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# Abstract

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Lithium-ion batteries (LIBs) are pivotal in modern energy storage systems, powering applications ranging from portable electronics to electric vehicles (EVs) and grid-scale storage. Despite their widespread use, challenges such as limited energy density, performance degradation under high rates, and reduced stability at extreme conditions hinder their full potential. This study focuses on addressing these limitations through advanced electrolyte design and cathode optimization, emphasizing the integration of boron-containing additives and the development of stable interphases.

The research highlights the importance of cathode-active materials (CAMs) such as layered oxides, including $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ (NMC111) and nickel-rich variants like $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811), in achieving high energy densities. While these materials offer excellent performance, they face challenges such as transition metal dissolution, interfacial instability, and structural degradation during prolonged cycling. These issues underscore the need for optimized electrolytes capable of forming robust cathode-electrolyte interphases (CEIs) to mitigate degradation and enhance overall battery performance.

To address these challenges, boron-containing compounds were investigated as key components in electrolyte formulations. Mesityldimethoxyborane (MDMB) was introduced as a multifunctional electrolyte component to improve lithium-ion transport and interfacial stability. By modifying the solvation structure and reducing anion mobility, MDMB enhanced ionic conductivity and facilitated the formation of a boron-rich CEI. This interphase effectively stabilized the cathode, minimized side reactions, and improved cycling performance under high current densities. Electrochemical impedance spectroscopy (EIS) and computational modeling validated MDMB's role in optimizing electrolyte dynamics, demonstrating reduced overpotential and enhanced lithium-ion transference.

Building on this foundation, ethylene glycol mesityl borane (EGMB), a novel cyclic boric ester, was synthesized and incorporated as a functional additive to improve battery performance under extreme conditions. EGMB exhibited significant benefits, forming a CEI enriched with boron and fluorine. This robust interphase not only improved mechanical and chemical stability but also mitigated oxygen release and transition metal dissolution, which are common issues with Ni-rich cathodes. The enhanced CEI facilitated high lithium-ion conductivity, resulting in improved discharge capacities and extended cycle life, even under ultrahigh voltages (up to 4.8 V), fast charging, and wide temperature ranges. Electrochemical evaluations confirmed EGMB’s ability to enhance compatibility with NMC cathodes, achieving high capacity retention and Coulombic efficiency over extended cycling.

The research demonstrates that boron-based additives or electrolyte component can effectively address critical issues in LIBs, including interfacial instability and poor lithium-ion transport. By tailoring electrolyte formulations to incorporate boron-containing compounds, this work provides a pathway to enhance the durability, safety, and performance of LIBs in demanding applications. These findings contribute to the advancement of next-generation LIBs capable of meeting the growing energy demands of modern technology while maintaining operational stability across diverse conditions.

This study underscores the transformative potential of electrolyte engineering in overcoming the limitations of current LIB technologies. By integrating innovative boron chemistry and interfacial design strategies, this research paves the way for the development of high-performance energy storage systems suitable for a broad range of applications, from consumer electronics to electric mobility and renewable energy solutions.

**Keywords**: Lithium-ion battery, electrolyte, additive, boron compounds, high voltage.