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Cathode materials for next-generation high energy density battery cells

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Among cathodes currently investigated for high-energy battery cells, three compositions stand as the most promising ones, which are $Li1.1Ni0.35Mn0.55O2$ (R3m + C2/m), $LiNi0.5Mn1.5O4$ (Fd3m) and $LiNi0.8Mn0.1Co0.1O2$ (R3m). The three compositions have little or no cobalt, so being cheaper and more sustainable than current state-of-art materials, and maximize the energy stored at the cell level via 1) delivering high discharge capacity as for the R3m phase, or 2) increasing charge voltage ˃ 4.5 V as for $LiNi0.5Mn1.5O4$. Each phase reacts singularly with Li, involving cation disordering, oxygen sublattice rearrangement and phase transformation, depending on its nominal composition and degree of de-lithiation, among other parameters. Interestingly, in some instances, the three phases relate to each other as a function of battery cell ageing. For example, COBRA Li-rich oxides (R3m + C2/m) oxidize to a highly disordered layered oxide first (R3m) and eventually transforms into a spinel phase (Fd3m) after deep cycling. Monitoring and understanding structural changes via high-throughput microscopy techniques is a significant challenge but necessary for developing cathode materials with an extended cycle life beyond 2000 cycles.

So far, we have collected structural information for the materials during battery cell cycling using post-mortem and operando studies. In the frame of four European projects, 1) COBRA [H202:875568], 2) IntelLiGent [HORIZON; 101069765], 3) ADVAGEN [HORIZON:?] and 4) SPINMATE [HORIZON: 101069712] working with the cathode materials herein presented, we would like to complement results with high-resolution microscopy and spectroscopy analyses to characterize the structure and chemical composition at the nano-domain level.

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