Optimization of Ion Transport in High-Energy Composite Cathodes

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

PI: Y. S. Meng (UCSD)

Technical Approach:

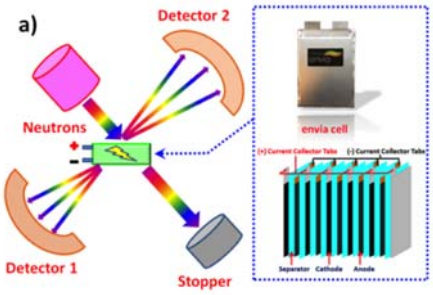
- A systematic study of electrode/electrolyte interfaces with power suite of analytical tools: neutron/x-ray diffraction (ND/XRD), electron energy loss spectroscopy (EELS), X-ray photoelectron spectroscopy (XPS) and first principles computation (FP)

Status:

- Completed study on layer-layer (LL) composite cathodes
- Developed protocol for silicon/carbon based composites.

Technology:

- Developed *operando* neutrc diffraction to quantify the oxygen evolution and transition metal migration
- Used EELS and XPS to probe and diagnose the Si SEI chemical compositions
- Succeeded in surface modification to enhance ion transport in Li rich Mn rich layered oxides



Operando Neutron Diffraction set up to probe lithium dynamics and transition metal migration in real time in porch cells.

Objectives:

- Probe and control the atomic-level kinetic processes in classes of high energy composite electrodes, including both high voltage cathode and Si-based anode.
- Pin down the mechanism of ion migration and determine the optimum bulk compositions and surface characteristics for high rate and long life
- Help the synthesis efforts to produce the materials at large scale with consistently good performance

Deliverables: Modifying and controlling the oxygen activities in LL composites; Atomistic level understanding of the surface chemical composition and morphology changes in Si without and with additives and coatings.

Funding:

Duration: 4 yrs (Yr 4)

FY16 Budget: $259K (DOE)

Milestones:

- **Q1:** Investigate the mechanism of improved performance in high voltage Li rich Mn rich layered oxides with LLTO coating.
- **Q2:** Quantify the SEI characteristics of ALD and MLD coated silicon anode upon long cycling with combination of STEM/EELS and XPS
- **Q3:** Go/No-Go Milestone: Complete the efforts on investigation of surface modification and morphology control for Li rich Mn rich layered oxides. Criteria: Discontinue studies if the voltage retention does not get improved by 50% in 100 cycles.
- **Q4:** Identify the optimum surface modification and morphology control of silicon/carbon anode with >87% first cycle capacity retention and > 99% columbic efficiency