THE UNIVERSITY OF BRITISH COLUMBIA

Chemistry
Faculty of Science

FOURTH YEAR MEETING

& THESIS OUTLINE

Exploration of Crystal Nucleation Phenomena Through Molecular Simulation

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Date	**Time**	**Location**
Monday, October 4th 2021	11:00 AM	CHEM D317

1 Analysis of the relative stability of lithium halide crystal structures: Density functional theory and classical models

- This project is a explores the relative energetics of low-lying lithium halide crystal structures using both density functional theory and pairwise classical models.
- There is a large amount of work associated with this project, I expect it will occupy approximately 1/4 to 1/3 of the thesis.
- **Status: 100 % complete.** This project is published.[1].

2 Bayesian Optimization for Lithium Halide Forcefields: Exploring the Limits of Pairwise Additive Potentials for Molecular Simulation

- This project employs a machine learning technique, Bayesian optimization, for finding pairwise lithium halide forcefields that reproduce known experimental or theoretical quantities.
- **Status: 90 % complete.** All relevant project code, most data collection, and most data analysis is complete.

3 The NiAs Crystal Structure of LiI: Low Energy, but Never Observed

- This project combines aspects of both chapter 1 and 2, employing the high-quality reference data we produced in chapter 1 with the methodology from chapter 2 to explore why the ($T = 0$, $P = 0$) energy of LiI in the NiAs structure is lower than LiI in the rocksalt structure, yet NiAs is not observed experimentally.
- **Status: 70 % complete.** Relevant project code is complete and much of the data is collected. A few more simulations are required.

4 Convolutional Neural Networks with Steinhart Order Parameters: Machine Learning for Structure Detection in Molecular Simulation

- This project came out of the need to distinguish different lithium halide crystal structures in simulation. It employs neural networks for local crystal structure detection.
- **Status: 80 % complete.** Relevant project code is complete. Still need to decide on an interesting simulation to showcase this project, then write it up.

5 Competitive Nucleation of LiX Crystal Structures

- This project is still in progress, but will use aspects of several previous chapters to explore competitive nucleation in LiX crystal structures.
- **Status: 20 % complete.**

Expected date of program completion: September 2022.

[1] Scheiber, H. O., and G. N. Patey. The Journal of Chemical Physics 154.18 (**2021**): 184507