Design and Synthesis of Advanced High-Energy Cathode Materials

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

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Technical Approach:

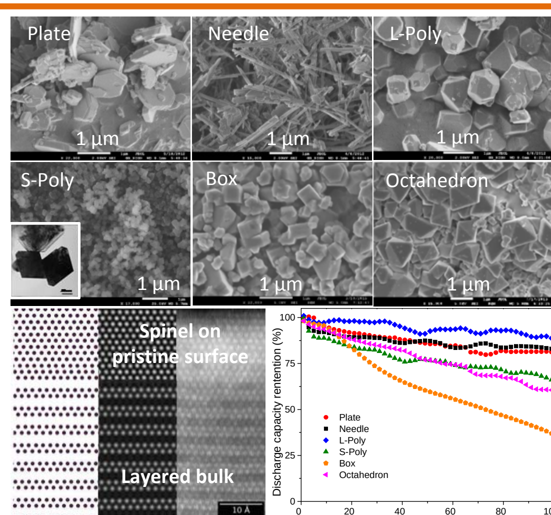
- Synthesize single-crystal model systems and use them to gain fundamental understanding on kinetic barriers and instabilities in high-energy cathode materials.
- Perform advanced *ex situ* and *in situ* diagnostic studies at both single-crystal and electrode levels for insights on material's optimization.

Status:

- Revealed that surface properties of pristine LMR-NMC particles differ from that of the bulk and they are facet dependent.
- Demonstrated the critical role of pristine surface on a range of side reactivities and overall stability of the LMR-NMC cathodes.

Technology:

- A combination of model system construction and advanced diagnostic studies.
- Engineering of active particles, especially surface properties, for enhanced cathode performance and stability.



Objectives:

- Establish correlations between material's physical properties and electrode performance/stability.
- Identify optimal bulk and surface properties for minimum side reactions and maximum Li transport.
- Develop designer materials for next-generation cathodes.

Deliverables:

- Identification of properties and processes that limit the performance of electrode materials.
- Synthesis of advanced cathode materials with improved energy density, rate capability, and safety.

Funding:

Duration: 4 yrs (Yr 4); FY16 Budget: $500K (DOE)

Milestones:

- Q1: Establish synthesis-structure-electrochemical property relationships in high-voltage Li-TM-oxides.
- Q2: Downselect alternative high-energy cathode materials for further investigation. Go/No-Go criteria: material delivers at least 200 mAh/g capacity in the voltage window of 2-4.5 V.
- Q3: Determine Li concentration and cycling dependent transition-metal movement in and out of oxide particles. Examine the mechanism.
- Q4: Identify key surface properties and features hindering stable cycling of Li-TM-oxides at high voltages.