NMR and MRI Studies of SEI, Dendrites, and Electrode Structures

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

PI/Co-PI: Clare P. Grey (Cambridge)

Objective: To determine the effect of voltage and additives (FEC) on the composition of the Si SEI

To synthesize and test new inorganic coatings to increase the Coulombic efficiency seen on cycling Si

Identify correlations between SEI structure and thickness and Li metal dendrite formation

To determine the local and long range structures formed on cycling Na and Li anode materials

Impact:

 Improved SEI leading to increased Coulombic efficiencies; Strategies to reduce Li/Na dendrite formation; rational strategies for improving anode performance

Accomplishments:

- Synthesis of ¹³C-labelled FEC
- Multinuclear NMR characterization of SEI on Si with ¹³C-FEC
- DNP studies of SEI on Si with different additives
- Prepared P-N coatings on Si
- New glass cell built to facilitate MRI/dendrite studies
- Na dendrite growth at different current densities investigated and compared to Li
- Characterization of new Na cathode materials
- Characterization of Sn anodes for Na ion batteries

¹H-¹³C CP NMR and DNP experiments show the presence of cross-linking peaks when FEC is used as an additive in LP30 suggesting the molecular basis for increased SEI stability on Si



FY 18 Milestones:

- Q1. Multinuclear NMR studies of SEI on Si with ¹³C-FEC
- Q2. MRI/dendrite studies of two ionic liquids
- Q3. DNP studies of SEI on Si with different additives (e.g. FEC) and coatings (e.g. phosphazenes)
- Q4. Multinuclear NMR studies of phase chemistries during (dis)charge of active materials in Na-ion batteries

FY18 Deliverables:

New elastomeric battery coatings; SEI composition with coatings/FEC; Parameters that dictate dendrite growth, Na phase chemistries during cycling

Funding:

FY17: \$275K, FY17: \$275K, FY16: \$283K