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Compositional Analysis of Heterostructural Ti-Doped Li1.2Mn0.8O2 Cathode Materials during the Computational and Experimental Crystal Growth Processes

This study investigates the structural and morphological properties of pure and titanium-doped Li1.2Mn0.8O2 cathode materials through integrated computational modelling and experimental techniques. Titanium doping was chosen due to its ability to enhance structural stability, reduce capacity fading, and mitigate voltage decay in lithium-rich manganese oxides.. Molecular dynamics simulations reveal that Ti doping improves local atomic ordering, as evidenced by radial distribution function analysis showing reduced Mn-O bond distortion compared to undoped samples. Experimentally, Li1.2Mn0.8O2 and its Ti-doped variants (6% and 10%) were synthesized via a co-precipitation method. X-ray diffraction (XRD) analysis confirmed phase purity and reduction in the spinel variant that is brought about by Mn-migration. The particle size distribution analysis showed a reduction in agglomeration with optimal 6% Ti doping, corroborated by scanning electron microscopy (SEM) imaging that revealed more uniform spherical morphology. These findings highlight Ti's dual role as both a structural stabilizer through strengthened Mn-O-Ti bonding networks and a morphological modifier via surface energy manipulation during crystal growth. The integrated approach demonstrates that Ti doping influences particle size distribution, structural stability, and morphology, and revealed the optimal Ti-concentration to be implemented for improving these anomalities. By aligning with emerging strategies for LRMO optimization through controlled cation doping, this study provides quantitative insights into dopant concentration effects on both atomic-scale structure and microscale morphology. It establishes a framework for the rational design of high-stability, manganese-rich cathode materials through targeted elemental substitution, addressing broader challenges in the field of lithium-ion battery technology.

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Primary author: KGOEDI, Moloko Emmanuel (University of limpopo)

Co-authors: MASEDI, Cliffton (University of Limpopo); NGOEPE, Noko (UL); NGOEPE, Phuti Esrom (University of LImpopo); LEDWABA, Raesibe (University of Limpopo)

Presenter: KGOEDI, Moloko Emmanuel (University of limpopo)

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