Systematic study of Zr4+, Nb5+and Mo6+doping in LiNi0.8Mn0.1Co0.1O2 (NMC811) cathodes prepared from a commercial Ni0.8Mn0.1Co0.1(OH)2 precursor: Structural and electrochemical perspectives

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Abstract Lithium-ion batteries (LIBs) are widely used in energy storage due to their high energy density, long cycle life, and scalability. Nickel-rich lithium nickel manganese cobalt oxides (Ni-rich NMCs) are promising cathode materials owing to their high energy density. However, their application is limited by low stability, leading to capacity loss at high delithiated states and safety concerns. In this study, layered LiNi0.8Mn0.1Co0.1O2 (NMC811) cathode was doped with high oxidation state elements (Zr, Nb, and Mo), known for strong transition metal--oxygen (TM-O) bond energies. These dopants can hinder oxygen release and improve the chemical stability of Ni-rich cathodes. The materials were synthesized via a solvent solution method. X-ray diffraction (XRD) confirmed a single-phase layered structure without impurity peaks, and all doped samples showed an increased I(003)/I(104) intensity ratio, indicating reduced cation mixing. No significant changes in particle morphology were observed due to the low dopant level (1 wt%). Electrochemical tests showed that Zr-and Mo-doped samples delivered higher initial discharge capacities and better cycling stability. Notably, Zr-doped NMC (ZrNMC) retained 71.6% of its capacity after 100 cycles at 0.1 C, compared to 49.6% for pristine NMC. Electrochemical impedance spectroscopy (EIS) revealed that ZrNMC exhibited lower charge transfer resistance during cycling, suggesting improved ion transport. These results indicate that doping with high oxidation state elements is an effective strategy to enhance the structural and electrochemical performance of Ni-rich NMC cathodes, making them more viable for next-generation LIB applications.

Keywords **Author Keywords:** Lithium-ion batteries; Ni-rich cathodes; High oxidation state dopants; Zr doping; Nb doping; Mo doping
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Data will be made available on request.

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