PART 2

MATERIAL DESIGN

QUANTUM ESPRESSO INSTALLATION

TUTORIAL A-Z

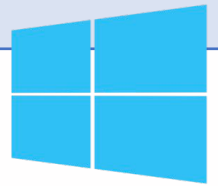
Install QE

Ubuntu/Linux

- sudo apt install
  - gfortran
  - libblas-dev
  - liblapack-dev
  - libfftw3-dev
  - libopenmpi-dev
- download & install QE
- add QE to path

Windows/MacOS

- download & install
  - VirtualBox
  - Ubuntu
  - QE
- alternative:
  - VirtualBox
  - MateriApps Live



Tools

- Text editor
  - Notepad++
  - Gedit, Emacs, dll..
- Graph plot
  - Gnuplot
  - Origin, Excel
- Crystal visualization
  - VESTA
  - XCrysden

Structure QE

Quantum ESPRESSO = op**E**n-**S**ource **P**ackage for **R**esearch in **E**lectronic **S**tructure, **S**imulation, and **O**ptimization

INPUT

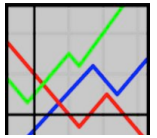
- Input.in

PROSES

- pw.x

OUTPUT

- Output.out



GNUPLOT

```
$ pw.x < input.in > output.out
```

Running QE

Handson #

1. Structures Optimization
2. Electronic Structures
3. Phonon Structures
4. Thermoelectric properties