Advancing Solid-State Interfaces in Li-ion batteries

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

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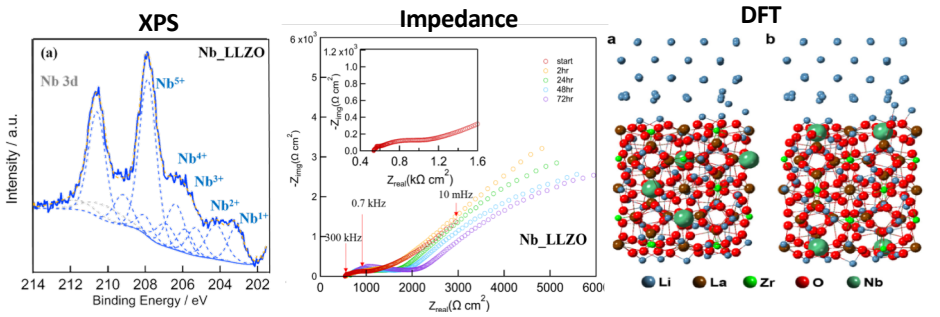
Objective:

The project objectives are multifaceted, including the development of a new mechanically and chemically stable and Li ion conductive (≥2 x 10^{-4} S/cm at 298K) solid electrolyte (S_{EL}) for a solid-state battery encompassing a metal Li anode, Li-oxide-based cathode and nonflammable crystalline and amorphous solid electrolytes that can operate at cathode potentials > 5V (denoted as a S_{Li}-S_{EL}-S_C system)

Impact:

Protective organic and inorganic compounds can enhance the stability of interface, improve Li ion interfacial transport, minimize dendrite formation and increase safety in Li ion batteries.

- Demonstrated that stability of Li and LLZO interface strongly depends on both surface chemistry and dopant type.
- Established correlation between interfacial stability and interfacial impedance.



Observed reduction of Nb in Nb-doped LLZO with XPS core level spectra after Li deposition on clean Nb-LLZO surface, corresponding time dependent impedance increase of Li_Nb-doped LLZO_Li symmetric cells at room temperature and DFT optimized structures with Nb dopants (a) distributed in the bulk and (b) segregated towards the surface for Nb-doped LLZO in contact with Li.

Accomplishments (FY18):

- Used state-of-the-art XPS method for exploring intrinsic chemical stability of Li-solid electrolyte interface
- Demonstrated orientation-dependent interaction between Li and LLTO: orientation with more Li-intercalation path found to be more unstable
- Determined the window of structural stability of LLZO upon UHV annealing
- Extended the interface stability study from oxide solid-electrolyte (LLTO, LLZO) to glass electrolyte (LPS)
- Introduced new computational tools for characterizing interaction of lithium and solid electrolytes (LLTO, LLZO)

FY19 Milestones:

- Understanding the impact of LLZO dopants (Nb vs. Al) on interfacial reactivity and stability (Q1)
- Determine the impact of solid electrolyte crystallinity (epitaxial vs. amorphous) on interfacial stability (Q2)
- Distinguish chemical vs. electrochemical reactivity at the interface and bulk with Li/S_{EL}/$LiCoO_2$ full cells (Q3)
- Gain knowledge to enable predictive modeling of realistic interfaces in solid-state batteries by DFT characterization (Q4)

FY19 Deliverables: Quarterly reports, new approaches for characterization and modeling interfaces

Funding:

— FY19: $400,000 , FY18: $400,000 , FY17: $400,000