High Voltage Electrolyte Based on Fluorinated Compounds for High Energy Li-ion Chemistry

Abstract

Lithium ion batteries have dominated the portable electronics market and have the potential to dominate large-scale battery applications including hybrid and electric vehicles, as well as grid storage, because of their high energy and power densities. It is well known that conventional electrolytes show poor anodic stabilities above 4.5 V versus Li/Li$. As a result, high voltage electrolytes are essential for the development of next generation high energy lithium ion batteries. Both fluorinated electrolytes and additives can be introduced in to the electrolyte system. In this work, fluorinated electrolytes were used in both graphite-LiNi$_{0.5}$Co$_{0.2}$Mn$_{0.3}$O$_2$ (operated between 3.0 - 4.6 V) and graphite- LiNi$_{0.5}$Mn$_{1.5}$O$_4$ (operated between 3.5 - 4.9 V) full cell systems. The baseline electrolyte for all cells (referred to as Gen2) was composed of 1.2M LiPF$_6$ dissolved in a mixture of EC and EMC (3:7 in weight ratio). After a series of electrochemical tests, compared to the baseline electrolyte, the fluorinated electrolytes displayed significantly enhanced performance under both high cut off voltage and high temperature ($55^\circ$ C). The post test analysis results showed that the cycled electrode can not only reach a much more stable interface but also overcome the crystal structure change after long term cycling when the fluorinated electrolyte system was used. In addition to changing the solvent, a series of additives were designed, synthesized and evaluated for high-voltage Li-ion battery cells using a Ni-rich layered cathode material LiNi$_{0.5}$Co$_{0.2}$Mn$_{0.3}$O$_2$ (NCM523). The repeated charge/discharge cycling for NCM523/graphite full cells using Gen2 with 1 wt % of these additives as electrolytes was performed. Electrochemical performance testing and post analysis result demonstrated that our as selected or designed cathode additives can passivate the cathode and prevent the cathode from side reactions. The developed methodology could provide fundamental direction in the design and investigation of better electrolytes for the next generation lithium ion batteries.