Boron Based Anion Receptor as Electrolyte Additive for Li-Ion Batteries

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Additives are used for lithium-ion battery electrolytes in order to tailor the properties. Anion receptors (AR) are promising candidates in this context. They function as anion-binding agents, promote salt dissolution, and reduce ion-pairs, therefore increase the ionic conductivity [1,2]. ARs with many different chemistries and structures were studied in the past. The library of ARs spans from aza-ethers to boron and phosphorous based receptors. Among them, boron-based receptors have received the greatest interest for applications in Li-ion batteries. Inorganic components of the SEI that are in contact with electrolyte might be attacked and dissolved by the anion receptor. The LiF content in the SEI (solid electrolyte interphase) has been reported to decrease on addition [3,4].

In this work the effect of a boron based anion receptor, tris (hexafluoroisopropyle) borate (THFIPB), on the electrochemistry of graphite was investigated in the 1M $LiPF_6$ EC:DMC electrolyte (LP30). Capacity retention was significantly improved due to THFIPB addition. Cycling experiments at 0 and 50^{o}C demonstrated that THFIPB is compatible with operation in an extended temperature window, and improved practical capacity was demonstrated. Electrodes were characterized during cycling by *operando* XRD, and post mortem by SEM. The SEI forming process and the SEI composition was studied by DEMS, XPS and FTIR, and the addition of small amounts (25 mM) THFIBP was found to significantly affect the SEI formation. The onset potential for C_2H_4 formation is higher, in the presence of THFIPB, consistent with XPS data, which shows that the surface is left bare at higher potentials. The SEM micrographs indicate a more porous SEI with anion receptor, in agreement with the improved electrode kinetics demonstrated by electrochemical cycling.

The addition of anion receptor is known to accelerate defluorination of the anion [5], and corresponding formation of PF_5, which again decompose to POF_3 and HF in the presence of trace amounts of water. The XPS results show that oxygen surface groups are removed when exposed to electrolytes with THFIPB. It was further shown that the first cycle irreversible capacity loss (ICL) was reduced for the graphite after exposure to LP30 with THFIPB.

References:

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