Ionic transport in materials with substitutional disorder

Alexander Urban

Department of Chemical Engineering, Columbia University, United States
E-mail address: au2229@columbia.edu

Substitutional disorder can have a profound impact on the ionic transport properties of crystalline solids, such as the solid electrolytes of solid oxide fuel cells or cation-disordered cathode materials for lithium ion batteries (LIBs). However, the direct experimental investigation of disorder on the atomic scale is challenging, and (conventional) first-principles computational techniques cannot be directly applied to disordered materials.

Here we show how relatively simple computational models can provide useful insight into the interplay of substitutional disorder and ionic conduction in cation-disordered LIB cathode materials. Over the last years, computational modeling has contributed to the understanding of this new class of materials and has guided the discovery of several new high-energy density cathode materials.