Self-assembling rechargeable Li batteries from alkali and alkaline-earth halides

U.S. DEPARTMENT OF ENERGY
Energy Efficiency & Renewable Energy

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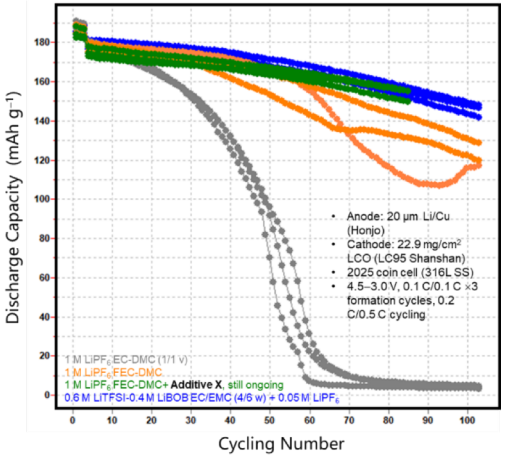
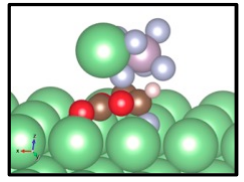
Objective: Investigate electrochemical formation of lithium halide based solid electrolyte films, with the goal of enabling and demonstrating self-assembling/self-healing batteries using lithium metal negative electrodes.

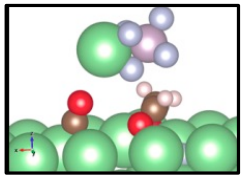
Impact:

- A self-forming solid electrolyte film process is ***simple and scalable***.
- Enables very high energy density cells (>350 Wh/kg) that could improve the driving range and reduce the cost of electric vehicles.

Cycling results for electrolytes with self-forming halide components, tested in $LiCoO_2$ - Li-metal full-cells







- Density Functional theory simulation of FEC decomposition in presence of $LiPF_6$ on Li metal

- Capacity retention of ~85% at 100 cycles for fluorinated electrolytes developed through theory and experiment, compared to baseline electrolyte

Accomplishments:

- Established quantitative theoretical criteria for reactivity of halogen-rich solvents and salts on lithium metal
- Validated selection criteria using Li-Li asymmetric cells that accurately quantify coulombic efficiency
- Delivered structural and chemical characterization results for baseline and self-healed halide films on Li metal
- Discovered several new fluorinated compounds with improved ability to self-form halide solid electrolyte films
- Demonstrated 83-85% capacity retention at 100 cycles in $LiCoO_2$-Li metal coin cells at C/5 charge, C/2 discharge, ≥ 3 mAh/cm^2, with 99.8-99.9% coulombic efficiency

FY19 Milestones:

- Deliver 12 baseline cells of >10 mAh capacity for DOE testing (Q1)
- Establish quantitative criteria for solid-electrolyte/liquid electrolyte combinations that exhibit self-healing functionality (Q2)
- Demonstrate Li-Li symmetric cells or Li-ion cells that meet criteria in M2.3, while cycling ≥5 mAh/cm^2 at C/5 rate over 100 cycles (Q3)
- Deliver 12 final cells of >10 mAh capacity for DOE testing (Q4)

FY19 Deliverables:

Deliver 12 final cells of >10 mAh capacity for DOE testing

Funding:

— FY19: $469,235, FY18: $462,912, FY17: $456,742