Large scale ab initio molecular dynamics simulations of liquid and solid electrolytes

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

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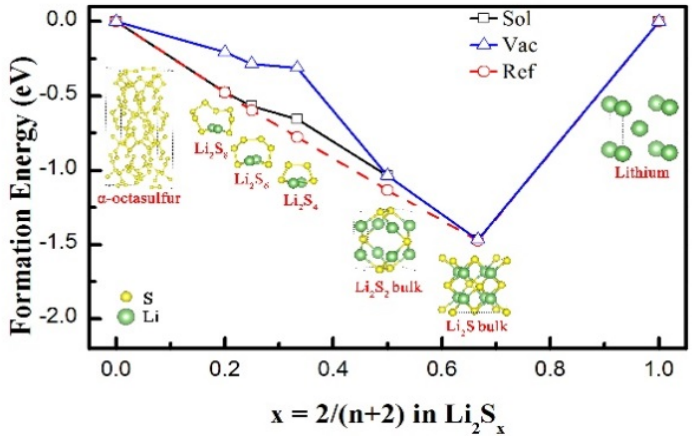
Objective: Develop the understanding of lithium sulfur battery process using ab initio simulations, help to discover new lithium sulfur cathode materials and mitigate the lithium polysulphide dissolution problem. Study the ion transport mechanism in solid electroltyes.

Impact: Remove the huddles in commercialization of LiS battery system, which has a potential energy capacity of ~2400 Wh/kg. Develop the understanding and designing principles for future battery development.

Recalibrate the Li_2S_n energy in the solvent electrolyte.



The energies of Li_2S_n are calculated using the implicit solvent model. Experimental voltages are used to fix the solvent model parameters.

Accomplishments: (FY18)

- Studied the use of 2D hexaaminobenzene as Li-S battery anode. Found it has a energy capacity of 1300 Wh/kg, and it is stable against the Li_2S_n dissolution.
- Investigated the mechanism of moisture instability of the solid electrolyte: $Li_{10}GeP_2S_{12}$ (LGPS). Proposed a new compound: $Li_{10}(GeS_4)(PO_4)_2$, which is stable against moisture, and has even large Li mobility than the original LGPS.
- Investigated a sandwich structure of 2D hexaaminobenzene as Li-S battery anode, to overcome the volumetric capacity problem for 2D materials. Developed a method to calculate its Li mobility.

FY 19 Milestones:

- Continue the study of sandwich Li-S anode structure, finalize the method to calculate the diffusion barrier in the amorphous system.
- Continue to study of solid electrolytes, especially for their surface stabilities and reconstructions.
- Develop thermodynamic integration method to calculate Li_2S_n properties in solvent

FY19 Deliverables: investigate one new cathode systems, one solid electrolyte

Funding:

— FY19: 225K, FY18: 225K