Nanostructured Design of Sulfur Cathodes for High Energy Lithium-Sulfur Batteries

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

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Technical Approach:

- Adsorption test and build relative models of Li_2S_x species on the surface of metal sulfides/oxides
- Explore different metal sulfides/oxides through electrochemical test and postmortem analysis
- Density functional theory (DFT) calculations to reveal the polysulfide capture and diffusion mechanism on the metal sulfides/oxides

Status:

- Demonstrated that the polysulfide capture on the surface of metal oxides is monolayered chemisorption
- Results indicate that the better surface diffusion leads to higher deposition efficiency of sulfur species on electrodes
- DFT calculations for polysulfide adsorption and diffusion on the metal sulfides are now in progress

Technology:

Combined DFT and experimental results to better understand surface adsorption and diffusion, and build metal sulfides/oxides selection criteria

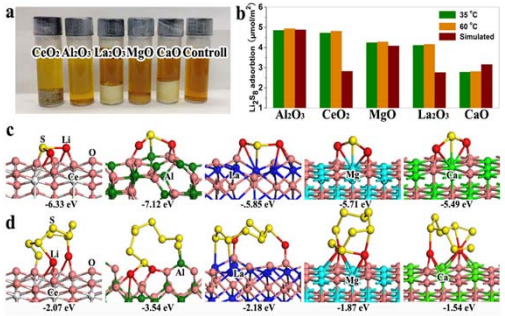

Figure: (a,b) Experimental and simulated adsorption of Li_2S_8 on different metal oxides. (c,d) Adsorption model of Li_2S and Li_2S_8 on different metal oxides.

Objectives:

- Perform Li_2S_8 adsorption test to the understand adsorption mechanism of sulfur species on different types of metal sulfides/oxides
- Give insight into the interaction mechanism between Li_2S_x species and metal sulfides/oxides through combined experiment-DFT computations
- Optimize and develop high-performance nanostructured sulfur cathodes

Deliverables: Build metal sulfides/oxides selection criterion based on the balance optimization between Li_2S_x adsorption and diffusion on metal sulfides/oxides surface for designing advanced cathode materials in Li-S batteries.

Funding:

Duration: 4 yrs (Yr 3)
FY15 Budget: $300K (DOE)

Milestones:

- **Q1:** Identify the adsorption mechanism between sulfur species and different types of metal sulfides/oxides
- **Q2:** Understand interaction mechanism through combined experiment-DFT computations
- **Q3:** Build cell for testing diffusion coefficient of Li_2S_x species on various types of metal sulfides/oxides
- **Q4:** Demonstrate and optimize the balance of surface adsorption and diffusion of Li_2S_x species on metal sulfides/oxides, enabling good performance of Li-S batteries.