First-principles Modeling and Design of Solid-State Interfaces for the Protection and Use of Lithium Metal Anodes

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

PI/Co-PI: Gerbrand Ceder UC Berkeley

Objective:

- Develop dendrite formation model including chemical composition of interfaces, mechanical properties, and species transport.
- Identify solid electrolyte materials based on interface stability and Li-ion conductivity
- Determine criteria for controlled Li deposition on anode surface.
- Asses Li deposition stability on candidate electrolyte materials

Impact:

- Improve lack of understanding of Li deposition and interface dynamics in advanced batteries.
- Li metal anodes with solid electrolytes greatly increases energy density and safety of current batteries.

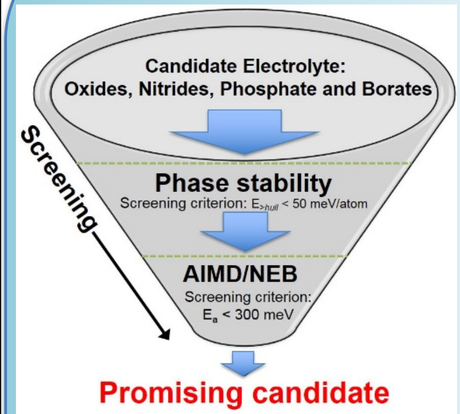


Fig1. Method adopted here to screen for promising electrolyte materials.

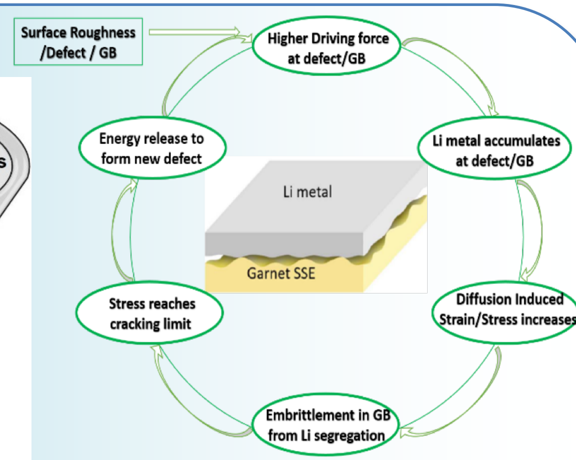


Fig2. Scheme of the formation and propagation of lithium dendrite during cycling.

Accomplishments:

- Screened solid electrolytes through large-scale material recognition based on ICSD and materials prediction.
- Used phase diagrams to assess chemical and electrochemical stable solid electrolytes.
- Developed a framework to study the stability of interface of solid electrolyte and Li Metal based on first principle calculations.
- Developed continuum method to predict dendrite formation and propagation based on multi-physical coupling method and fracture method.

FY 18 Milestones:

- 01/01/18. First principle calculations to screen for solid electrolytes with high Lithium conductivity.
- 04/01/18. First principle calculations of mechanical properties for candidate materials.
- 07/01/18. Continuum model to explain the formation of Lithium dendrite at the interface.
- 10/01/18. Continuum model to study the relation between Lithium dendrite growth and grain boundary and fracture.

FY18 Deliverables:

A framework of Computational method for prediction and suppression of dendrite growth in most solid electrolyte materials.

Funding: FY18: $300K (DOE) Duration: 3 years

New Lamination and doping Concepts for Enhanced Li – S Battery Performance

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

PI/Co-PI: Prashant N. Kumta (UPitt)/ Moni Kanchan Datta (UPitt)/ Oleg I. Velikokhatnyi (UPitt)

Objective:

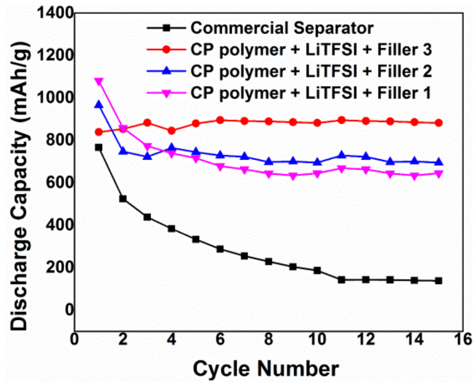
Successfully demonstrate generation of novel approaches using improved lithium ion conductor (LIC) coatings and doping strategies to improve performance of sulfur cathodes for Li-S batteries to achieve the EV everywhere blueprint target.

Impact:

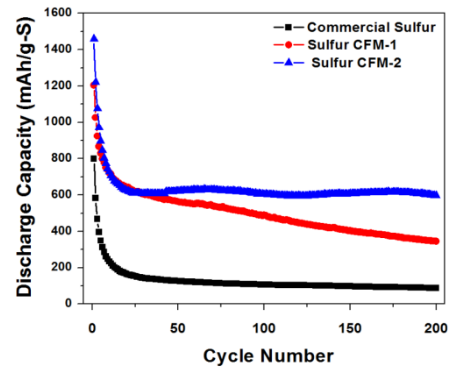
- LIC coatings and complex framework materials (CFM) will help retain polysulfides improving performance
- Theory and experiments will identify and develop doped LICs with much higher Li-ion conduction
- Novel dopants identified by theory and experiments will improve electronic conductivity, rate capability and cyclability

Improved Cycling Behavior

Composite Polymer (CP) Based Sulfur Batteries Showing No Fade



CFM Based Electrodes Demonstrating Minimal Fade Over 300 Cycles



Accomplishments:

- Demonstrate effectiveness of LIC materials in improving sulfur cathode cyclability (4-5 mAh/cm^2).
- Synthesis of high stability flexible sulfur nanowires (~0.003%fade/cycle) and complex framework materials (CFM) with stability over ~300 cycles.
- Development of polymeric LIC systems with doped oxide nanoparticles exhibiting stability over 100 cycles. Composite polymers (CPs) exhibits exception no fade characteristics for commercially obtained sulfur electrodes.
- Identification of doped inorganic LIC systems using first principles and corresponding synthesis of LIC materials displaying ~3 orders of improvement in ionic conductivity.

FY 17 Milestones:

- Synthesis of VACNT and LIC coated chemically synthesized nanosulfur based composite materials
- Design and engineer doped sulfur nanoparticles with improved electronic and ionic conductivity
- Design and engineer high capacity doped LIC coatings on doped nanosulfur

FY17 Deliverables: Quarterly reports, Full cells (4 mAh) meeting the desired deliverables

Funding:

— FY17: $416,687, FY16: $416,687, FY15: $416,687