

# Electrode Materials Design and Failure Prediction

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## Objective:

Develop computational models for understanding the various degradation mechanisms for next generation lithium ion batteries. In FY19, majority of the focus will be devoted to understanding the cathode solid-state-electrolyte interface.

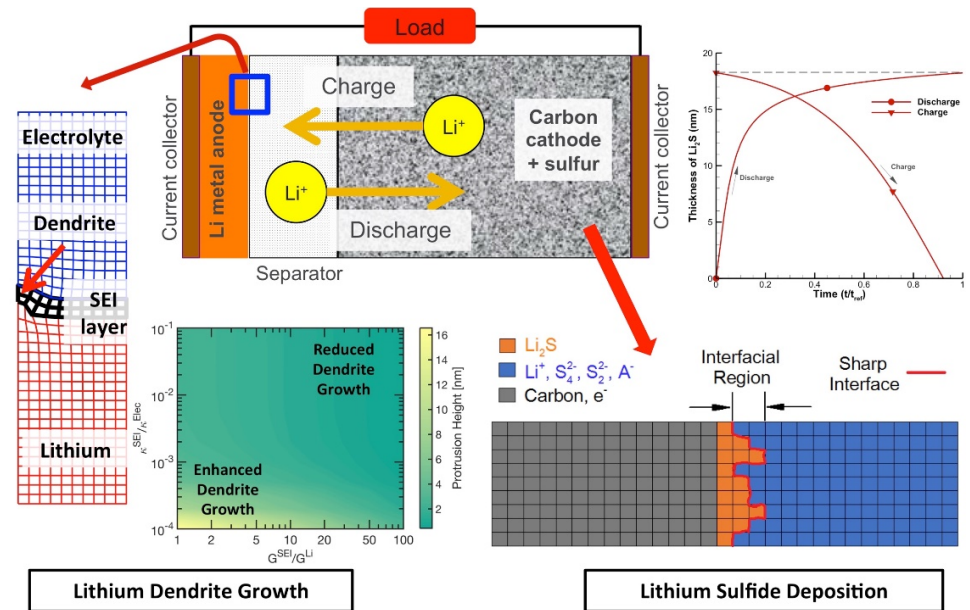
## Impact:

- Findings from this research will give a better understanding of the factors limiting the cycle life of solid state electrolyte lithium ion batteries on the cathode side.
- These results will enable the incorporation of cathode particles within solid state electrolytes.

## Accomplishments:

- Developed a computational model incorporating elastic-plastic deformation of lithium and electrolyte, which also solves for potential and concentration distribution.
- Increasing the yield strength and elastic modulus of polymer electrolytes can prevent growth of dendrites.
- Presence of inhomogeneity and mechanical stiffness of the solid-electrolyte-interphase layer, can have a significant impact on the growth of dendritic protrusions.
- Simulation of the  $\text{Li}_2\text{S}$  precipitation process reveals that, operation at high C-rates can lead to  $\text{Li}_2\text{S}$  accumulation, because its precipitation is faster than dissolution.

## Deposition Induced Degradation in Lithium Batteries.



## FY19 Milestones:

- Analyze the effect of delamination at the cathode/solid-state-electrolyte interface as a mode of degradation. (Q2)
- **Go/No-go:** Estimate SOC dependent impedance at cathode solid-state-electrolyte interface. If not possible, proceed with the impedance measured at fixed SOC. (Q4)

## FY19 Deliverables:

Computational framework to estimate delamination and impedance at cathode/solid-state-electrolyte interface.

## Funding:

— FY19: \$450k, FY18: \$450k, FY17: \$450k