Dendrite Growth Morphology Modeling in Liquid and Solid Electrolytes

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

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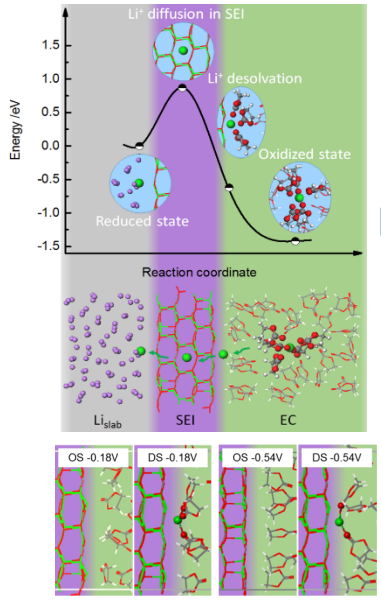
Objective:

- Develop a validated multi-scale model to predict Li dendrite morphology evolution in both liquid and solid electrolytes LIBs during electrodeposition and stripping, in order to accelerate the adoption of Li metal electrodes in current and emerging battery technologies.

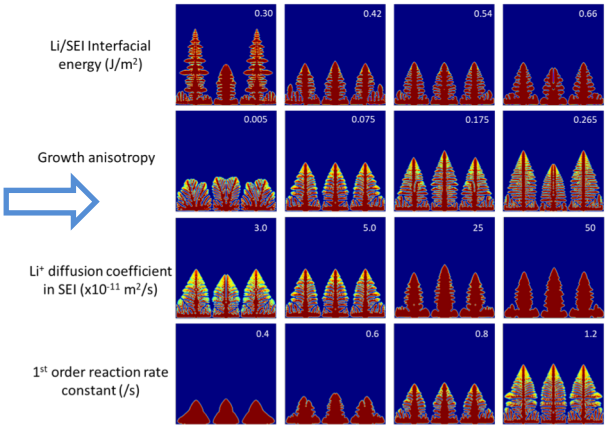
Impacts:

- Enable the design of durable and safe Li-anodes for high energy density Li-ion batteries that can meet DOE's target for EV applications >350 Wh/kg & <$100/kWh$_{use}$.
- The multiscale modeling approach can be applied to other battery systems and integrated with cell and pack design.

Energy Landscape for $Li^+(sol) + e^- \rightarrow Li^0$



SEI properties -- Li dendrite morphology map from phase field simulation.



De-solvation kinetics change with the applied voltage

Accomplishments:

- Connected the charge transfer kinetics and SEI properties with Li dendrite morphology in liquid electrolyte via a multiscale modeling approach.
- Revealed the charge transfer reaction kinetics at a Li/SEI/ electrolyte interface via DFTB simulations.
- Developed an implicit phase field model for Li dendrite growth in liquid electrolyte incorporating solid electrolyte interphase (SEI) effects.
- Developed in-situ optical microscope to capture critical parameters on dendrite growth and morphology evolution.

FY 18 Milestones:

- Identity the Li dendrite formation mechanisms inside solid electrolytes (at the surface & grain boundaries)
- Develop a multiphase multigrain phase-field model, that incorporates the mechanical and electrochemical driving forces for Li dendrite growth in polycrystalline solid electrolyte batteries
- Compare experiments and modeling results on the impact of solid electrolyte microstructure to Li morphology

FY17 Deliverables: A validated Li dendrite morphology model in solid electrolytes, Quarterly reports

Funding:

— FY18: $337,023; FY17: $352,104; FY16: N/A

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:

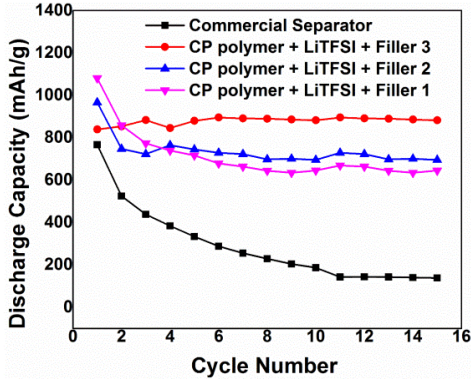
Successfully demonstrate generation of novel approaches using improved lithium ion conductor (LIC) coatings and doping strategies to improve performance of sulfur cathodes for Li-S batteries to achieve the EV everywhere blueprint target.

Impact:

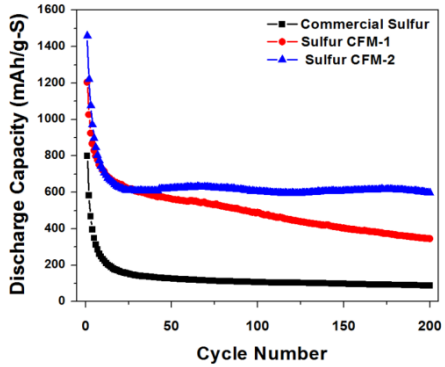
- LIC coatings and complex framework materials (CFM) will help retain polysulfides improving performance
- Theory and experiments will identify and develop doped LICs with much higher Li-ion conduction
- Novel dopants identified by theory and experiments will improve electronic conductivity, rate capability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