Sulfur-Containing SEI-formers – from DFT Predictions to Full Cell Assessments

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Efficient cycling of lithium-ion batteries (LIBs) requires stability of the electrolyte versus the electrodes. Unfortunately, the low potential of the graphite negative electrode is outside the thermodynamic stability range for many battery electrolyte solvents, including organic carbonates, why their usage relies on kinetic stabilization by the passivation layer, the solid electrolyte interphase (SEI), created on the surface. SEI is thus a key element with impact on cycle life, self-discharge, power density, etc. One way to improve LIBs is to better control the SEI formation, often made by adding special molecules, SEI-formers, to the electrolyte.

We here present a systematic study of several different sulfur-containing compounds (Fig. 1) as SEI-formers used in the standard LP30 battery electrolyte. The electrochemical analysis of the resulting electrolytes shows a notable difference in the reduction behavior and by XPS and IR spectroscopies we reveal the compositions of the corresponding formed SEI-layers. The experimental data are further interpreted using data from DFT calculations of reduction potentials and reaction paths to connect the additives' chemical structure to their SEI-forming properties. Finally, the electrolytes are cycled in graphite/LFP full cells to study the long-term stabilization properties of the SEI-layers formed.

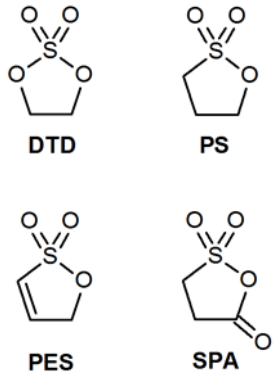

Fig. 1 Chemical structures of the studied SEI-forming additives.