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# Systematic study of $Zr^{4+}$ , $Nb^{5+}$ and $Mo^{6+}$ doping in $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) cathodes prepared from a commercial $Ni_{0.8}Mn_{0.1}Co_{0.1}(OH)_2$ 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  $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$  (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. © 2026 Elsevier B.V.

## Author keywords

High oxidation state dopants; Lithium-ion batteries; Mo doping; Nb doping; Ni-rich cathodes; Zr doping

## Indexed keywords

### Engineering controlled terms

Cathode materials; Cathodes; Chemical stability; Cobalt compounds; Electric discharges; Electrochemical impedance spectroscopy; Impurities; Ions; Lithium compounds; Molybdenum compounds; Nickel oxide; Niobium compounds; Oxidation; Oxygen; Semiconductor doping; Zirconium; Zirconium compounds

### Engineering uncontrolled terms

Doped sample; High oxidation state; High oxidation state dopant; Higher energy density; Ion batteries; Lithium ions; Mo-doping; Nb doping; Ni-rich cathode; Zr-doping

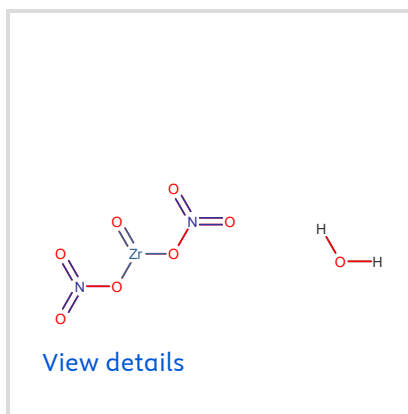
### Engineering main heading

Lithium-ion batteries

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