myMaster

by

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Abstract

The most important things

Acknowledgements

I acknowledge...

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Introduction

Here, I introduce the introduction

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State of the science

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Existing Models

[2]

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Simulation tools

3.1 LAMMPS

3.1.1 Input files

Lammps input files are a set of commands to be executed. Some commands are only valid in the right order. The structure of such a file is:

1. **Initialization:** Units, processors, boundary conditions, atom_style, pair_style
2. **Atom definition:** Either from input file (restart/data) or making a lattice or region and create a box and atoms.
3. **Settings:**
4. **Run:**

Most properties are already set with a standard value, which means that only non-standard properties has to be set.

atom_style atom_style decides what kinds of interactions are possible to implement.

All commands ar available from the LAMMPS documentation [3]. A very good beginners guide for LAMMPS [1]

Part III

Bibliography

[1] Albert C. Molecular dynamics simulations. http://puccini.che.pitt.edu/~karlj/Classes/CHE3935/MD_simulations.pdf.

[2] Randall T Cygan, Jian-Jie Liang, and Andrey G Kalinichev. Molecular models of hydroxide, oxyhydroxide, and clay phases and the development of a general force field. *The Journal of Physical Chemistry B*, 108(4):1255–1266, 2004.

[3] sandia.gov. Lammps input commands. http://lammps.sandia.gov/doc/99/input_commands.html, October 2013.