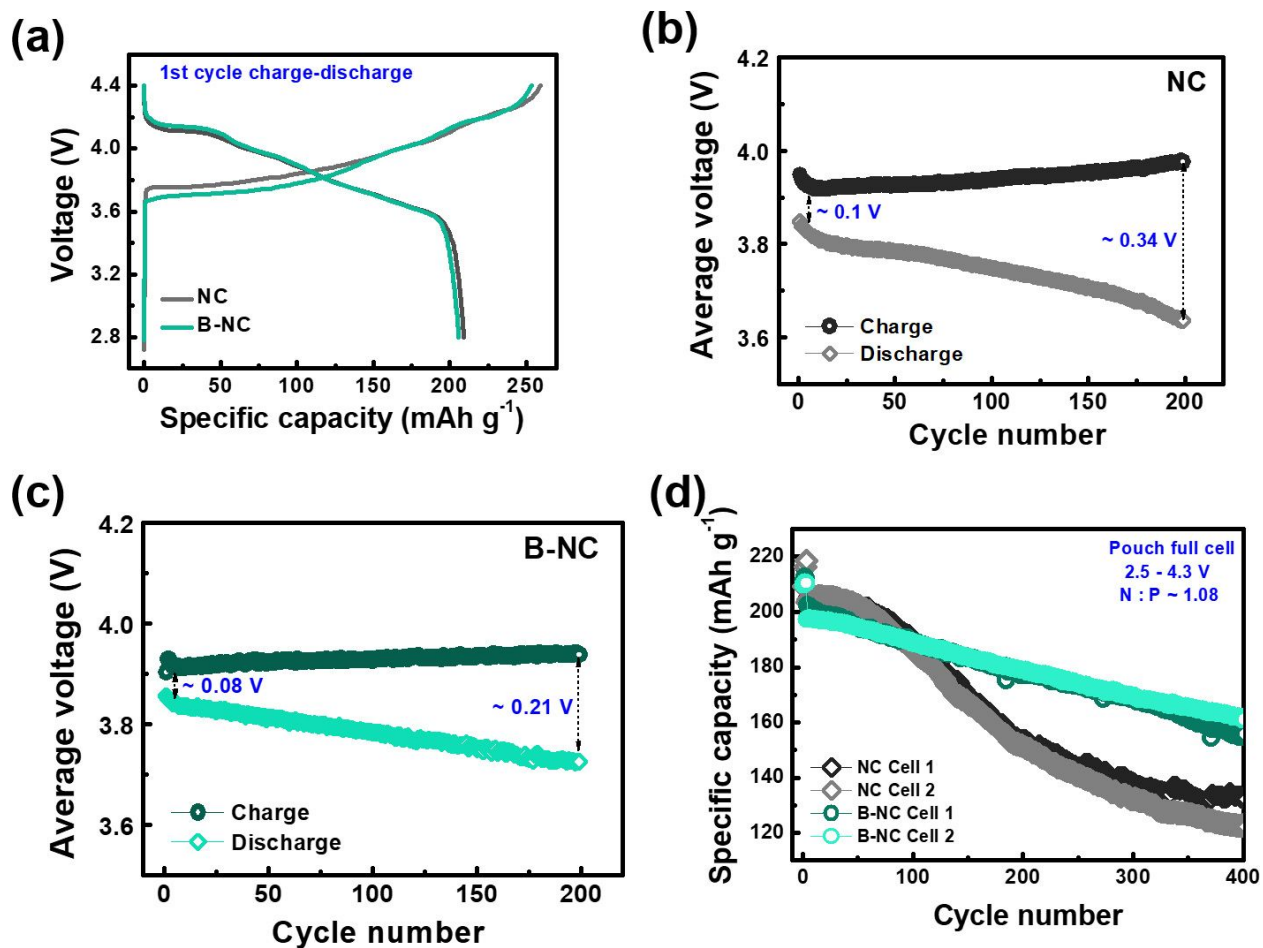


Figure S4. (a) First charge-discharge curves of fresh NC and B-NC. (b) and (c) Average charge/discharge voltage of NC and B-NC. (d) Extra pouch-full cell cycling data of NC and B-NC.

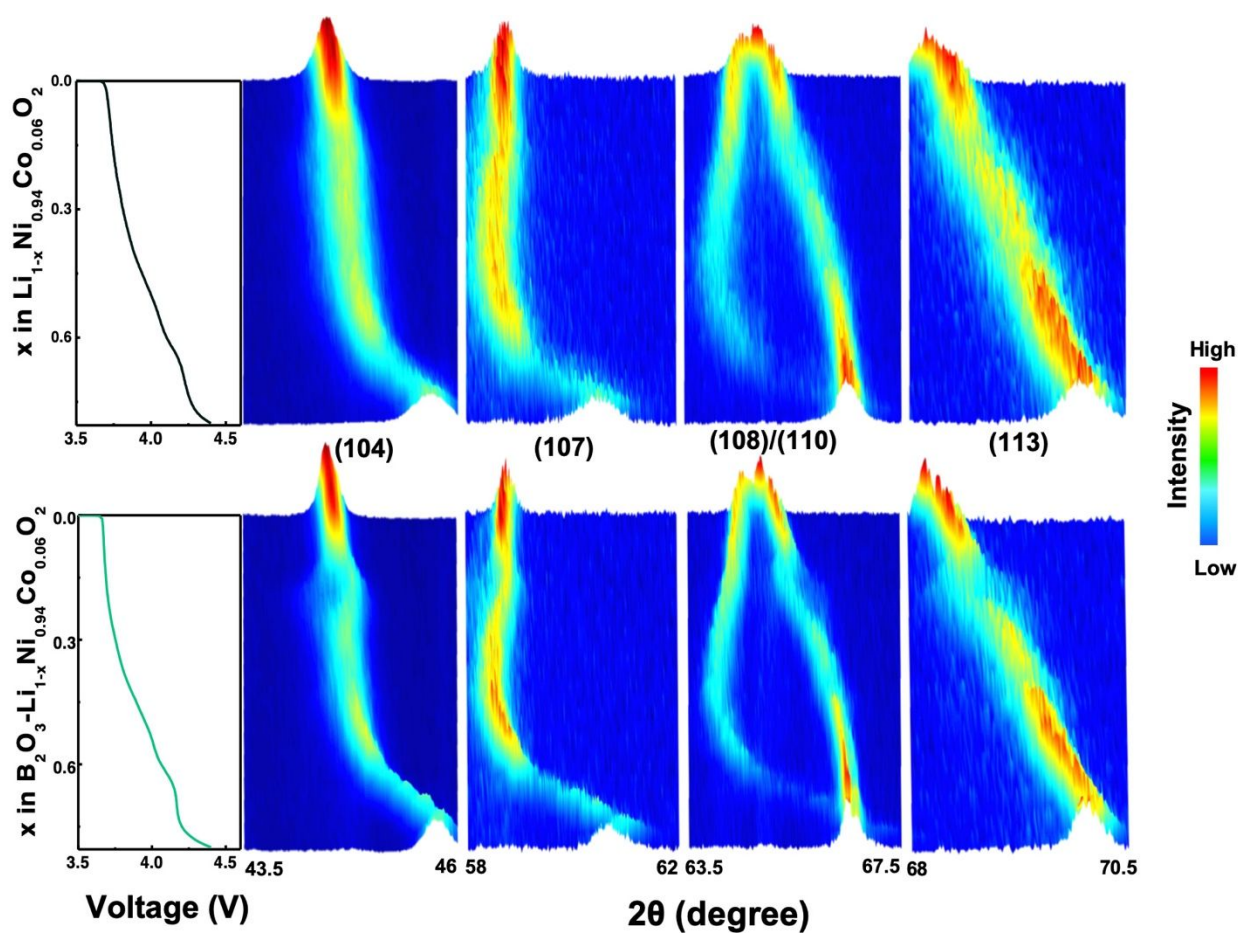


Figure S5. *In-situ* XRD contour plot of (104) - (110) diffraction peaks as a function of the state of delithiation.

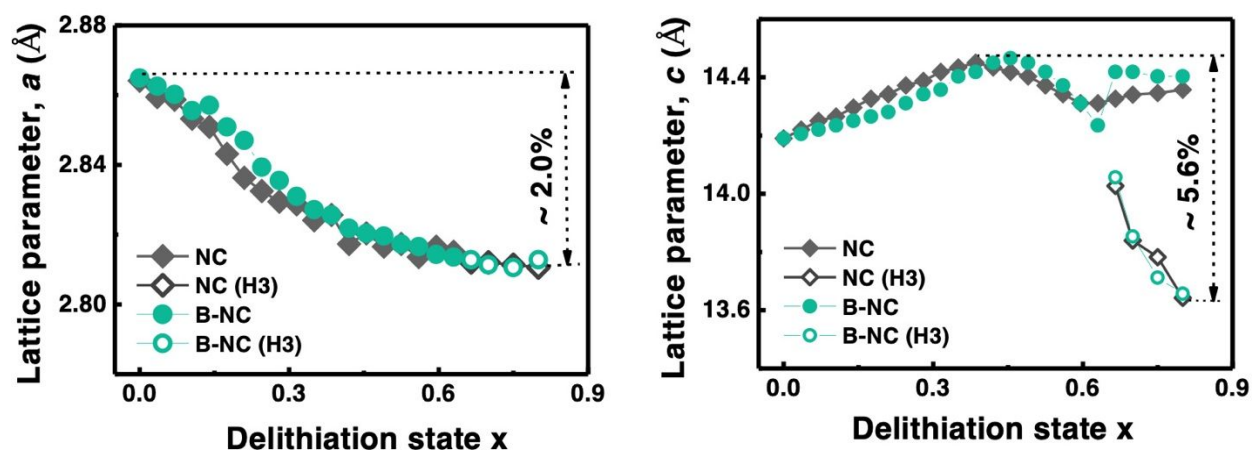


Figure S6. Evolution of the lattice parameters a and c as a function of state of delithiation x for fresh NC and B-NC samples upon charging (x in $\text{Li}_{1-x}\text{Ni}_{0.94}\text{Co}_{0.06}\text{O}_2$ and $\text{B}_2\text{O}_3\text{-Li}_{1-x}\text{Ni}_{0.94}\text{Co}_{0.06}\text{O}_2$).

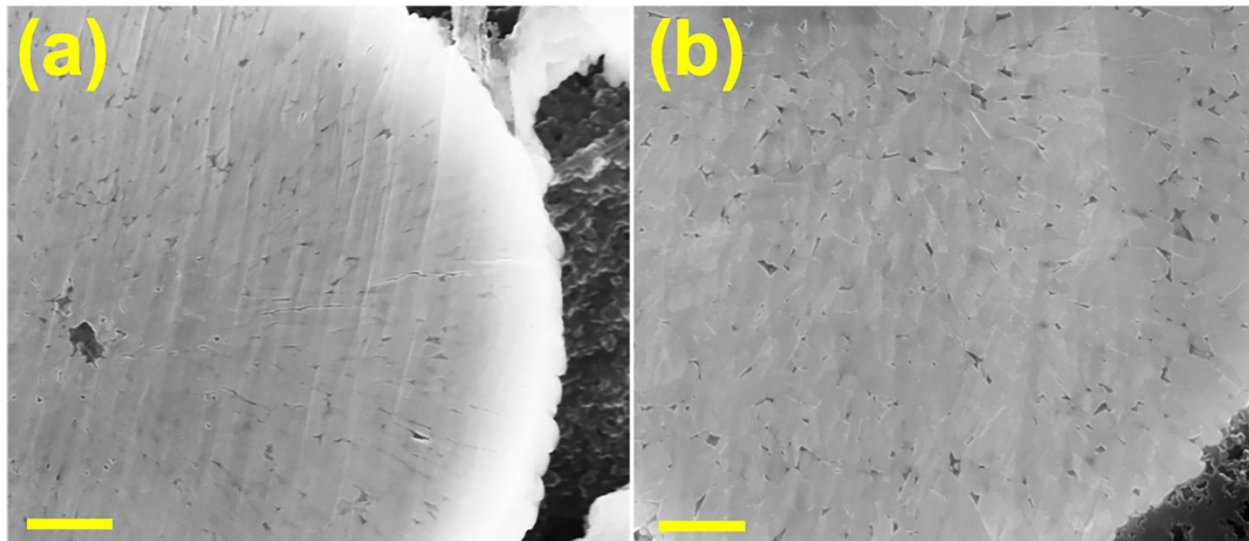


Figure S7. Cross-section SEM images for NC (a) and B-NC (b) after 400 cycles in pouch full cell. The scale bar in the images is 1 μ m

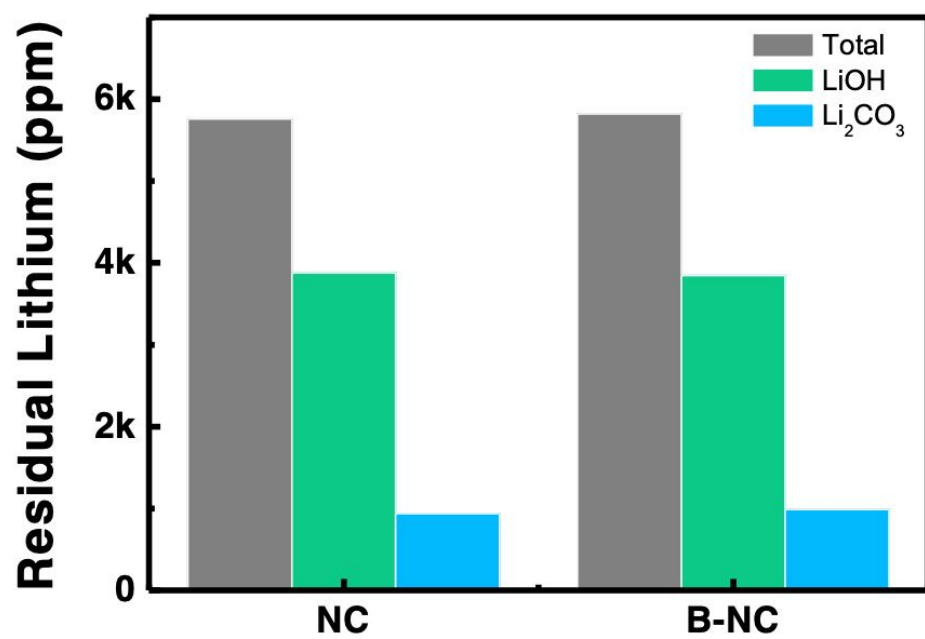


Figure S8. Content of the surface residual lithium of the fresh NC and B-NC

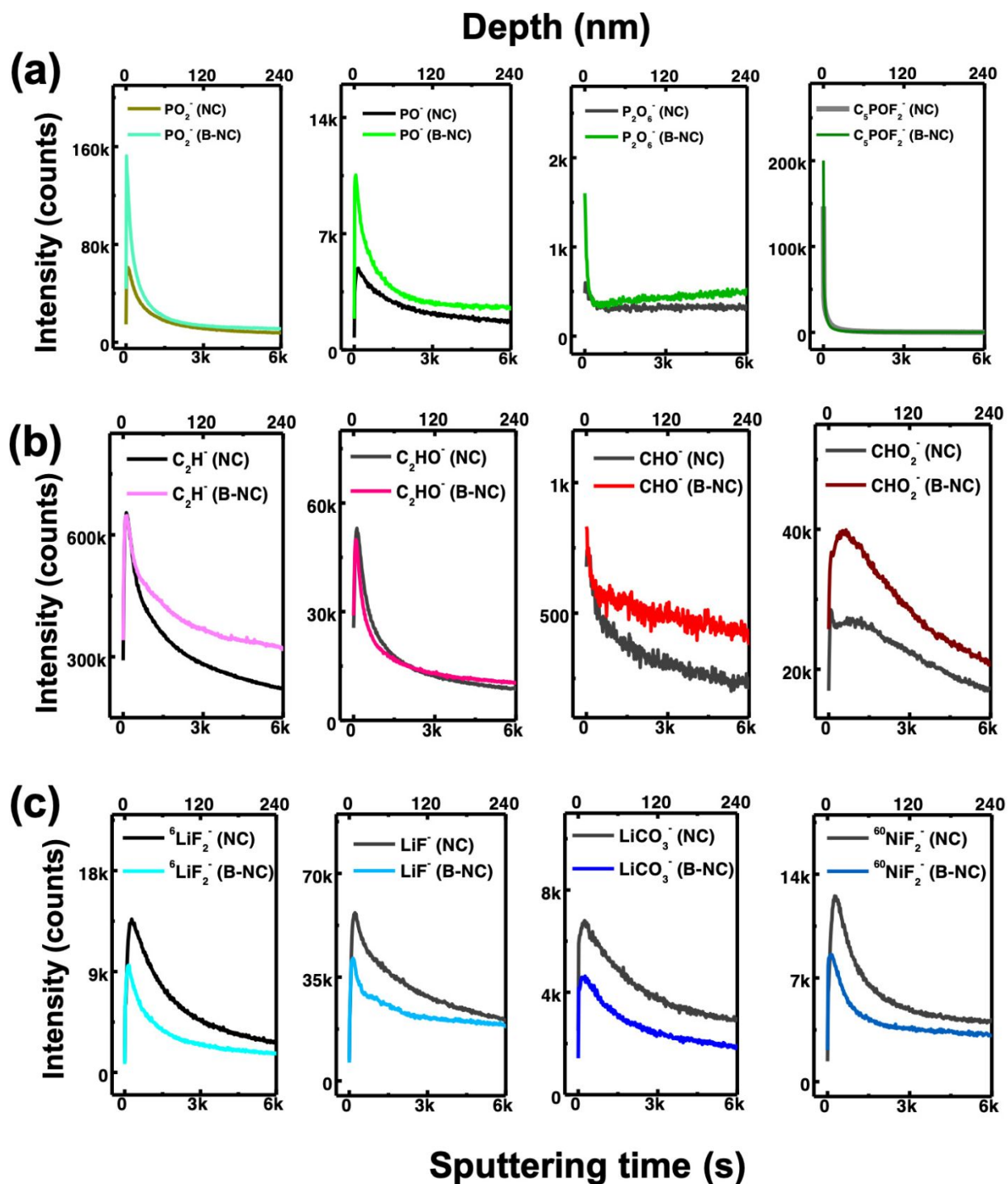


Figure S9. TOF-SIMS depth profiling of the representative cathode/electrolyte interphase (CEI) species for NC and B-NC. (a) and (b) Non-metal organic/inorganic species, (c) metal-based species.

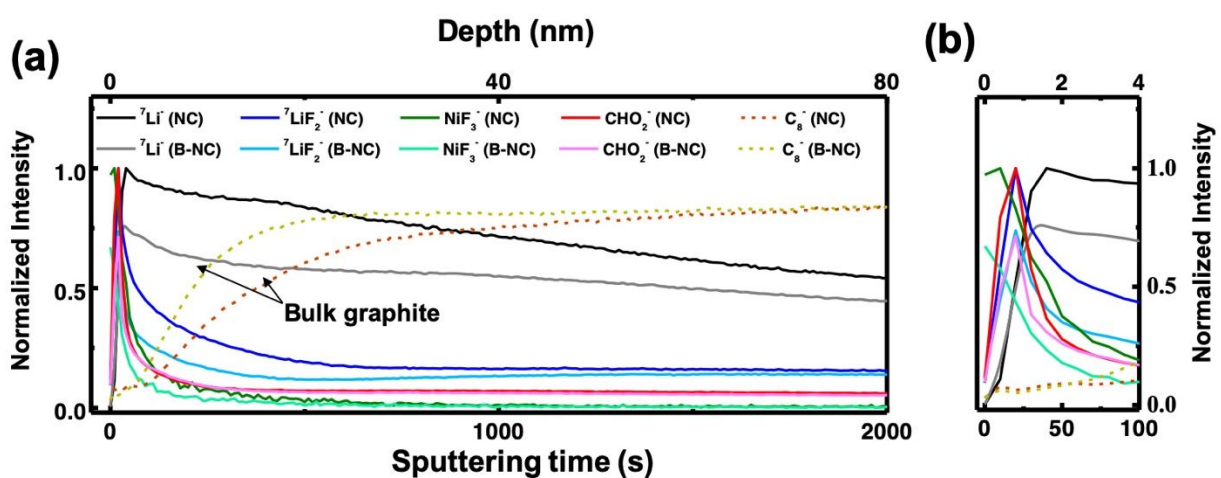


Figure S10. (a) TOF-SIMS depth profiling of the characteristic solid/electrolyte interphase (SEI) species in the graphite anodes paired with NC and B-NC samples after 400 cycles in pouch full cells, (b) the enlarged section of (a) for the first 100s sputtering. Note that the normalization of the species of ${}^7\text{Li}^+$, ${}^7\text{LiF}_2^+$, NiF_3^+ and CHO_2^+ in B-NC is on basis of the intensity of the corresponding species in NC.

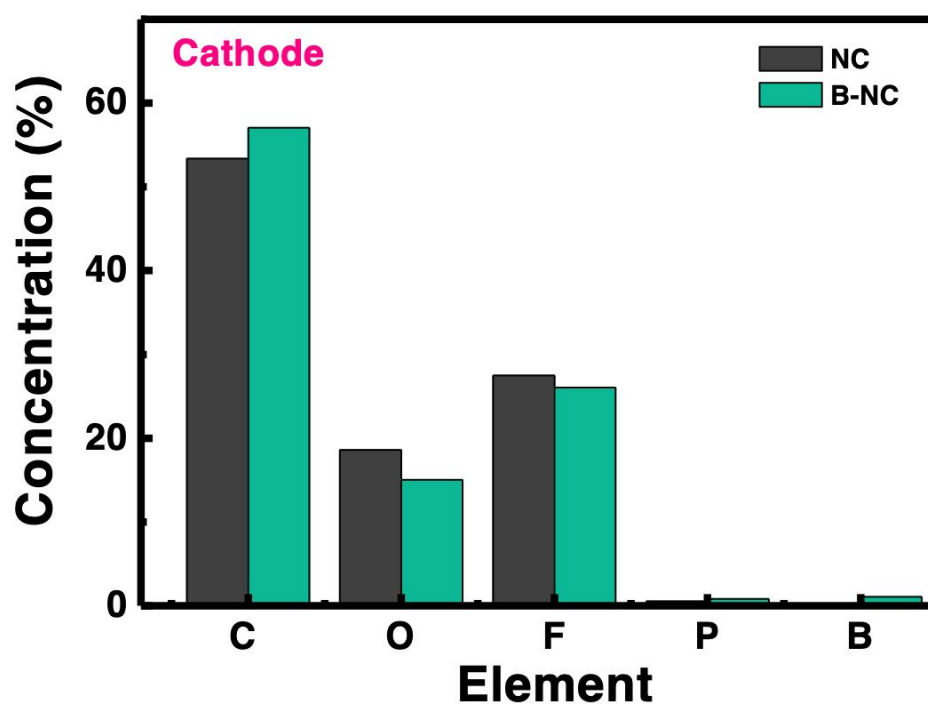


Figure S12. XPS element concentration harvested from the NC and B-NC cathodes after 400 cycles in pouch full cells.

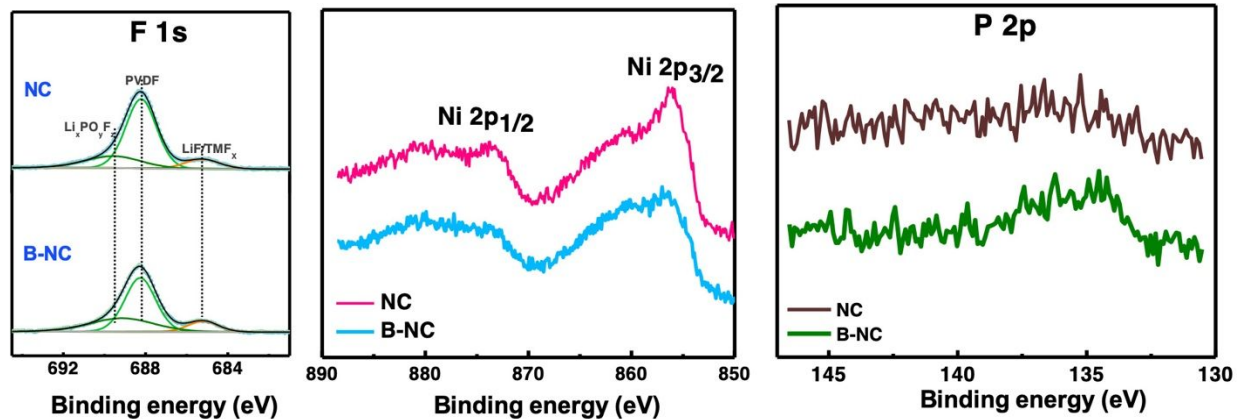


Figure S13. XPS F 1s, Ni 2p, and P 2p spectra obtained from the NC and B-NC cathodes after 400 cycles in pouch full cells.

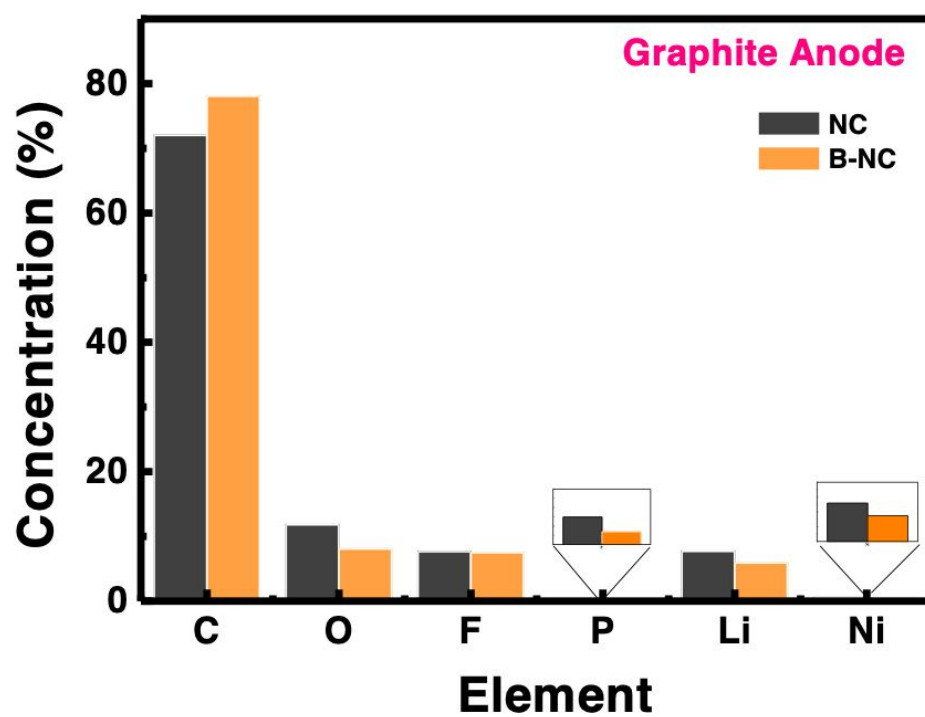


Figure S14. XPS element concentration harvested from the graphite anodes paired with NC and B-NC cathodes after 400 cycles in pouch full cells.

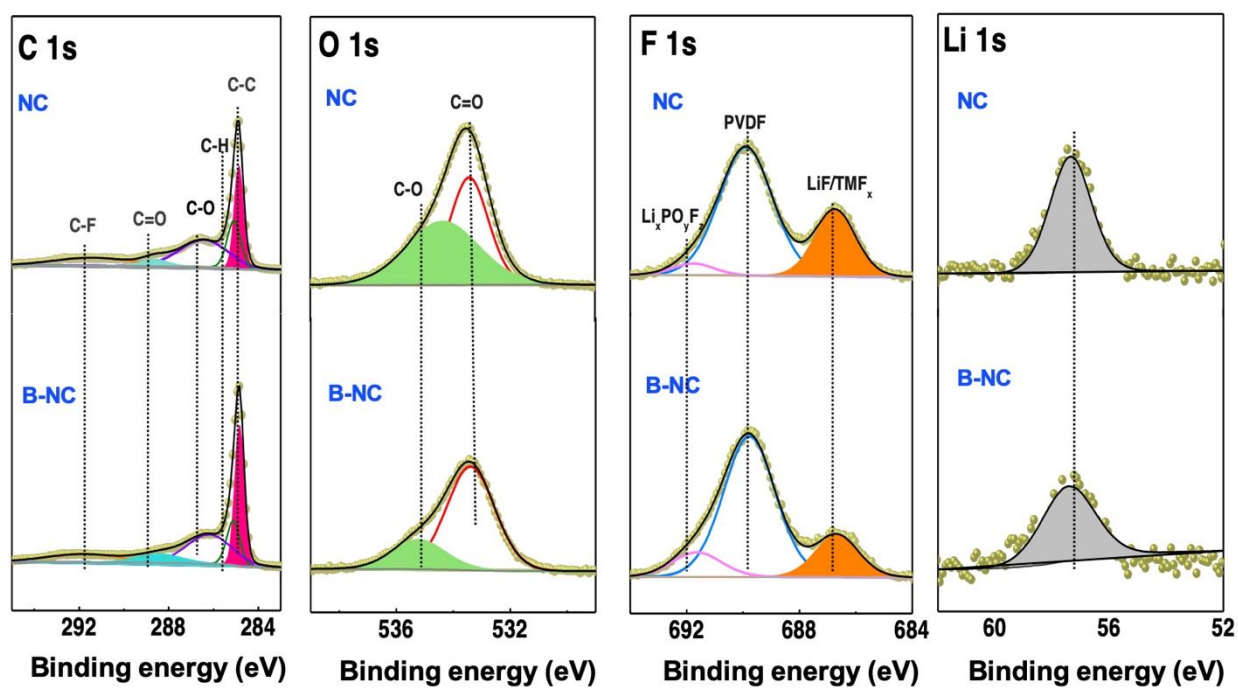


Figure S15. XPS C 1s, O 1s, F 1s, and Li 1s spectra obtained from the graphite anodes coupled with NC and B-NC cathodes after 400 cycles in pouch full cells.

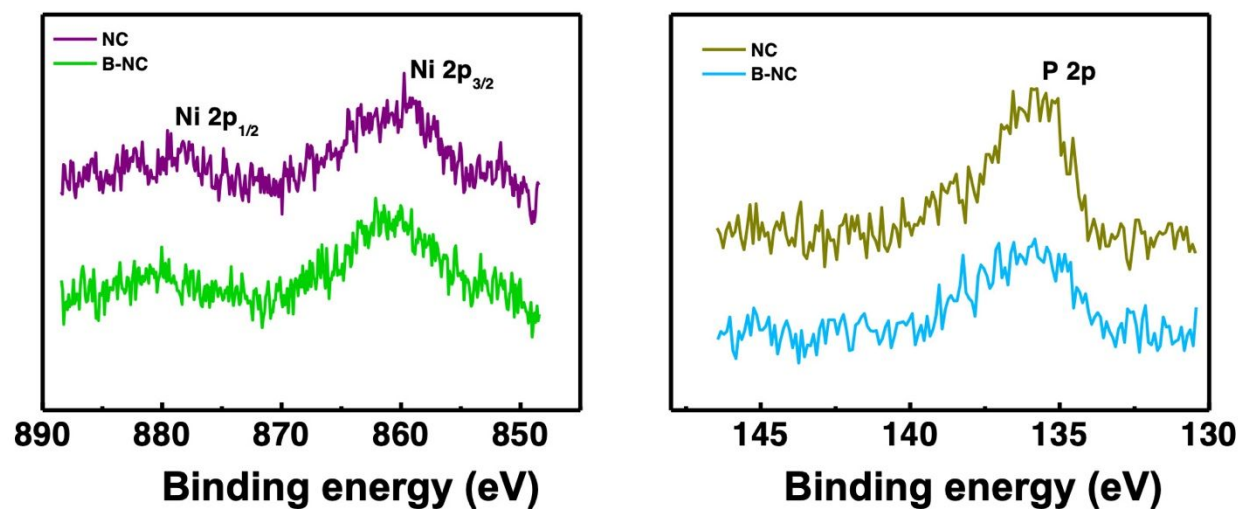


Figure S16. XPS Ni 2p and P 2p spectra obtained from the graphite anodes paired with NC and B-NC cathodes after 400 cycles in pouch full cells.

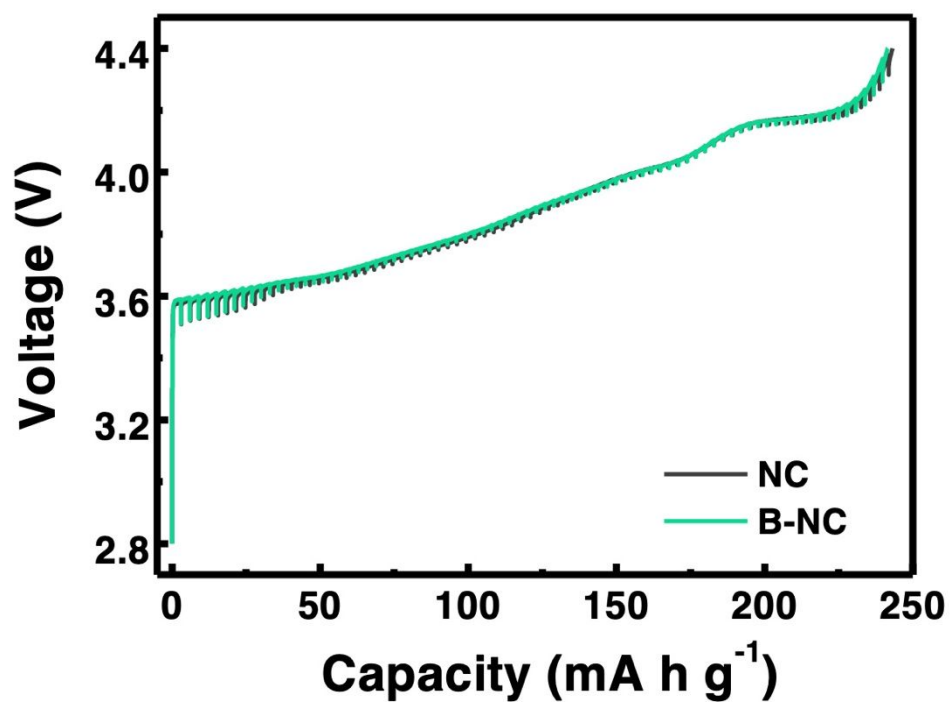


Figure S17. GITT curves of the fresh NC and B-NC upon charging.

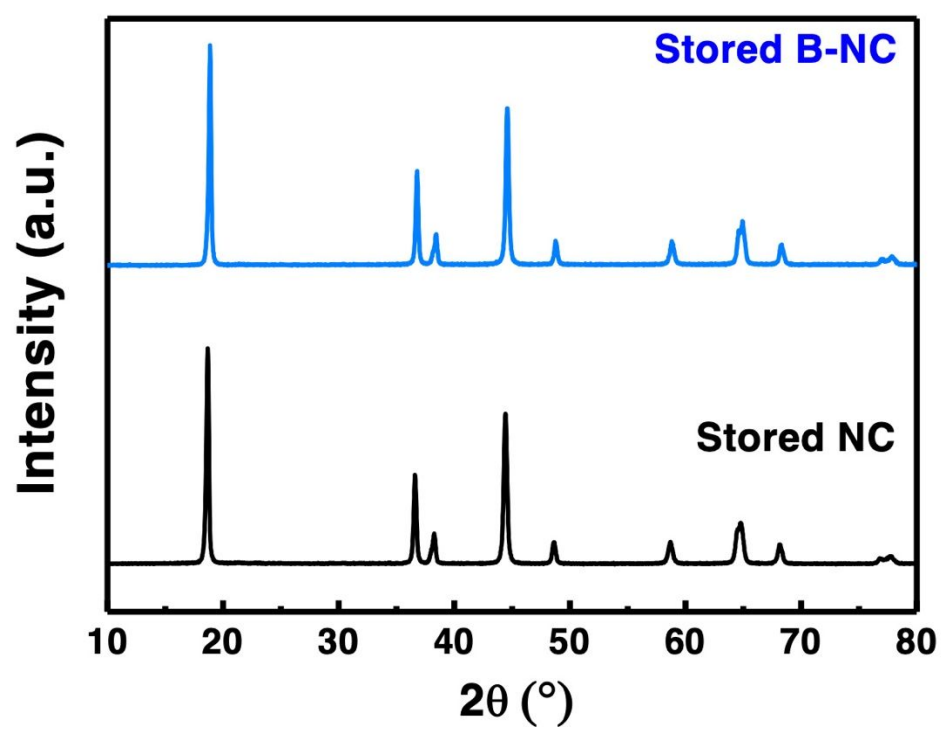


Figure S18. XRD patterns of the 30-day air stored NC and B-NC samples.

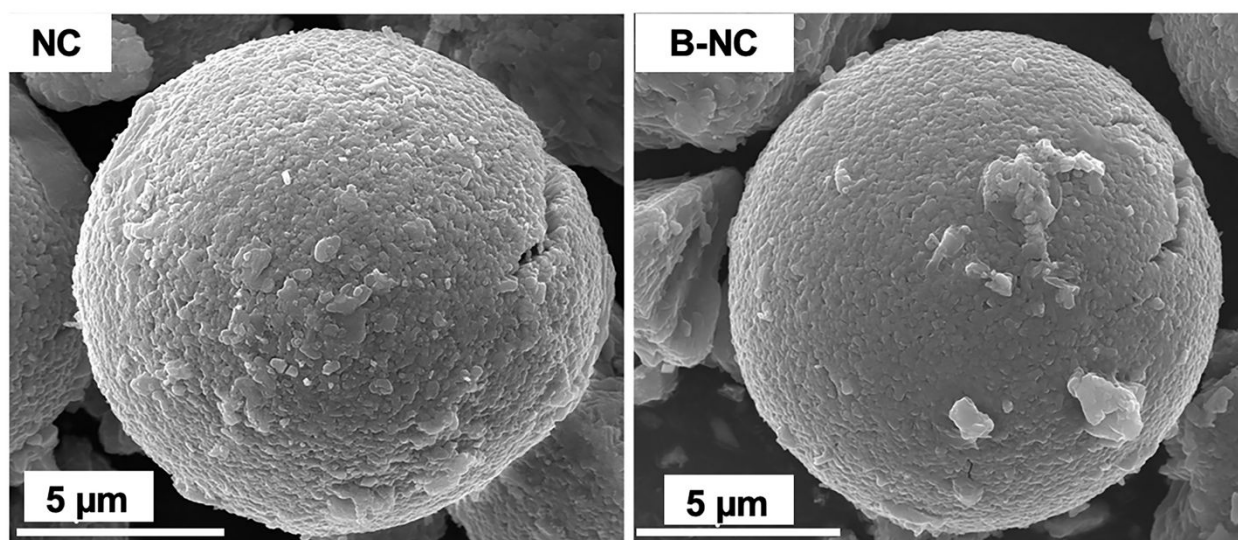


Figure S19. SEM images of the 30-day air stored NC and B-NC samples.

Table S1. Comparison of the lattice parameters and Li/Ni mixing for fresh NC and B-NC

Samples	<i>a</i>-axis (Å)	<i>c</i>-axis (Å)	<i>V</i> (Å³)	Li/Ni mixing
NC	2.8711(0)	14.1760(0)	101.2001(0)	1.8%
B-NC	2.8747(9)	14.1905(0)	101.5641(8)	2.0%