Predicting and Understanding Novel Li-ion Energy Storage Materials from First-principles

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

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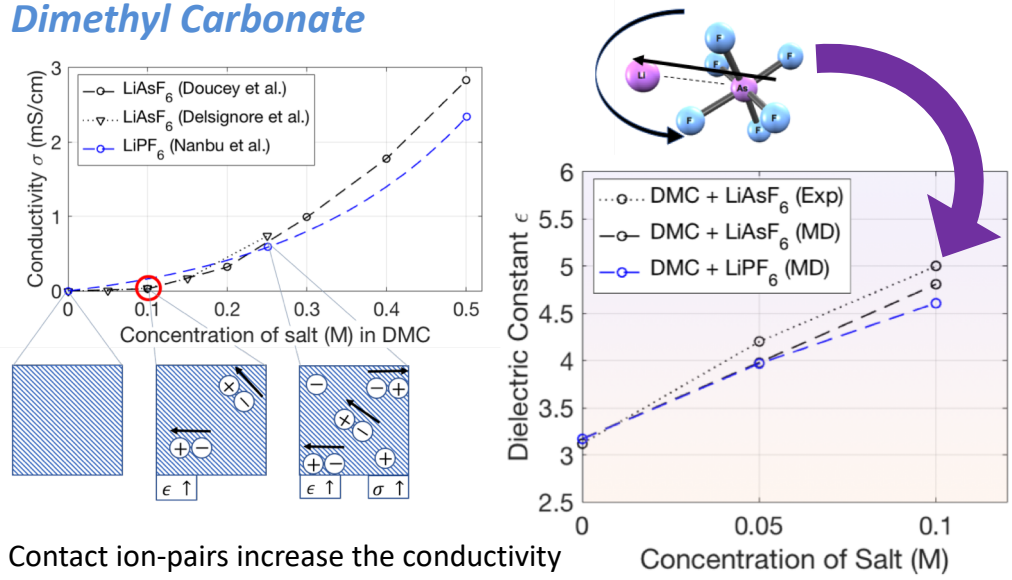
Objective:

To develop and understanding, at the atomic and molecular scale, of the Li-ion dynamics within the electrolyte and anode and to identify strategies for increased performance and cyclability.

Impact:

- Understanding the effect of contact-ion pairs on the dielectric constant for low permittivity electrolytes provides a framework to predict speciation for such systems
- Understanding Li transport in Si-anodes will allow high-throughput screening of dopants promoting mobility

The Dielectric Constant And Speciation of $LiPF_6$ in Dimethyl Carbonate



Contact ion-pairs increase the conductivity and dielectric constant of the electrolyte

Accomplishments:

- First computational framework to include dielectric constant contribution from contact-ion pairs
- New insight into speciation of salt in linear carbonate electrolytes
- Predicted the phase transformations of SiO_2 upon lithiation in the Si-anode and reversibility of Li_2O
- Showed the contribution of the native SiO_2 layer on passivation of Si
- **New Start** to screen for low-permittivity electrolyte blends to optimize for high conductivity
- **New Start** High throughput search to identify alloys or dopants to Si with high Li diffusivity

FY 18 Milestones/Deliverables:

- Validate computational model for $LiAsF_6$ in DMC
- Predict dielectric constant and speciation for $LiPF_6$ in DMC
- Present kinetic and and thermodynamic evaluations of the lithiation mechanisms of Si-anode

Go/No-Go milestone:

- Assess algorithm for modeling the dielectric constant of Li^+ electrolytes across different electrolyte systems

Funding:

— FY18: $350k, FY17: $350k, FY16: $350k