Understanding Frustration, Correlation, and Disorder in Materials for Energy Storage and Conversion

Brandon C. Wood,

Materials Science Division, Lawrence Livermore National Laboratory, California, USA

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Abstract: Complex ion dynamics are key to the functionality of many energy storage and conversion processes. However, such behavior is often very difficult to probe, particularly when the relevant materials are intrinsically disordered or form functional interfaces with a high degree of structural and chemical heterogeneity. In this regard, atomic-scale simulations have become a valuable tool, since they provide a way to isolate specific dynamical phenomena. In this talk, I will provide an overview of some of our recent computational efforts towards understanding complex ion dynamics in materials for energy applications using first-principles molecular dynamics. Examples will be drawn from our work on solid-state battery electrolytes, semiconductor materials for solar hydrogen production, and metal hydrides for hydrogen storage. In each of these instances, I will show how highly correlated motion and dynamical fluctuations in the broader structural environment impact key thermodynamic and kinetic properties. I will also discuss how frustration, correlation, and disorder are interrelated, and how they collectively give rise to emergent diffusion behavior with implications for device performance and stability.