

Fluorinated ether based electrolyte for high-energy lithium–sulfur batteries: Li⁺ solvation role behind reduced polysulfide solubility

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By employing new electrolytes, the polysulfide shuttle phenomenon, one of the main problems of lithium–sulfur (Li–S) batteries, can be significantly reduced. Here we present excellent coulombic efficiencies as well as adequate performance of high-energy Li–S cells by the use of fluorinated ether (TFEE) based electrolyte at low electrolyte loading. The altered reaction mechanism was studied with multiple techniques to explain the observed differences in the galvanostatic cell discharge profiles and to reveal whether the conversion involves polysulfide intermediate species – validated by *operando* sulfur K-edge XANES analysis. In addition, UV/Vis spectroscopy confirmed a reduced polysulfide solubility and diffusion for the new electrolyte, which arguably reduces the polysulfide shuttling and allows for better electrochemical performance. The molecular level origin for the lower voltage of the first discharge plateau was found to be poor Li⁺ ion solvation ability of the fluorinated ethers as analyzed by COSMO-RS computations for several electrolytes. By investigating different ratios of TFEE and DOL an optimal electrolyte composition was determined and used to construct a high-energy cell with excellent performance characteristics. Overall, this study enables us to claim that a shift of focus from traditional solvents to those with reduced polysulfide (or indeed Li⁺) solubility should reduce polysulfide shuttle and be a cheap and easy way for Li–S battery improvement.¹

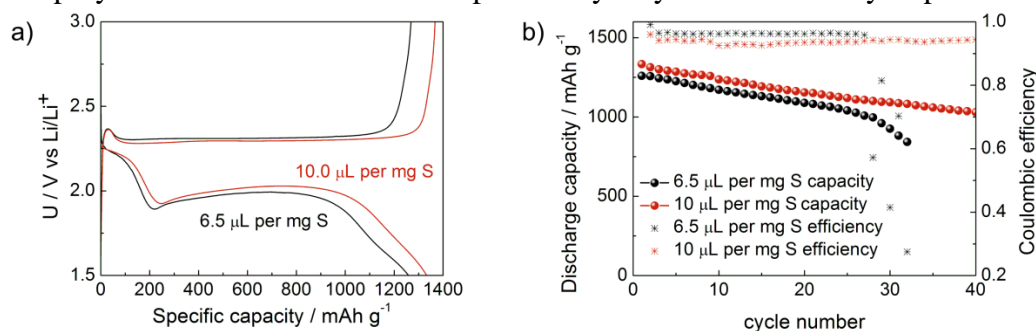


Figure 1: Discharge capacity and Coulombic efficiency for a high energy Li–S cell with 6.5 μL/mgS and 10 μL/mgS of 1 M LiTFSI TFEE:DOL 1:1 electrolyte.

References:

[1] S. Drvarič Talian, S. Jeschke, A. Vizintin, K. Pirnat, I. Arčon, G. Aquilanti, P. Johansson, R. Dominko, Chem. Mater. 29 (2017) 10037–10044.