Electrolyte/Binder for High Efficiency Li-S Batteries: New Materials Design and Computation

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

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Objective: Develop new electrolyte materials to help overcome the challenges of low active material utilization and poor cycle life to enable high efficiency Li-S batteries for vehicle application.

Impact:

- Enable improved materials utilization and longer cycle life in Li-S batteries
- Li-S batteries have the potential to power long-range, low cost electric vehicles

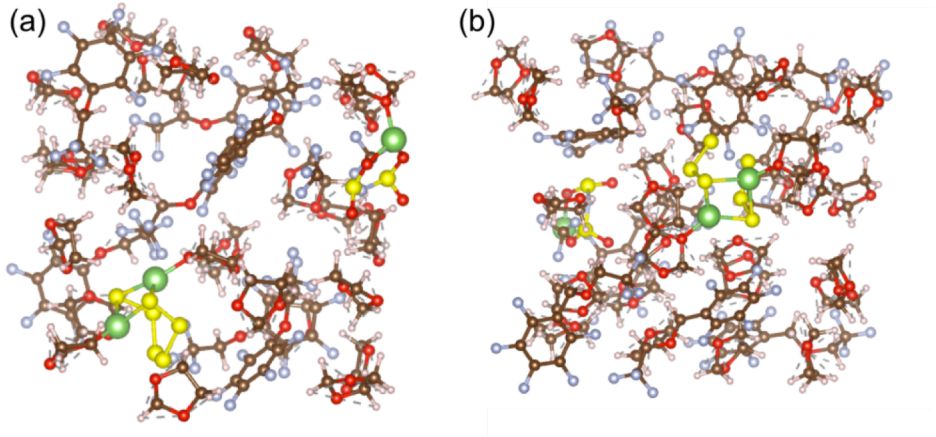

Figure: Snapshots from DFT calculations show Li_2S_4 species in the new electrolytes (a) TFE-PFPE:DOL and (b) TFE-PFBE: DOL [TFE-PFPE =pentafluoro(2,2,2-trifluoroethoxy)-benzene]; TFE-PFBE = ((pentafluoro(2,2,2-trifluoroethoxy) –methyl) -benzene)]

Accomplishments:

- Designed, synthesized, and tested new ether solvents containing a pentafluorophenyl group in the structure to act as an anion receptors strongly interact with polysulfides
- Ab initio molecular dynamics simulations of the structures and binding energies of lithium polysulfides (Li2Sx) in the proposed new ether solvents with pentafluorophenyl groups

FY19 Milestones:

- Design and synthesis of new fluorinated borate electrolytes and baseline studies
- Quantum chemical calculations of the chemical stability and reactivity properties of new borate additives
- Electrochemical characterization of performance of the new fluorinated borate electrolytes in lithium-sulfur cells

FY19 Deliverables: Quarterly reports, new electrolyte additives and binders

Funding: FY19: $500,000 FY18: $500,000