

mlplib

MLPLIB is a Python package for computational chemistry tools using Machine Learning potential.

Features

- Geometry optimization
- Molecular dynamics
- Phonon calculations
- Search for Crystal structure
- Future
 - NEB calculations

Usages

see [test/](#)

Installation

```
conda create -n mlplib_env python=3.9
conda activate mlplib_env
git clone https://github.com/nkitamuraQC/mlplib.git
cd mlplib
pip install -r requirements.txt
```

- Optional
 - Setting of PYTHONPATH