NMR and Pulse Field Gradient Studies of SEI and Electrode Structure

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

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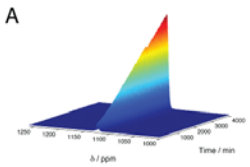
Technical Approach:

- NMR of local structure; *in situ* and *ex situ* NMR studies of Li^+ transport and structural changes

Status:

- Completed Si nanowire study
- Developed protocol for SEI studies
- Identified key organics in Si SEI.
- Developed new ^{23}Na NMR in situ metrology; applied to Na metal studies
- Correlated Li-air

Technology:



• **Dendrites –** Used imaging studies to correlate dendrite formation with Li^+-ion depletion (in electrolyte) at anode

• Demonstrated two regimes for Na plating with different nucleation/growth mechanisms that depend on rate. Na metal plating occurs even at the lowest currents (see growth of Na metal signal in Figure for 0.5 mA cm^{-2}).

• **Si SEI** – Multinuclear NMR methodology has been developed

• Clear ^{13}C NMR signatures of major Si SEI components identified

• **In situ metrologies –** Li – sulphur – used ^7Li NMR studies to determine new phase diagram for Li – S – electrolyte.

• Developed method for probing Li dynamics during cycling

• **Li air** – Redox mediator LiI results in the reversible formation of LiOH

Objectives:

- Identify major SEI components, and their spatial proximity, and how this changes with cycling
- Develop coatings for negative and positive electrodes – and understand their effect on SEI formation.
- Use in situ NMR metrologies to investigate Li and Na dendrite formation, and the role that additives and different electrolytes play in controlling Li/Na morphology

Deliverables: Understanding of structural changes in Si/high voltage cathodes. Molecular level understanding of the SEI

Funding:

Duration: 4 yrs (Yr 4)

FY16 Budget: $313K

Milestones:

• **Q1:** Identify the major carbon-containing break down products that form on graphene platelets

• **Q2:** Establish the difference between extrinsic and P-doped silicon nanowires.

• Go/No-Go: If no difference in performance of P-doped wires established after the 1st cycle, terminate project.

• **Q3:** Complete SEI study of Si nanoparticles by NMR spectroscopy. Develop NMR methodology to examine cathode SEI

• **Q4:** Produce first optimized coating for Si electrode.