

研究论文

## 新型成膜电解液添加剂亚硫酸丁烯酯的电化学行为

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**摘要** 合成制备了一种新的环状亚硫酸酯类有机溶剂——亚硫酸丁烯酯(BS). 量子化学计算结果表明, 亚硫酸丁烯酯有机溶剂分子的总能、LUMO值比碳酸丙烯酯有机溶剂的低, 具有较强的得电子能力, 不易被氧化. 其作为添加剂与碳酸丙烯酯(PC)混合应用于锂离子电池中, 可有效地抑制PC在石墨电极中的共插入, 能显著改善循环性能.

**关键词** [亚硫酸丁烯酯](#) [电解液](#) [石墨电极](#) [锂离子电池](#) [固体电解质相界面膜](#)

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## Electrochemical Behavior of Butylene Sulfite as Novel Film-forming Electrolyte Additive for Lithium Ion Batteries

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**Abstract** As a novel organic solvent electrolyte material, sulfites possess high a antioxidation and electrochemical stability. Butylene sulfite with cyclic structure was synthesized. The total energy and the frontier molecular orbital energy of the organic butylene sulfite and propylene carbonate molecules were calculated. The LUMO energy and the total energy of the propylene carbonate molecule were lower than that of the butylene sulfite molecule. It is clearly indicated that the butylene sulfite molecule can easily accept electrons and bears a high reaction activity. Even in additive amounts(volume fraction 5%) butylene sulfite is suppressing co-intercalation of propylene carbonate(PC) into graphite. The formation of a stable passivating film on the graphite surface was believed to be the reason for the improved cycle performance for lithium ion battery.

**Key words** [Butylene sulfite](#) [Electrolyte](#) [Graphite electrode](#) [Lithium ion battery](#) [Solid electrolyte interface film](#)

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