Exploratory studies of novel sodium-ion battery systems

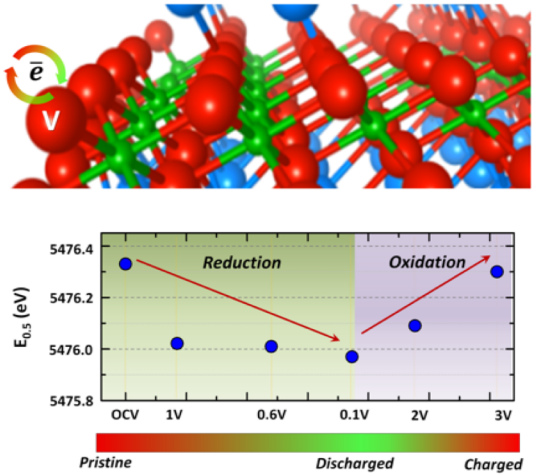
U.S. DEPARTMENT OF ENERGY
Energy Efficiency & Renewable Energy

PI/Co-PI: Xiao-Qing Yang (BNL) and Seongmin Bak (BNL)

- ***Objective:***
- To develop new advanced in situ material characterization techniques and apply these techniques sodium-ion battery systems).
- To provide guidance in development of Na-ion batteries systems with high energy and power density, low cost, good safety characteristics and long life.
- ***Impact:***
- The results of this project will accelerate the deployment of electrical vehicles.

Title of Graph:

Na-Ion Intercalation and Charge Storage Mechanism in Two-Dimensional Vanadium Carbide: V_2C



Accomplishments:

- Completed the in situ hard x-ray absorption studies at vanadium K-edge of one type of Maxene material V_2C as new anode material for sodium ion batteries
- Completed the soft x-ray absorption studies at vanadium L-edge, carbon and oxygen K-edge of one type of Maxene material V_2C.
- Completed the synchrotron based x-ray absorption at Cu and Mn k-edge for a new $NaCuMnO_2$ cathode material for Na-ion batteries during charge-discharge cycling.

FY 18 Milestones:

- Q1: Complete XRD and XAS studies and of new $NaCrS_2$ layer structured cathode materials during charge-discharge cycling.
- Q2: Complete the XRD studies with Rietveld refinement of $Na_3VP_3O_9N$, ad well as XAS investigation of this new cathode material .
- Q3: Complete the synchrotron based in situ x-ray diffraction studies of $Na_{0.66}Mn_{0.6}Ni_{0.2}Mg_{0.2}O_2$ as new cathode material for Na-ion batteries.
- Q4: Complete the synchrotron based x-ray absorption near edge structure (XANES) studies of $Na_{0.66}Mn_{0.6}Ni_{0.2}Mg_{0.2}O_2$ as new cathode material for Na-ion batteries during charge-discharge cycling .
- ***FY18 Deliverables:*** Develop and apply synchrotron based XRD, XAS and TXM techniques to study the structural changes of new electrode materials for Na-ion batteries.

Funding:

— FY18: $100,000, FY17: $500,000, FY16: $500,00

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:

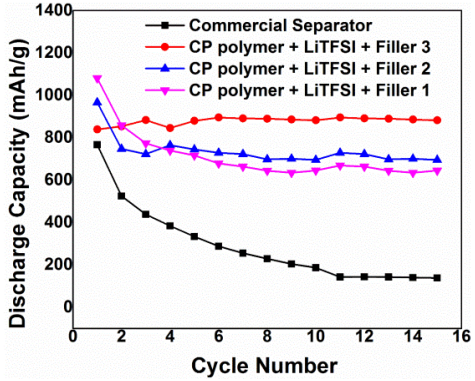
Successfully demonstrate generation of novel approaches using improved lithium ion conductor (LIC) coatings and doping strategies to improve performance of sulfur cathodes for Li-S batteries to achieve the EV everywhere blueprint target.

Impact:

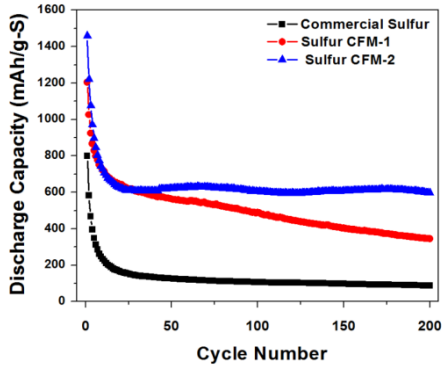
- LIC coatings and complex framework materials (CFM) will help retain polysulfides improving performance
- Theory and experiments will identify and develop doped LICs with much higher Li-ion conduction
- Novel dopants identified by theory and experiments will improve electronic conductivity, rate capability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