

Dysprosium (Dy) Doping on the High Voltage Spinel $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ Cathode Materials for li-ion Batteries.

Batteries, supercapacitors, fuel cells, and capacitors stand out as the most promising electrochemical energy storage systems due to their attributes, including high energy density, minimal self-discharge, and the absence of a memory effect. The high-voltage spinel $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ (LMNO) is highly regarded as a promising energy storage material for the next generation of lithium batteries due to its ability to achieve high energy densities. The limited electronic conduction of most transition metal oxides restricts their specific capacitance and charge-discharge rate. To overcome these limitations, researchers often doped transition metal oxides with Dy. This study utilized an iterative genetic algorithm approach and first-principles calculations to investigate the structural, electronic, and mechanical properties of the lithium manganese-nickel oxide spinel material family. Our attempt involved modifying the conventionally used cathode material $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ by doping Rare earth Dy on Mn sites. The unpaired 4f electronic configuration and the variation in ionic sizes make them well-suited for doping into other materials for a variety of applications. As a result, researchers found that REE-doping maintained the cubic spinel structure, reduced particle size, and enhanced the cyclic performance of resulting batteries. Overall, of the rare-earth elements studied, Dysprosium (Dy) is crucial for batteries. Its presence in battery materials can enhance performance, capacity, and lifespan.

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Session Classification: Poster