Advancing Solid-State Interfaces in Li-ion Batteries

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

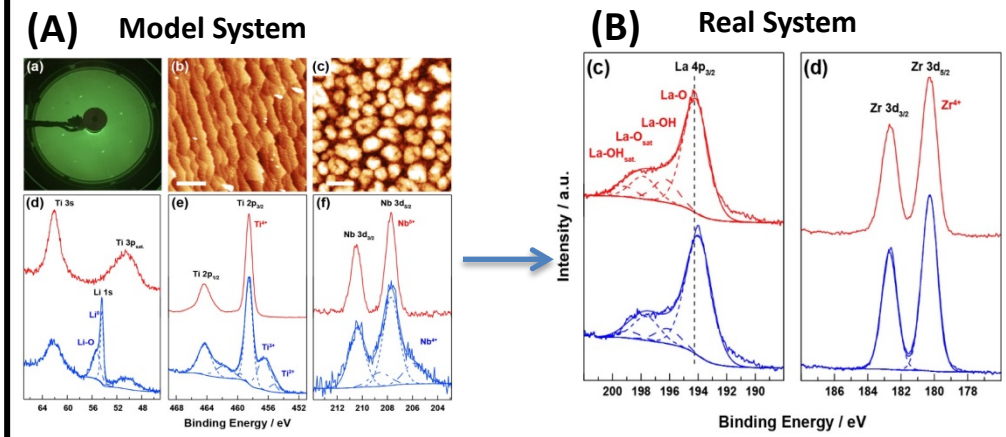
PI/Co-PI: PI/Co-PI: Nenad M Markovic(ANL), Larry A. Curtiss ANL)

- ***Objective:*** Develop mechanically and chemically stable Li-selective solid "membranes" in organic electrolytes (S_{Li}-S_M-E_{EL}) and conductive solid electrolytes for a solid-state battery (S_{Li}-S_{EL}-S_C) capable of protecting the metal Li anode during the discharge process.

Impact:

- Protective organic and inorganic compounds can lead to enhanced stability of interface, improve Li ion interfacial transport, minimize dendrite formation and increase safety in Li ion batteries.

Chemical and morphological interfacial interactions of Li with solid electrolytes : from model to real systems



A - illustrates structural and chemical characterization of STO(001) surface both before and after Li deposition. **B** - illustrates Li interaction with Nb:LLZO system

Accomplishments:

- Developed state-of-the-art experimental and computational techniques capable of exploring chemical stability and reactivity of S_{Li}-S_{EL}-S_C systems.
- Established first ever stability-/reactivity-function relationships for studying interaction of Li metal anode with a model Nb doped $SrTiO_3$ (STO) single crystal solid electrolyte.
- Used the knowledge from model systems to understand Li interaction with a real ($Li_{6.5}La_3Zr_{1.5}Nb_{0.5}O_{12}$, LLZO) solid electrolyte.
- Understanding of morphological and chemical stability of Li-Nb:STO(hkl) and Li-Nb:LLZO via DFT calculations

FY 18 Milestones:

- Development of well defined single crystal LLZO interfaces to assess factors that govern the interfacial and bulk properties of the Li/LLZO system.
- Investigate other relevant crystalline oxides and glassy materials as a potential solid electrolytes.
- Explore the interaction of solid electrolytes with well-characteriaed cathode oxide materials (LiCoO2)

FY18 Deliverables: Quarterly reports, new approaches for characterization and modeling interfaces

Funding:

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

OVERCOMING INTERFACIAL IMPEDANCE IN SOLID-STATE BATTERIES

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EXAMPLE

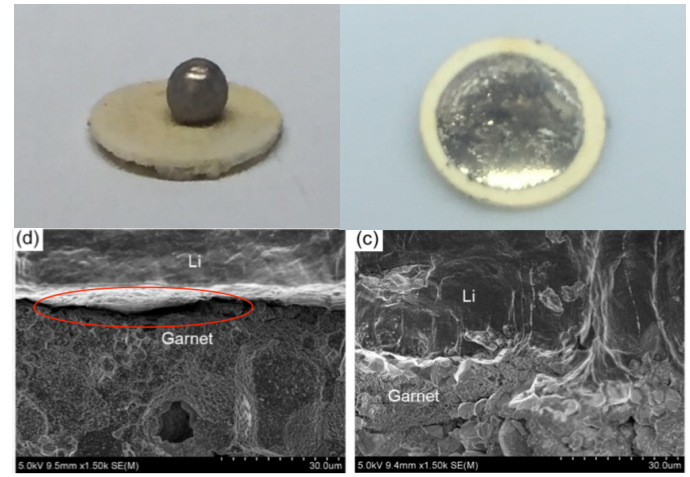
PI/Co-PI: Eric Wachsman (UMD)/ Liangbing Hu (UMD) / Yifei Mo (UMD)

Objective: Develop a multifaceted and integrated (experimental and computational) approach to reduce interfacial impedance of garnet-based solid-state Li ion batteries (SSLiBs).

Impact:

- Overcome primary issue with garnet electrolyte SSLiBs, interfacial impedance, thus enabling an entirely new safer (non-flammable) battery platform
- Enable highest capacity Li-metal anodes with no dendrites for higher energy density batteries (~500 Wh/kg)

Li Metal Wetting of Solid-State Electrolyte



Developed surface treatment to allow Li-metal wetting thus dramatically reducing interfacial impedance

Accomplishments: (FY16)

- First comprehensive investigation of interface impedance in garnet based SSLiBs
- Determined interfacial impedance as function of electrolyte/electrode contact area in 3D controlled solid state structures
- Developed computational models to investigate interfacial ion transport with interlayers
- Developed multiple efficient interlayer solutions to decrease interfacial impedance
- Demonstrated low interfacial impedance (~10 Ω cm^2) between both electrolyte and Li-metal anode and between electrolyte and cathode

FY 17 Milestones:

- Demonstrate full cells with NMC cathode
- Demonstrate full cells with Sulfur cathode
- Develop models to investigate interfacial transport for Li-S and Li-NMC SSLiBs
- Achieve full cell (Li-S or Li-NMC) performance of 350-450 Wh/kg and 200 cycles

FY17 Deliverables: Submission of 12 improved cells for government testing and evaluation

Funding:

— FY17: $401,634, FY16: $401,635 FY15: $409,608