

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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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 Pr_2NiO_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