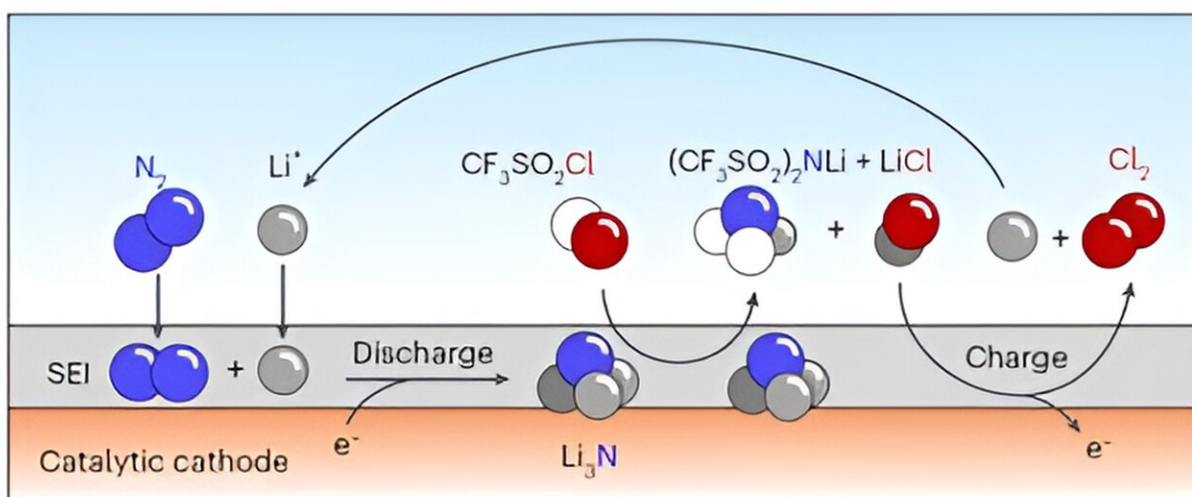


Researchers achieve electrosynthesis of LiTFSI and N-containing analogs via looped Li-N₂ battery

January 16 2024, by Liu Jia



Schematic representation illustrating the cascade LiTFSI synthesis in a Li-N₂ battery. Credit: Prof. Wang Yaobing's group

Lithium bis(trifluoromethanesulfonyl)imide, commonly known as LiTFSI, and its analogs, are critical electrolytes for lithium batteries and solar cells. However, the commercialization of LiTFSI through thermal chemical synthesis relies on the use of NH₃ intermediates, which involves multiple catalytic and purification processes, leading to substantial carbon emissions. Therefore, developing a method for the direct synthesis of LiTFSI from N₂ under mild conditions becomes

particularly important.

In a study [published](#) in *Nature Catalysis*, Prof. Wang Yaobing's team from Fujian Institute of Research on the Structure of Matter of the Chinese Academy of Sciences proposed a cascade electrochemical synthesis strategy based on Li–N₂ batteries, and achieved efficient electrochemical synthesis of various nitrogen-containing compounds, including LiTFSI.

The specific strategy includes catalytically reducing N₂ to Li₃N during discharge, acylating Li₃N to form LiTFSI and the byproduct LiCl, and oxidizing LiCl during charging to complete the synthetic cycle.

The researchers demonstrated the electrocatalytic reduction of N₂ to Li₃N through techniques such as X-ray diffraction and low-temperature transmission electron microscopy, and confirmed the feasibility of the S–N acylation reaction between Li₃N and CF₃SO₂Cl through [nuclear magnetic resonance](#), [mass spectrometry](#), and Fourier transform infrared spectroscopy. Based on the color change of methyl orange from red to colorless during the charging process, they proved that the byproduct LiCl was oxidized to Cl₂.

The experimental results indicated that, under optimized conditions, the catalytic reduction efficiency from N₂ to Li₃N reached 53.2%, the conversion efficiency from N₂ to LiTFSI was 48.9%, and the energy efficiency of electrochemical synthesis of LiTFSI reached 3.0%.

In addition, the researchers utilized a flow cell device to achieve continuous electrochemical synthesis of LiTFSI, demonstrating the practical significance of this strategy in production. By expanding the substrate scope, they provided a pathway for the direct electrochemical synthesis of analogs with different N–X bonds (X = S, C, etc.) and metal cations (Li⁺, Zn²⁺, etc.), proving the scalability of the strategy.

This study presents a comprehensive electrochemical synthesis scheme for the practical production of nitrogen-containing chemicals, which offers a promising approach to synthesizing high-end electrolytes with enhanced nitrogen atom efficiency.

More information: Xiang Zhang et al, Cascade electrosynthesis of LiTFSI and N-containing analogues via a looped Li–N₂ battery, *Nature Catalysis* (2024). [DOI: 10.1038/s41929-023-01067-3](https://doi.org/10.1038/s41929-023-01067-3)

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