Multi-scale Modeling of Solid State Electrolytes for Next Generation Lithium Batteries

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

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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

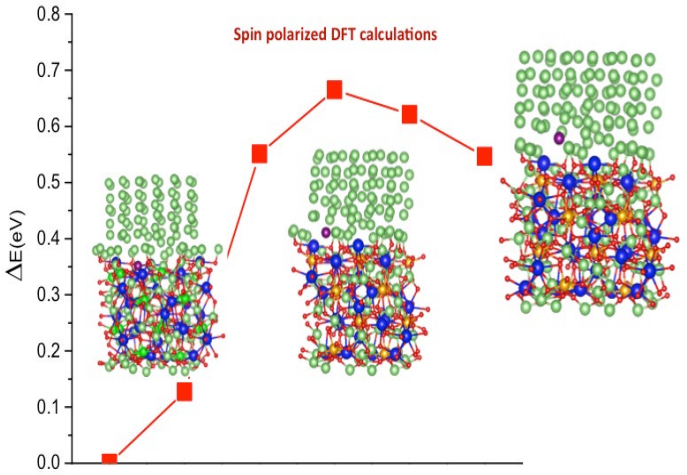

Figure: Energy barrier obtained from density functional theory lithium atom migration from LLZO to lithium metal. The magnitude of the barrier obtained is 0.65 eV.

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.

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