Dendrite Growth Morphology Modeling in Liquid and Solid Electrolytes

PI/Co-PI: Yue Qi (Michigan State U.)/ Long-Qing Chen (Penn State U.) / Xingcheng Xiao and Qinglin Zhang(GM)

- *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.

Impact:

- 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.

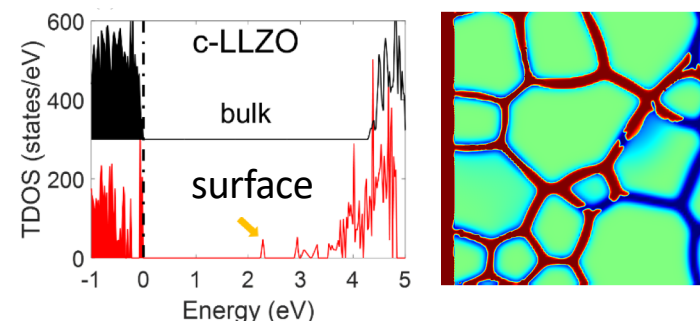In liquid electrolyte

In solid electrolyte

Accomplishments:

- Developed an atomistic-informed phase-field model to predict Li dendrite growth in liquid electrolytes while incorporating solid electrolyte interphase (SEI) effects.
- Revealed the fundamental difference between Li and Mg plating morphology is the desolvation energy and the equilibrium exchange current.
- Identified the Li-dendrite formation in solid electrolytes is due to the electronic conductive internal defects, such as pore and crack surfaces.
- Incorporated the microstructure of the solid electrolyte and coupled mechanical-electrochemical driving forces to simulate dendrite growth in solid electrolytes.
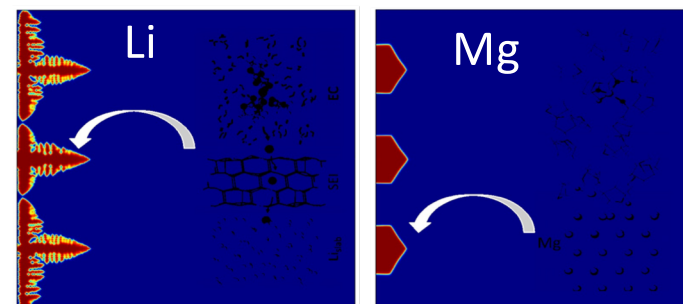
FY19 Milestones:

- A fully coupled Li/SEI/liquid electrolyte dendrite morphology model is developed (Q1)
- Reveal the relationship between Li/SEI properties and dendrite morphology (Q2)
- Determine the effect of multicomponent SEI layer on dendrite morphology (Q3)
- Guide the design of artificial SEI coating on Li metal (Q4)

FY19 Deliverables:

A validated Li dendrite morphology model in solid and liquid electrolytes, Quarterly reports

Funding:

— FY19: 310,816; FY18: $337,023; FY17: $352,104;