Modeling Ion Transport in Solid-State Electrolytes: From the Perspective of Potential Energy Surfaces

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Ion transport in solid-state electrolytes limits the performance of safe, high energy density solid state batteries. Improving these materials requires reliable predictions of ionic conductivity and mechanistic insight into how chemistry, structure, and disorder control ion diffusion, which in turn demands efficient modeling approaches that overcome the time and length scale limitations of molecular dynamics.

In this talk, I will present our work on cost efficient multiscale tools for modeling ion diffusion in solid state electrolytes. The approach applies topological and geometric analysis of the potential energy landscape to identify ion sites, diffusion pathways, and transport bottlenecks, and couples this with efficient statistical models to predict ionic diffusivities in electrolyte materials with ab initio molecular dynamics accuracy at a fraction of the computational cost. The framework also generates physically interpretable energy landscape descriptors – such as migration barrier distributions and network connectivity – that directly connect structure to ionic transport and performance, and enable physics based machine learning models for accelerated materials discovery.

I will further discuss insights from our calculations, including the effects of ion substitution and configurational entropy on the effective free energy landscape for lithium transport, and outline ongoing efforts to extend this methodology to non crystalline electrolytes e.g. polymer based systems and multiphase composites.

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