リチウム金属電池の性能向上のためのイオン液体におけるアニオン駆動型の配位構造
Anion-Driven Coordination in Ionic Liquid Electrolytes for Enhanced Li Metal Battery

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研究成果概要

Modifying the coordination structure of electrolytes provides an effective approach to mitigate issues at the lithium metal surface, such as dendrite formation and the instability of the solid electrolyte interphase (SEI). This research investigates the impact of incorporating anions with varying donor numbers, specifically $[PF6]^-$ and [OTf]– (trifluoromethanesulfonate), into $[FSA]^-$-based ionic liquids (where $[FSA]^-$ refers to bis(fluorosulfonyl)amide) on coordination dynamics and interfacial behavior. The introduction of $[PF6]^-$ and $[OTf]^-$ anions modifies the clustering and interactions of ionic components within the electrolyte, shedding light on their relationship with interfacial and electrochemical properties. Both theoretical and experimental findings indicate that by mixing different anions, a favorable coordination structure with low (de)coordination energy and efficient electrochemical processes can be achieved. This strategy promotes the formation of a stable solid electrolyte interphase, which enhances the Li deposition and dissolution processes, suppresses dendrite formation, and ultimately leads to improved cycle stability and capacity retention in Li metal batteries paired with $LiFePO_4$.

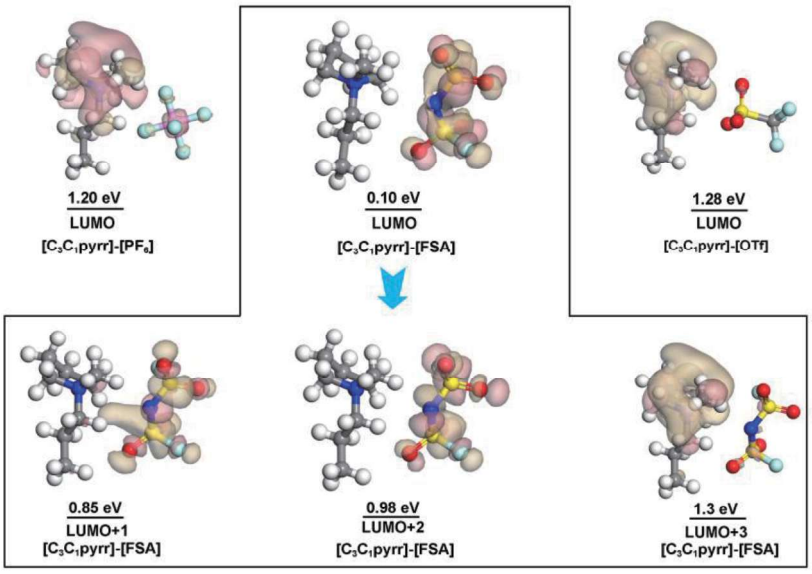

Figure 1. The molecular orbitals and energy levels of cations interacting with different anions.

発表論文（謝辞なし）

1. S. Wu, Y. Nishigaki, J. Hwang, Kazuhiko Matsumoto, *Chem. Eng. J.* 508 (2025) 160927.