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Deciphering the complexity of Li-rich layered oxides (LRLO) by synchrotron-based techniques

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In the last decades, remarkable industrial and academic research efforts have been focusing on lithium-ion batteries (LIBs) for portable electronics and electric vehicles (EV). Generally speaking, LIBs are more expensive than other battery chemistries, but they provide the highest power and energy densities as well as longer cycle. This technology requires further development in terms of safety and performance to establish itself also in the automotive market. Thus, new materials and chemistries at the positive/negative electrode sides as well as at the electrolyte side are necessary to overcome the state-of-the-art and the commercial benchmarks. Over-stoichiometric Li-rich layered oxides (LRLO) materials are a family of promising positive electrode materials with large specific capacity and high working potential. The eco-friendly Co-free LRLOs have attracted a lot of attentions, thanks to the improved sustainability, reduced costs and outstanding performance (250 mAh g-1). The crystal structure and cation ordering of LRLO are a matter of controversy. In the literature the structure of these materials is identified as solid solution, with an $R\bar{3}m$ crystal structure with partial supercell ordering of lithium ions, or as a nano-mosaic constituted of coexisting solid-solution phases with $R\bar{3}m$ and $C2/m$ structures. Overall, extensive defectivities play a key role in the breakdown of the cation ordering in the $C2/m$ lattice that degrades in the $R\bar{3}m$ one. This structural ambiguity/instability is at the origin of the capacity and voltage fading in batteries originating from undesired lattice transformations.

The resilience of the LRLO lattice can be finely tuned by a careful optimization of the transition metals blend and overlithiation. This complex balance allows to enhance the electrochemical performance in batteries in parallel with the removal of cobalt.

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