Characterization and Computational Modeling of Structurally-Integrated Electrodes

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

PI/Co-PI: Michael Thackeray /Jason Croy (ANL)

Technical Approach:

•Utilize DOE user facilities and beyond to provide insights into the atomic-scale processes that govern composite electrode performance and degradation

Status:

•Explored stability of Li_2TiO_3 structures as possible stabilizers in integrated, composite electrodes

•Initiated computational studies on Co-based spinels as integrated structures in layered-layered-spinel electrodes

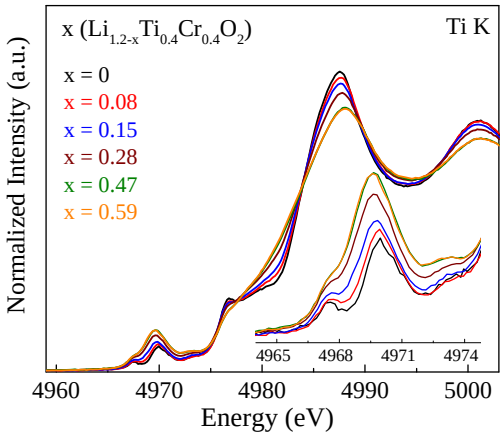
Objectives:

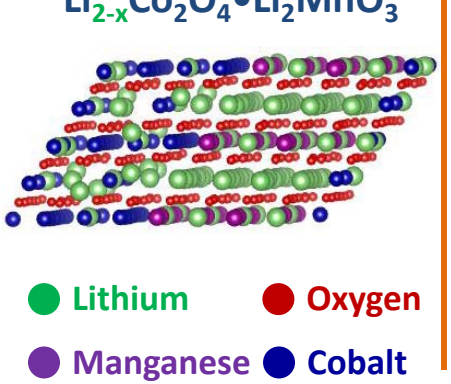
•Exploration of the fundamental, atomic-scale processes that are most relevant to the challenges of next-generation, energy-storage technologies

•Capitalize on unique facilities to advance the field through collaborations and multi-disciplinary efforts

•Characterize and model structurally-integrated electrodes with layered-layered and spinel character

Technology: Atomic-scale understanding of Li_2TiO_3-based structures, and modeling of Co-based spinels, in integrated electrodes





Deliverables: Understanding of structure-property relationships that govern advanced composite cathodes

Funding:

Duration: 3 yrs (Yr 1)
FY16 Budget: $300K

Milestones: ongoing Q1-4

•Characterize bulk and surface properties of structurally-integrated electrode materials using DOE's User Facilities at Argonne (APS, EMC, ALCF) and facilities elsewhere

•Use complementary theoretical approaches to further the understanding of the structural and electrochemical properties of layered-layered-spinel electrodes and protective surface layers

•Analysis, interpretation, and dissemination of collected data for publication and presentation