Phosphorus Pentoxide Additive for Lithium-ion Batteries

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FULL DESCRIPTION

Background

Chemical and electrochemical instability between lithium (Li) metal anode and the liquid Li-ion electrolytes result in mossy Li deposit causing severe volume expansion, low Li deposition-stripping efficiency, formation of dead Li and fast depletion of electrolyte. All of these lead to short cycle life and safety concerns. Current strategies to implement Li metal anode use solid-state Li-ion electrolytes including inorganic or organic Li-ion conductors. The disadvantages of solid-state electrolytes include poor producibility, poor stability and low conductivity. The other strategy to implement Li metal anode is to use a new type of liquid electrolytes named localized high concentration electrolytes (LHCEs). The disadvantage of the LHCEs is the expensive co-solvents which are also not readily available.

Technology

Prof. Juchen Guo and his research team at UCR have discovered the use of phosphorous pentoxide (P2O5) as an additive to modify the conventional carbonate solvents-based lithium hexa-fluoro-phosphate (LiPF6) electrolytes. P2O5 as an additive, stabilizes the electrolyte/electrode interphases by mitigating the hydrogen fluoride (HF) induced side reactions. The P2O5 additive not only improves the Li metal deposition morphology for a denser deposition layer but also alleviates the transition metal dissolution and NMC622 particle cracking problems.

I

\[
\text{Li}^+ \left[ F_2 \text{P} \text{F} \text{F} \right] \xrightarrow{\text{HF}} \text{LiF} + \text{F}_2 \text{P} \text{F} \text{F} \xrightarrow{\text{H}_2 \text{O}} \text{HPO}_2 \text{F} \rightarrow \text{HF} + \text{H}_2 \text{O} \xrightarrow{\text{HPO}_2 \text{F}} \text{PO}_3 \text{F} \rightarrow \text{F}\text{OP} \text{OH}
\]

II

\[
\text{PO}_3 \text{F} + 6 \text{HF} \rightarrow 2 \text{F}\text{OP} \text{OH} + 2 \text{F} \text{OP} \text{OH}
\]

III

\[
4 \text{F} \text{OP} \text{OH} + \text{P}_2 \text{O}_{10} + \text{DEC} \rightarrow 2 \text{F} \text{O} \text{P} \text{O} \text{CO}_2 + \text{F} \text{P} \text{O} \text{OH} + \text{LiPF}_6
\]
Mechanisms of P$_2$O$_5$ additive: (I) Decomposition of LiPF$_6$ electrolyte induced by H$_2$O to produce HF and difluorophosphoric acid (HPO$_2$F$_2$); (II) HF scavenging reaction of P$_2$O$_5$; (III) Reactions of products from (II) with P$_2$O$_5$ to generate new species beneficial to the Li metal anode.

Cycling performance of 0.4 Ah Li||NMC622 pouch cell (50 µm Li anode and 3 mAh/cm$^2$ cathode areal capacity) in lean electrolyte (electrolyte to capacity ratio = 3 g per Ah) at C/10 charging and C/3 discharging.

ADVANTAGES

▶ Mitigation of lithium metal corrosion.
▶ Greatly improved cell performance because of mitigation of HF induced side reactions and improved Li metal deposition.
▶ Improved cycle life - the cycle life of a 0.4 Ah Li-NMC622 pouch cell improved from 30 cycles to more than 200 cycles with 87.7% capacity retention.
▶ Li-NMC622 cathode resistance stays relatively stable.

SUGGESTED USES

Rechargeable lithium-ion batteries

STATE OF DEVELOPMENT

Inventors have developed and demonstrated a proof-of-concept, rechargeable Li-metal batteries using this new electrolyte.

INVENTOR INFORMATION

▶ Please visit Prof. Guo's research group website to learn more about their research.
▶ Please review all inventions by Prof. Guo and his team at UCR.

RELATED MATERIALS

▶ Performance Leap of Lithium Metal Batteries in LiPF6 Carbonate Electrolyte by a Phosphorus Pentoxide Acid Scavenger

RELATED TECHNOLOGIES

▶ New Recycling Methods For Li-Ion Batteries

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