



 $\spadesuit$ 

Database API

Tools

Cluster system

Cloud system

Usage guide

Reference

Tools

- ► Fully automatic calculation system of electronic structure by Firstprinciples
- nap (Nagoya Atomisticsimulation Package)
- ► Compound Prediction App
- ► Specific Heat Prediction App
- ▶ API Tools

LINK

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

Home > Tools > nap (Nagoya Atomistic-simulation Package)



# 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.

### Contact details for inquiries

Ryo Kobayashi

E-mail: kobayashi.ryo=nitech.ac.jp ([ = ] --> [ @ ])

Department of Physical Science and Engineering, Nagoya Institute of Technology

10 (Materials research by Information Integration" Initiative 情報統合型物質・材料開発イニシアティブ



This site explains the content and usage of the data platform constructed by Ml2l, that is being conducted as the JST Innovation Hul