Characterization and Computational Modeling of Structurally Integrated Electrodes

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

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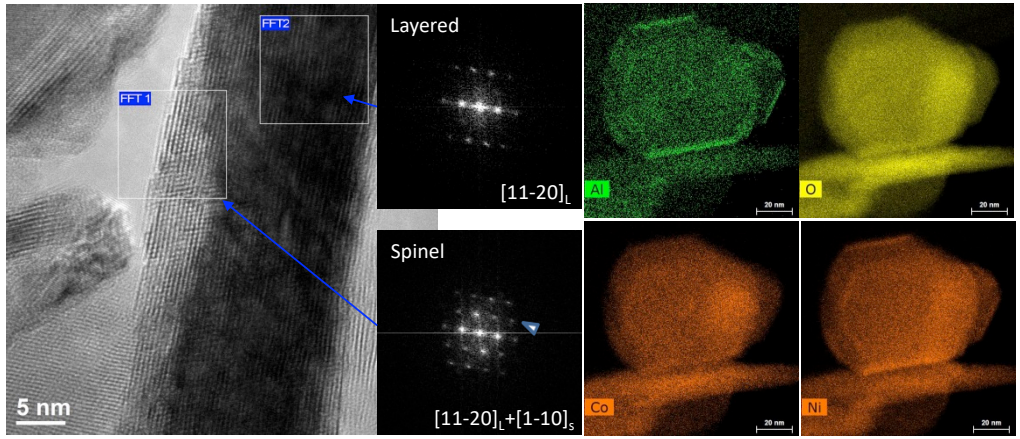
Objective:

- Evaluate atomic-scale electrochemical processes and structures that are most relevant to next-generation, lithium-ion battery technologies
- Capitalize on unique experimental facilities and theoretical approaches to advance the field through collaborations and multi-disciplinary efforts

Impact:

Advancement of DOE goals for PHEV and EV batteries through detailed understanding of structure-electrochemical property relationships and degradation mechanisms

Surface-Modified Layered-Layered-Spinel Particles



Accomplishments:

- A series of $Li_{1.25-x}(Ni_{0.28}Mn_{0.53}Co_{0.19})O_{2.25-\delta}$ ($0 \leq x \leq 0.25$), layered-layered-spinel (LLS) oxides, containing various spinel contents, has been analyzed by combined Rietveld refinement of synchrotron X-ray and neutron diffraction data
- HRTEM studies of LLS cathodes show preferential formation of spinel domains in the near-surface region of LLS particles, suggesting a compositional dependence
- STEM-EDX studies suggest facet-dependent segregation of of elements on surface-modified, LLS particles
- The properties of low-temperature, Ni-doped, $LiCoO_2$-based spinels were examined via DFT calculations

FY 18 Milestones:

- Characterization of complex materials relevant to energy storage applications, including bulk, surface, and interface structures
- Development of new theoretical tools that enable detailed descriptions of the local, atomic environments that govern electrochemical responses in these complex materials
- Combined theoretical/experimental analysis, interpretation, and dissemination of collected data for publication and presentation

FY18 Deliverables:

Quarterly reports; An understanding of structure-property relationships that govern complex energy-storage materials

Funding:

— FY18: TBD, FY17: $500K, FY16: $500K