

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.

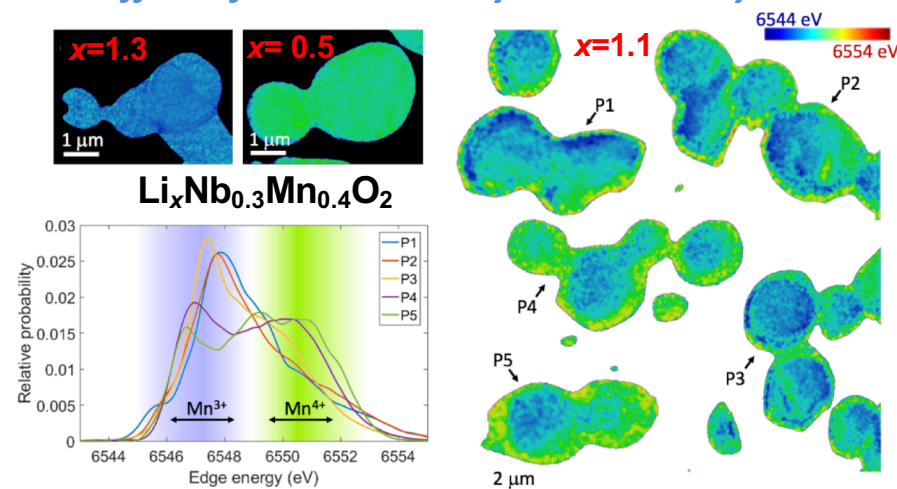
Impact:

- 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.

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.

Effect of local chemistry on Li mobility



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