Solving Atomic Structure using Statistical Mechanical Searches on X-ray scattering derived Potential Energy Surfaces

by

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Introduction

This is the introduction to the thesis.

Chapter 1

The importance of atomistic structure

1.1 Atomic Structure Experiments

TEM/STEM

In-Situ Experiments

X-ray Total Scattering

In-Situ Experiments

1.2 Computationally Extracting Structure from Measurements

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Exotic Simulations

Chapter 2

Statistical Mechanical Potential Energy Surface Minima Search

The general strategy of my work is to use statistical mechanical ensembles to search potential energy surfaces (PESs) which include information about the atomic structure. This information will come from experimental data or computational sources like Density Functional Theory or Embedded Atom Method calculations.

Chapter 3

Potential Energy Surfaces