Electrolyte additives for lithium ion battery

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ABSTRACT

Electrolyte additives is very importance for enhancement the durability of lithium ion battery. Electrolyte additives for cathode materials as borane and borate compounds with various fluorinated aryl or alkyl groups as anion receptors, tris(pentafluorophenyl) borane (TPFPB), triphenyl borate (TPBO) and trimethyl borate (TMBO) etc, are investigated as electrolyte additives in lithium ion batteries ($LiFePO_4$ cathode, 1M $LiPF_6$ EC-DMC 1:1 electrolyte) at 25 and 60°C. Some of the electron deficient boron sites on borane or borate compounds anion receptors can promote the dissolution of salt (as $LiPF_6$, LiF etc) in several solvents. According to the study results, tris(pentafluorophenyl) borane has the ability to improve the cycle performance of $LiFePO_4$ at high temperature. The observed improved cycling performance and improved lithium ion transport are attributed to decreased LiF content in the SEI film. TPBO shows formation of a thick surface/electrolyte interface (SEI) which hampers ion flow and does not protect the electrode from degradation. TMBO performance improves with increasing concentration, also suppresses thermal decomposition of the electrolyte and formation of the SEI film. An electrolyte additive with boron-nitrogen-oxygen groups for high voltage (5 V) $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) electrode is investigated by electrochemical performance, material analysis and density function theory first principles calculation (DFT). The Methylboronic acid MIDA ester (ADM) additive in ethylene carbonate and dimethyl carbonate (EC/DMC) electrolyte for LNMO cathode shows a paramount discharge capacity retention of 96% (15% in without additive) after 25 cycles at 75 mA g^{-1} and 40°C. By characterizations, the results interpret that the ADM additive decomposes and participates in the reaction pathway of cathode electrolyte interface (CEI) formation, which are more protective and resistant to electrolyte oxidative decompositions, and more potent in maintaining the structural integrity of nickel (Ni), manganese (Mn), and PF_6^-.

The structural variation of solid electrolyte interphase (SEI) layer with electrolyte additive LiPO2F2 on graphite (FSN) anode plays an important role in the performance of Li-ion battery during operation, which is still poorly understood. Small-angle neutron scattering (SANS) is an effective and accurate in characterizing the SEI structure in the bulk sample. The present study performs the accurate SANS model analysis to quantitatively evaluate the thickness, composition, coverage (interface area) and even morphological change of SEI layer on FSN anode at the nano-scale length. The SEI formation and subsequent variation in these structural parameters with charge time revealed by SANS are correlated with the battery performance. This in-depth SANS analysis could provide insight into the mechanism.

Keywords: Lithium ion battery, electrolyte additive, solid electrolyte interphase, cathode electrolyte interphase.