# The formation of residual Li compounds on Ni-rich NCM cathodes and their effect on the electrochemical performance in LPSCl-based ASSBs

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Nickel-rich $LiNi_xCo_yMn_{(1-x-y)}O_2$ (NCM-type) lithium transition metal oxides have attracted a significant interest as a cathode material in lithium ion batteries due to their high energy density and low cobalt content, however, their reactivity with air during storage/handling and how this affects the electrochemical performance had been overlooked until the recent years. Exposure to air (which consists of $H_2O$ and $CO_2$) during storage/handling can lead to formation of LiOH, $LiHCO_3$, $Li_2CO_3$ and also basic transition metal hydroxides/carbonates.[1,2] The formation of such residual lithium compounds can also cause structural changes near the surface of cathode particles after leaving highly delithiated regions.[3] Therefore, it is crucial to understand how such residual lithium compounds are formed during the synthesis and post-synthesis storage. It is also very important to understand how these compounds affect the electrochemical performance.

In all-solid-state batteries (ASSBs), the presence of $Li_2CO_3$ can positively affect the electrochemical performance in sulfide-based solid electrolytes,[4,5] however, there has been no dedicated study which aimed to understand relationship between the cell electrochemical performance and the presence of residual lihium compounds -with a focus on the type of compounds present. In this study, we prepare $LiNi_{0.83}Mn_{0.06}Co_{0.11}O_2$ single crystal powders with different residual lithium amounts and types, by either carefully controlling the washing procedures, or post-processing conditions (e.g. heat treatment parameters). The ambient air exposure conditions (e.g. with different humidity and $CO_2$ concentrations) are further used to change surface properties of powders during storage. Alternatively, NCM powders were also coated with lithium compounds such as $Li_2CO_3$ using external lithium sources.

Characterization of such NCM powders will be presented in this talk. Valuable insights which we gain from a number of analytical techniques such as XPS, TOF-SIMS, TGA-MS, FIB-SEM, acid titration and XRD will be presented. Later, the relationship between the residual lithium compound type (and amount) and the electrochemical performance will be discussed (in ASSB cells with LPSCl-based sulfide solid electrolyte).

**References**

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Burak Aktekin received his B.Sc (2010) and M.Sc (2013) in Metallurgical and Materials Engineering Department in Middle East Technical University. He then joined Uppsala University where he worked on the high voltage spinel positive electrodes for LiBs. His research activities covered (post)synthesis modifications of cathode materials, electrode and cell preparation in different formats, as well as a study of liquid (and polymer) electrolytes. Having obtained his PhD in 2019 and following a brief postdoctoral period at Uppsala University, Dr. Aktekin joined J. Janeks's research group at the Institute of Physical Chemistry, Justus Liebig University Giessen where he is working on interfaces in solid-state batteries. Dr. Aktekin has experience in a wide range of analytical tools within the context of battery research.

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