

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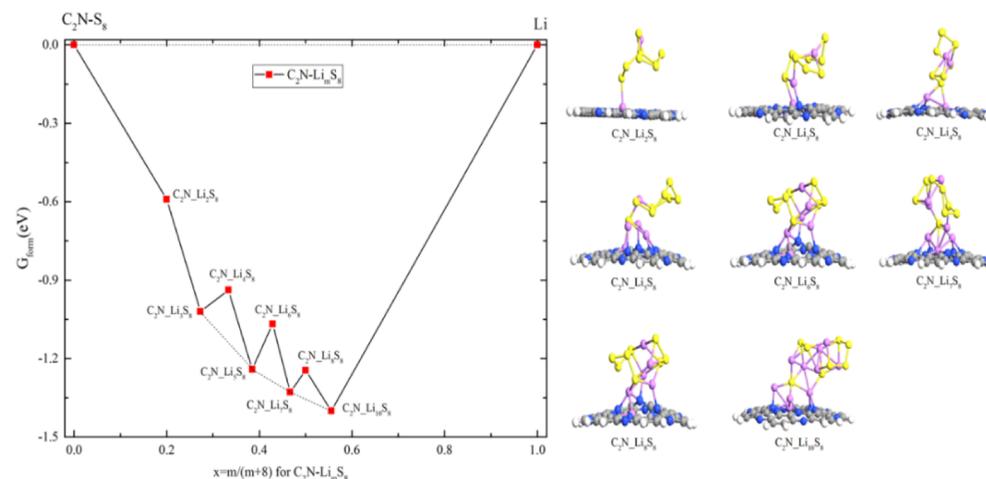
**Objective:** Develop the understanding of lithium sulfur battery process using ab initio simulations, help to discover new lithium sulfur cathode materials and mitigate the lithium polysulphide dissolution problem. Study the ion transport mechanism in solid electrolytes.

**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.

### Accomplishments: (FY17)

- Studied the use of 2D C<sub>2</sub>N nanosheet as the potential LiS cathode material. Discovered that the anchoring of Li<sub>n</sub>S<sub>m</sub> cluster to C<sub>2</sub>N can thermodynamically overcome the dissolution of the lithium polysulphide, and show that C<sub>2</sub>N can be a good cathode material.
- Studied the use of partially oxidized black phosphorus as Li cathode. Such a system can be considered as a hybrid lithium air system, with a large theoretical capacity of ~1500 Wh/kg.
- Calculated the binding configuration and binding energy between the lithium polysulphide and transition metal embedded in carbon nitride 2D materials.

### C<sub>2</sub>N nanosheet as possible LiS battery cathode



The energies of Li<sub>n</sub>S<sub>8</sub> binding to the C<sub>2</sub>N substrate (left) and binding configuration (right).

### FY 18 Milestones:

- Continue study of using carbon nitride, or other 2D nanosheets for LiS cathode material
- Using molecular dynamics to investigate the stability of Li<sub>n</sub>S<sub>m</sub> cluster binding to the substrate
- Develop thermodynamic integration method to calculate Li<sub>2</sub>S<sub>n</sub> properties in solvent
- Study ion diffusion mechanism in solid electrolyte

**FY18 Deliverables:** investigate two new cathode systems, one solid electrolyte

### Funding:

— FY18: 225K, FY17: 225K