

## Development of High Energy Lithium-Sulfur Batteries

### Introduction

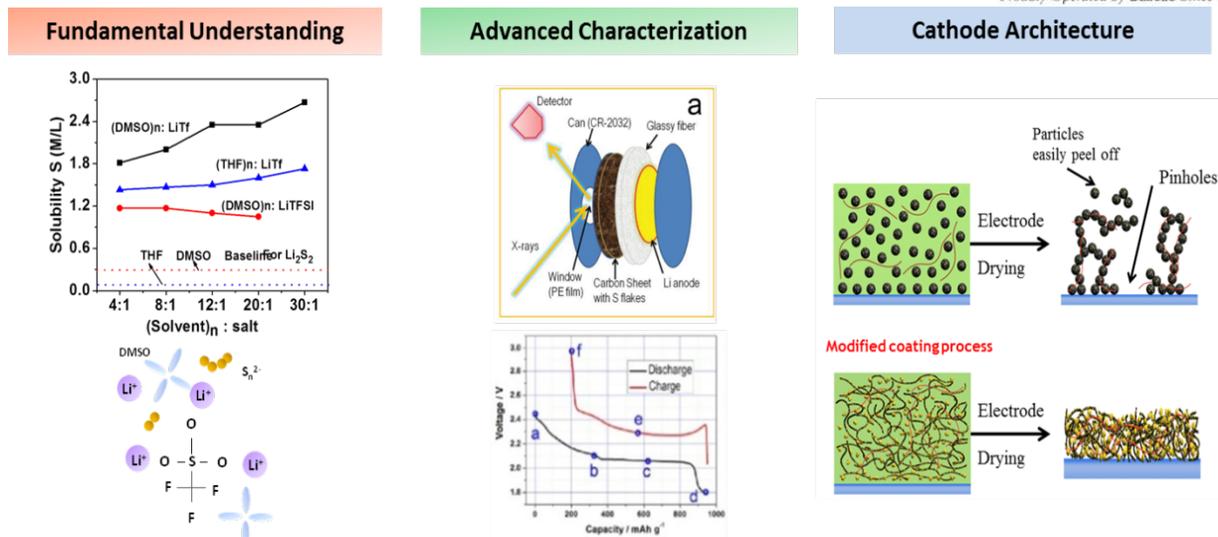
Ever increasing demand on large-scale energy storage technologies, particularly for sustainable transportation and sustainable power grid require a cost-effective, high energy and power battery technology. Lithium sulfur (Li-S) battery is a promising candidate that can potentially store more energy per weight than the state of the art lithium ion battery. It uses low cost and nontoxic sulfur as cathode. However, the challenge with Li-S battery is that the electrochemical reactions involve soluble polysulfide species that cause instability and unreliability of Li-S batteries, e.g. cycling, low efficiency, and self-discharge etc. Fundamental mechanism understanding, material innovation and electrode architecture design are crucial for development of high performance Li-S batteries for different practical applications.

### Project Objective

The objective of this project is to investigate the fundamental chemistry of lithium polysulfides and develop new functional electrode materials and architectures for high energy, low cost Li-S batteries. Modulating the solvating structure of lithium polysulfide molecules in organic electrolytes will be explored to control the dissolution of polysulfide species. New cathodes with different functional groups were proven to enable the thick sulfur loading and the electrochemical stability of the Li-S cells. The redistribution of sulfur among sulfur cathode and the whole Li-S cell upon cycling will be characterized to provide new fundamental insight and valuable guidance for the development of Li-S battery.

### Main Achievements

- Identified the factors that govern the solubility of polysulfide species in organic Li-S electrolyte.
- Demonstrated a liquid-phase Li-S redox flow battery.
- Developed an in-situ X-ray Fluorescence microscopy combined with XAS technique to observe the dissolution/redistribution and chemical state changes of sulfur electrode in real time.
- Developed molecular doping approach of carbon hosts to fabricate functional thick cathodes.



**Figure 1.** Solubility of lithium polysulfides and the interaction between anions/cations/solvent molecules (DMSO as an example) in different electrolytes (Left); Charge/discharge curve of a Li-S cell designed for in-situ characterization (Middle); Optimized materials and process for a uniform coating of Li-S battery cathode (Right).

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## Publications

1. J. Chen, D. Wu, E. Walter, M. Engelhard, P. Bhattacharya, H. Pan, Y. Shao, F. Gao, J. Xiao, J. Liu, Molecular-confinement of polysulfides within mesoscale electrodes for the practical application of lithium sulfur batteries, *Nano Energy* 2015, 13, 267.
2. H. Pan, X. Wei, W. A. Henderson, Y. Shao, J. Chen, P. Bhattacharya, J. Xiao, J. Liu, On the Way Toward Understanding Solution Chemistry of Lithium Polysulfides for High Energy Li-S Redox Flow Batteries, *Advanced Energy Materials* 2015, 5, DOI: 10.1002/aenm.201500113
3. X. Yu, H. Pan, Y. Zhou, P. Northrup, J. Xiao, S. Bak, M. Liu, K.-W. Nam, D. Qu, J. Liu, T. Wu, X.-Q. Yang, Direct Observation of the Redistribution of Sulfur and Polysulfides in Li-S Batteries During the First Cycle by In Situ X-Ray Fluorescence Microscopy, *Advanced Energy Materials* 2015, 5, DOI: 10.1002/aenm.201500072