First Principles Calculations of Existing and Novel Electrode Materials

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

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Technical Approach:

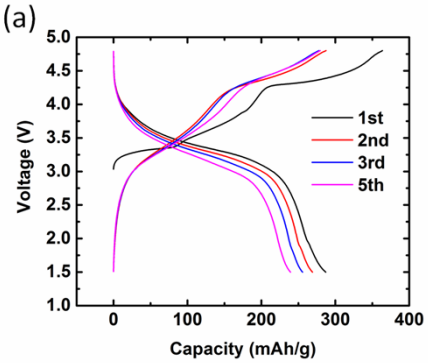
- Use first principles calculations to understand capacity limitations in electrode materials.
- Combine Nudged Elastic Band calculations with percolation models to predict Li transport and capacity of partially disordered materials.
- Develop predictive approach to investigate oxygen charge transfer in Li-excess materials

Status:

- Developed transport and voltage models for Li-excess materials. Developed model for oxygen oxidation and for disorder in synthesized materials. Demonstrated viability of disordered materials.

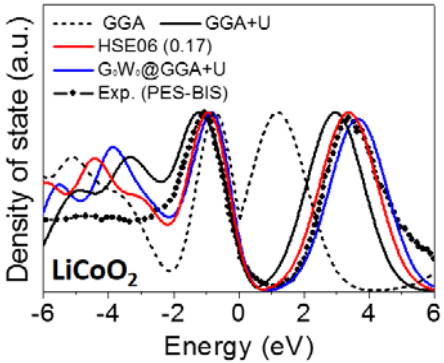
Technology:

- Disordered materials with high capacity and low volume change



Objectives:

- Identify the structure of layered Li-cathodes that leads to high capacity.
- Develop predictive modeling of oxygen charge transfer and oxygen loss.
- Develop high-capacity Li and Na cathodes



Deliverables: Three ordered states in Na_xMO_2 that can be verified with experiments, voltage curve of Li_2MO_3 compounds, method for predicting oxygen charge transfer in Li-excess compounds.

Funding:

Duration: 4 yrs (Yr 4)
FY16 Budget: $356K (DOE)

Milestones:

- **Q1:** Go/No-Go: Model to predict compositions that will disorder as synthesized Criteria: No-go if model can not reproduce exp data..
- **Q2:** At least one Ti-based compound with high capacity .
- **Q3:** Predictive model for the voltage curve (slope) of cation-disordered materials.
- **Q4:** Modeling capability for materials with substantial oxygen redox capability.