Model-System Diagnostics for High-Energy Cathode Development

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

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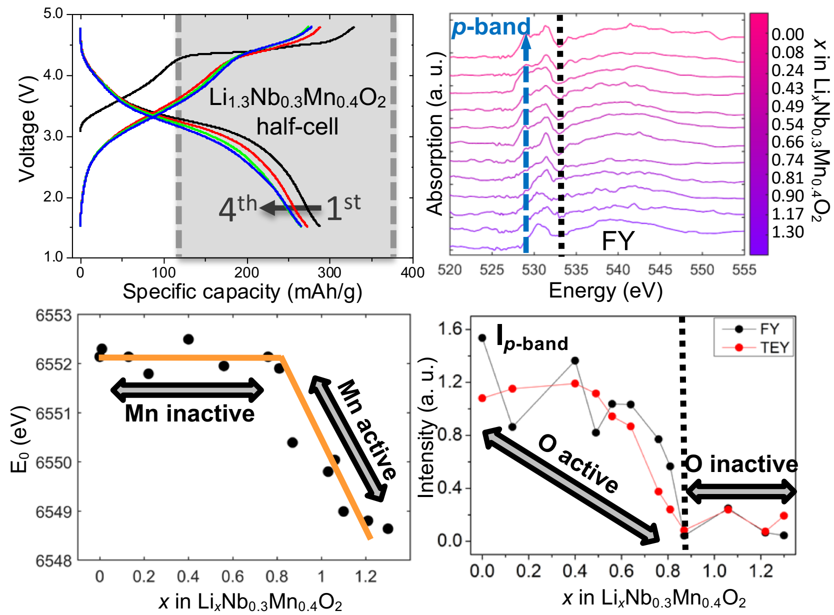
Objective:

- 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.

Redox chemistry in high-capacity Li-excess cathodes



Accomplishments:

- Developed techniques to synthesize model single crystals of novel Li-excess oxide cathodes with high capacities.
- Obtained new understanding on redox chemistry and charge compensation mechanism in high-capacity Li-TM oxide cathodes.
- Elucidated oxygen sub-lattice activities at high voltages and obtained critical insights for designing better-performing Li-TM oxide cathodes.
- Developed and evaluated surface engineering approaches to promote stable high-voltage cycling of oxide cathodes.
- Obtained key understanding of phase transformation mechanism and kinetic barriers in intercalation cathodes.

FY 18 Milestones:

- Understand effect of O redox on structural reversibility.
- Determine O redox kinetics and effect on cathode rate capability.
- Investigate surface reactivity and its impact on cycling stability and safety of Li-excess TM oxides.
- Go/No-Go: Design oxide chemistry and particle morphology to control O activities at high voltages. Criteria: If reversible O redox and lattice O loss can be decoupled.

FY18 Deliverables: Reveal the impact of O redox activities on performance and stability of Li-TM oxide cathodes.

Funding:

— FY18: 550K, FY17: $550K, FY16: $550K