Advanced in situ Diagnostic Techniques for Battery Materials

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

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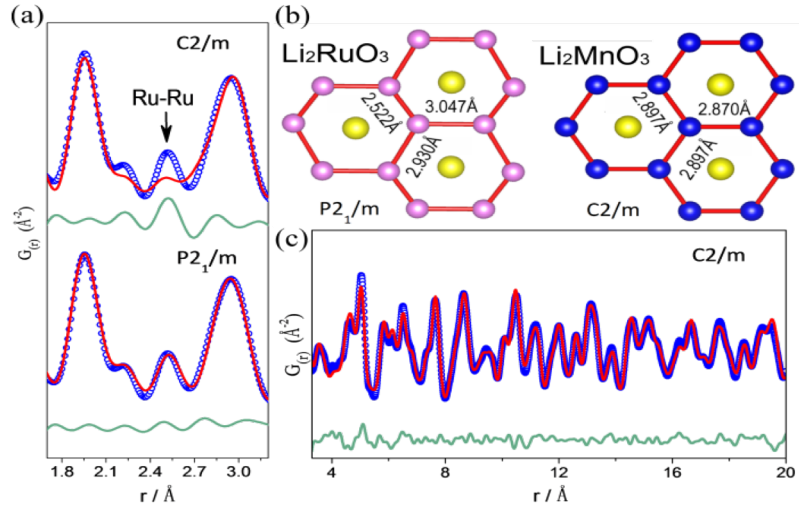
Objective:

- Develop new advanced in situ material characterization techniques
- Support the development of new cathode and anode materials for the next generation of lithium-ion batteries for plug-in hybrid electric vehicles

Impact:

- The results of this project will be used for the development of technologies that will significant increase the energy density, cycle life and reduce the cost..

Title of Graph: X-ray PDF developed at BNL has the capability to detect short bond of Ru-Ru in $Li_2Ru_{0.5}Mn_{0.5}O_3$ cathode material



Accomplishments:

- Developed and applied synchrotron based x-ray "Pair Distribution Function" (PDF) and neutron PDF techniques to study the high energy density cathode materials for Li-ion batteries
- Developed and applied transmission X-ray microscopic (TXM) both in full frame and nano-probe scanning TXM to study high Ni content NCM cathode materials.
- Developed and applied synchrotron based insitu XRD and XAS in combination with 3-D STEM tomography to study high energy density cathode materials for Li-ion batteries

FY 17 Milestones:

- Q1: Complete the *in situ* TXM studies of $LiCoO_2$ cathode materials during high voltage charge-discharge cycling
- Q2: Complete the neutron diffraction studies of $LiCoO_2$ as high energy density cathode material at high voltage charge
- Q3: Complete the pair distribution function (PDF) studies of $LiCoO_2$ using both x-ray (x-PDF) and neutron (n-PDF)
- Q4: Complete the experimental design, data collection and analysis of three dimensional (3D) STEM tomography studies of high energy density $Li_{1.2}Ni_{0.15}Co_{0.1}Mn_{0.55}O_2$ cathode materials

FY17 Deliverables: Develop and apply synchrotron based x-ray PDF, XRD, XAS, and TXM, as well as STEM and neutron based PDF techniques to study new cathode materials.

Funding:

— FY18: $150,000, FY17: $600,000, FY16: $600,00

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:

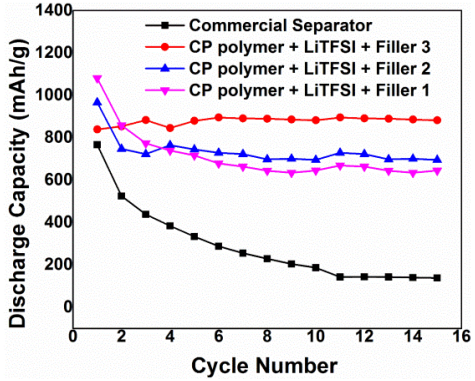
Successfully demonstrate generation of novel approaches using improved lithium ion conductor (LIC) coatings and doping strategies to improve performance of sulfur cathodes for Li-S batteries to achieve the EV everywhere blueprint target.

Impact:

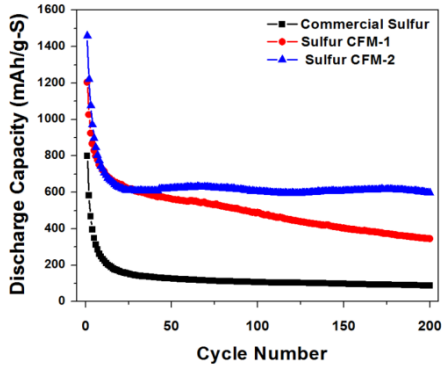
- LIC coatings and complex framework materials (CFM) will help retain polysulfides improving performance
- Theory and experiments will identify and develop doped LICs with much higher Li-ion conduction
- Novel dopants identified by theory and experiments will improve electronic conductivity, rate capability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