Predicting and Understanding Novel Electrode Materials from First Principles

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**Technical Approach:**
- Computational *ab initio* atomistic modeling methods
- High-throughput computations and data mining

**Status:**
- Elucidated excellent potential for high Li-ion mobility in the Li excess materials, coupled to the state-of-charge. Poor rate capability in these materials is likely due to surface passivation and/or poor particle-particle level transport.

**Technology:**

1) Investigations of the charge-discharge mechanisms in the Li-excess materials

2) Pristine Li$_2$MnO$_3$ have competitive Li-ion mobility in the bulk

**Objectives:**
- Predict new chemistries, crystal structures and morphologies for improved electrode materials

<table>
<thead>
<tr>
<th>Tech</th>
<th>Objective</th>
<th>Properties</th>
<th>Status</th>
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<tbody>
<tr>
<td>Understanding of the Li excess materials</td>
<td>Improve capacity and voltage retention</td>
<td>Structural and chemical instability leads to poor voltage and capacity retention</td>
<td>Identified process for performance fade in Li$_x$MnO$_3$</td>
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<tr>
<td>The Materials Project Battery App</td>
<td>Accelerate novel materials development</td>
<td>3600+ Li ion intercalation materials, algorithms, etc made available</td>
<td>&gt; 17,000 registered users, incl. the battery community</td>
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**Deliverables:**
- (1) Understanding of the underlying mechanism for performance decay in the Li-excess materials, (2) computed data and algorithms for electrode materials design available on the Materials Project.

**Funding:**
- Duration: 4 yrs (Yr 4)
- FY16 Budget: $287K (DOE)

**Milestones:**
- **Q1:** Mn mobilities as a function of Li content in layered Li$_x$MnO$_3$ and related defect spinel and layered phases
- **Q2:** Surface facets calculated and validated for Li$_2$MnO$_3$
- **Q3:** Calculate stable crystal facets. Determine whether facet stabilization is possible through morphology tuning. **Go/No-Go:** Stop this approach if facet stabilization can not be achieved.
- **Q4:** Li mobilities as a function of Li content in layered Li$_x$MnO$_3$ and related defect spinel and layered phases

**Fig. 1.** Comprehensive investigations of the Li-ion extraction mechanisms for inter-layer (top) and intra-layer (bottom) Li migration in Li$_x$MnO$_3$.

**Fig. 2.** The Li-ion migration path (top) and activation energy barriers (bottom) of Li$_x$MnO$_3$. Inset tetrahedrons present the saddle point configuration of Mobile Li.