Task 3.5 – First-Principles Calculations of Existing and Novel Electrode and Solid Electrolyte Materials

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

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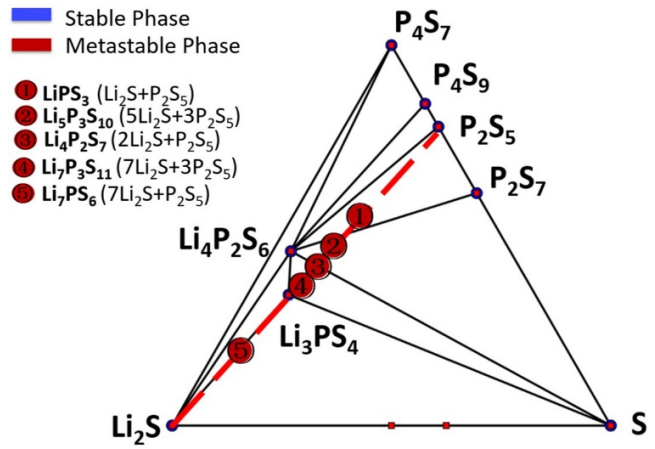
Objective:

- Determine the design principles needed to create solid state electrolytes with high Li-ion conductivity for solid-state batteries, while also achieving stability against common Li-ion cathodes and Li metal anodes

Impact:

- Understanding of factors that control Li-ion motion in crystalline and amorphous solids
- Strategies to create stable interfaces against Li
- Long Cycle-life solid state batteries

Calculated Phase Diagram of Li-S-P



Accomplishments:

- This is a new direction for this project. We have performed initial calibration and testing of methods to predict phase stability and conductivity in Li-P-S sulfide electrolytes
- Methods to predict interfacial reactivity
- Initial phase diagram of Li-P-S

FY19 Milestones:

Q1. Li_2S-P_2S_5 phase diagram for solid state electrolytes: solid phases correctly modeled
Q2. Amorphous phase structure modeled correctly in Li-P-S
Q3. Model Li-ion transport in amorphous Li-P-S
Q4: understanding on which structural and compositional features make LPS an excellent ionic conductor

FY19 Deliverables: Study on Li-ion transport in Li-P-S systems. Papers and Presentations

Funding:

— FY19: 400K