Predicting and Understanding Novel Electrode Materials from First Principles

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

PI: Kristin A. Persson (LBNL)

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

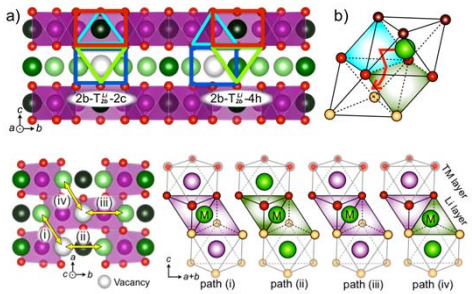

Fig. 1. Comprehensive investigations of the Li-ion extraction mechanisms for inter-layer (top) and intra-layer (bottom) Li migration in Li_2MnO_3.

2) Pristine Li_2MnO_3 have competitive Li-ion mobility in the bulk

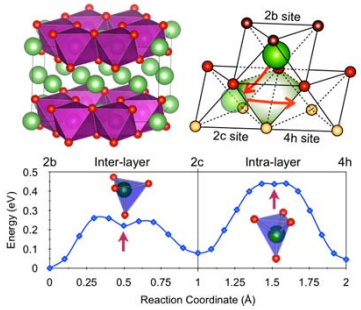

Fig. 2. The Li-ion migration path (top) and activation energy barriers (bottom) of Li_2MnO_3. Inset tetrahedrons present the saddle point configuration of Mobile Li.

Objectives:

Predict new chemistries, crystal structures and morphologies for improved electrode materials

Tech	Objective	Properties	Status
Understanding of the Li excess materials	Improve capacity and voltage retention	Structural and chemical instability leads to poor voltage and capacity retention	Identified process for performance fade in Li_2MnO_3
The Materials Project Battery App	Accelerate novel materials development	**3600**+ Li ion intercalation materials, algorithms, etc made available	> 17,000 registered users, incl. the battery community

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_xMnO_3 and related defect spinel and layered phases
- **Q2:** Surface facets calculated and validated for Li_2MnO_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_xMnO_3 and related defect spinel and layered phases