Identification of Efficient and Stable Electrochemical Interfaces for Li-S Batteries

**PI/Co-PI:** Perla Balbuena (Texas A&M University)/Jorge Seminario (Texas A&M University)

- **Objective:** Investigate and demonstrate solid electrolyte candidates and optimal interfaces for a Li/S battery capable of achieving an energy density ≥500 Wh/Kg while achieving a 1,000-cycle life.

**Impact:**
- Highly-accurate computational approach will guide optimal material screening cutting down trial and error experimentation costs and time
- Integrated computations and experiments help understanding and characterization of interfacial phenomena

**Accomplishments:**
- New Start

**FY 18 Milestones:**
- Interfacial stability of solid electrolytes on Li-metal surface
- Ionic/electronic transport at Li-metal/solid electrolyte interfaces
- Discharge/charge reactions of S/C cathode and Ionic/electronic transport in presence of solid electrolyte
- Solid electrolyte materials optimization

**FY18 Deliverables:** Characterization of selected solid electrolytes at the interfaces of Li-metal and S-C cathode

**Funding:**
- FY18: $400,000
OVERCOMING INTERFACIAL IMPEDANCE IN SOLID-STATE BATTERIES

**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)

**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 cm²) 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