



# Quantum ESPRESSO and BoltzTraP2



**EDI SUPRAYOGA**

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National Research and Innovation Agency (BRIN)

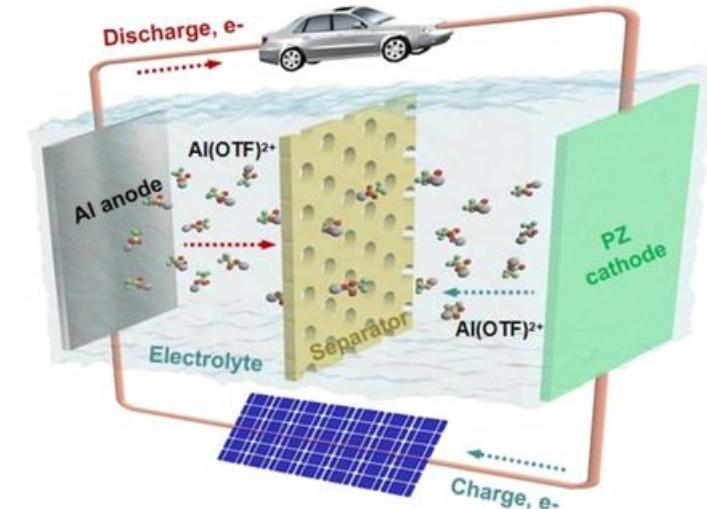
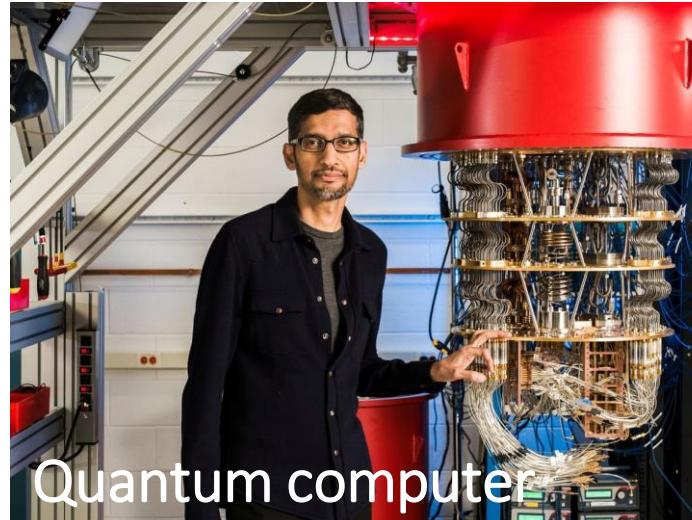
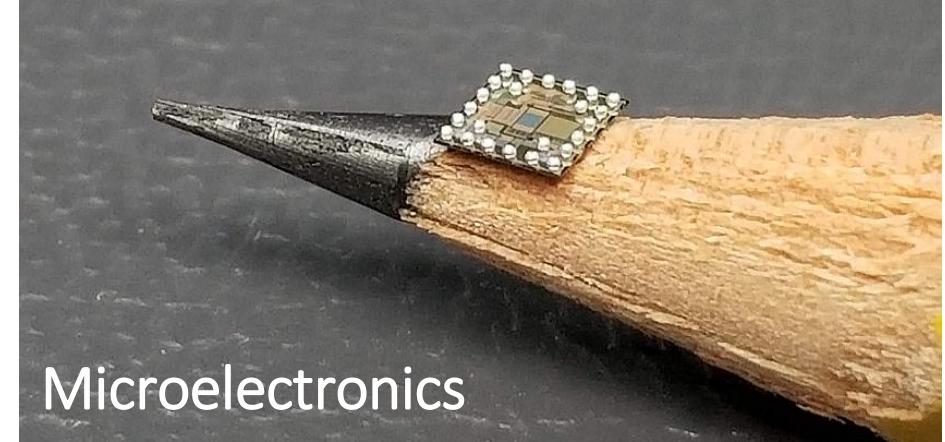


# QUANTUM ESPRESSO INTRODUCTION

PART #1

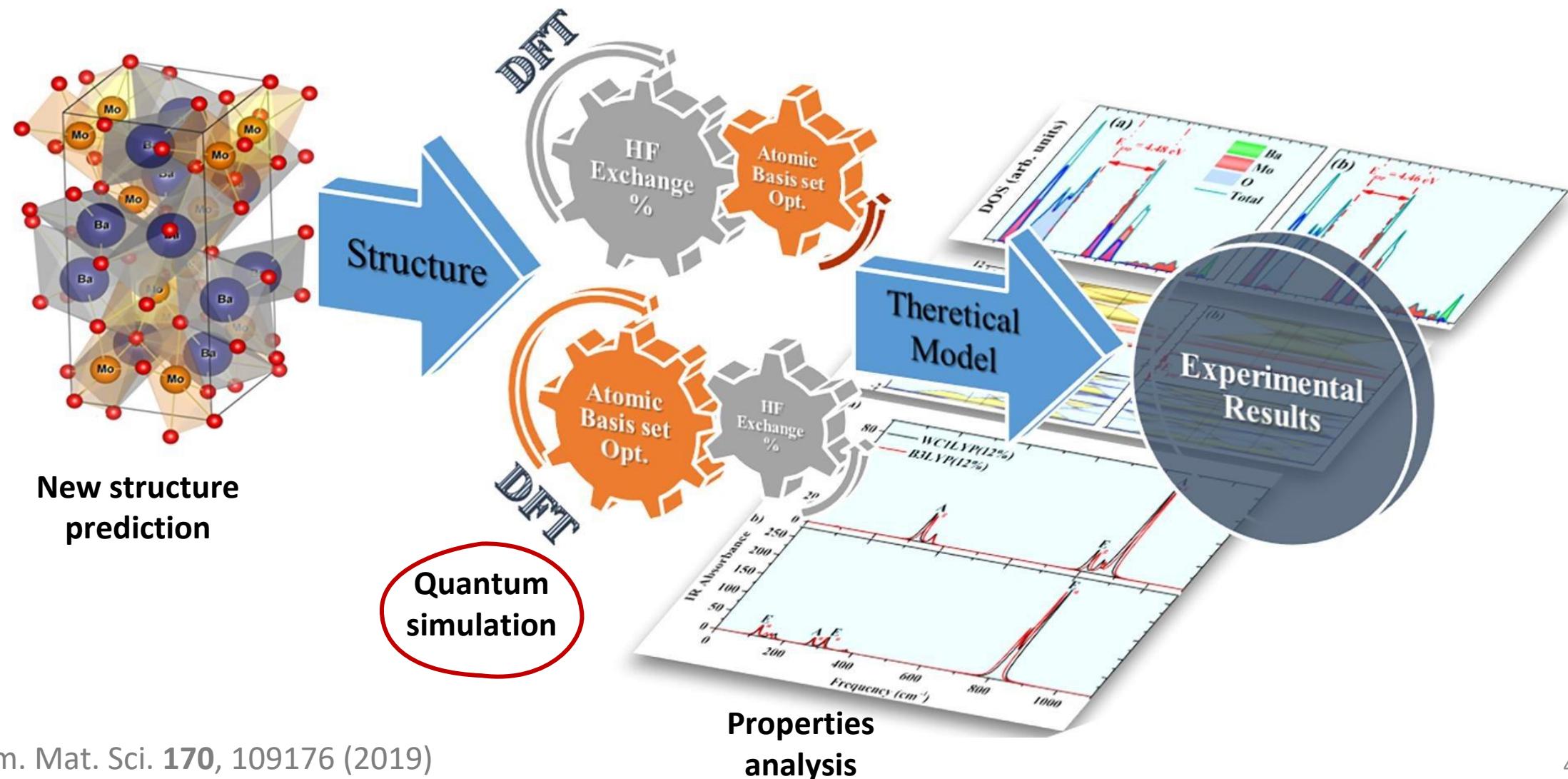


# Motivation: Materials everywhere..



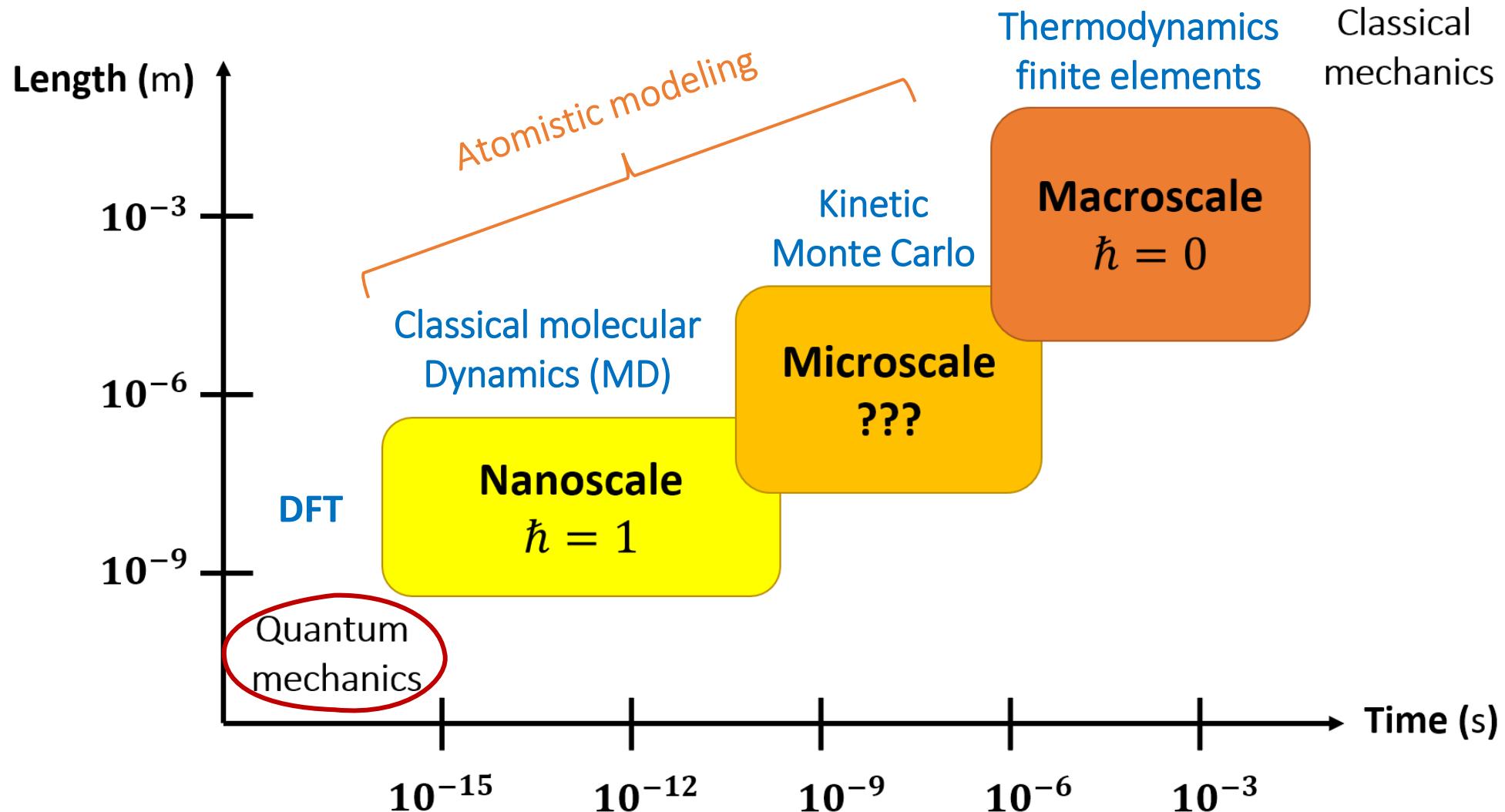


# Materials Discovery





# Time & Length scale





# Fundamental physics and approximation

In Quantum Mechanics:

- A group of particles can be represented by a **wave function**  $\psi(\mathbf{r}, t)$
- The evolution of the wave function with respect to time is described by **Schrödinger equation**

$$i\hbar \frac{d}{dt} \psi(\mathbf{r}, t) = \mathcal{H}\psi(\mathbf{r}, t)$$

too complicated to be solved  
even by a supercomputer



Erwin Schrödinger  
(1933)

Example of approximation:

## Electron:

Time independent Schrödinger eq.

$$\mathcal{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

## Ion:

Classical mechanics (Newton)

$$\vec{F} = m\vec{a}$$



# Born-Oppenheimer approximation

- Ions are considered to be classical particles in **fixed position**
- The **role of ions** as providers of **external potential** that influences the movement of electrons

$$\mathcal{H}_{\text{BO}} = - \sum_{i=1}^n \frac{\hbar^2}{2m_e} \nabla_i^2 + \sum_{i < j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \sum_i \sum_{\alpha}^N \frac{Z_{\alpha} e^2}{|\vec{r}_i - \vec{R}_{\alpha}|} + \sum_{\alpha < \beta}^N \frac{Z_{\alpha} Z_{\beta} e^2}{|\vec{R}_{\alpha} - \vec{R}_{\beta}|}$$



J. Robert  
Oppenheimer

➡ still complicated even it  
has been approximated

Solving the Schrödinger equation gives us:

- **Electron wave function**, is a function of electron position (*depending on ion position*)
- **Eigen Energy** Value, which includes the kinetic energy of the electron and other interactions related to the electron (*but does not include the kinetic energy of the ion*)



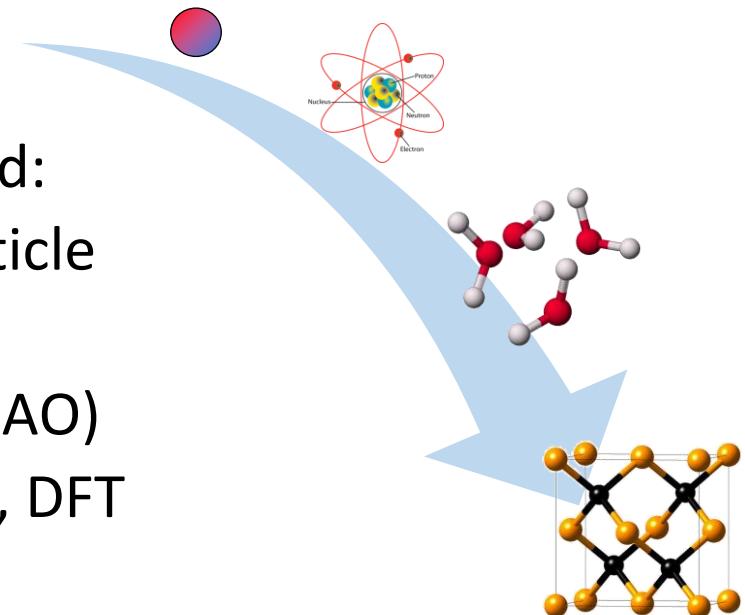
# Electronic structure calculation method

what to solve?

$$i\hbar \frac{d}{dt} \psi(\mathbf{r}, t) = \mathcal{H}\psi(\mathbf{r}, t) \quad \text{Or} \quad \mathcal{H}\psi = E\psi$$

The approximation form must recognize the material studied:

- **Particle** → Schrödinger eq. still solvable for few particle
- **Atom** → consider electrons – ion interaction
- **Molecule** → linear combination of atomic orbitals (LCAO)
- → Bloch theorem, periodicity, tight-binding, DFT
- **Amorph** → Molecular dynamics (MD)
- Etc.



Mathematical tools that often appear: **Calculus** and **Matrix Algebra**



# DFT software



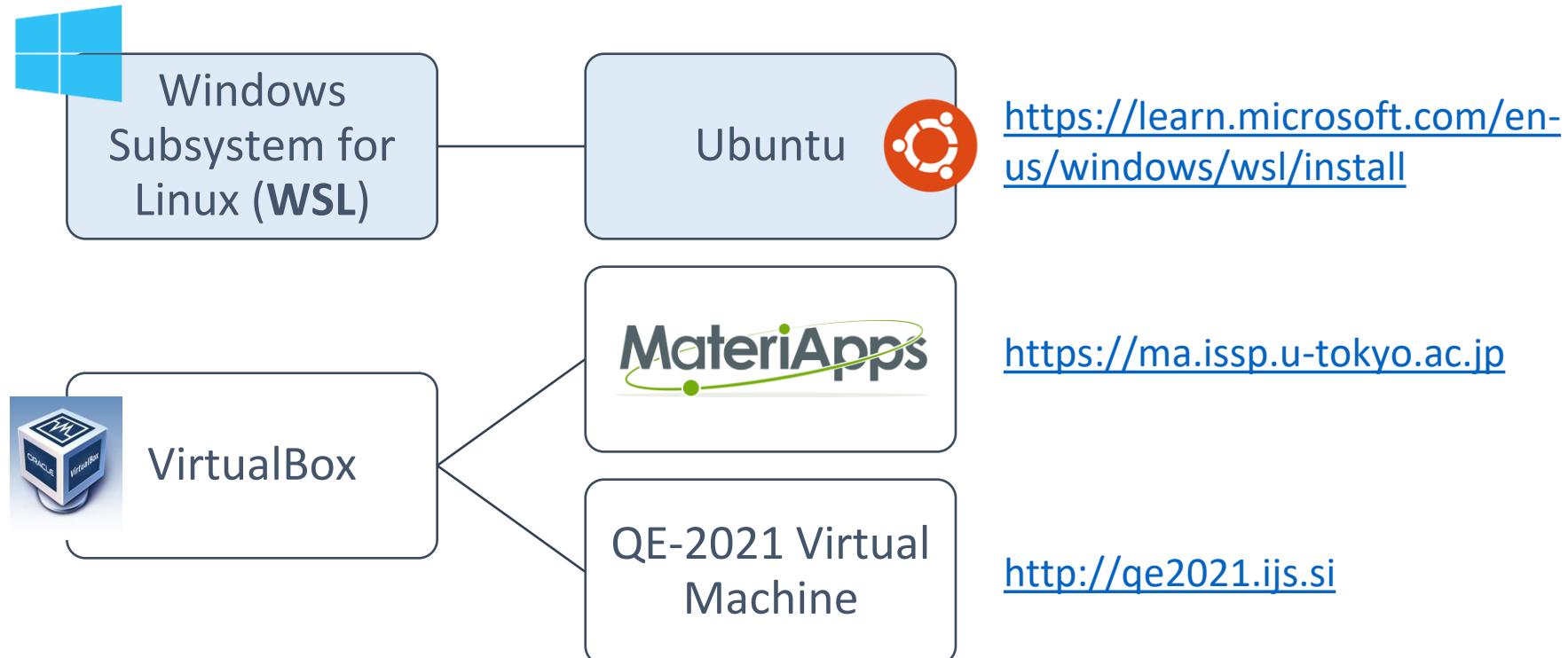


# QUANTUM ESPRESSO INSTALLATION

PART #2



# QE Installation (Windows)





# QE Installation (Linux)



## 1 Update list of repositories

```
$ sudo apt update  
$ sudo apt upgrade
```

## 2 Important development tools and libraries

```
$ sudo apt install git wget build-essential g++  
gfortran liblapack-dev libfftw3-dev libopenmpi-dev
```

## 3 Quantum ESPRESSO and Wannier90

```
$ sudo apt install quantum-espresso wannier90
```

## 4 Additional tools

```
$ sudo apt install xcrysden gnuplot  
$ sudo apt install python3-dev jupyter-server  
$ sudo apt install python3-numpy python3-scipy python3-sympy python3-matplotlib
```



# Useful Resources

- **How to obtain CIF File**
  - AFLOW (<http://aflowlib.org>)
  - Materials Project (<https://materialsproject.org>)
- **How to generate QE Input**
  - PWgui (<http://www-k3.ijs.si/kokalj/pwgui/>)
  - BURAI (<https://nisihara.wixsite.com/burai>)
  - Materials Cloud (<https://www.materialscloud.org/home>)
- **How to Running QE**
  - AiiDA (<https://www.materialscloud.org/work/aiidalab>)
  - Exabyte (<https://exabyte.io>)
  - HPC BRIN (<https://hpc.brin.go.id>)

## Tools

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



# QUANTUM ESPRESSO

## SCF CALCULATION

PART #3



# Kohn-Sham equations

## INPUT

### Model:

unit cell  
lattice vectors  
basis

### Physical approx:

xc-approximation  
GGA, LDA, ...

### Numerical approx:

energy cut-off  
k-points grid  
SCF procedure

## RUN

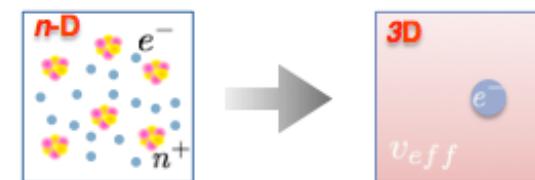


Solve Kohn-Sham equations

## OUTPUT

### Physical quantities:

charge density  
total energy  
KS wavefunctions  
KS energies



$$\left[ -\frac{1}{2} \nabla^2 + V_{ion}(r) + V_H[n(r)] + V_{XC}[n(r)] \right] \psi_i(r) = \varepsilon_i \psi_i(r)$$

External nuclear potential

Hartree potential

Exchange-correlation potential



# Input File

QE-SSP/gr/scf/scf.in

```
1 &CONTROL
2 calculation = 'scf'
3 pseudo_dir = '../pseudo/'
4 outdir = '../tmp/'
5 prefix = 'gr'
6 /
7 &SYSTEM
8 ibrav = 4
9 a = 2.4623
10 c = 10.0
11 nat = 2
12 ntyp = 1
13 occupations = 'smearing'
14 smearing = 'mv'
15 degauss = 0.02
16 ecutwfc = 60
17 /
18 &ELECTRONS
19 mixing_beta = 0.7
20 conv_thr = 1.0D-6
21 /
22 ATOMIC_SPECIES
23 C 12.0107 C.pbe-n-rrkjus_psl.0.1.UPF
24 ATOMIC_POSITIONS (crystal)
25 C 0.333333333 0.666666666 0.500000000
26 C 0.666666666 0.333333333 0.500000000
27 K_POINTS (automatic)
28 12 12 1 0 0 0
```

## &CONTROL

Line	Syntax	Meaning	Default
2	calculation	Task to be calculated ('scf', 'nscf', 'relax', 'vc-relax', 'bands', etc.)	'scf'
3	pseudo_dir	Directory containing pseudopotential files	current directory
4	outdir	Temporary (tmp) folder to save output data	current directory
5	prefix	Filenames of output data in tmp folder	'pwscf'



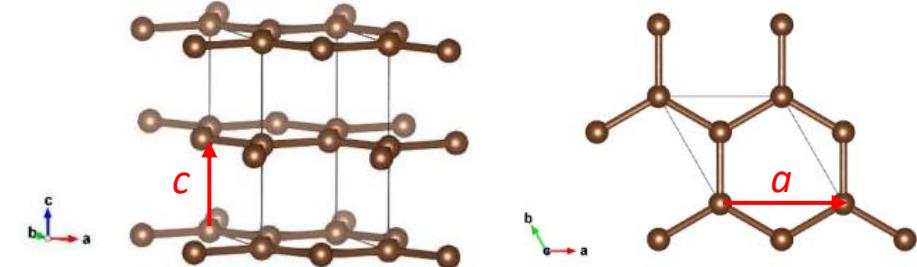
# Input File

## QE-SSP/gr/scf/scf.in

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26 C 0.666666666 0.333333333 0.500000000
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28 12 12 1 0 0 0

```



## &SYSTEM

Line	Syntax	Meaning	Default
8	ibrav	Bravais lattice index	required
9,10	a,c	Lattice constant (in Angstrom)	required
11	nat	Number of atoms per unit cell	required
12	ntyp	Number of types of atoms	required
13	occupations	'smearing' for the case of metal, 'fixed' for insulator with gap	-
14	smearing	Smearing method	'gaussian'
15	degauss	Value of the Gaussian spreading (Ry) for BZ integration in metal	0.0
16	ecutwfc	Cut-off energy (Ry)	required



# Input File

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```

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24 ATOMIC_POSITIONS (crystal)
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26 C 0.66666666 0.33333333 0.500000000
27 K_POINTS (automatic)
28 12 12 1 0 0 0

```

ibrav	Structure	Lattice vectors
0	Free	Lattice vectors are given in card CELL_PARAMETERS
1	Cubic P	$v_1 = a(1, 0, 0), v_2 = a(0, 1, 0), v_3 = a(0, 0, 1)$
2	Cubic F	$v_1 = \frac{a}{2}(-1, 0, 1), v_2 = \frac{a}{2}(0, 1, 1),$ $v_3 = \frac{a}{2}(-1, 1, 0)$
3	Cubic I	$v_1 = \frac{a}{2}(1, 1, 1), v_2 = \frac{a}{2}(-1, 1, 1),$ $v_3 = \frac{a}{2}(-1, -1, 1)$
-3	Cubic I	$v_1 = \frac{a}{2}(-1, 1, 1), v_2 = \frac{a}{2}(1, -1, 1),$ $v_3 = \frac{a}{2}(1, 1, -1)$
4	Hexagonal and Trigonal P	$v_1 = a(1, 0, 0), v_2 = a(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0),$ $v_3 = a(0, 0, \frac{c}{a})$
5	Trigonal R, 3-fold axis c	$v_1 = a(x, -y, z), v_2 = a(0, 2y, z),$ $v_3 = a(-x, -y, z)$ , where $x = \sqrt{\frac{1-c}{2}}$ , $y = \sqrt{\frac{1-c}{6}}, z = \sqrt{\frac{1+2c}{3}}, c = \cos \gamma$
-5	Trigonal R, 3-fold axis (111)	$v_1 = \frac{a}{\sqrt{3}}(u, v, v), v_2 = \frac{a}{\sqrt{3}}(u, v, v),$ $v_3 = \frac{a}{\sqrt{3}}(v, v, u)$ , where $u = z - 2\sqrt{2}y$ and $v = z + \sqrt{2}y$ with $y, z$ as for case ibrav = 5
6	Tetragonal P	$v_1 = a(1, 0, 0), v_2 = a(0, 1, 0), v_3 = a(0, 0, \frac{c}{a})$
7	Tetragonal I	$v_1 = \frac{a}{2}(1, -1, \frac{c}{a}), v_2 = \frac{a}{2}(1, 1, \frac{c}{a}),$ $v_3 = \frac{a}{2}(-1, -1, \frac{c}{a})$
8	Orthorhombic P	$v_1 = (a, 0, 0), v_2 = (0, b, 0), v_3 = (0, 0, c)$



# Input File

QE-SSP/gr/scf/scf.in

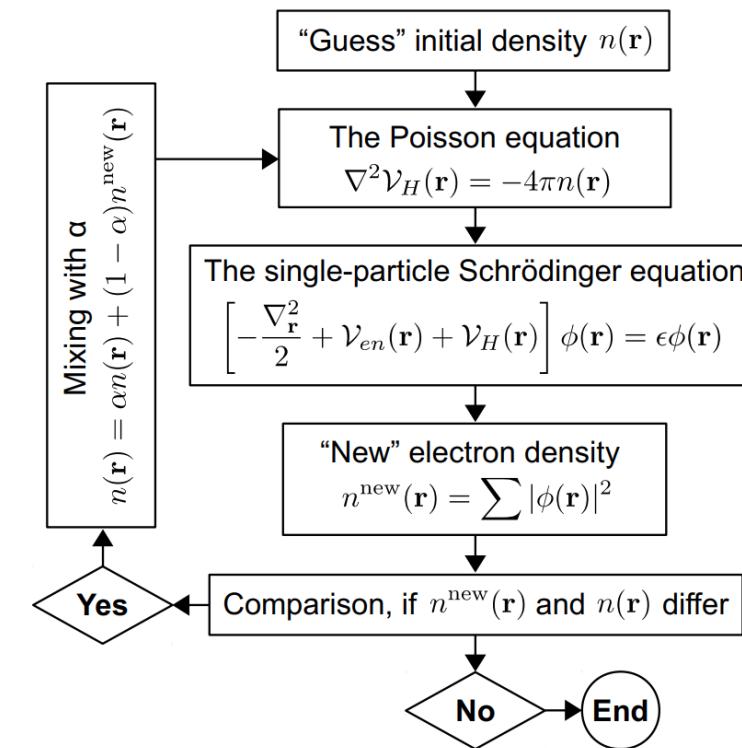
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15 degauss = 0.02
16 ecutwfc = 60
17 /
18 &ELECTRONS
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20 conv_thr = 1.0D-6
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24 ATOMIC_POSITIONS (crystal)
25 C 0.333333333 0.666666666 0.500000000
26 C 0.666666666 0.333333333 0.500000000
27 K_POINTS (automatic)
28 12 12 1 0 0 0

```

## &ELECTRONS

Line	Syntax	Meaning	Default
19	mixing_beta	Mixing factor for self-consistency	0.7
20	conv_thr	Convergence threshold for scf	1.D-6





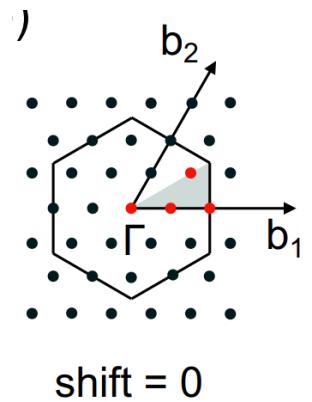
# Input File

QE-SSP/gr/scf/scf.in

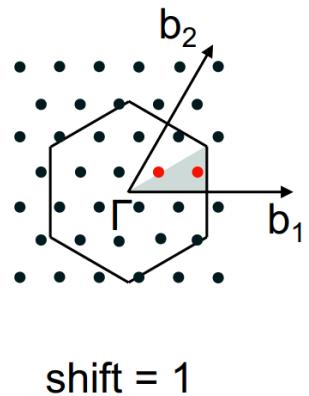
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28 12 12 1 0 0 0

```

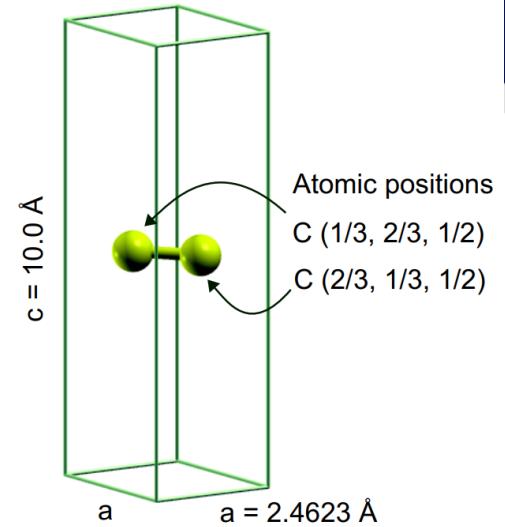


shift = 0



shift = 1

Hexagonal lattice (ibrav = 4)



Line	Syntax	Meaning
22,23	ATOMIC_SPECIES	A <i>mandatory input card</i> includes name, mass, and pseudopotential used for each atomic species present in the system.
24-26	ATOMIC_POSITIONS	A <i>mandatory input card</i> includes type and coordinates of each atom in the unit cell.
27,28	K_POINTS	A <i>mandatory input card</i> includes information of the $k$ -points used for Brilloin-zone integration.



# How to get pseudopotential

<http://www.quantum-espresso.org/pseudopotentials/>

ANY FUNCTIONAL		ANY TYPE		Apply Filter	
ANY PP LIBRARY		OTHER OPTIONS			
1 H				2 He	
3 Li	4 Be			5 B	6 C
11 Na	12 Mg			7 N	8 O
19 K	20 Ca			9 F	10 Ne
37 Rb	38 Sr	21 Sc	22 Ti	13 Al	14 Si
55 Cs	56 Ba	23 V	24 Cr	15 P	16 S
87 Fr	88 Ra	25 Mn	26 Fe	17 Cl	18 Ar
*	57-70	27 Co	28 Ni	19 Ga	20 Ge
		29 Cu	30 Zn	31 As	32 Se
		31 Ga	32 Ge	33 Br	34 Kr
		33 Ge	34 As	35 Se	36 Br
		35 Sn	36 Sb	37 Te	38 I
		37 In	38 Cd	39 Po	40 At
		39 Pd	40 Ag	41 Bi	42 Rn
		41 Rh	42 Ru	43 Pt	44 Au
		43 Nb	44 Tc	45 Os	46 Ir
		45 Mo	46 Ru	47 Hg	48 Tl
		47 Tc	48 Rh	49 Pt	50 Au
		48 Ru	49 Rh	51 Hg	52 Tl
		49 Nb	50 Ru	51 Os	52 Ir
		50 Mo	51 Rh	53 Hg	54 Tl
		51 Tc	52 Ru	53 Os	54 Ir
		52 Ru	53 Rh	55 Hg	56 Tl
		53 Nb	54 Ru	56 Os	57 Ir
		54 Mo	55 Rh	57 Hg	58 Tl
		55 Tc	56 Ru	58 Os	59 Ir
		56 Ru	57 Rh	59 Hg	60 Tl
		57 Nb	58 Ru	60 Os	61 Ir
		58 Mo	59 Rh	61 Hg	62 Tl
		59 Tc	60 Ru	62 Os	63 Ir
		60 Ru	61 Rh	63 Hg	64 Tl
		61 Nb	62 Ru	64 Os	65 Ir
		62 Mo	63 Rh	65 Hg	66 Tl
		63 Tc	64 Ru	66 Os	67 Ir
		64 Ru	65 Rh	67 Hg	68 Tl
		65 Nb	66 Ru	68 Os	69 Ir
		66 Mo	67 Rh	69 Hg	70 Tl
		67 Tc	68 Ru	70 Os	71 Ir
		68 Ru	69 Rh	71 Hg	72 Tl
		69 Nb	70 Ru	72 Os	73 Ir
		70 Mo	71 Rh	73 Hg	74 Tl
		71 Tc	72 Ru	74 Os	75 Ir
		72 Ru	73 Rh	75 Hg	76 Tl
		73 Nb	74 Ru	76 Os	77 Ir
		74 Mo	75 Rh	77 Hg	78 Tl
		75 Tc	76 Ru	78 Os	79 Ir
		76 Ru	77 Rh	79 Hg	80 Tl
		77 Nb	78 Ru	80 Os	81 Ir
		78 Mo	79 Rh	81 Hg	82 Tl
		79 Tc	80 Ru	82 Os	83 Ir
		80 Ru	81 Rh	83 Hg	84 Tl
		81 Nb	82 Ru	84 Os	85 Ir
		82 Mo	83 Rh	85 Hg	86 Tl
		83 Tc	84 Ru	86 Os	87 Ir
		84 Ru	85 Rh	87 Hg	88 Tl
		85 Nb	86 Ru	88 Os	89 Ir
		86 Mo	87 Rh	89 Hg	90 Tl
		87 Tc	88 Ru	90 Os	91 Ir
		88 Ru	89 Rh	91 Hg	92 Tl
		89 Nb	90 Ru	92 Os	93 Ir
		90 Mo	91 Rh	93 Hg	94 Tl
		91 Tc	92 Ru	94 Os	95 Ir
		92 Ru	93 Rh	95 Hg	96 Tl
		93 Nb	94 Ru	96 Os	97 Ir
		94 Mo	95 Rh	97 Hg	98 Tl
		95 Tc	96 Ru	98 Os	99 Ir
		96 Ru	97 Rh	99 Hg	100 Tl
		97 Nb	98 Ru	100 Os	101 Ir
		98 Mo	99 Rh	101 Hg	102 Tl
		99 Tc	100 Ru	102 Os	103 Ir
		100 Ru	101 Rh	103 Hg	104 Tl
		101 Nb	102 Ru	104 Os	105 Ir
		102 Mo	103 Rh	105 Hg	106 Tl
		103 Tc	104 Ru	106 Os	107 Ir
		104 Ru	105 Rh	107 Hg	108 Tl
		105 Nb	106 Ru	108 Os	109 Ir
		106 Mo	107 Rh	109 Hg	

## PSEUDO SEARCH RESULTS

### Pseudopotential File

#### Si.blyp-hgh.UPF

Pseudopotential type: NORMCONS  
Method: Goedecker-Hartwigsen-Hutter-Teter  
Functional type: Becke-Lee-Yang-Parr (BLYP) exch-corr  
non relativistic  
  
Origin: Hartwigsen-Goedecker-Hutter PP  
Author: Goedecker/Hartwigsen/Hutter/Teter  
Generated in analytical, separable form. Converted from CPMD format using cpmd2upf v.5.0.1.  
Uploaded by marsamos  
Classification unverified

#### Si.pbe-rrkj.UPF

Pseudopotential type: NORMCONS  
Method: Rappe Rabe Kaxiras Joannopoulos  
Functional type: Perdew-Burke-Ernzerhof (PBE) exch-corr  
scalar relativistic  
  
Origin: Original QE PP library  
Author: Andrea Dal Corso  
Generated by Andrea Dal Corso code (rrkj3)  
Uploaded by Erica Vidal  
Classification controlled by Paolo Giannozzi

#### Si.pbe-van\_gipaw.UPF

Pseudopotential type: ULTRASOFT  
Method: Rappe Rabe Kaxiras Joannopoulos  
Functional type: Perdew-Burke-Ernzerhof (PBE) exch-corr  
Is Gipaw  
scalar relativistic  
  
Origin: Original QE PP library  
Generated by "atomic" code by A. Dal Corso (QE distribution)  
Uploaded by Erica Vidal  
Classification controlled by Paolo Giannozzi

## Si.pbe-rrkj.UPF

- ▶ type of exchange-correlation functional
- ▶ type of pseudopotential



# How to Run

```
1 | $ cd ~/QE-SSP/gr/scf/  
2 | $ mpirun -np 4 pw.x < scf.in > scf.out
```

```
3 | $ cat scf.out
```



## QE-SSP/gr/scf/scf.out

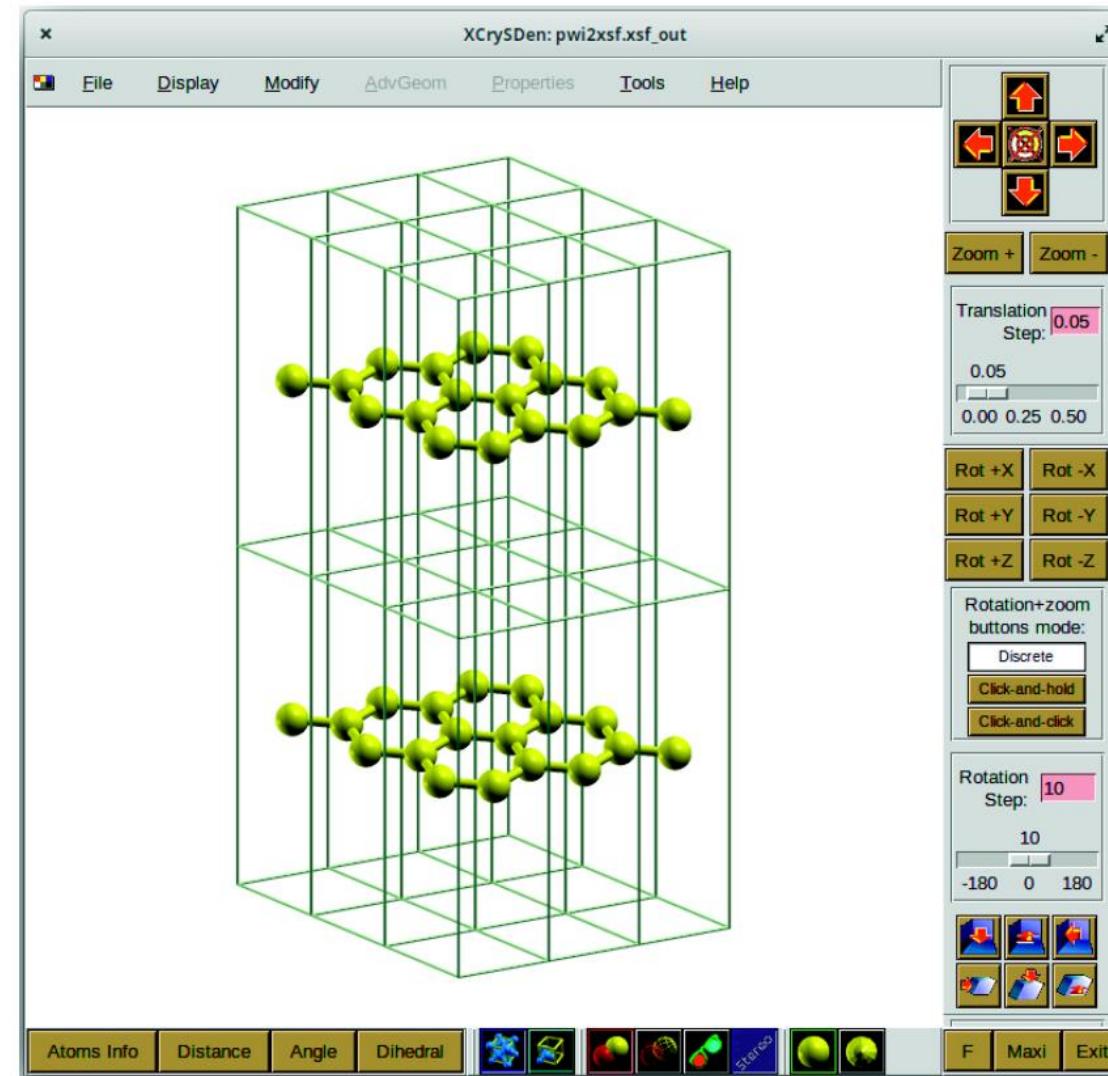
```
!      total energy          =      -23.90991271 Ry  
Harris-Foulkes estimate    =      -23.90991328 Ry  
estimated scf accuracy     <      0.00000084 Ry  
  
The total energy is the sum of the following terms:  
  
one-electron contribution =      -90.80734321 Ry  
hartree contribution      =       47.24141117 Ry  
xc contribution           =      -8.30684749 Ry  
ewald contribution        =      27.96304915 Ry  
smearing contrib. (-TS)   =      -0.00018232 Ry  
  
convergence has been achieved in 13 iterations
```

```
4 | $ grep ! scf.out
```



# How to Check

5 | \$ xcrysden &





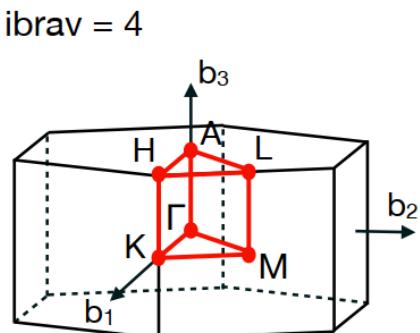
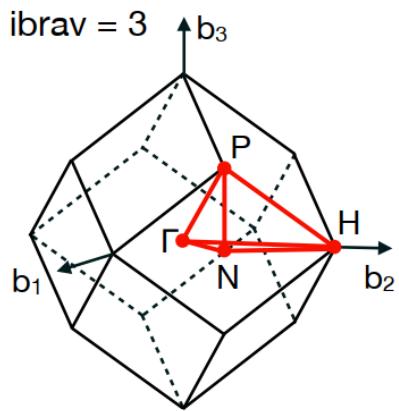
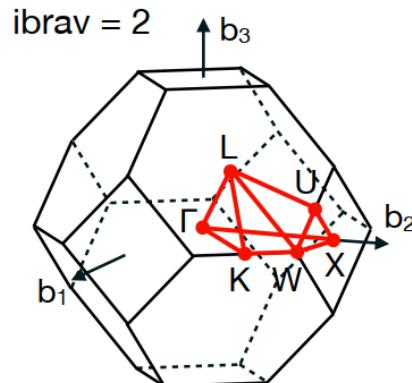
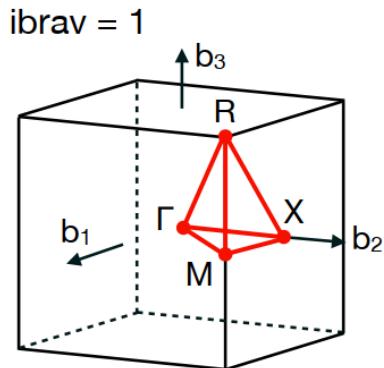
# QUANTUM ESPRESSO BANDS CALCULATION

PART #4



# Bands calculation

1 | \$ cd ~/QE-SSP/gr/bands/



QE-SSP/gr/bands/nscf.in

```

1 &CONTROL
2 calculation      = 'bands'           ← non-SCF
3 pseudo_dir       = '../pseudo/'      calculation
4 outdir          = '../tmp/'          ←
5 prefix           = 'gr'
6 /
7 &SYSTEM
8 ibrav            = 4
9 a                 = 2.4639055825
10 c                = 15.0
11 nat              = 2
12 ntyp             = 1
13 nbnd             = 16
14 occupations     = 'smearing'
15 smearing         = 'mv'
16 degauss          = 0.020
17 ecutwfc          = 40
18 /
19 &ELECTRONS
20 mixing_beta      = 0.7
21 conv_thr         = 1.0D-6
22 /
23 ATOMIC_SPECIES
24 C 12.0107 C.pbe-n-rrkjus_psl.0.1.UPF
25 ATOMIC_POSITIONS (crystal)
26 C 0.3333333333 0.6666666666 0.5000000000
27 C 0.6666666666 0.3333333333 0.5000000000
28 K_POINTS (crystal_b)
29 4
30 gG 40
31 K 20
32 M 30
33 gG 0

```

Selected special k-point  
coordinates



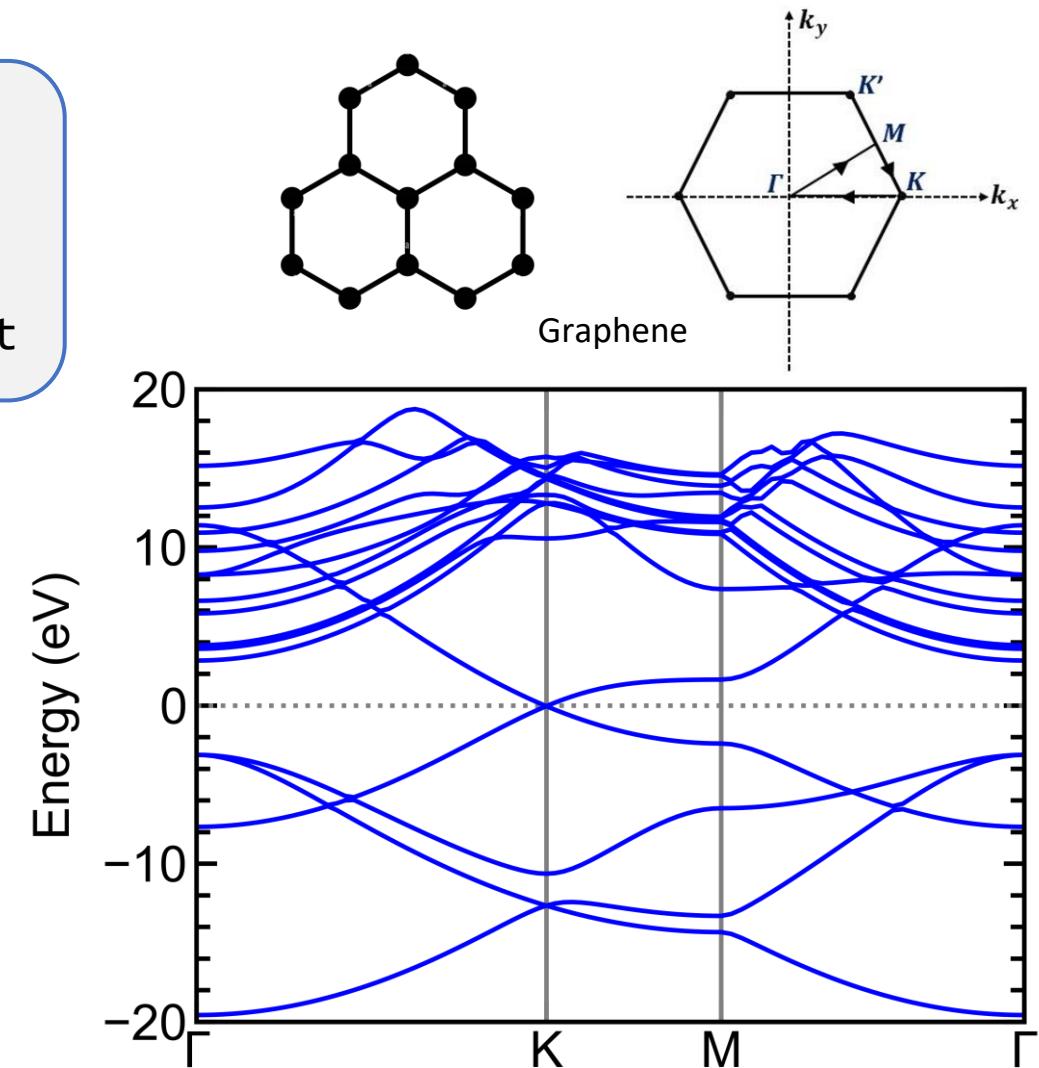
# Electronic energy dispersion

```
1 $ cd ~/QE-SSP/gr/bands/  
2 $ mpirun -np 4 pw.x <scf.in> scf.out  
3 $ mpirun -np 4 pw.x <nscf.in> nscf.out  
4 $ mpirun -np 4 bands.x <bands.in> bands.out
```

## QE-SSP/gr/bands/bands.in

```
1 &BANDS  
2 outdir = '../tmp/'  
3 prefix = 'gr'  
4 filband = 'gr.bands' ← Name of data file  
5 /
```

```
5 $ jupyter-lab plot-bands.ipynb
```



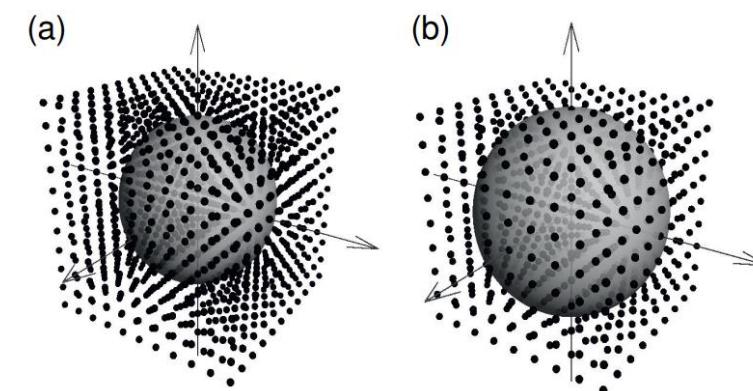


# Electronic density of states

QE-SSP/gr/edos/nscf.in

```
1 &CONTROL
2 calculation      = 'nscf'           ← non-SCF calculation
3 pseudo_dir       = '../pseudo/'
4 outdir          = '../tmp/'
5 prefix          = 'gr'
6 /
7 &SYSTEM
8 ibrav           = 4
9 a               = 2.4639055825
10 c              = 15.0
11 nat             = 2
12 ntyp            = 1
13 nbnd            = 16
14 occupations    = 'tetrahedra'     ← Linear tetrahedron method
15 ecutwfc         = 40
16 /
17 &ELECTRONS
18 mixing_beta     = 0.7
19 conv_thr        = 1.0D-6
20 /
21 ATOMIC_SPECIES
22 C 12.0107 C.pbe-n-rrkjus_psl.0.1.UPF
23 ATOMIC_POSITIONS (crystal)
24 C 0.333333333 0.666666666 0.500000000
25 C 0.666666666 0.333333333 0.500000000
26 K_POINTS (automatic)
27 48 48 1 0 0 0   ← High density k-point
```

```
1 $ cd ~/QE-SSP/gr/edos/
```



QE-SSP/gr/edos/dos.in

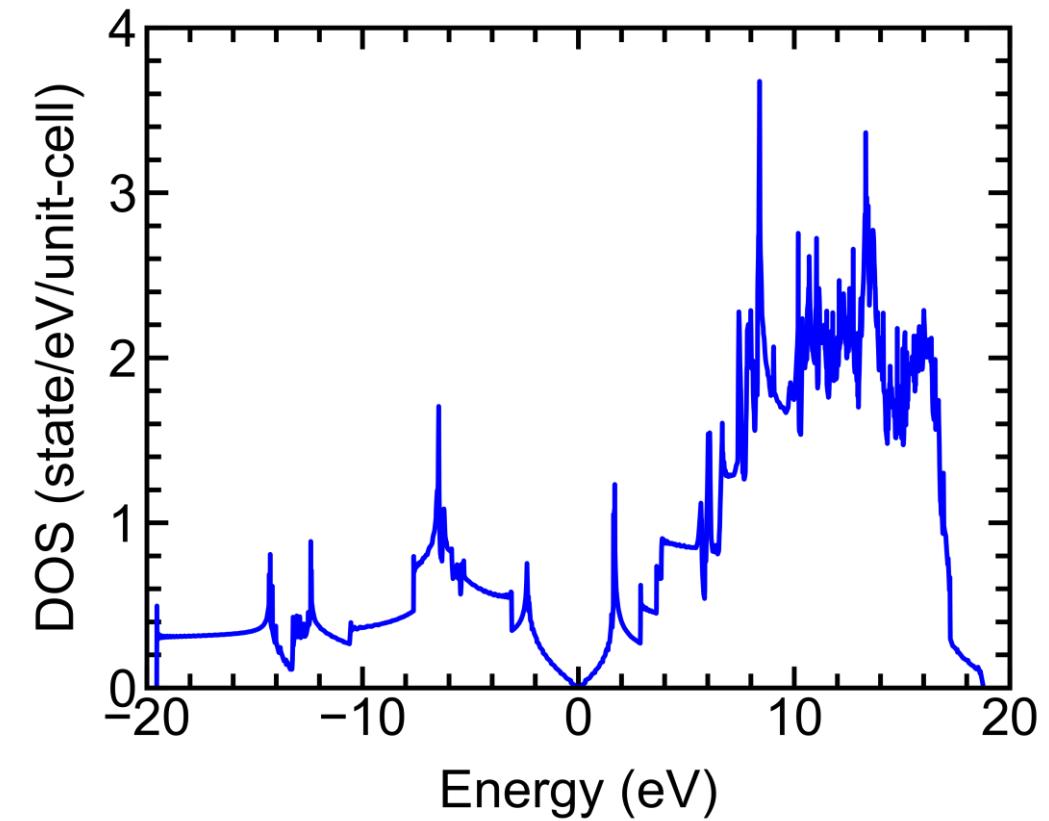
```
1 &DOS
2 outdir = '../tmp/'
3 prefix = 'gr'
4 fildos = 'gr.dos'
5 /
```



# Electronic density of states

```
1 | $ cd ~/QE-SSP/gr/edos/  
2 | $ mpirun -np 4 pw.x <scf.in> scf.out  
3 | $ mpirun -np 4 pw.x <nscf.in> nscf.out  
4 | $ mpirun -np 4 dos.x <dos.in> dos.out
```

```
5 | $ jupyter-lab plot-dos.ipynb
```





# BoltzTraP2

## CRASH COURSE

PART #5



# Electronic transport calculation

Linearized Boltzmann transport formalism + Relaxation Time Approximation

TE Kernel:

$$\mathcal{L}_i = \int_{-\infty}^{\infty} \mathcal{T}(E)(E - \mu)^i \left( -\frac{\partial f}{\partial E} \right) dE , i = 0, 1, 2$$

Electrical conductivity:

$$\sigma = q^2 \sum_{j=1}^{N_B} \mathcal{L}_{0,j}$$

Seebeck's coefficient:

$$S = \frac{1}{qT} \frac{\left( \sum_{j=1}^{N_B} \mathcal{L}_{1,j} \right)^2}{\sum_{j=1}^{N_B} \mathcal{L}_{0,j}}$$

Thermal conductivity:

$$\kappa_e = \frac{1}{T} \left( \sum_{j=1}^{N_B} \mathcal{L}_{2,j} - \frac{\left( \sum_{j=1}^{N_B} \mathcal{L}_{1,j} \right)^2}{\sum_{j=1}^{N_B} \mathcal{L}_{0,j}} \right)$$

Derivative of Fermi-Dirac distribution function

Transport Distribution Function:

$$\mathcal{T}(E) = v^2(E) \tau(E) D(E)$$

Carrier velocity:

$$v^2(E) = \frac{v_g^2}{2} = \frac{1}{2\hbar^2} \left( \frac{dE}{dk} \right)^2$$

Relaxation time:

$$\tau(E) = \frac{C}{D(E)}$$

Density of states

Power Factor:

$$PF = S^2 \sigma$$

TE figure of merit:

$$ZT = \frac{S^2 \sigma}{\kappa_e + \kappa_{ph}} T$$



# BoltzTrap2 installation

## Requirements

- Python v3.5 or higher
- Python Package Index (pip)

## BoltzTrap2 Installation

```
$ pip install boltztrap2
```

```
$ pip install pyfftw vtk
```

## pip Installation

```
$ sudo apt install python3-pip
```

## required

```
$ sudo apt install cmake  
$ pip install numpy cython
```

## Add PATH

```
$ nano ~/.bashrc  
# add to the last line:  
Export PATH=/home/.local/bin:$PATH
```

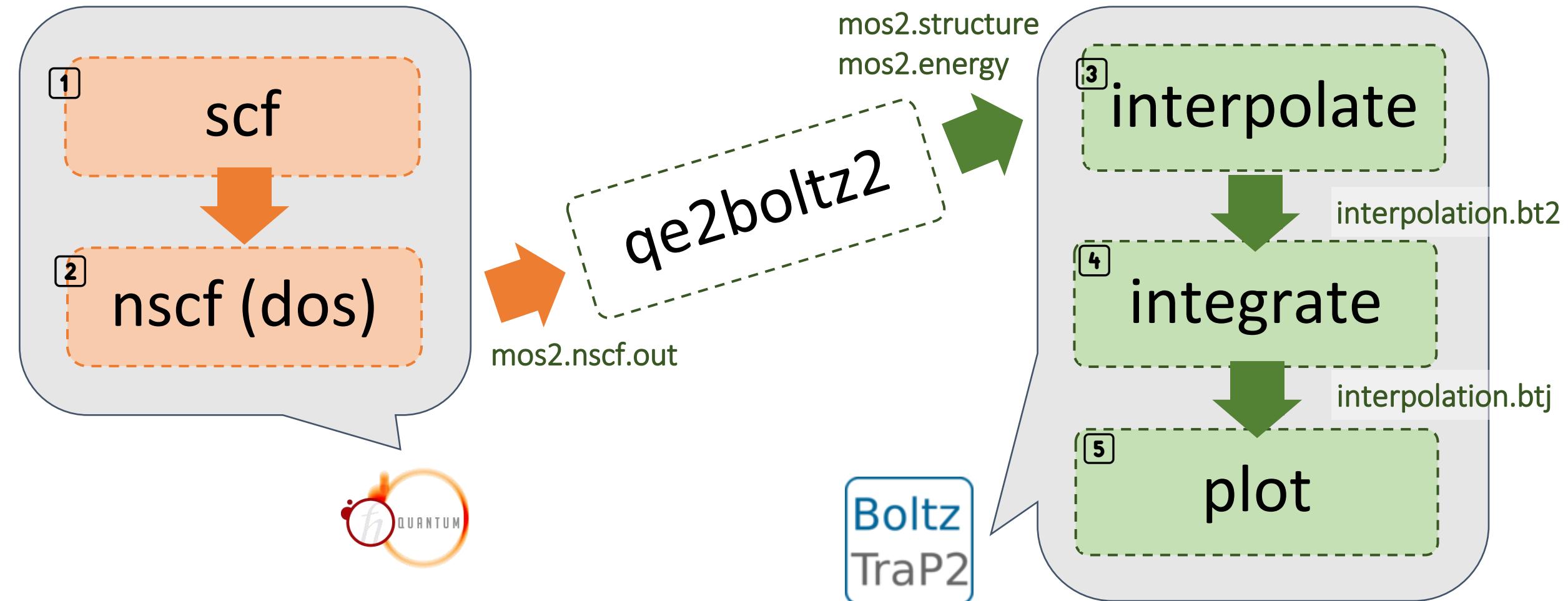
Boltz  
Trap2

[https://gitlab.com/sousaw/  
BoltzTrap2](https://gitlab.com/sousaw/BoltzTrap2)

btp2



# Computing transport properties





# Computing transport properties

## 1. Grab the Fermi energy:

```
$ grep Fermi mos2.nscf.out
```

## 2. Convert QE to BoltzTraP2:

```
$ qe2boltz2.py mos2 pw 0.0786 0
```

## prefix

pw  
dos

Efermi

## nbnd\_exclude (lowest energy)

### 3. Interpolate band energy:

```
$ btp2 interpolate -m 5 -e -0.5 ./
```

how fine the  
interpolation is

# Minimum energy

## PATH to 'nscf.out'



# Computing transport properties

## 4. Calculate Onsager coeff.:

```
$ btp2 integrate interpolation.bt2 300:500:50
```

JSON output file

$T_{\min} : T_{\max} : T_{\text{step}}$

Temperature range:  
 $300 \text{ K} \leq T \leq 500 \text{ K}$

$$\mathcal{L}_i = \int_{-\infty}^{\infty} \mathcal{T}(E)(E - \mu)^i \left( -\frac{\partial f}{\partial E} \right) dE \quad (i = 0, 1, 2)$$

Output files:

- JSON format: `interpolation.btj`
- Old BoltzTraP format: `.trace`, `.condtens`, `.halltens`

$$\begin{aligned}\sigma &= q^2 \mathcal{L}_0 \\ S &= \frac{1}{qT} \frac{\mathcal{L}_1}{\mathcal{L}_0} \\ \kappa_e &= \frac{1}{T} \left( \mathcal{L}_2 - \frac{(\mathcal{L}_1)^2}{\mathcal{L}_0} \right)\end{aligned}$$



# Computing transport properties

5. Plot the result:

```
$ btp2 plot -u -c '["xx", "zz"]' -s 50 interpolation.btj s
```

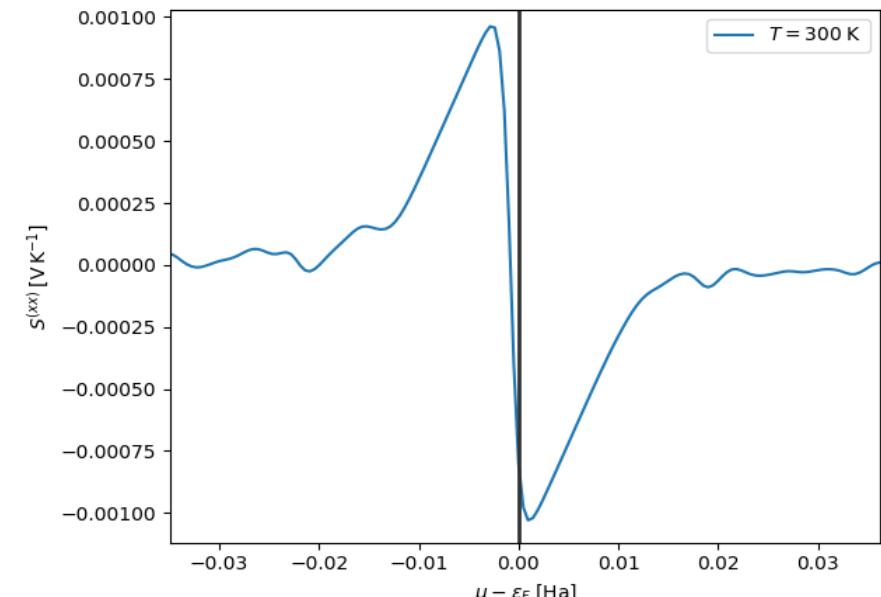
-u : plot as function of  $\mu$   
-T : plot as function of T

-c '["xx"]'  
component  
to be plotted

-s 50  
number of  
subsampling

JSON output file

Seebeck



<https://gitlab.com/sousaw/BoltzTraP2/-/wikis/tutorial>



# More tutorials? just look at my channel...

The screenshot shows a YouTube channel page for 'Edi Suprayoga'. The channel has 1.23K subscribers and 38 videos. The bio indicates the user is a Physics & Computation Enthusiast. Below the channel info, there are tabs for Home, Videos, Playlists (which is selected), and Community. A search bar is at the top right. The main content area displays four playlists: 'BoltzTraP2 + Quantum Espresso' (Part 1 INSTALLATION), 'Workshop/Kolokium', 'Phonopy + QE', and 'BURAI 1.3'. Each playlist card includes a thumbnail, title, and a 'View full playlist' link at the bottom.

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Created playlists

BoltzTraP2 + Quantum Espresso

Part 1 INSTALLATION

4 videos

Workshop/Kolokium

Uniaxial Strain-Induced Electronic Properties Alteration of Monolayer MoS<sub>2</sub>

A. Setiawan<sup>1</sup>, I. P. Handayani<sup>2\*</sup>, Engineering Physics, Institute of Chemical Engineering, Research Center for Physics, Nuclear Research Center, Bandung Institute of Technology, Indonesia

4 videos

Phonopy + QE

Online Tutorial on Thermal Analysis using Phonopy

7 videos

BURAI 1.3

TUTORIAL QUANTUM ESPRESSO WITH BURAI

PLAY ALL

9 videos

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View full playlist

View full playlist

[https://www.youtube.com/watch?v=24\\_eyLI3nf&list=PLIRLJRX4nclWt7HgpDlLFqjyXNO2AdVYO&pp=gAQBiAQB](https://www.youtube.com/watch?v=24_eyLI3nf&list=PLIRLJRX4nclWt7HgpDlLFqjyXNO2AdVYO&pp=gAQBiAQB)