LATEX Template for Thesis

A dissertation submitted to the Graduate School

of the University of LATEX

in partial fulfillment of the requirements for the degree of

Doctorate of Philosophy

in the Department of Chemistry

of the College of Arts and Sciences

by

Your Name

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Abstract

ABSTRACT

To all suffering PhD students.

Acknowledgment

ACKNOWLEDGMENT

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List of Abbreviations

CHARMM Chemistry at Harvard Macromolecular Mechanics

LAMMPS Large-scale Atomic/Molecular Massively Parallel Simulator

NAMD Nanoscale Molecular Dynamics

Chapter 1

Introduction

1.1 Molecular dynamics packages

CHARMM[1], LAMMPS[3] and NAMD[2].

1.2 Organization of thesis

Figure 1.1: Image credit: https://www.latex-project.org/

Chapter 2

Logo of CHARMM

2.1 Methods

Figure 2.1: Image credit: https://embnet.vital-it.ch

2.2 Conclusions

Chapter 3

Logo of LAMMPS

3.1 Methods

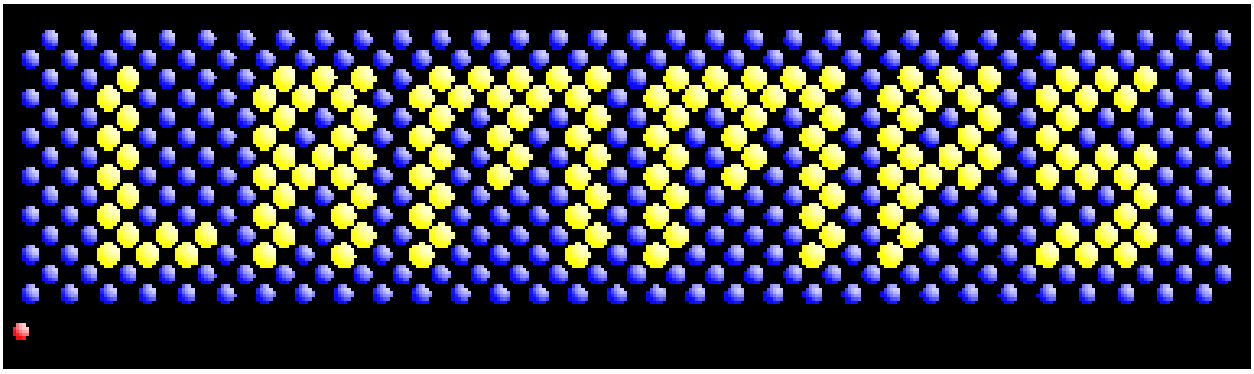

Figure 3.1: Image credit: https://lammps.sandia.gov/

3.2 Conclusions

Chapter 4

Logo of NAMD

4.1 Methods

Figure 4.1: Image credit: https://www.ks.uiuc.edu/Research/namd/

4.2 Conclusions

Chapter 5

Conclusions

Table 5.1: Chapters of molecular dynamics package names

Chapter	name
2	CHARMM
3	LAMMPS
4	NAMD

Bibliography

[1] Bernard R Brooks, Robert E Bruccoleri, Barry D Olafson, David J States, S a Swaminathan, and Martin Karplus. Charmm: a program for macromolecular energy, minimization, and dynamics calculations. *Journal of computational chemistry*, 4(2):187–217, 1983.

[2] James C Phillips, Rosemary Braun, Wei Wang, James Gumbart, Emad Tajkhorshid, Elizabeth Villa, Christophe Chipot, Robert D Skeel, Laxmikant Kale, and Klaus Schulten. Scalable molecular dynamics with namd. *Journal of computational chemistry*, 26(16):1781–1802, 2005.

[3] Steve Plimpton. Fast parallel algorithms for short-range molecular dynamics. *Journal of computational physics*, 117(1):1–19, 1995.