Interfacial Processes – Diagnostics

U.S. DEPARTMENT OF Energy Efficiency & Renewable Energy

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Technical Approach:

- Apply in situ and ex situ advanced spectroscopy and imaging probes to characterize physico-chemical phenomena on electrochemical interfaces and Interphases in composite electrodes and battery cells
 - Design and employ new experimental methodologies to study Li-ion materials and cell components
 - Use model single crystal/particle electrodes to determine the mechanism and kinetics of detrimental processes

Status:

Pioneered the use of near-field FTIR spectroscopy and imaging for direct chemical analysis of SEI layer. Determined the mechanism of transition metal dissolution in LMNO and LMNC electrodes.



Develop and deploy novel and unique multi-probe diagnostic systems to study model systems and prototype Li-ion cells

Objectives:

- Unveil the structure and reactivity at hidden or buried interfaces and interphases that determine battery performance and failure modes
- Obtain detailed insight into the dynamic behavior of molecules, atoms, and electrons at electrode/electrolyte interfaces of high voltage Ni-rich NCM cathode materials
 - Understand basic properties and function of interfaces, provide remedies to interface instability.
 - Establish clear connections between diagnostics, theory/modeling, materials synthesis, and cell development efforts
 - o Characterize degradation modes

Deliverables:

- Understanding of the underlying principles that govern the function and operation of battery materials, electrodes and cells.
- Develop and apply novel NFIR experimental methodologies.

Fundina:

Duration: 4 yrs (Yr 1) FY16 Budget: \$450K (DOE)

Milestones:

- Q1: Build and test binder- and carbon-free model NMC electrodes.
- Q2: Complete preliminary characterization of interfacial activity of the baseline NMC material in organic carbonate electrolytes
- Q3: Determine relationship between surface reconstruction and surface layer formation during cycling in NMC electrodes
- Q4: Go/No-Go: Demonstrate feasibility of in situ near-filed FTIR microscopy and spectroscopy to study interfacial phenomena at Libattery electrodes Criteria: Stop development of *in situ* NSOM, if the experiments fail to deliver adequate sensitivity, selectivity and specificity.