

Supplementary Information:

Investigation of the Electrochemical Performance and Structural Stability of O6-Type Lithium-Rich Layered Oxide as a Positive Electrode Active Material for Improved Lithium Battery Performance

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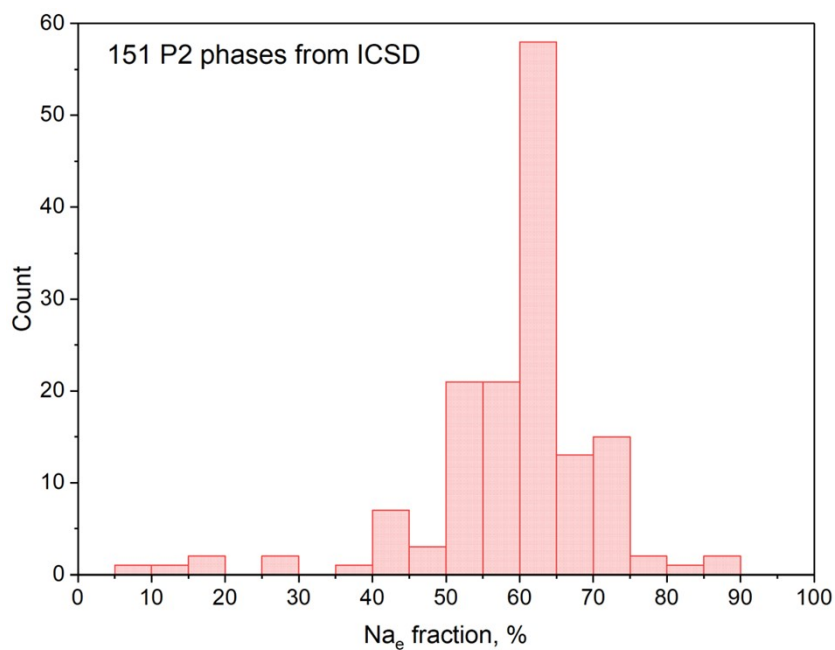


Figure S1. Analysis of the Na_e site occupancy for the 152 sodium phases of P2-type structures reported in the Inorganic Crystal Structure Database (<https://icsd.products.fiz-karlsruhe.de/>).

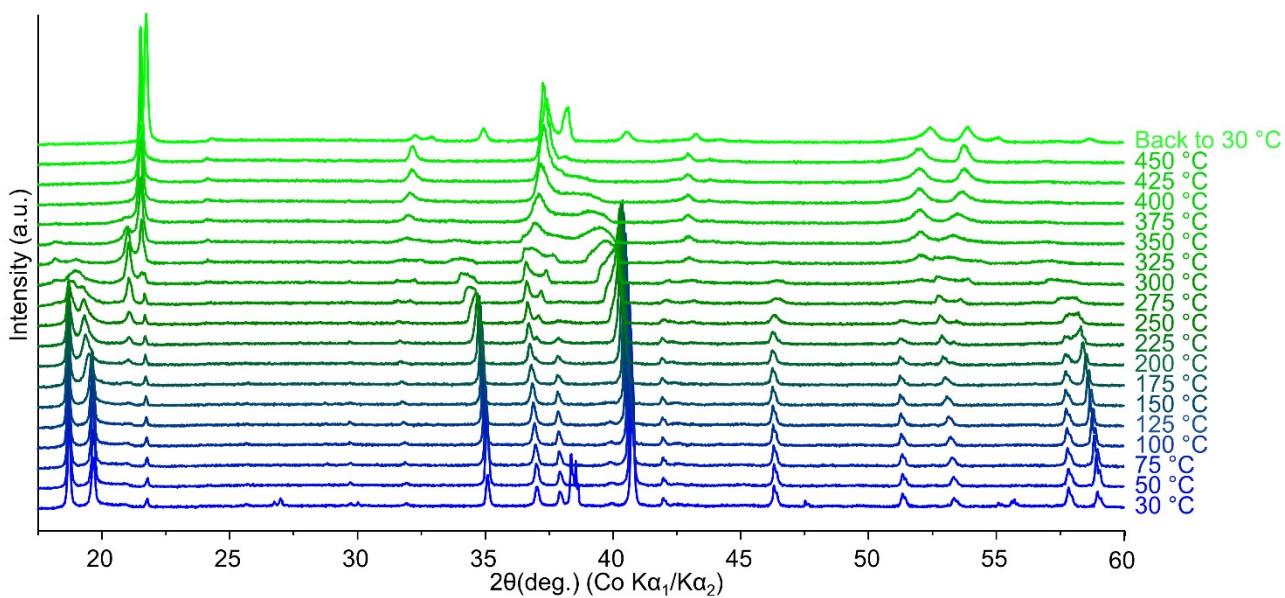


Figure S2. Variable temperature X-ray diffraction patterns recorded during the ion exchange reaction between “P2-Na_{5/6}Li_{1/6}Ni_{1/6}Mn_{4/6}O₂” and LiCl.

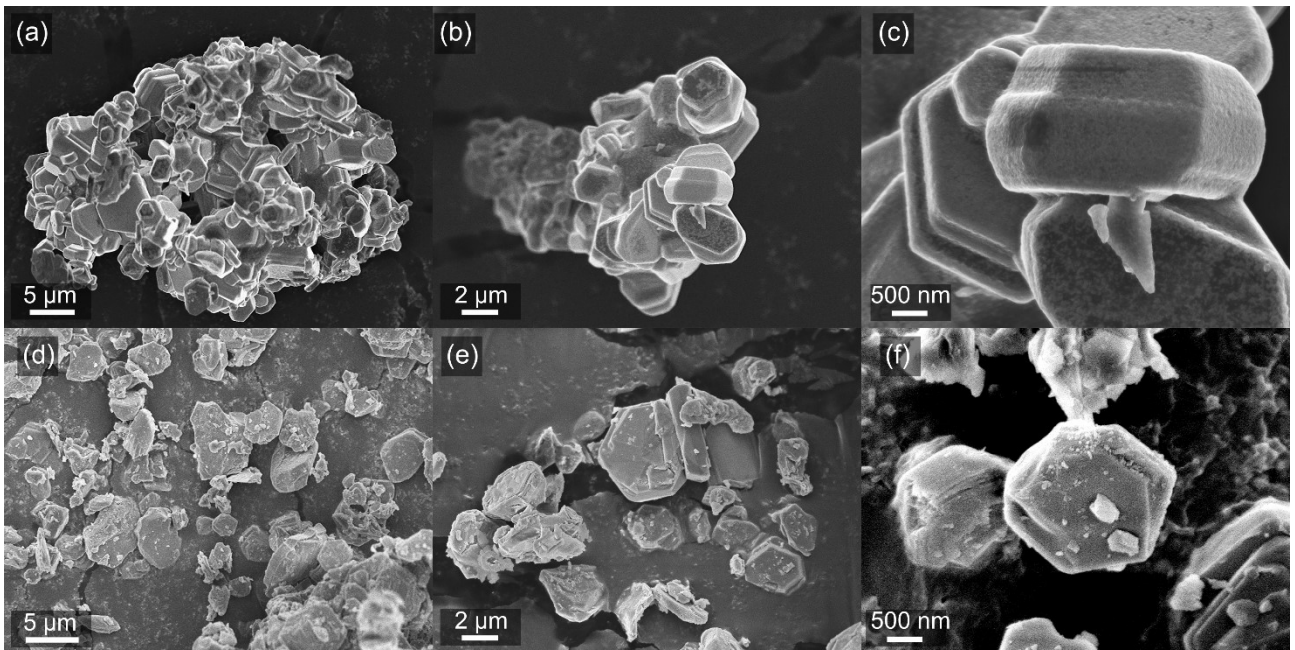


Figure S3: Scanning electron microscopy images of particles of: (a), (b) and (c) the “P2- $\text{Na}_{5/6}\text{Li}_{1/6}\text{Ni}_{1/6}\text{Mn}_{4/6}\text{O}_2$ ” phase; (d), (e) and (f) the “O6- $\text{LiNi}_{1/6}\text{Mn}_{4/6}\text{O}_2$ ” phase.

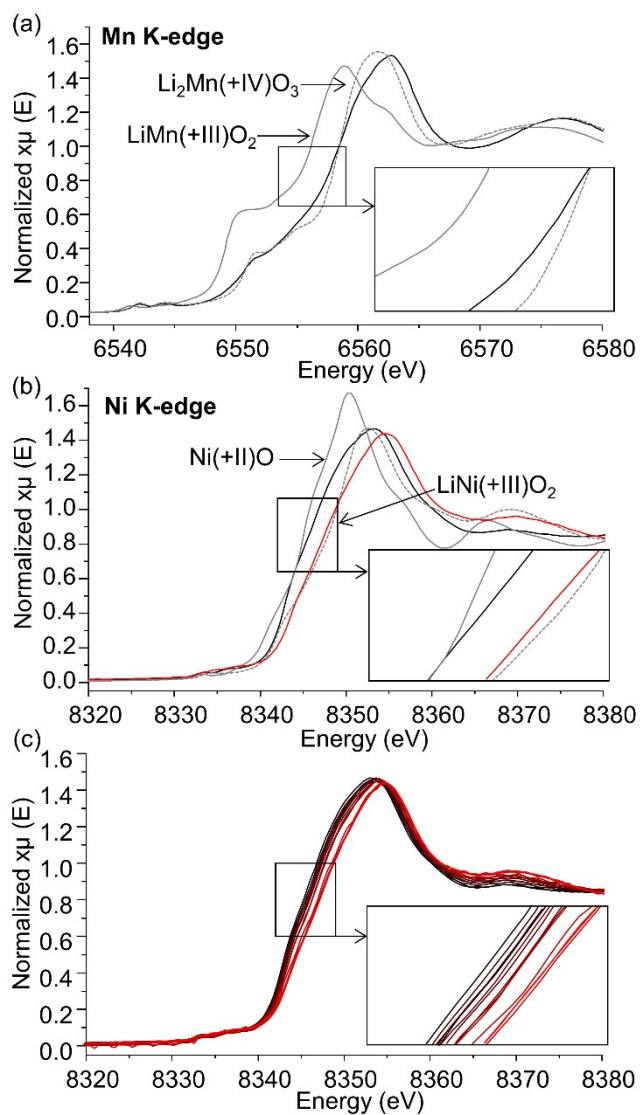


Figure S4. (a) and (b) Spectra recorded at the Mn and Ni K-edges, respectively, for the pristine “O6- $\text{LiNi}_{1/6}\text{Mn}_{4/6}\text{O}_2$ ” (in black) and for the O6 phase obtained after the deintercalation of 0.3 moles of Li^+ ions per formula unit (in red in (b)). Spectra for different reference compounds containing Mn^{3+} or Mn^{4+} ions and Ni^{2+} and Ni^{3+} ions are also shown. (c) *Operando* X-ray absorption spectroscopy experiment during the deintercalation of 0.3 moles of Li^+ ions per formula unit.

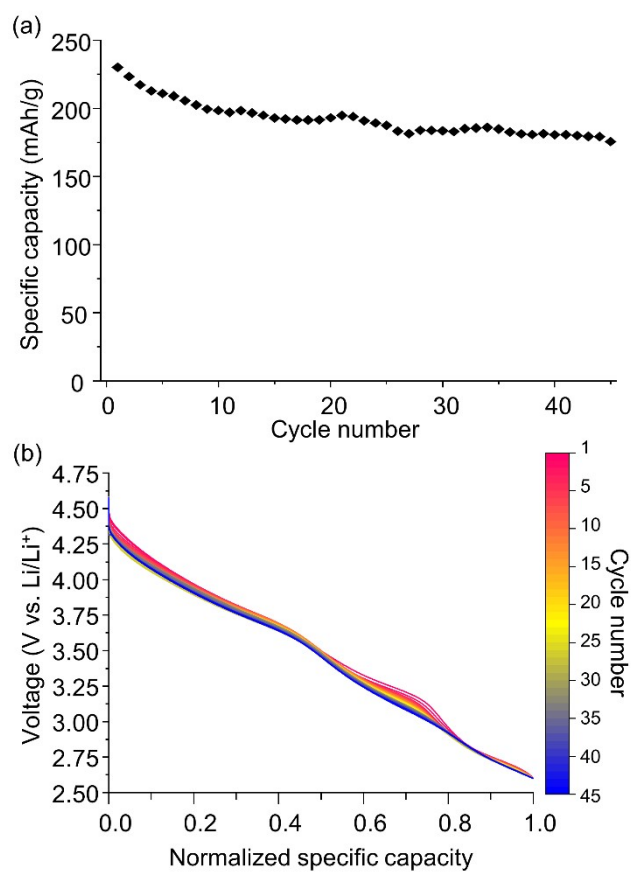


Figure S5. 45 galvanostatic cycles of charge and discharge of a lithium battery cell using the “O6- $\text{LiNi}_{1/6}\text{Mn}_{4/6}\text{O}_2$ ” phase at the positive electrode. (a) Evolution of the discharge specific capacity as a function the cycle number. (b) Evolution of the cell voltage V as a function of the normalized specific capacity of the battery.