Ab initio molecular dynamics computations have provided the interface structure of a LLZO solid electrolyte with a Li surface. Monte Carlo simulations have been used to obtain LLZO grain boundary structures for use in calculation of exchange current densities for continuum models. The Young’s modulus at grain-interior and grain-boundary region for LLZO solid electrolytes has been calculated for input to continuum level models.

**PI/Co-PI:** Anh T. Ngo (Argonne), Larry A. Curtiss (Argonne), and Venkat Srinivasan (Argonne).

**Objective:** Multi-scale modelling to obtain an in-depth understanding of the interaction of electrodes and solid electrolytes to help develop highly efficient solid state electrolytes batteries for vehicle applications.

**Impact:**
- Development of stable and effective solid-state electrolytes as a replacement for the commercially used organic liquid electrolytes to improve safety and energy density in lithium ion batteries.
- The use of solid electrolytes provides a path to prevent dendrites in Li-metal anodes, thereby leading to batteries with significant higher energy density.

**Accomplishments:**
- Ab initio molecular dynamics computations have provided the interface structure of a LLZO solid electrolyte with a Li surface.
- Monte Carlo simulations have been used to obtain LLZO grain boundary structures for use in calculation of exchange current densities for continuum models.
- The Young’s modulus at grain-interior and grain-boundary region for LLZO solid electrolytes has been calculated for input to continuum level models.

**FY19 Milestones:**
- Computation of elastic-conductivity properties of interfaces between LLZO and lithium as function of applied electric field for input into multiscale modelling.
- Investigation of structure and stability of solid state electrolytes interfaces with anode and cathode surfaces for input into multiscale modelling.
- Continuum level modeling of solid state electrolytes to improve their stability and conductivity properties using atomistic inputs.

**FY19 Deliverables:** Quarterly reports, Journal publications.

**Funding:** FY19: $300,000 FY18: $300,000