Addressing Internal "Shuttle" Effect: Electrolyte Design and Cathode Morphology

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

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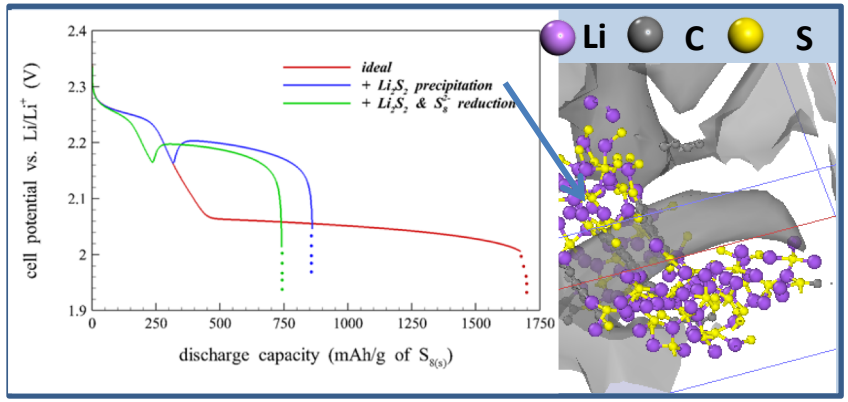
- ***Objective:*** (i) Predict *in-situ* formation of an anode passivation layer; (ii) Evaluate strategies to minimize polysulfide shuttle with advanced cathode structure design

Impact:

- Integrated experiments and computations for evaluation of alternative electrolyte chemistries, and design, fabrication, and test of improved cathode architectures
- Develop an improved understanding of the Li/S chemistry and ways to control undesired interfacial effects.

Cathode performance influenced by carbon-sulfur morphology



Accomplishments:

- Characterization of reactions and SEI formation at the anode in presence of soluble polysulfides
- Synthesis and characterization of composite C-S structures, theoretical elucidation of discharge reactions as a function of cathode morphology
- Identification of the role of the Li_2S_2 and Li_2S deposition morphology as a key issue leading to a predominantly insulating film or inducing pore blockage.
- Prediction of alternative materials for retention of soluble polysulfides at the cathode side.
- Identification of charge mechanisms in Li_2S_2 and Li_2S via formation of hole polaron species at S anion sites.

FY 18 Milestones:

- Characterize Li_2S_2 and Li_2S deposition morphology using atomistic and mesoscopic modeling as a function of cathode structure, sulfur loading, and current rate
- Effects of S-containing electrolytes on cathode performance

FY18 Deliverables:

Estimates of optimum cathode microstructure and S loading

Funding:

— FY18: $0, FY17: $379,466, FY16: 325,189; FY15:$285,345