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Influence of Ti-dopant during Crystal Growth of Li-rich Layered $\text{Li}_{1.2}\text{Mn}_{0.8}\text{O}_2$ Cathode Materials using co-precipitation synthesis route

The outstanding energy density and capacity exhibited by lithium-rich manganese-based layered oxide (LRLO) cathode materials have positioned them as emerging strong contenders for future lithium-ion battery systems. Their optimal utilisation is hindered by several challenges, such as Mn-migration and oxygen loss, contributing to structural reconstruction resulting in voltage fading and poor electrochemical performance. This inability to retain a layered phase during cycling is a challenge that disrupts the ability to maintain a consistent conductive ion flow (lithium). Herein, Ti doping was introduced into $\text{Li}_{1.2}\text{Mn}_{0.8}\text{O}_2$ cathodes to monitor its influence on the crystalline internal microstructure, polymorph content control to later contribute towards the cycling retention, and Li^+ kinetics. The Ti concentrations of 2,4,6,8, and 10% were introduced using the co-precipitation method applied in the synthesis of the metal hydroxide precursor. The scanning electron microscopy (SEM) imaging revealed spherical morphology of particles with 3-20 microns. Compositional analysis of the various doped samples obtained through the XRD spectra showed that Ti-doped LrLO (6% Ti) has achieved high polymorphic content of layered-layered cathode materials as desired, with 80,5% Li_2MnO_3 and 3,4 % LiMnO_2 and only 15% spinel content. On the other hand; the samples containing 4, 8, and 10% Ti content demonstrated higher spinel contents of 24.1, 22.3, and 25.9 %, respectively. Overall, across all samples, the Li_2MnO_3 polymorphs exist in greater quantities above an impressive 75% yield, followed by spinel above 15% and whereas LiMnO_2 has a minimum of as little as 0.2%. This dominance of the Li_2MnO_3 variant shows that when Ti is doped to replace a part of Mn, the Jahn–Teller effect is weakened, and a stable layered structure is formed. This may be ascribed to the fact that, unlike Mn, Ti–O bond energy is higher, and it does not participate in the redox reactions. Our findings provide a suitable element doping strategy for regulating the voltage decay and cycle retention of LrLO, thus promoting their real-world application in future batteries.

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None

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