Advanced Microscopy and Spectroscopy for Probing and Optimizing Electrode-Electrolyte Interphases in High Energy Lithium Batteries

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

PI: Y. Shirley Meng (University of California San Diego)

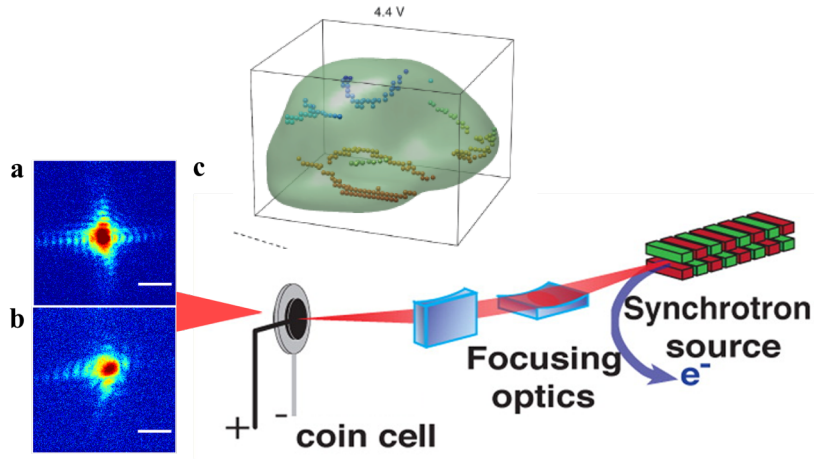
- ***Objective:***

The proposed diagnostic tools will ultimately lead to quantitative understanding careful manipulation of the anion activities (anion redox and oxygen evolution) in both the bulk structure and interfaces in lithium excess layered oxide materials to improve energy density, stabilize the operation voltage

- ***Impact:***

The insights and knowledge provided by the characterization tools will have the critical importance of enabling a major breakthrough in commercial applications for high voltage and high energy density cathode material for lithium ion batteries used for vehicle applications

Our approach intends to investigate the anion activities in single particle Li–excess cathode materials using operando imaging and spectroscopic analysis



Accomplishments:

- XPS and DEMS characterization confirms anion redox activities in Li excess layered oxides.
- BCDI measurements on Li-excess single NMC particle demonstrate significantly higher amount of defects such as stacking faults, compared with classical layered oxides.
- STEM/ EELS characterization of Li-excess single NMC particle confirms that the layer-to-spinel transformation is largely confined to the surface 2-5nm.

FY 18 Milestones:

- Benchmark electrode performance of bulk and surface modified Li-excess NMC
- XPS characterization of CEI of and DEMS characterization of anion evolution on modified Li-excess NMC
- BCDI imaging of modified Li-excess NMC single particle
- Propose strategies to optimize the anion activities in Li excess NMC cathode materials.

FY18 Deliverables:

Characterizing single particle behavior of modified Li-excess layered NMC materials

Funding:

— FY18 ($360K BMR funding, $40K cost share) same in FY17

New Lamination and doping Concepts for Enhanced Li – S Battery Performance

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

PI/Co-PI: Prashant N. Kumta (UPitt)/ Moni Kanchan Datta (UPitt)/ Oleg I. Velikokhatnyi (UPitt)

Objective:

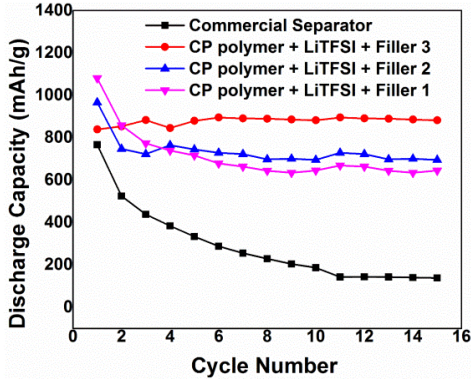
Successfully demonstrate generation of novel approaches using improved lithium ion conductor (LIC) coatings and doping strategies to improve performance of sulfur cathodes for Li-S batteries to achieve the EV everywhere blueprint target.

Impact:

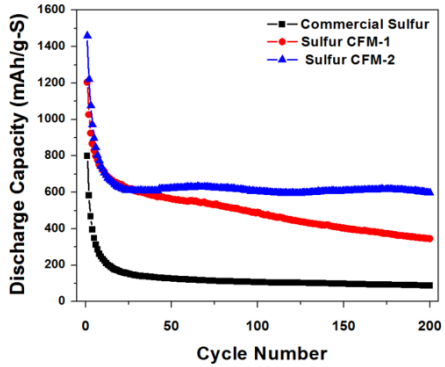
- LIC coatings and complex framework materials (CFM) will help retain polysulfides improving performance
- Theory and experiments will identify and develop doped LICs with much higher Li-ion conduction
- Novel dopants identified by theory and experiments will improve electronic conductivity, rate capability and cyclability

Improved Cycling Behavior

Composite Polymer (CP) Based Sulfur Batteries Showing No Fade



CFM Based Electrodes Demonstrating Minimal Fade Over 300 Cycles



Accomplishments:

- Demonstrate effectiveness of LIC materials in improving sulfur cathode cyclability (4-5 mAh/cm^2).
- Synthesis of high stability flexible sulfur nanowires (~0.003%fade/cycle) and complex framework materials (CFM) with stability over ~300 cycles.
- Development of polymeric LIC systems with doped oxide nanoparticles exhibiting stability over 100 cycles. Composite polymers (CPs) exhibits exception no fade characteristics for commercially obtained sulfur electrodes.
- Identification of doped inorganic LIC systems using first principles and corresponding synthesis of LIC materials displaying ~3 orders of improvement in ionic conductivity.

FY 17 Milestones:

- Synthesis of VACNT and LIC coated chemically synthesized nanosulfur based composite materials
- Design and engineer doped sulfur nanoparticles with improved electronic and ionic conductivity
- Design and engineer high capacity doped LIC coatings on doped nanosulfur

FY17 Deliverables: Quarterly reports, Full cells (4 mAh) meeting the desired deliverables

Funding:

— FY17: $416,687, FY16: $416,687, FY15: $416,687