

Supporting Information

Structural underpinnings of the enhanced cycling stability upon Al-substitution in $\text{LiNi}_{0.45}\text{Mn}_{0.45}\text{Co}_{0.1-y}\text{Al}_y\text{O}_2$ positive electrode materials for Li-ion batteries

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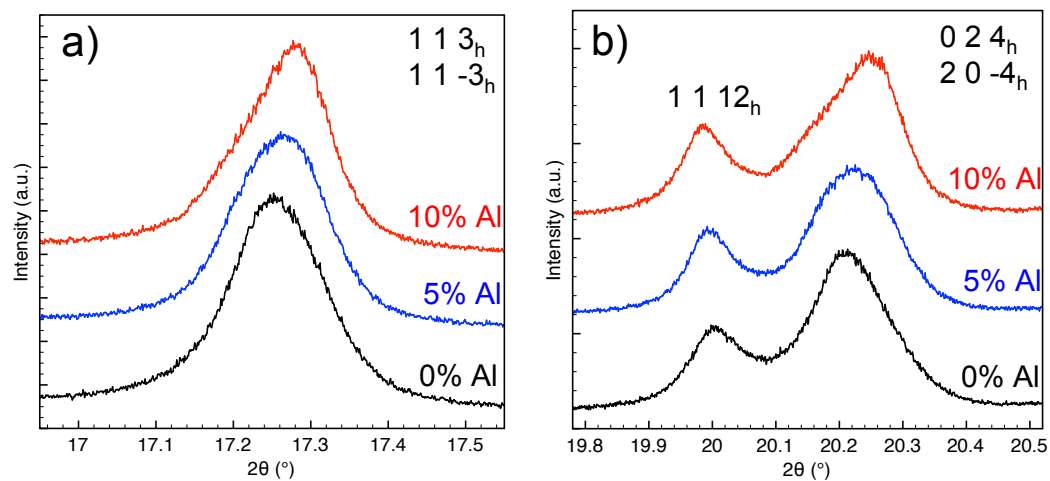


Figure S1: Peak splitting is observed with high values of Al-substitution, indicating a structural distortion within the transition metal planes.

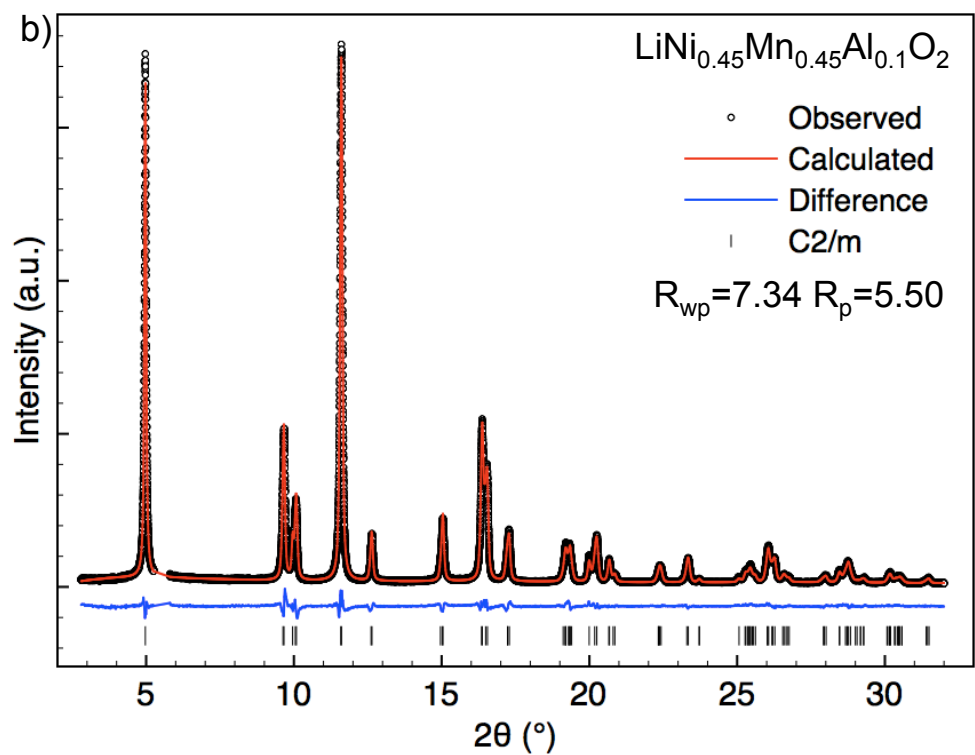
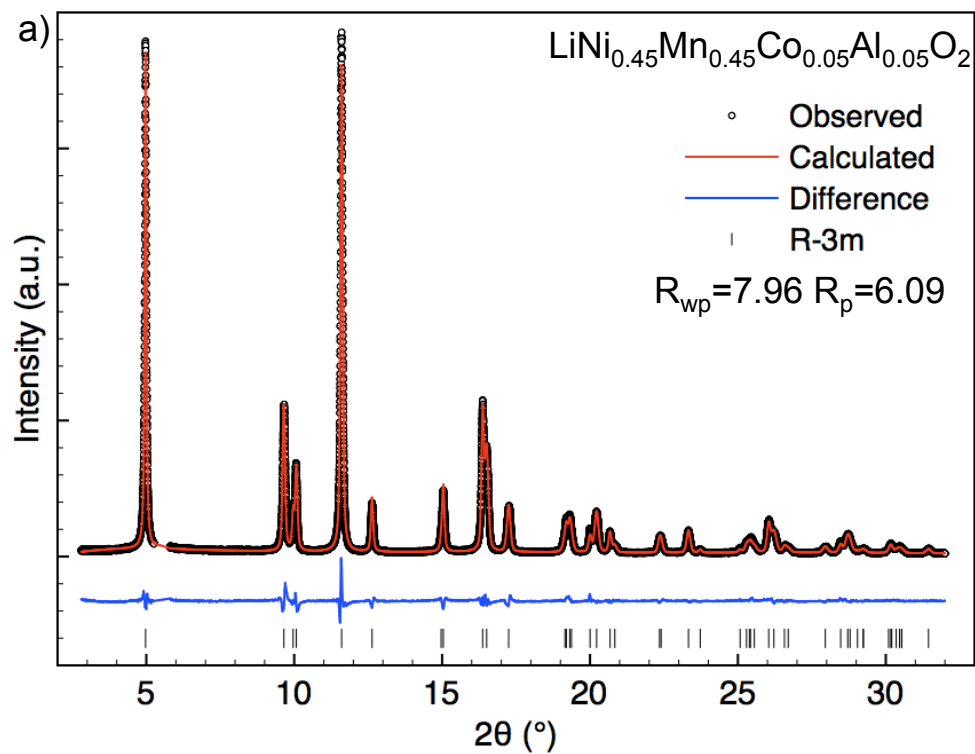


Figure S2: High-resolution XRD patterns and Rietveld refinements for $\text{LiNi}_{0.45}\text{Mn}_{0.45}\text{Co}_{0.1-y}\text{Al}_y\text{O}_2$ with a) $y=0.05$ and b) $y=0.10$.

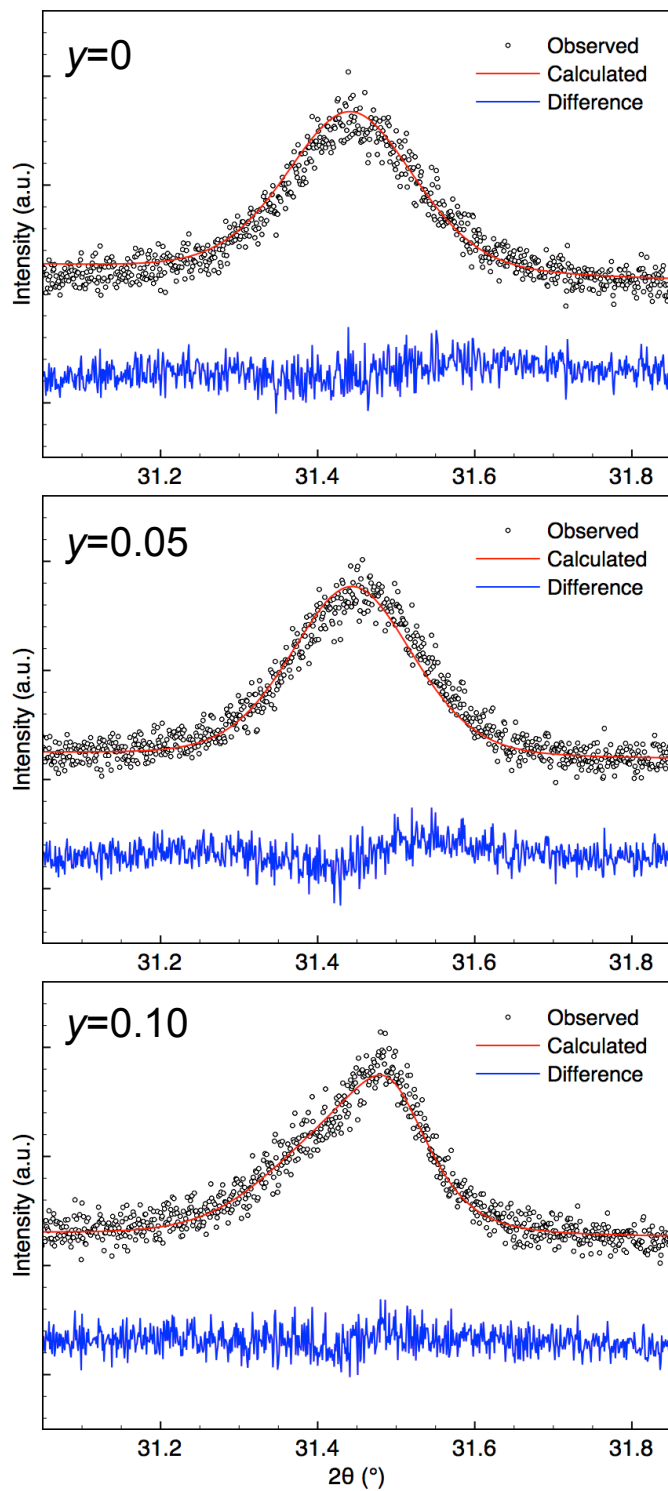


Figure S3: Magnification of the 1 2 11 reflection ($R\bar{3}m$) showing the Rietveld fits for a) $y=0$, b) $y=0.05$ and c) $y=0.10$. $R\bar{3}m$ symmetry was used in (a) and (b), while $C2/m$ was used for (c).

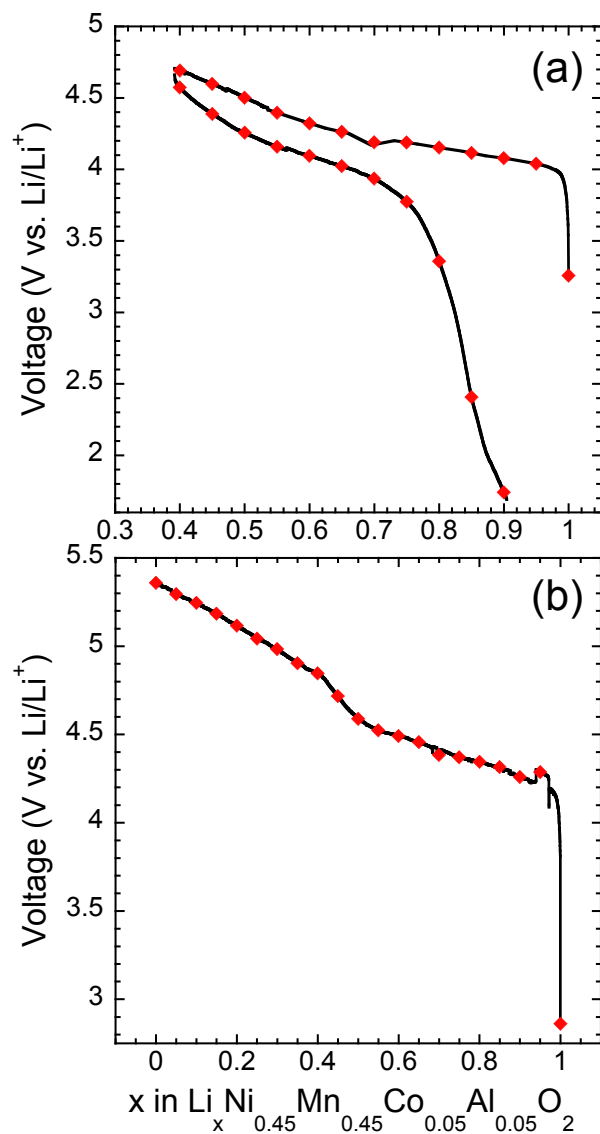


Figure S4: Voltage vs. x in $\text{Li}_x\text{Ni}_{0.45}\text{Mn}_{0.45}\text{Co}_{0.05}\text{Al}_{0.05}\text{O}_2$ ($y=0.05$) for the first cycle during *in situ* XRD testing. Pouch cells were a) cycled, b) fully charged. The points at which diffraction data is presented are indicated.

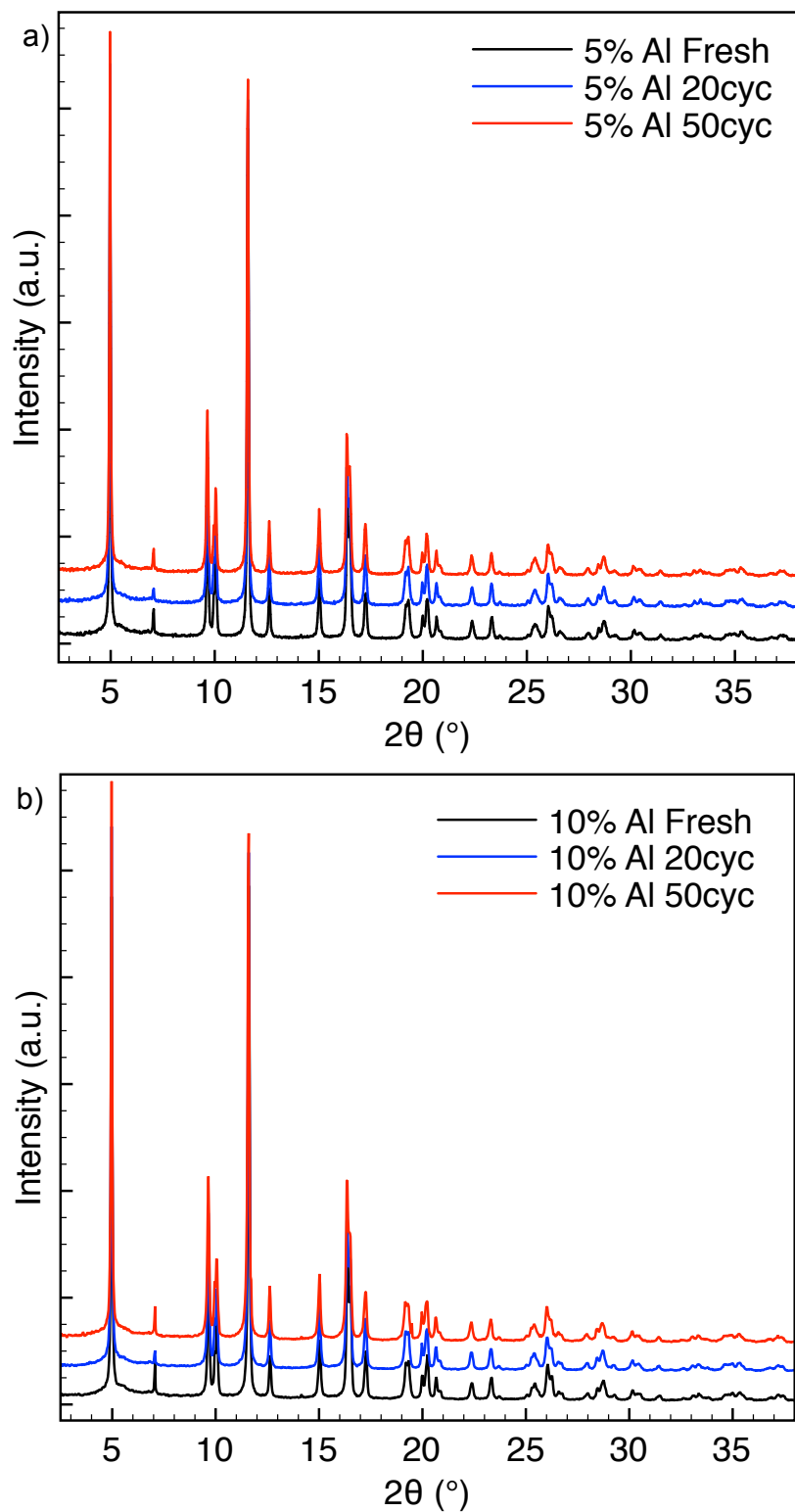


Figure S5: High-resolution XRD patterns of fresh and cycled $\text{LiNi}_{0.45}\text{Mn}_{0.45}\text{Co}_{0.1-y}\text{Al}_y\text{O}_2$ electrodes with a) $y=0.05$ and b) $y=0.10$. The small peak at $\sim 7^\circ$ 2θ is due to graphite.