Model-System Diagnostics for High-Energy Cathode Development

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

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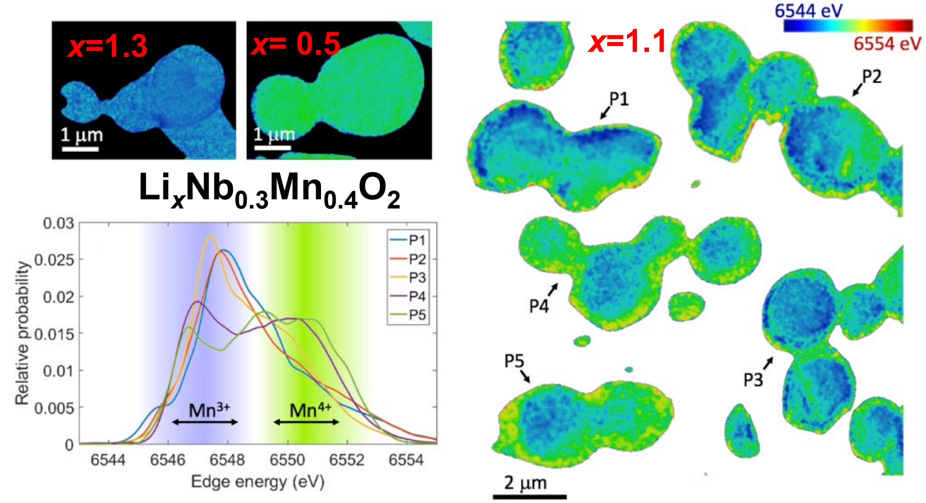
Objective:

- Identify performance- and stability-limiting properties and processes in high-energy/high-voltage cathodes.
- Design bulk and surface properties of cathode materials to minimize side reactions and maximize Li transport kinetics.
- Synthesize new and improved materials for next-generation lithium-ion batteries.

Impact:

- Fundamental knowledge gathered from model-system based studies will guide electrode material engineering.
- The use of non-empirical, rational-design approach will develop materials with improved commercial viability for EV batteries.

Effect of local chemistry on Li mobility



Correlation of local structural ordering, Li diffusion pathway and chemical reaction propagation in rock-salt TMO cathodes.

Accomplishments:

- Determined total capacity, kinetic properties, capacity fade, voltage fade and hysteresis as a function of O redox activities in Li-excess TM oxide (TMO) cathodes.
- Elucidated chemical and structural changes associated with TMO cycling involving O redox.
- Revealed the effect of local chemistry on Li diffusion pathways and reaction mechanisms.
- Developed a densification mechanism elucidating performance degradation resulting from a combination of TM reduction and deterioration in Li percolation network.
- Demonstrated the use of cation-site chemistry to balance capacity and stability in Li-excess rock-salt cathodes.

FY 19 Milestones:

- Understand the interplay between cationic and anionic redox processes in model Li-excess TMO cathodes (Q1).
- Characterize interfacial processes and surface changes (Q2).
- Evaluate the effect of particle size/morphology on oxygen redox chemistry and kinetics (Q3).
- Develop design strategies to improve performance of anion-active oxide cathodes (Q4).

FY19 Deliverables: Understand the underlying failure mechanisms associated with performance issues in Li-TM oxides involving anion redox.

Funding:

— FY19: $500K, FY18: $500K, FY17: $550K