Examples_QE

Example jobs for QuantumEspresso can be found in a GitHub repository.

Examples in the above repository were created mainly for those who want to learn first-principles calculations. Basic calculations such as DOS and band structure can be practiced.

Prerequisite

To use python scripts prepared, the following libralies need to be installed in advance while the python scripts are not absolutely necessary to run QE jobs.

- python
- pymatgen
- seekpath
- pyyaml

These python libralies can be installed with the following command. If you have troubles, you can skip this part.

```
pip install pymatgen seekpath seekpath pyyaml
pip install pymatgen --upgrade
```

> **NOTE:** If you don't have python on your computer, you need to install python. Anaconda is a useful installer of a set of different python libraries: https://www.anaconda.com/products/distribution.

Download of this repository

```
git clone https://github.com/masato1122/Examples_QE.git
```

If you don't have `git` command, download a zip file and unzip under the directory you like.

Band structure

`./examples/band_structure` contains an example to calculate the electron band structure of silicon.

Move to this directory in your terminal with `cd ./Examples_QE/examples/band_structure` and follow the description written in https://github.com/masato1122/Examples_QE/tree/main/examples/band_structure.

Phonon dispersion

will be uploaded...