Addressing Internal "Shuttle" Effect: Electrolyte Design and Cathode Morphology Evolution in Li-S Batteries

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

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Technical Approach:

- *Ab initio* and mesoscale modeling of anode and cathode interfacial reactions.
- Synthesis, characterization and multiscale modeling of composite C/S cathode structures and properties; electrochemical tests of full cells.

Status:

- Characterized anode interfacial reactions in presence of polysulfides (PS); effect of electrode porosity as a function of C/S ratio on electrochemical behavior.
- Theoretical and experimental analysis of materials for PS retention.

Technology:

Theoretical-experimental approach for developing a better understanding of the effects of electrode micro & mesostructures and interfacial chemistry on electrochemical behavior.

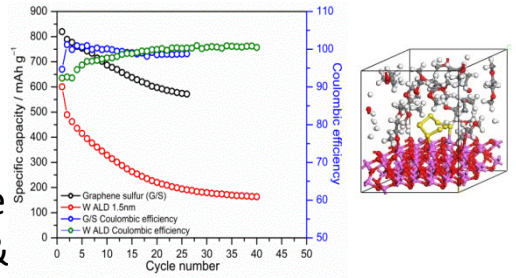

Fig. 1. Specific capacity and Coulombic efficiency of modified (red/blue) and non-modified (black/green) C/S cathodes

Objectives:

- Overcome the lithium-metal anode deterioration issues through protection/stabilization strategies: i) in-situ chemical formation of a protective passivation layer; ii) advanced cathode electrode design

Deliverables: Li/S cell operating for at least 500 cycles at an efficiency > 80%.

Funding:

Duration: 3 yrs (Yr 2)
FY16 Budget: $330K (TAMU, $220K; Purdue, $110K)

Milestones:

- **Q1:** Complete coin cell testing of various C/S electrodes.
- **Q2:** Using electrochemical and transport modeling gain an understanding of the mesoscopic interfacial reactions.
- **Q3:** Complete evaluation of deposition-induced stress and mechanical interplay.
- **Q4:** Go/No-Go: Determination of SEI nucleation and growth at the PS/Li anode interface. Criteria: Determine reasons for electrolyte failure or success.