Effect of Transition Metal Doping on the Electrochemical Performance of NCM811 Cathodes

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Ni-rich $LiNi_xCo_yMn_zO_2$ (NCM) cathodes have been the subject of considerable research due to their high capacity and potential application in lithium-ion batteries for electric vehicles. Among these materials, $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ (NCM811) has emerged as a promising candidate for next-generation energy storage solutions [1]. However, the intrinsic structural and cycling stability issues associated with Ni-rich cathodes necessitate the development of effective strategies to enhance their performance and longevity. Doping with extrinsic multivalent cations has been established as a viable method to address the stability concerns of Ni-rich NCM cathodes. In light of this, our study presents a comprehensive investigation of developing an efficient screening methodology for doping NCM811 cathodes with a range of cations, including Mg^{2+}, Al^{3+}, Ti^{4+}, Zr^{4+}, Ta^{5+} and W^{6+}[2, 3].

The methodology is founded on a "top-down" approach, whereby a precursor layer containing the dopant is coated onto the cathode material, followed by the diffusion of the dopant into the particles during heat treatment at elevated temperatures. This approach facilitates the rapid identification of potential dopants for Ni-rich cathode materials, paving the way for further optimization and realising high-capacity, stable cathode materials. Furthermore, the research delves into the impact of the oxidation states of the dopants on the electrochemical, morphological, and structural properties of the Ni-rich NCM cathodes. Through a series of galvanostatic cycling measurements, it is observed that cathodes doped with high oxidation state dopants, particularly Ta^{5+} and W^{6+} display superior performance compared to their undoped counterparts and those doped with low oxidation state dopants [2, 3]. Additionally, physicochemical measurements and analyses reveal distinct differences in the grain geometries and crystal lattice structures of the various cathode materials, which contribute to their diverse electrochemical performance characteristics and correlate with the oxidation states of their dopants.

Taken together, the findings of this study offer valuable insights into the role of dopant oxidation states in the enhancement of Ni-rich NCM cathode materials, as well as a streamlined method for identifying suitable dopants for high-capacity, stable NCM811 cathodes. Ultimately, this research has the potential to significantly advance the development of high-performance lithium-ion batteries for electric vehicle applications, thereby contributing to the broader goals of energy sustainability and environmental conservation.

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