

Advanced in situ Diagnostic Techniques for Battery Materials

U.S. DEPARTMENT OF

ENERGY

Energy Efficiency & Renewable Energy

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

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

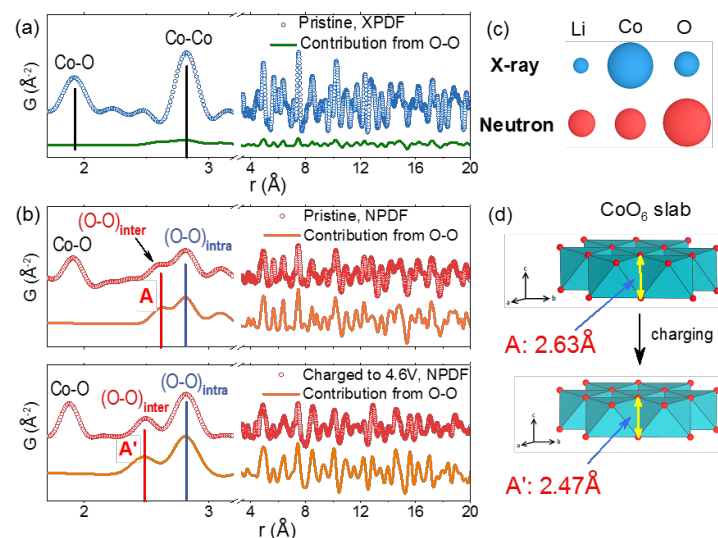
Impact:

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

Accomplishments:

- Completed studies of LiCoO_2 , a widely used commercial cathode material using TXM technique
- Completed studies of ion exchange synthesis mechanism of $\text{Li}_2\text{Mg}_2\text{P}_3\text{O}_9\text{N}$.
- The correlations between transition metal chemistry and structure in $\text{Li}_2\text{Ru}_{0.5}\text{Mn}_{0.5}\text{O}_3$ has been investigated in a wide voltage window.
- The complexities of structural changes in layered oxide cathode materials during fast charge–discharge cycling and heating were investigated using synchrotron based XRD and XAS, as well as TEM.

Title of Graph: xPDF (a) and nPDF (b) data of pristine and charged samples. (c) The relative scattering power for X-ray and for neutron scattering. (d) The change of the shortest O-O pair distance after charge



FY 19 Milestones:

- Q1: Complete the ex situ soft x-ray absorption (sXAS) studies at oxygen K-edge of novel organic disulfide cathode materials
- Q2: Complete the ex situ soft x-ray absorption (sXAS) studies at sulfur K-edge of novel organic disulfide cathode materials.
- Q3: Complete x-ray absorption spectroscopy (XAS) studies of sulfur electrode harvested from failed pouch cells after multiple cycling.
- Q4: Complete x-ray absorption spectroscopy (XAS) studies of sulfur electrode harvested from failed high energy Li/S pouch cells after multiple cycling.

FY19 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:

— FY19: \$500,000, FY18: \$500,000, FY16: \$600,00