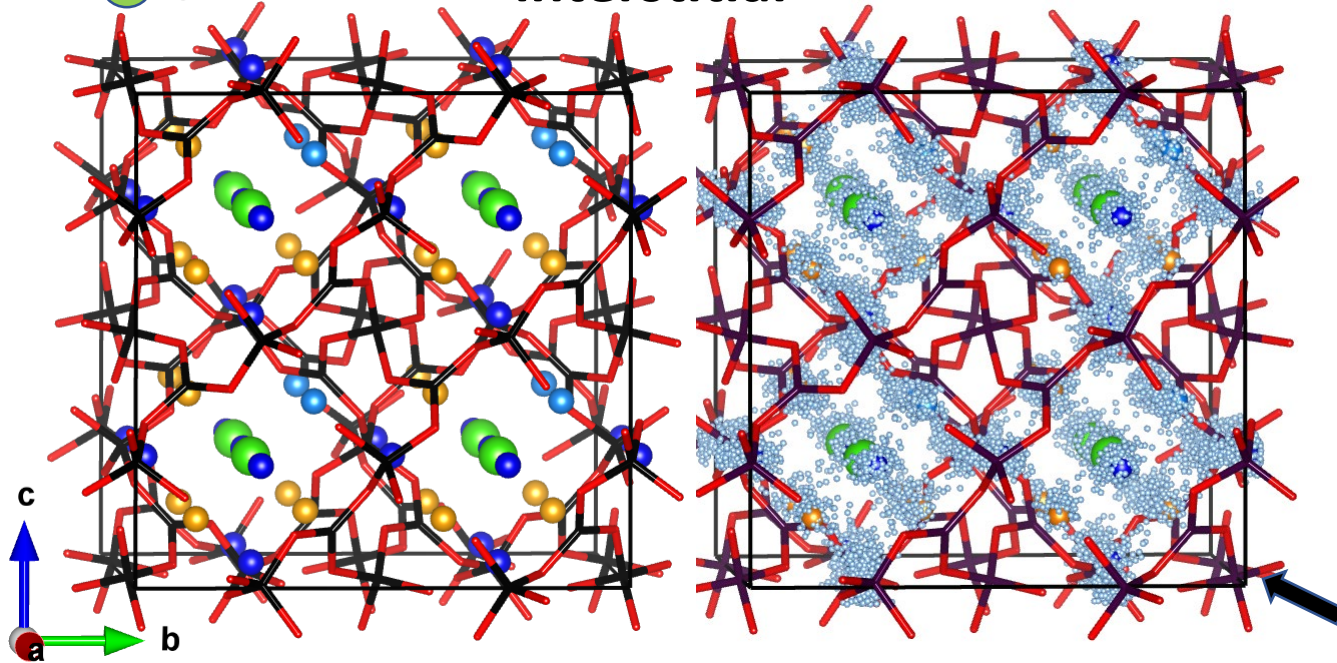


# Materials simulation research – example study of ideal solid electrolytes for all-solid-state batteries from Ph. D. work of Dr. Yan Li

● Cl ● Li ● interstitial



Li boracite in its ideal crystal form

Superposed Li ion positions from MD simulation at 1200K

B-O framework

## Research focus areas –

- Using existent software methods to study properties of known and predicted materials, particularly those associated with all-solid-state batteries
- Developing software to extend capabilities of materials simulations – <http://pwpaw.wfu.edu>

## Opportunities for student participation

- All students interested in materials simulations and materials software development are encouraged to contact [natalie@wfu.edu](mailto:natalie@wfu.edu). It is possible to participate in this research as a beginner or to build from previous experience.

Links: [Research links for N. A. W. Holzwarth](#)  
[Webpage for N. A. W. Holzwarth](#)  
[WFU Physics webpage](#)