Tools

- Fully automatic calculation system of electronic structure by First-principles
- nap (Nagoya Atomistic-simulation Package)
- Compound Prediction App
- Specific Heat Prediction App
- API Tools

LINK

- MateriApps
- Toki no Mori Wiki - Machine learning (Japanese only)

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nap (Nagoya Atomistic-simulation Package)

Overview

- A classical molecular dynamics (MD) package that includes the following programs:

pmd	parallel MD program
fitpot	parameter optimization program for some force fields including neural-network and Morse potentials
nappy	python scripts for pre/post-processing for pmd and fitpot

- Fortran language is used for pmd and fitpot, Python language for nappy.

Requirements

- macOS or Linux OS
- OpenMPI
- Python 2.x

Download

- nap: Nagoya Atomistic-simulation Package : Github
- Manual website

Licence

This software is released under the MIT License.

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