Tips for how to shell

Basic shell commands

{…}: variable
#: command out
>: command to be typed in the terminal

```
# to see contents in the current directory
> ls

# to see the current absolute path
> pwd

# to change the current directory
> cd {absolute or relative path of a directory}
# to got to the login {home} directory
# cd
# to go to the upper directory
> cd ..

# to see the contents of a file
> cat {filename}
> more {filename}
> less {filename}

# to see the contents of a file which includes a given text
> grep {text} {filename}

# to see the last part of a file
> tail {filename}
# to see the last part of a file while the simulation is running
> tail -f {filename}
```

How to call QE command (pw.exe)

You may not want to type "/home/qe/pw.exe" each time. To call "pw.exe" command from anywhere on your computer, the path in which pw.exe is located, namely "/home/qe/pw.exe", needs to be added in PATH. More concretely, you need to add "export PATH=$PATH:/home/qe/pw.exe" in your .bash_profile.

Go to the home (login) directory.

```
> cd
```

Open ".bash_profile" file with an eidtor (emacs, vim, …) and add the following line.

```
export PATH=$PATH:/home/qe
```

With this line, the directory in which QE command, e.g. "pw.exe" or "pw.x", are located is added in "PATH".
Make sure that the line is added in ".bash_profile".

```
> cat .bash_profile | grep PATH
…
export PATH=$PATH:(directory you added, for example, /home/qe)
…
```

Then, close and reopen the terminal and check if "pw.exe" command work anywhere in your terminal as below.

```
> pw.exe (or pw.x for Mac or Linux)

   Program PWSCF v.7.1 starts on 11Dec2022 at 15:56:19
     Git branch: develop
     Last git commit: 9ddde6fa44e0fb1c7debb78532a4b581a6ef82fd
     Last git commit date: Fri Oct 28 07:34:35 2022 +0000
     Last git commit subject: Merge branch 'fix_hubbardocc' into 'develop'

   This program is part of the open-source Quantum ESPRESSO suite
   for quantum simulation of materials; please cite
       "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);
       "P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);
       "P. Giannozzi et al., J. Chem. Phys. 152 154105 (2020);
        URL http://www.quantum-espresso.org",
   in publications or presentations arising from this work. More details at
   http://www.quantum-espresso.org/quote

   Parallel version (MPI), running on     1 processors

   MPI processes distributed on     1 nodes
   0 MiB available memory on the printing compute node when the environment starts

   Waiting for input...
```

Calculation of electron band structure

You can find examples for QuantumEspresso (QE) in a GitHub. If you can use “git” command, you can download examples from your terminal, otherwise you need to download the zip file.

Go to the directory where you want to download examples.

```
> cd (any directory you want, for example, “…/work”)
```

Download examples from GitHub.

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

Check if “Examples_QE” was properly downloaded or not.

```
> ls
Examples_QE  ***  ***
```

Move to the directory for band structure calculation.

```
> cd ./Examples_QE/examples/band_structure
```

You can find the same description in https://github.com/masato1122/Examples_QE. To start the band structure calculation, follow the process written in HERE.