

# Task 3.7 – First-Principles Modeling and Design of Solid-State Interfaces for the Protection and Use of Lithium-Metal Anodes

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## *Objective:*

- Determine the design principles that control the solid electrolyte/Li electrode interfaces and create more stable Li/solid-electrolyte combinations

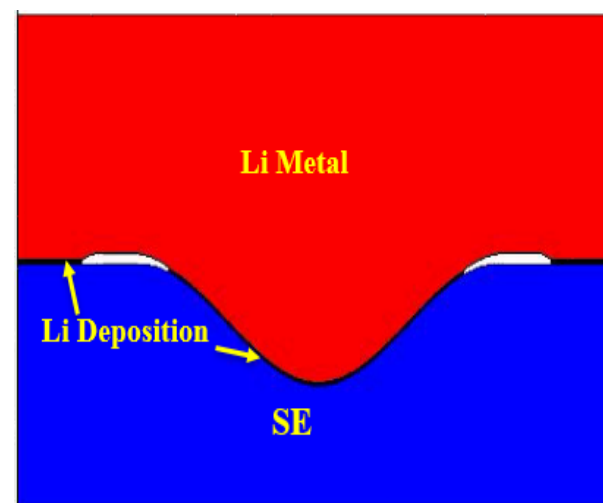
## *Impact:*

- Understanding of the complex evolution of Li-metal/solid electrolyte interfaces during electrochemical cycling.
- More reliable all solid-state batteries with Li metal anodes

## *Accomplishments:*

- Developed models that integrate electrochemical transport and mechanical behavior of the electrodes
- Demonstrated that surface roughness of solid state conductor combined with plasticity of Li metal leads to growth of porosity of metallic anode

## *Deposition of Li metal with surface roughness*



## *FY19 Milestones:*

- Q1. high-throughput framework to screen solid state electrolytes materials s.
- Q2. fracture models for crack propagation in SSE: perfect crystal with cracks
- Q3. fracture models for crack propagation in SSE: perfect crystal with with grain boundaries
- Q4: fracture models for crack propagation in SSE as a pressed/porous electrolyte

*FY19 Deliverables:* Insight and design rules for Li metal anode in SSB. Papers and Presentations

## *Funding:*

— FY19: 300K; FY18: 300K