Novel Chemistry: Lithium Selenium and Selenium Sulfur Couple

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

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• **Objective:** The objective of this project is to develop a series of novel S_xSe_y cathode materials for rechargeable lithium batteries with high energy density and long cycle life as well as low cost and high safety.

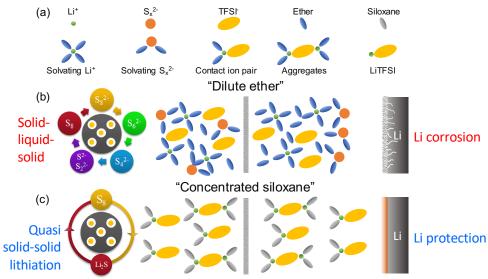
Impact:

- The high electronic conductivity of Se can help to improve the reversible capacity, cycle stability and rate capability as well as areal loading of S_xSe_y cathodes
- Exploration of advanced electrolytes can suppress polysulfides/polyselenides shuttle and improve reversible Li stripping/plating for metallic Li batteries

Accomplishments(FY18):

- Investigated the impact of novel concentrated siloxane electrolytes and confirm the suppression of polysulfides/polyselenides shuttle
- Elucidated the quasi solid-solid lithiation mechanism of Li/Se and Se-S systems in the concentrated siloxane electrolytes by Operando X-ray absorption spectroscopy
- Understood the interactions between concentrated siloxane electrolytes and polysulfides by advanced computational simulation
- Enabled highly reversible Li plating/stripping by concentrated siloxane electrolytes
- Achieved 100% coulombic efficiency for metallic Li/S

Tuning electrolytes structure to enable a 100% coulombic efficiency metallic Li/Se-S battery



FY19 Milestones:

- Interfacial understanding on cycled Li metal in different electrolytes (Q1)
- Leakage current measurement of Li-Se and Se-S systems in different electrolytes (Q2)
- Computational understanding on the interactions of cations/anions with solvents in electrolytes (Q3)
- Rational cathode design for high areal loading (>6 mg/cm²) Li-Se and Se-S systems (Q4)

FY19 Deliverables: Quarterly reports, new cathodes coupled with new electrolytes *Funding:*

– FY19: \$500K, FY18: \$500K, FY17: \$500K