First Principles Modeling of SEI Formation on Bare and Surface/Additive Modified Silicon Anode

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

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Technical Approach:

- *Ab initio* modeling SEI layer formation and evolution as a function of lithiation on bare, oxide-covered, SEI-covered and artificially coated Li_xSi_y surfaces.
- Determining e^- and ion transfer mechanisms via *ab initio* modeling.

Status:

- Demonstrated SEI growth mechanism via instability of SEI components.
- Analyzing alternative electrolyte formulations.

Technology:

Effective additives/solvents (such as VC, FEC) yield SEI decomposition **products** that are relatively **stable** under cycling; thus resulting in **controlled** SEI growth.

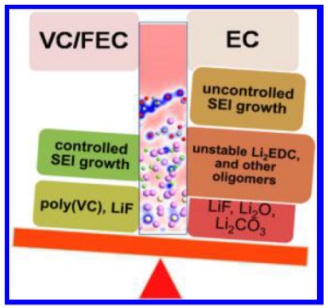

Fig. 1. Schematic illustration of the expected behavior of efficient (VC/FEC) vs. less efficient (EC) solvents/additives.

Objectives:

- Develop fundamental understanding of molecular processes leading to electrolyte decomposition and SEI formation on Si anodes
- Develop rational selection of additives and/or coatings

Deliverables: Understanding of SEI growth. Alternative electrolyte and/or coating formulations.

Funding:

Duration: 4 yrs (Yr 4)
FY16 Budget: $357.5K (TAMU: $200K, SNL: $157.5K)

Milestones:

- **Q1:** Identification of SEI formation mechanisms through alucone coatings on lithiated Si surfaces.
- **Q2:** Quantification of chemical and electrochemical stability of various SEI components. Evaluation of voltage effects on SEI products stability.
- **Q3:** Identification of alternative candidate electrolyte and coating formulations.
- **Q4:** Go/No-Go: Test candidate electrolyte formulations using KMC model and experimentally via collaborations. Criteria: Comparison with current best formulations.