SSRSE 05

The impact of a newly synthesized zwitterionic additive on the electrolyte performance of lithium-ion batteries

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Lithium-ion batteries (LIBs) have emerged as a crucial technology for powering sustainable transportation systems in the future. However, their large-scale application is hindered by serious safety concerns, particularly when LIBs are exposed to thermal, mechanical, or electrical abuse conditions [1,2]. The high energy density of LIBs, which is attributed to the use of volatile and flammable organic solvents in the electrolyte, poses significant safety risks [3,4]. Since the electrolyte is a critical component that interconnects all vital parts of the battery, it notably impacts numerous technological and chemical aspects of LIBs. To address these safety challenges, researchers have proposed several modifications to the electrolyte, including substituting the organic solvent or adding functional additives such as ionic liquids (ILs).

These modifications offer promising solutions for enhancing the safety and reliability of LIBs, thereby paving the way for their wider application in sustainable transportation systems.

The current demand for lithium-ion battery electrolytes entails developing electrolytes that can perform multiple functions simultaneously, such as stabilization and functionalization of the electrode materials such as stabilizing the electrode materials and functionalizing the electrode. In this context, electrochemical testing was conducted to compare the stability of the electrolyte containing the newly synthetised zwitterionic compound 1-butylsulfonate-3-methylimidazole ($C_1C_4imSO_3$) as an electrolyte additive. The study utilized electrolytes 1.0 M $LiPF_6$ in EC/DEC = 50/50, battery-grade solutions of lithium hexafluorophosphate salt in ethylene carbonate, and diethyl carbonate mixture. The results were evaluated based on the electrochemical performance of the electrolyte with the additive and compared to those of commercially used electrolytes. In addition to voltammetric results, molecular dynamic (MD) simulations and density functional theory (DFT) calculations were employed to reveal the essential mechanism between selected additive and electrolyte.

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