

SOLVING ATOMIC STRUCTURE USING STATISTICAL MECHANICAL SEARCHES ON  
X-RAY SCATTERING DERIVED POTENTIAL ENERGY SURFACES

by

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## DEDICATION

## ACKNOWLEDGMENTS

# ABSTRACT

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## LIST OF FIGURES

# INTRODUCTION

This is the introduction to the thesis.

# CHAPTER 1

## ATOMIC STRUCTURE: EXTRACTION AND APPLICATION

### 1.1 ATOMISTIC EXPERIMENTS

### 1.2 ATOMISTIC SIMULATIONS

How do I combine/separate the Ensemble, PES and PDF math/computation sections?

# CHAPTER 2

## ATOMIC PAIR DISTRIBUTION FUNCTION: THEORY AND COMPUTATION

### 2.1 THEORY

#### **Derivation**

### 2.2 COMPUTATION

#### **HPC and GPUs**

##### **GPUs and vectorization**

##### **Map from ij space to k space**

##### **Periodic Boundary Conditions**

### 2.3 EXPERIMENT

### 2.4 DATA PROCESSING WORKFLOW

# CHAPTER 3

## STATISTICAL MECHANICAL ENSEMBLES AND POTENTIAL ENERGY SURFACES

### 3.1 ENSEMBLES

**Hamiltonian Monte Carlo**

No-U-Turn-Sampling

**Grand Canonical Monte Carlo**

Configurational Biasing

# CHAPTER 4

## BENCHMARKING

### 4.1 PDF

#### **Au55**

### 4.2 PDF WITH ADPS

# CHAPTER 5

## ANNEALING AND AGGREGATION OF 2NM

### AU NANOPARTICLES

5.1 EXPERIMENTS

5.2 DATA PROCESSING

5.3 DATA ANALYSIS

5.4 SIMULATION

5.5 STRUCTURAL ANALYSIS

5.6 CONCLUSIONS

# CHAPTER 6

## PHASE CHANGES AND ANNEALING DYNAMICS OF $\text{Pr}_2\text{NiO}_4$ AND ITS DERIVATIVES

6.1 EXPERIMENTS

6.2 DATA PROCESSING

6.3 DATA ANALYSIS

6.4 SIMULATION

6.5 STRUCTURAL ANALYSIS

6.6 CONCLUSIONS



CHAPTER 7

CONCLUSION