

# QUANTUM ESPRESSO AND WANNIER90 CRASH COURSE

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<https://quantumresearch.id>

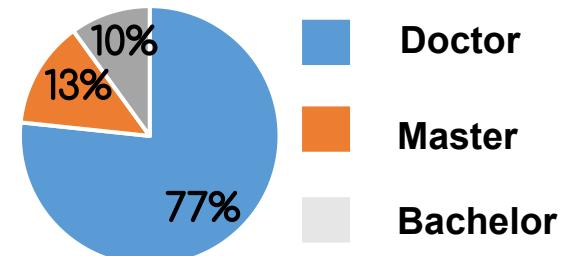




# BRIN Research Center for Quantum Physics



# OF RESEARCHERS:  
35 persons



further info:  
[quantumresearch.id](http://quantumresearch.id)

# “QuMaT” Research Group



## Quantum Matter Theory

Leader



Edi  
Suprayoga



Ahmad Ridwan  
Tresna Nugraha



Eddwi Hesky  
Hasdeo



M Shoufie  
Ukhtary



Muzakkiy  
P. M. Akhir

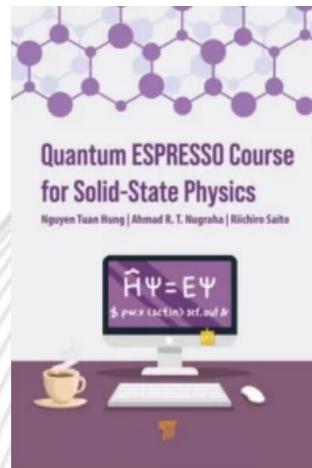


Choirun Nisaa  
Rangkuti

Research scopes:  
fundamental excitations and  
quasiparticles such as  
electrons, spins, photons, phonons,  
magnons, plasmons, and their  
interactions with each other

Publication outputs  
(last 5 years)

> 60 international journals  
1 textbook



## COLLABORATION



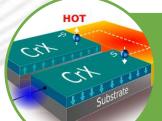
e-ASIA JRP

(2022 – 2025)

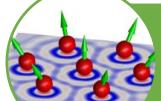
# Current FOCUS



Topological materials



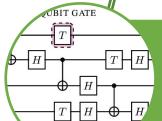
Nanoscale energy transport



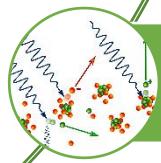
Skyrmions in magnetic materials



Quantum battery and state transfer



Open quantum systems



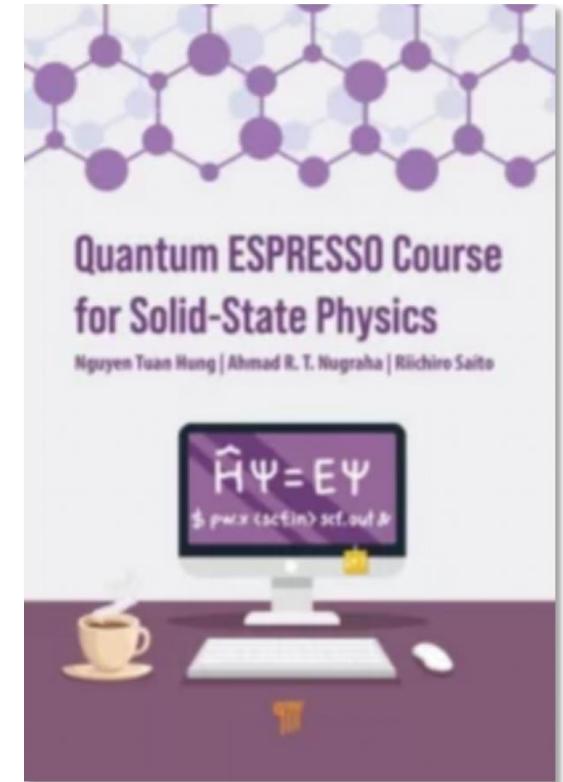
Light-matter interactions

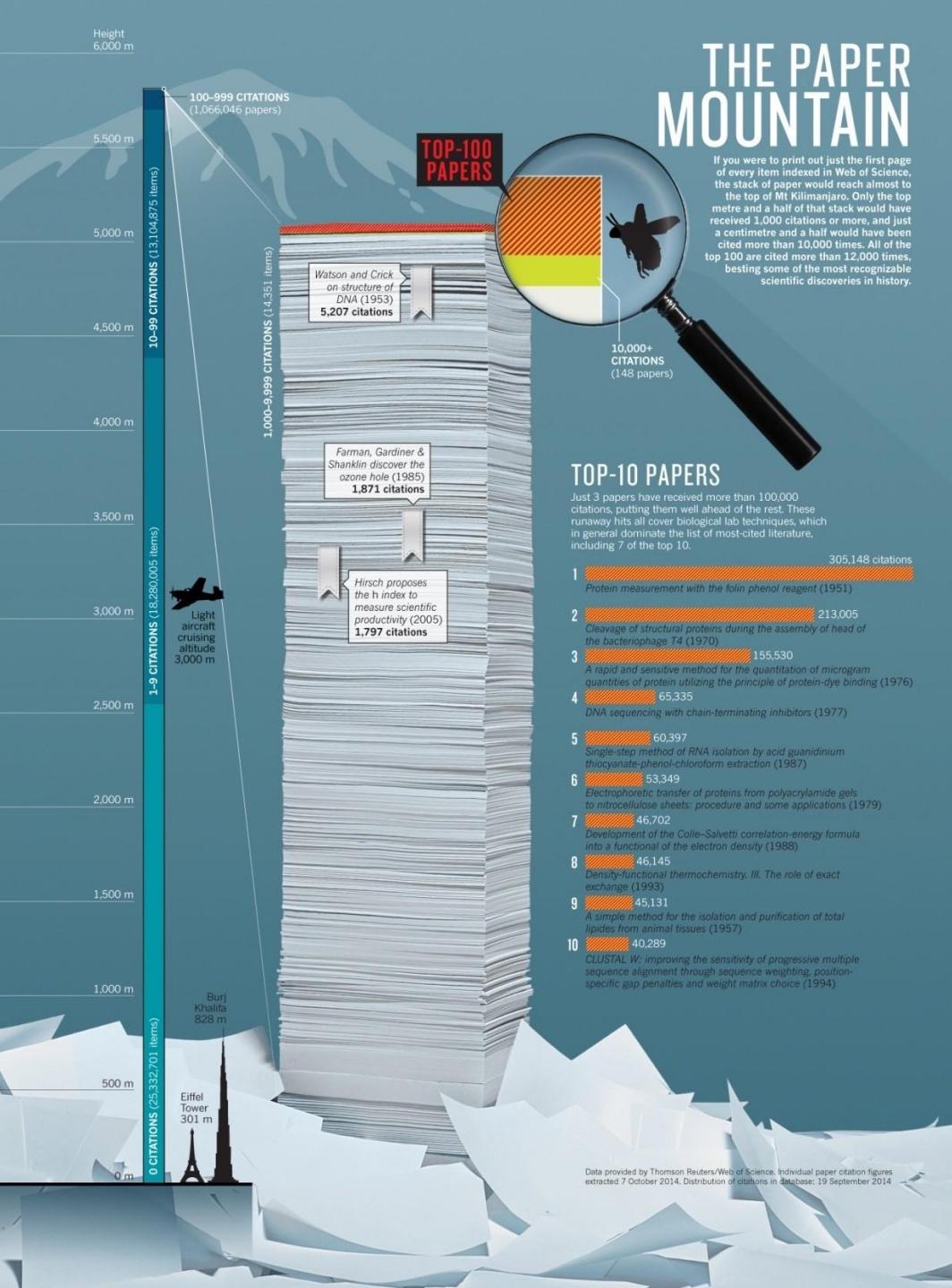


# Contents

- Short intro. to density-functional theory (DFT)
- How to run and use Quantum ESPRESSO (QE)
- Some applications for your motivations in research
- Challenges and future prospects

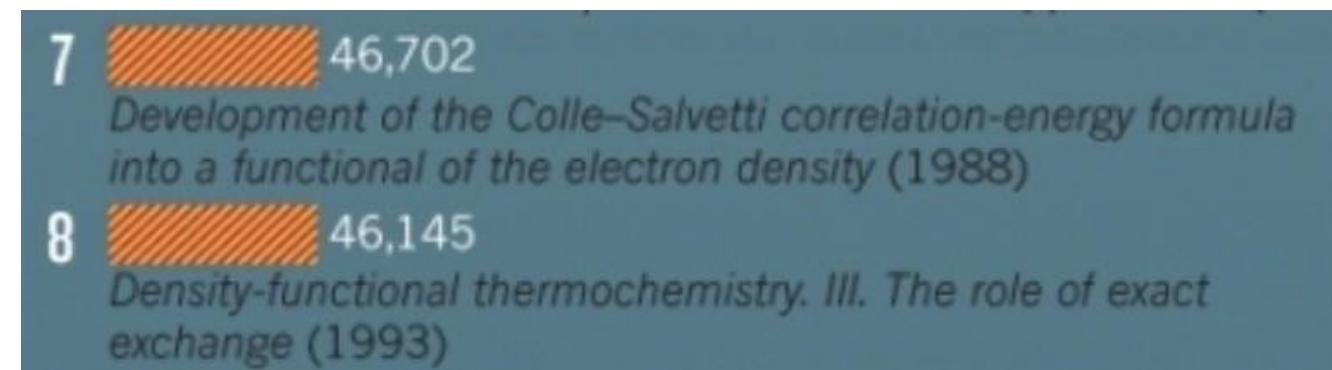
special thanks to N. T. Hung and R. Saito (Tohoku University) who together with ARTN developed a QE textbook and various QE workshops in Japan, Vietnam, and Indonesia





# Impact of DFT

**THE TOP 10 PAPERS:** 2 papers on density-functional theory (DFT) in the top 10 most cited papers in the entire scientific literature, ever. **NATURE, OCT 2014**



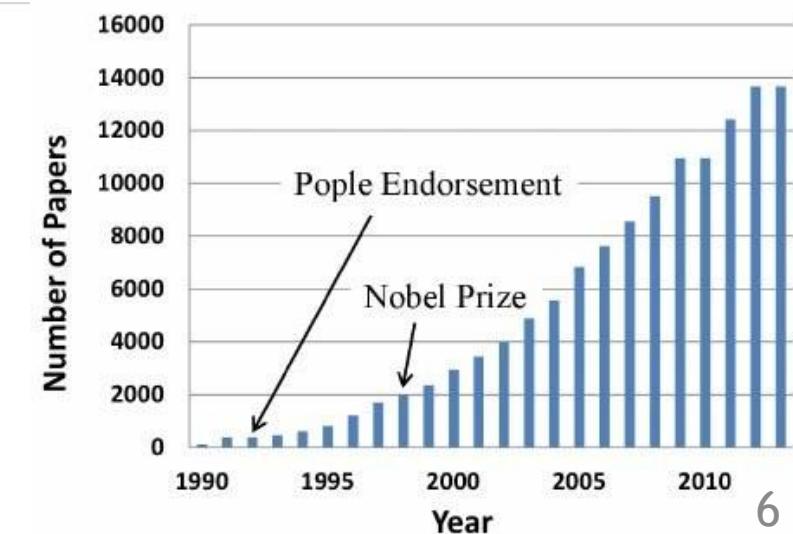
## The Nobel Prize in Chemistry 1998



Walter Kohn  
Prize share: 1/2



John A. Pople  
Prize share: 1/2



# MOST CITED PAPERS IN THE HISTORY OF APS

	Journal	# cites	Title	Author(s)
1	PRL (1996)	78085	Generalized Gradient Approximation Made Simple	Perdew, Burke, Ernzerhof
2	PRB (1988)	67303	Development of the Colle-Salvetti Correlation-Energy ...	Lee, Yang, Parr
3	PRB (1996)	41683	Efficient Iterative Schemes for Ab Initio Total-Energy ...	Kresse and Furthmuller
4	PR (1965)	36841	Self-Consistent Equations Including Exchange and Correlation ...	Kohn and Sham
5	PRA (1988)	36659	Density-Functional Exchange-Energy Approximation ...	Becke
6	PRB (1976)	31865	Special Points for Brillouin-Zone Integrations	Monkhorst and Pack
7	PRB (1999)	30940	From Ultrasoft Pseudopotentials to the Projector Augmented ...	Kresse and Joubert
8	PRB (1994)	30801	Projector Augmented-Wave Method	Blochl
9	PR (1964)	30563	Inhomogeneous Electron Gas	Hohenberg and Kohn
10	PRB (1993)	19903	Ab initio Molecular Dynamics for Liquid Metals	Kresse and Hafner
11	PRB (1992)	17286	Accurate and Simple Analytic Representation of the Electron ...	Perdew and Wang
12	PRB (1990)	15618	Soft Self-Consistent Pseudopotentials in a Generalized ...	Vanderbilt
13	PRB (1992)	15142	Atoms, Molecules, Solids, and Surfaces - Applications of the ...	Perdew, Chevary, ...
14	PRB (1981)	14673	Self-Interaction Correction to Density-Functional Approx. ...	Perdew and Zunger
15	PRB (1986)	13907	Density-Functional Approx. for the Correlation-Energy ...	Perdew
16	RMP (2009)	13513	The Electronic Properties of Graphene	Castro Neto et al.
17	PR (1934)	12353	Note on an Approximation Treatment for Many-Electron Systems	Moller and Plesset
18	PRB (1972)	11840	Optical Constants on Noble Metals	Johnson and Christy
19	PRB (1991)	11580	Efficient Pseudopotentials for Plane-Wave Calculations	Troullier and Martins
20	PRL (1980)	10784	Ground-State of the Electron-Gas by a Stochastic Method	Ceperley and Alder

Red colors are papers related to DFT

Apr 2019

Generalized Gradient Approximation Made Simple

John P. Perdew, Kieron Burke, and Matthias Ernzerhof  
Phys. Rev. Lett. **77**, 3865 – Published 28 October 1996; Erratum Phys. Rev. Lett. **78**, 1396 (1997)

Article	References	Citing Articles (130,981)	PDF	Export Citation
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Generalized Gradient Approximation (GGA)  
Improves accuracy of DFT

Self-Consistent Equations Including Exchange and Correlation Effects

W. Kohn and L. J. Sham  
Phys. Rev. **140**, A1133 – Published 15 November 1965

Physics

Article	References	Citing Articles (46,542)	PDF	Export Citation
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Kohn-Sham equation  
Numerical codes for DFT is possible

Inhomogeneous Electron Gas

P. Hohenberg and W. Kohn  
Phys. Rev. **136**, B864 – Published 9 November 1964

Physics

Article	References	Citing Articles (38,993)
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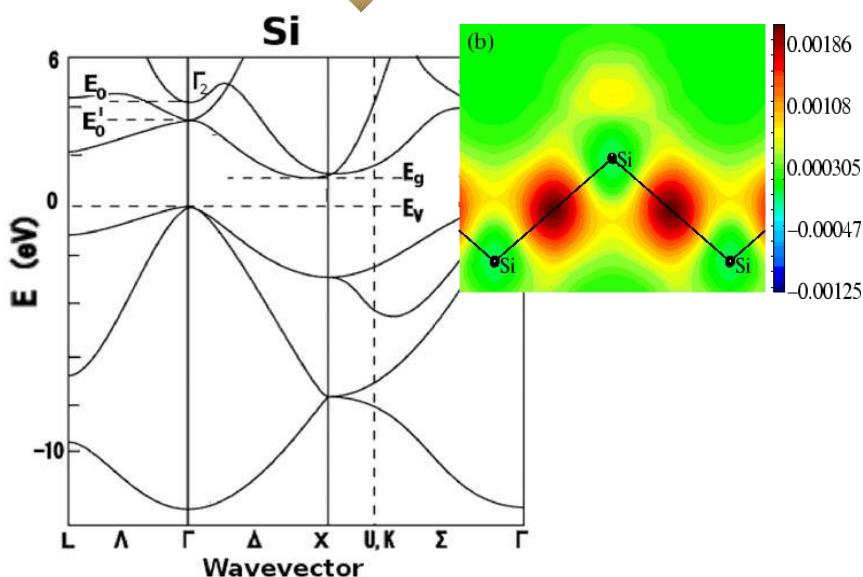
Hohenberg–Kohn theorems  
Starting point of the concepts of DFT

# What is DFT?

Simply saying:

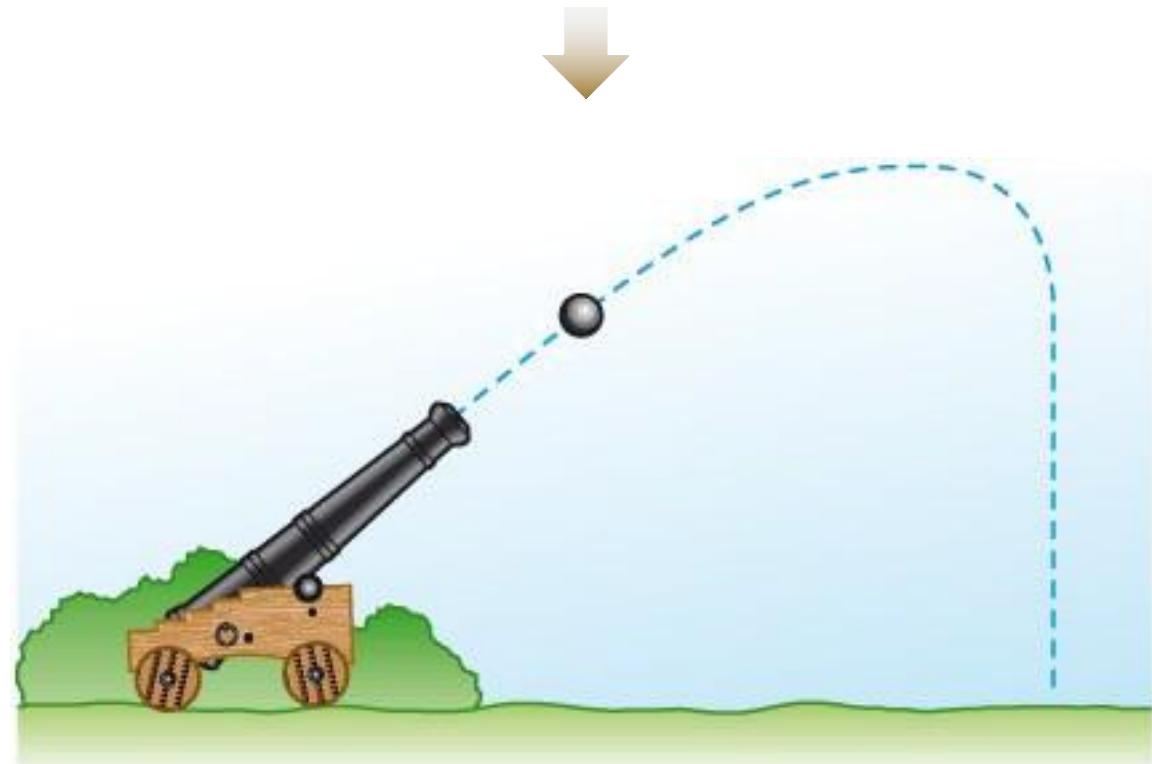
DFT is a method for solving the Schrödinger equation

$$\hat{\mathcal{H}}\Psi = E\Psi$$



The Newton equation

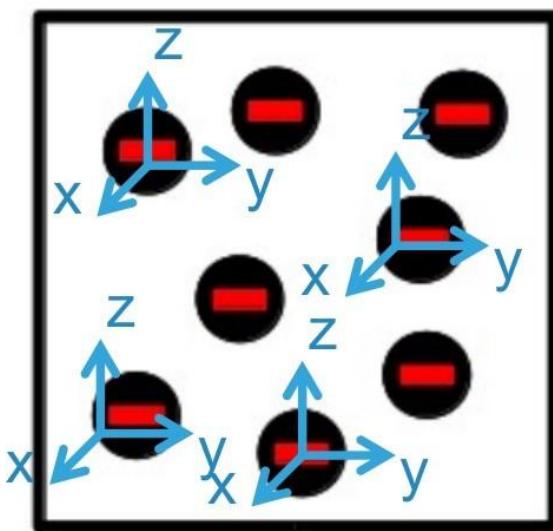
$$F = ma$$



# The Idea of DFT - Electron Density

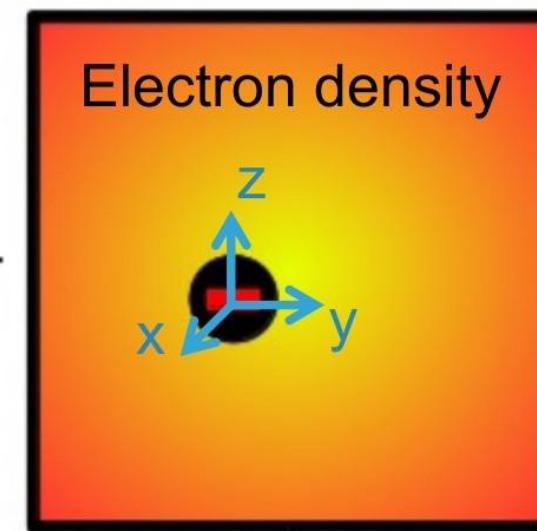


Just store data  
for Si case:  
 $\sim 5000^{84}$  numbers



3N-dimensional  
partial differential equation (PDE)

Reduction of dimensionality



3-dimensional PDE



$5000^3$  numbers



The idea can work when the two models are equivalent

# The Hohenberg-Kohn (H-K) Theorems

## The first H-K theorem

**Theorem:** There is a one-to-one correspondence between an external potential  $\mathcal{V}_{en}(\mathbf{r})$  and an electron density  $n(\mathbf{r})$  [Hohenberg and Kohn (1964)].

## The second H-K theorem

A universal functional for the energy  $E[n(r)]$  can be defined in terms of the density. The exact ground state is the global minimum value of this functional.

Inhomogeneous Electron Gas

P. Hohenberg and W. Kohn

Phys. Rev. **136**, B864 – Published 9 November 1964

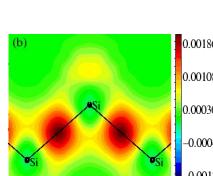


Article

References

Citing Articles (38,993)

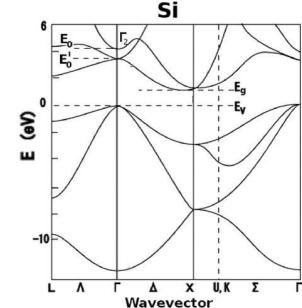
Density-functional theory



$n(r)$

Electron density

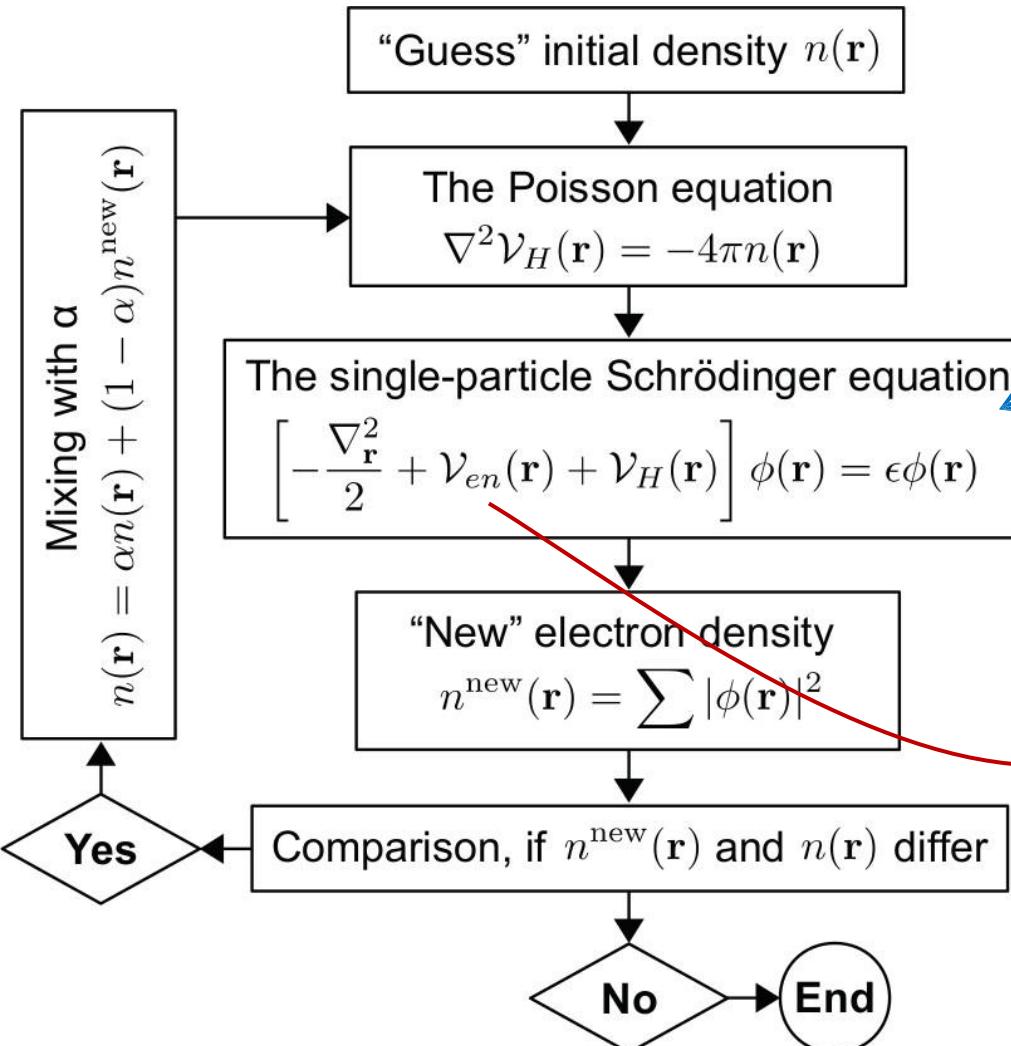
$E[n(r)]$



Materials Properties

# How to Know $n(r)$ ?

## Self-consistent field (SCF) method



Self-Consistent Equations Including Exchange and Correlation Effects

W. Kohn and L. J. Sham  
Phys. Rev. **140**, A1133 – Published 15 November 1965

Physics

Article

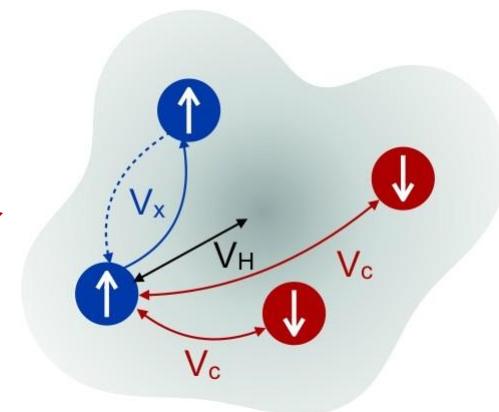
References

Citing Articles (46,542)

PDF

Export Citation

## The Kohn-Sham equation



The Pauli principle  
to avoid overlap  
(exchange -  $V_x$ )

Keeping to lower the  
Coulomb repulsion  
(correlation -  $V_c$ )

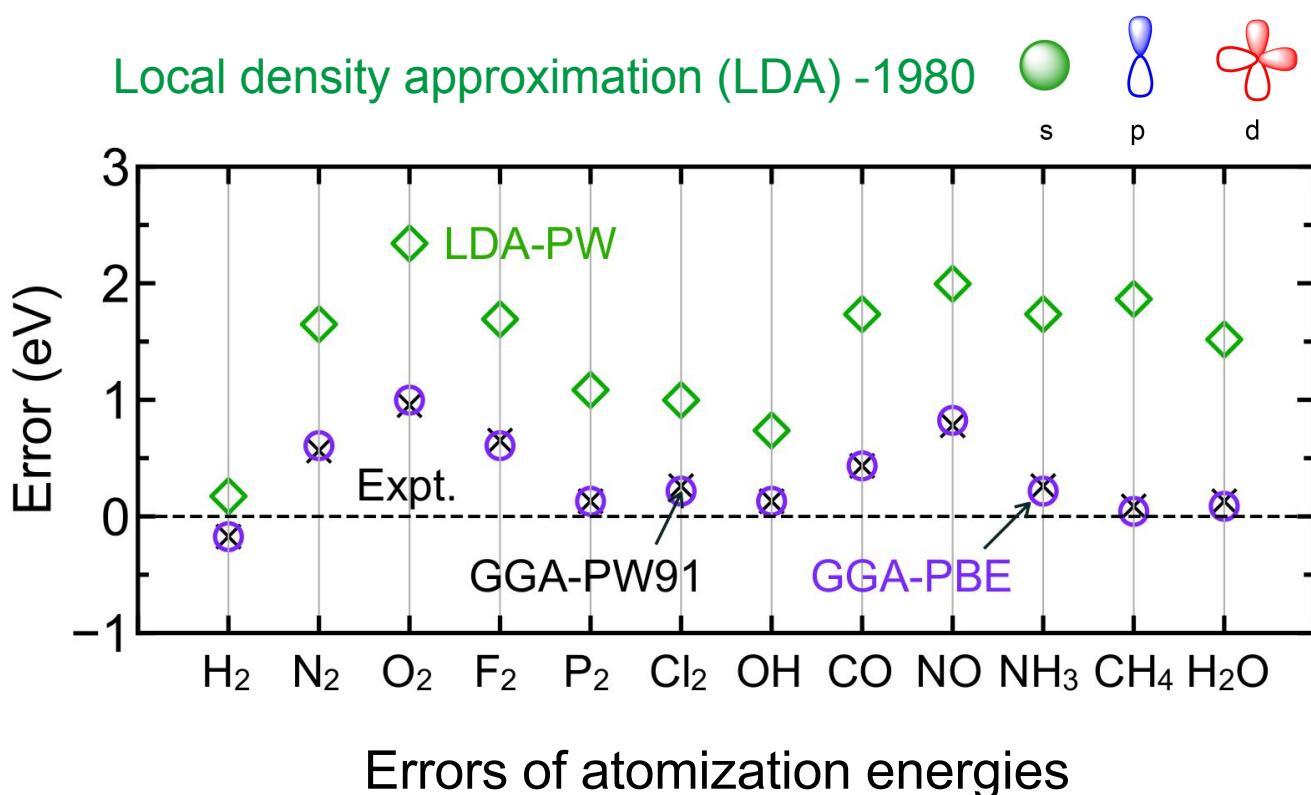
Exchange-correlation potential  
(Unknown functional)

# How to Deal with Unknown Functional?

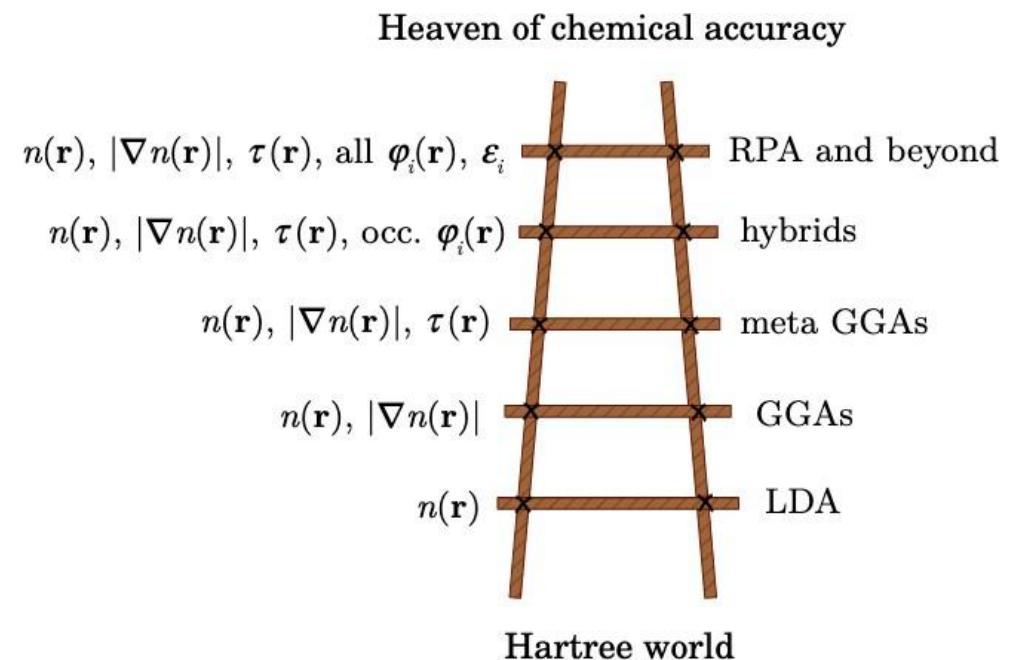
Generalized Gradient Approximation Made Simple

John P. Perdew, Kieron Burke, and Matthias Ernzerhof

Phys. Rev. Lett. **77**, 3865 – Published 28 October 1996; Erratum Phys. Rev. Lett. **78**, 1396 (1997)



It takes 30 years to introduce a good approximation functional



# Which Codes for DFT?

Trends in atomistic simulation engines

Citation Data 2022							
Code	Methods	Tags	Installation	Cost	Source	Citations ↓	Trend
Gaussian	WFM DFT	PBC AE GTO PP	Source Binary	\$	🔒	14700	↗
VASP	DFT WFM	PBC PAW PP PW	Source	\$	🔒	13100	↗
Quantum ESPRESSO (QE)	DFT S	PBC PP PW	Source NGC conda DNF Macports APT SingularityHub AUR Nix Spack EasyBuild Yum	⚡	🔓	3380	↗
CASTEP	DFT WFM	PBC PAW PP PW	Source Binary	⚡🎓	🔒	2820	↗
ORCA	WFM DFT	AE GTO PP	Binary	⚡🎓	🔒	2570	↗
WIEN2k	DFT WFM	PBC AE LAPW	Source	\$	🔓	1460	↗
Discovery Studio	FF DFT	Binary	\$	🔒		1220	↗

<https://atomistic.software/>

Chemical Sciences and Materials @ 2022 (PRACE)

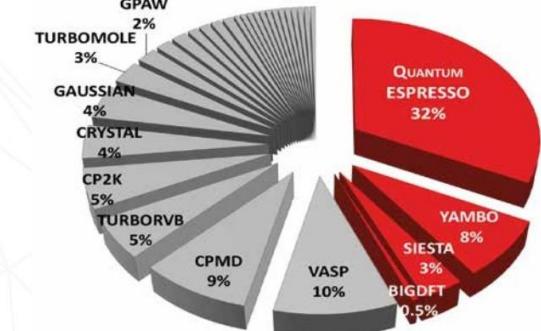
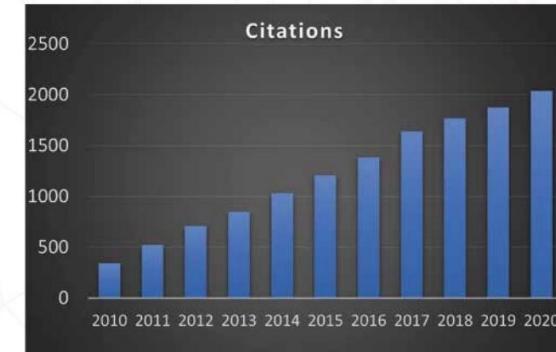


Fig1a

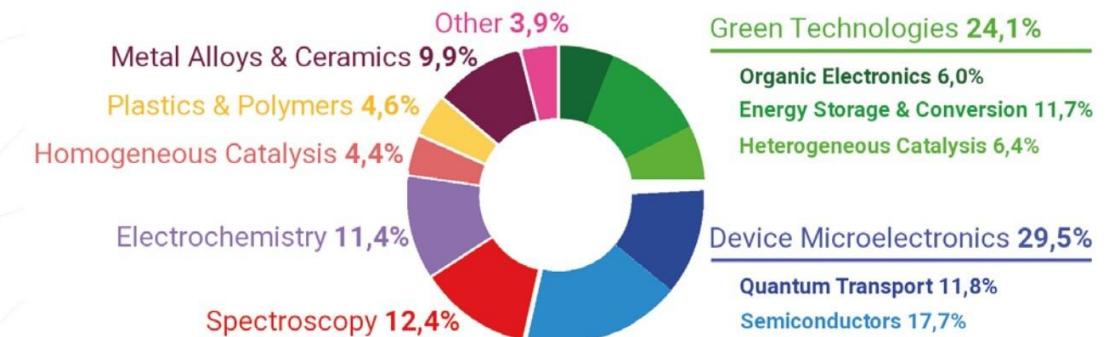


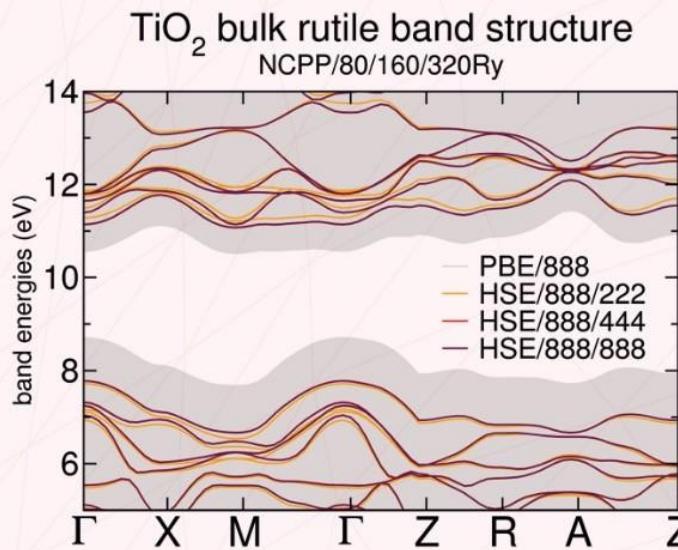
Fig1b

# Some Features of QE

Quantum ESPRESSO is a bundle of codes for DFT and beyond DFT

## PWSCF:

- ◆ Solution of Kohn-Sham equations with different methods
- ◆ Energies, forces, stress of molecules and materials
- ◆ Born-Oppenheimer molecular dynamics
- ◆ Band structures (e.g. Fig2a) and DOS
- ◆ Magnetic properties



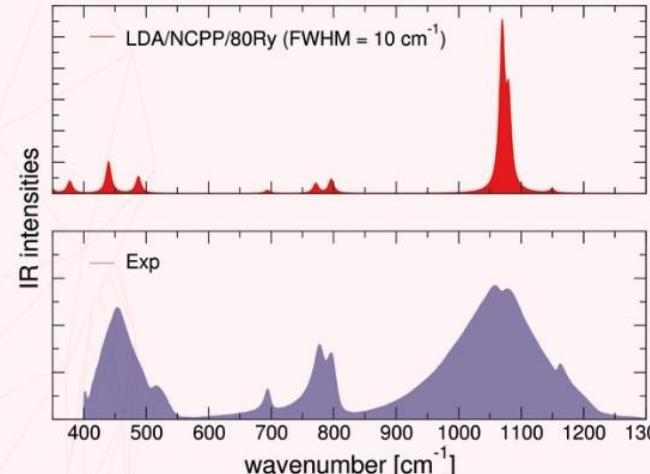
## CP:

- ◆ Car-Parrinello molecular dynamics
- ◆ Phonon frequencies
- ◆ IR and Raman spectra (e.g. Fig2b, Fig2c)
- ◆ Dielectric properties

## Phonon:

- ◆ Phonon frequencies
- ◆ IR and Raman spectra (e.g. Fig2b, Fig2c)
- ◆ Dielectric properties

## Quartz IR spectrum



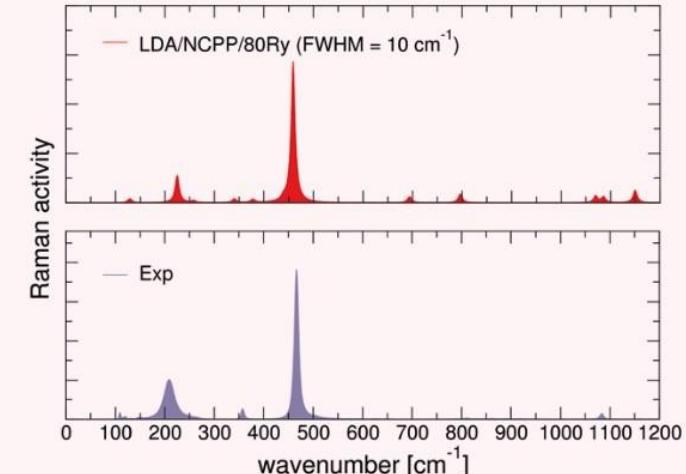
## TDDFPT:

- ◆ UV-Vis absorption
- ◆ Electron energy loss spectroscopy
- ◆ Spin wave spectroscopy

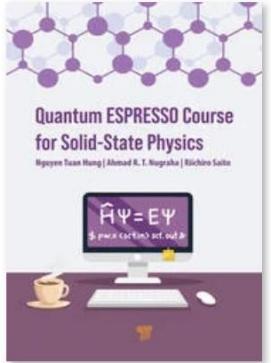
## NEB:

- ◆ Reaction paths

## Quartz Raman spectrum



# Recommended way to learn QE



Book

## Quantum ESPRESSO Course for Solid-State Physics

By Nguyen Tuan Hung, Ahmad R.T. Nugraha, Riichiro Saito

Edition 1st Edition

First Published 2022

eBook Published 29 December 2022

Pub. Location New York

Imprint Jenny Stanford Publishing

DOI <https://doi.org/10.1201/9781003290964>

Pages 372

eBook ISBN 9781003290964

Subjects Engineering & Technology, Mathematics & Statistics, Physical Sciences



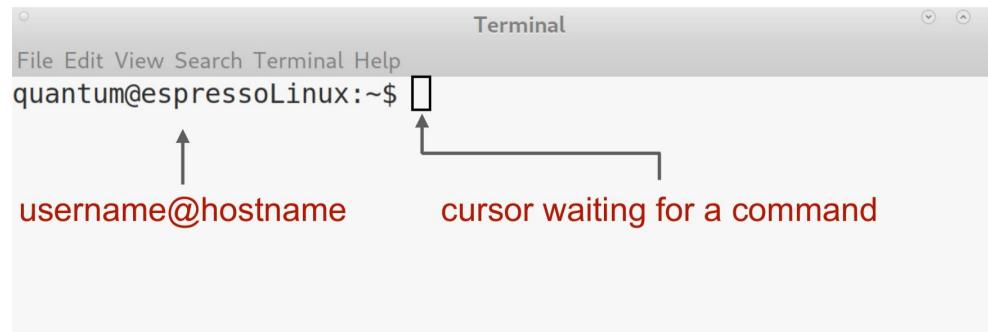
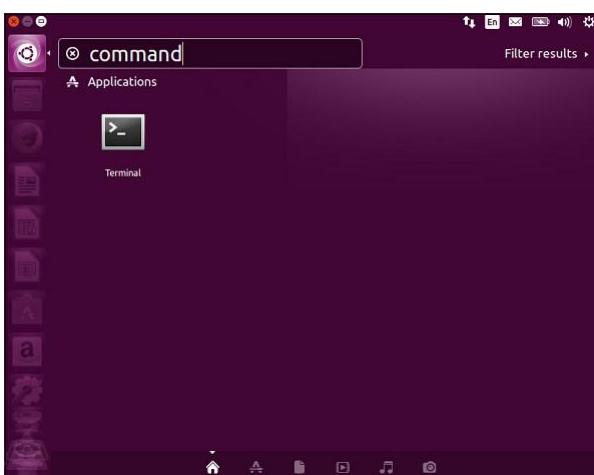
Unpublished, preprint  
version for Chap. 3

<https://bit.ly/QE-anmsqm2024>

Scripts/codes ready to run: <https://github.com/nguyen-group/QE-SSP>

Alternative fork/clone: <git clone https://github.com/artnugraha/QE-SSP.git>

# How to Install QE



## Quick installation of QE:

Step 1: Update system:

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

Step 2: Install quantum-espresso

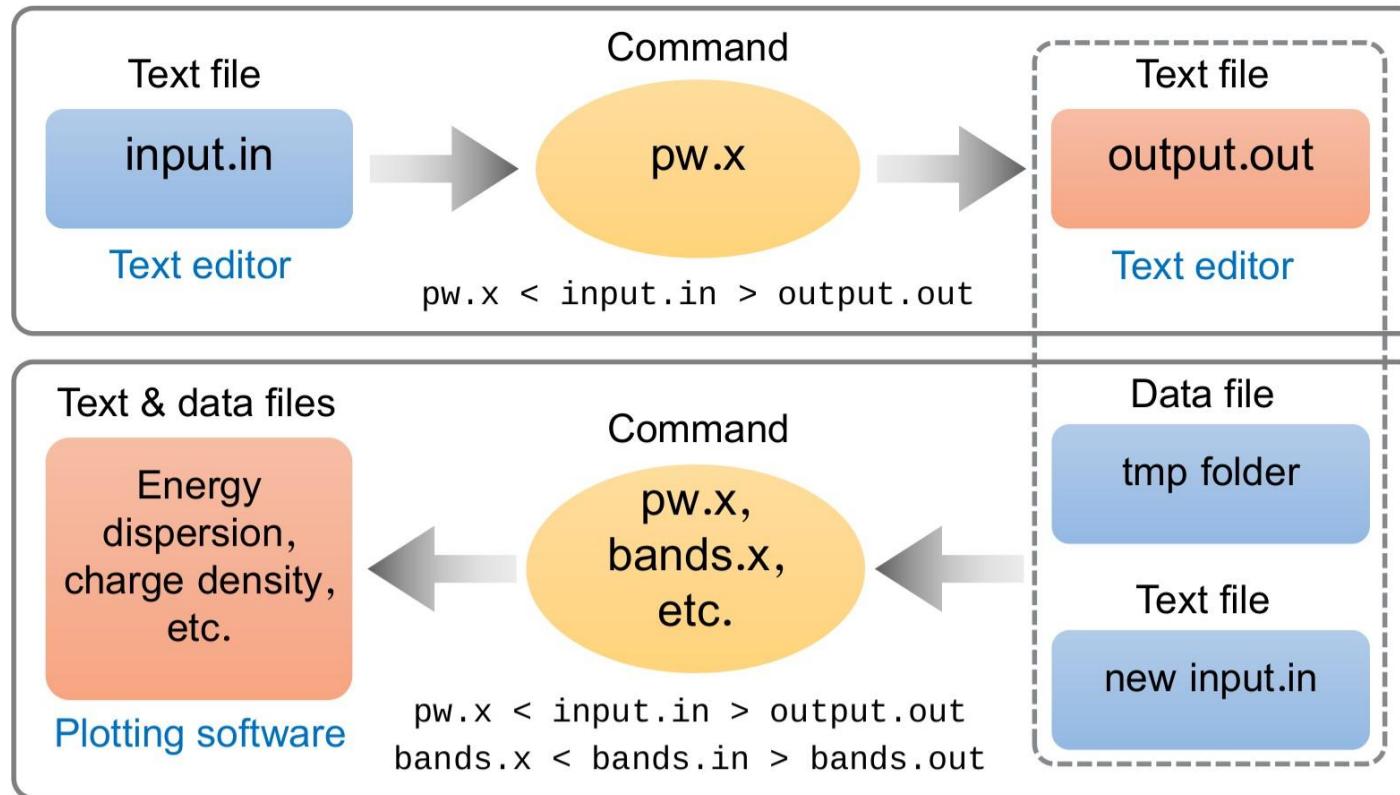
```
$ sudo apt install quantum-espresso
```

Step 3: Install some useful tools

```
$ sudo apt install python3-dev python3-numpy python3-matplotlib  
$ sudo apt install jupyter gnuplot xcrysden git
```

You can also install in MacOS or Windows

# QE Basic Workflow



## Some most important commands: in QE

Command	Purpose
pw.x	SCF and NSCF calculations
bands.x	band structure post-processing
dos.x	DOS postprocessing
epsilon.x	optical properties calculation
ph.x	phonon calculation

Download input files for examples

\$ git clone <https://github.com/artrnugraha/QE-SSP.git>

# Let's Do An Example without Knowing Everything

## SCF calculation only:

Go to folder of the example

```
$ cd ~/QE-SSP/gr/scf/
```

Run the example

```
$ pw.x < scf.in > 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

## Energy dispersion (SCF - NSCF - bands):

Go to folder of the example

```
$ cd ~/QE-SSP/gr/bands/
```

Run the example

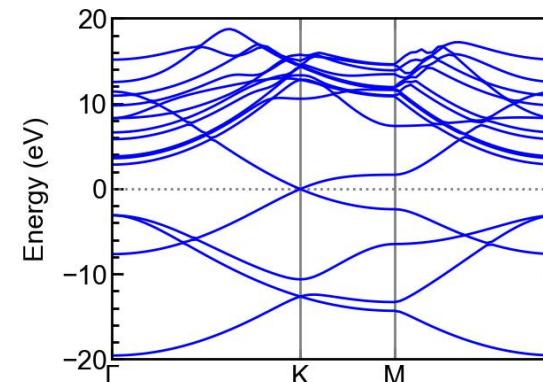
```
$ pw.x < scf.in > scf.out
```

```
$ pw.x < nscf.in > nscf.out
```

```
$ bands.x < bands.in > bands.out
```

Plot gr.bands.gnu

```
$ jupyter notebook plot-bands.ipynb
```



## 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
```

Generalized gradient approximation (GGA)

output data  
(charge density, etc.)

name of project

The screenshot shows a web browser window with the URL [pseudopotentials.quantum-espresso.org/legacy\\_tables/ps-library/c](https://pseudopotentials.quantum-espresso.org/legacy_tables/ps-library/c). The page title is "Pseudo search results - QUANTUM ESPRESSO". The main content area displays search results for pseudopotential files. The first result is "C.pbe-n-kjpaw\_psl.1.0.0.UPF", which is described as an UPF file from the PS Library by ADC, generated using the "atomic" code by A. Dal Corso v.6.3. It is a PAW type pseudopotential for Carbon (C) using the PBE functional, with Non Linear Core Correction and Scalar relativistic options. The second result is another "C.pbe-n-kjpaw\_psl.1.0.0.UPF" entry, also from the PS Library by ADC, generated using the "atomic" code by A. Dal Corso v.6.3MaX.

Pseudopotential File

C.pbe-n-kjpaw\_psl.1.0.0.UPF

Origin: PS Library

Author: ADC

Generated using "atomic" code by A. Dal Corso v.6.3

Pseudopotential type: PAW

Functional type: PBE

Non Linear Core Correction

Scalar relativistic

C.pbe-n-kjpaw\_psl.1.0.0.UPF

Origin: PS Library

Author: ADC

Generated using "atomic" code by A. Dal Corso v.6.3MaX

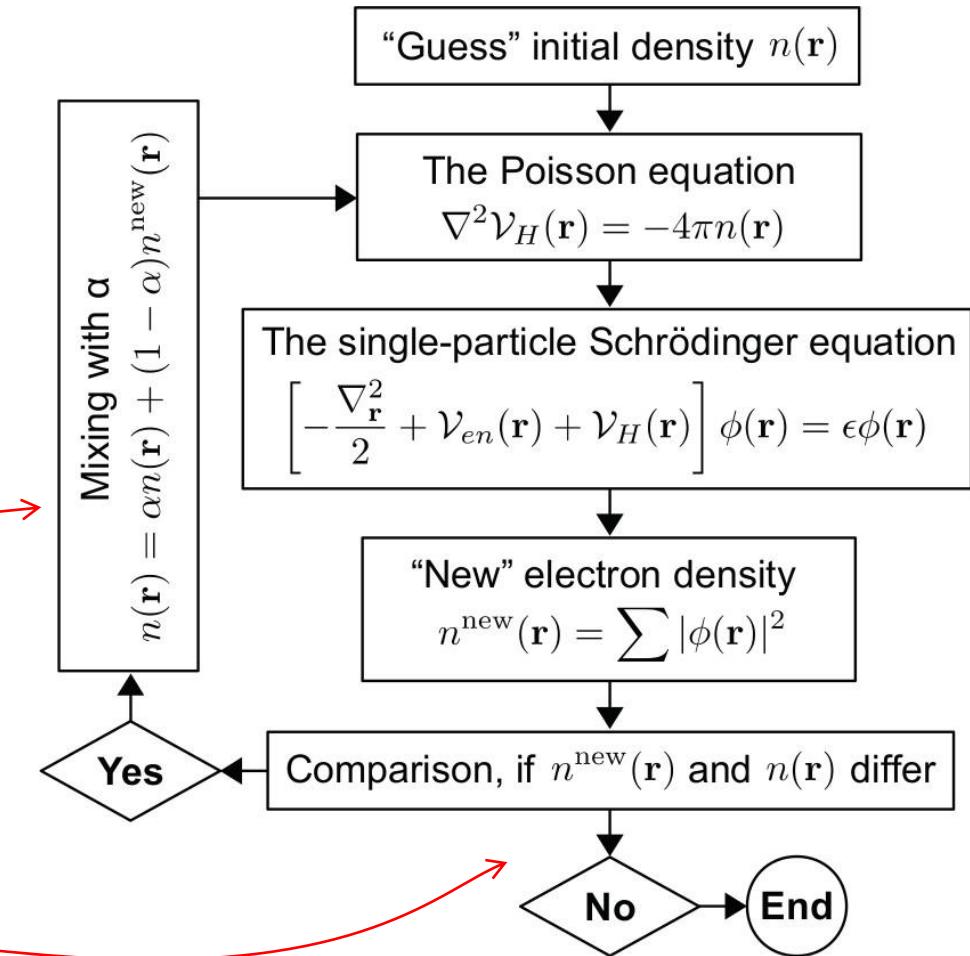
## QE-SSP/gr/scf/scf.in

```

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

```

## Self-consistent field method



## 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
```

Generalized gradient approximation (GGA)

output data  
(charge density, etc.)

name of project

The screenshot shows a web browser window with the URL [pseudopotentials.quantum-espresso.org/legacy\\_tables/ps-library/c](https://pseudopotentials.quantum-espresso.org/legacy_tables/ps-library/c). The page title is "Pseudo search results - QUANTUM ESPRESSO". The main content area displays two entries for pseudopotential files:

Pseudopotential File
C.pbe-n-kjpaw_psl.1.0.0.UPF
Origin: PS Library
Author: ADC
Generated using "atomic" code by A. Dal Corso v.6.3
Pseudopotential type: PAW
Functional type: PBE
Non Linear Core Correction
Scalar relativistic
C.pbe-n-rrkjus_psl.1.0.0.UPF
Origin: PS Library
Author: ADC
Generated using "atomic" code by A. Dal Corso v.6.3MaX

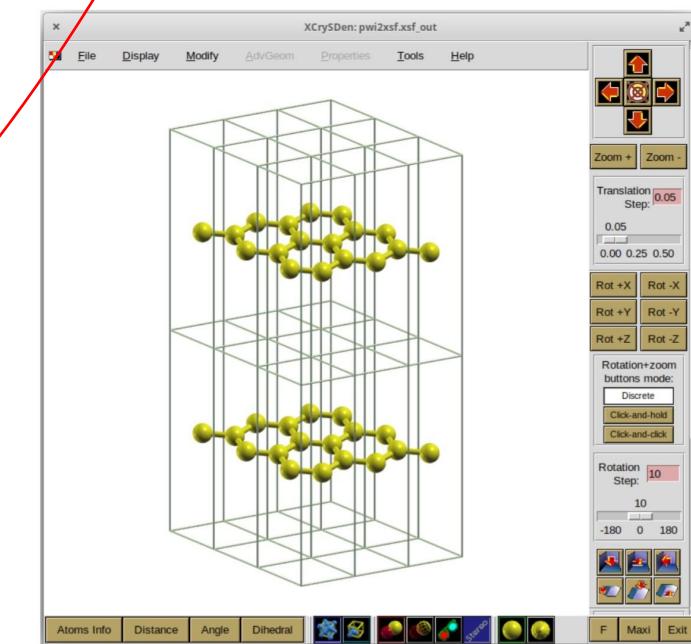
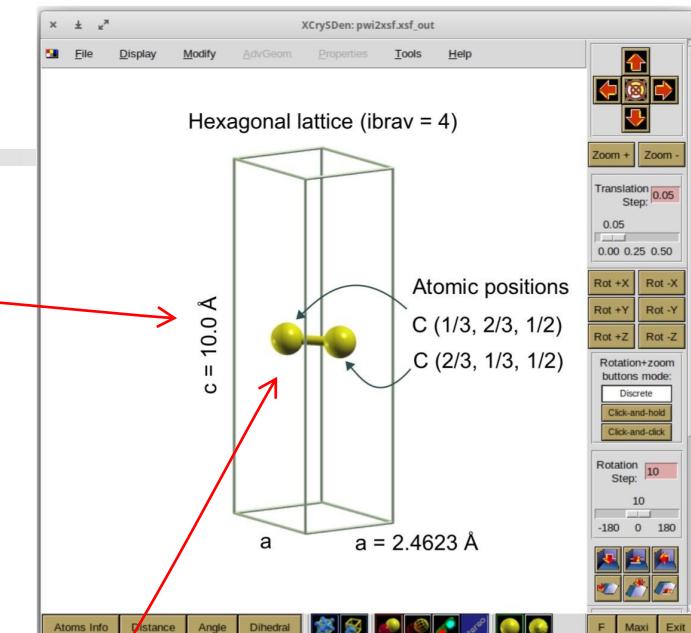
## QE-SSP/gr/scf/scf.in

```

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

```

atomic structure of  
graphene



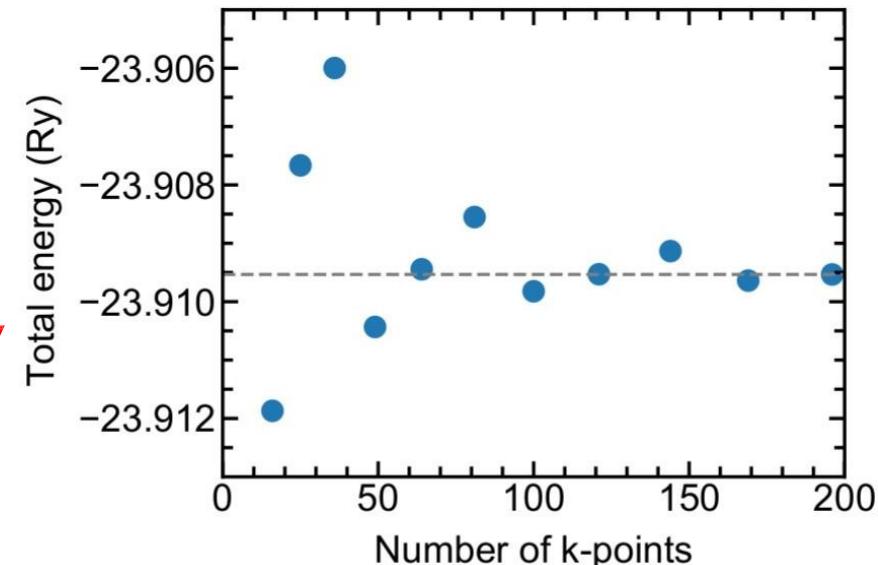
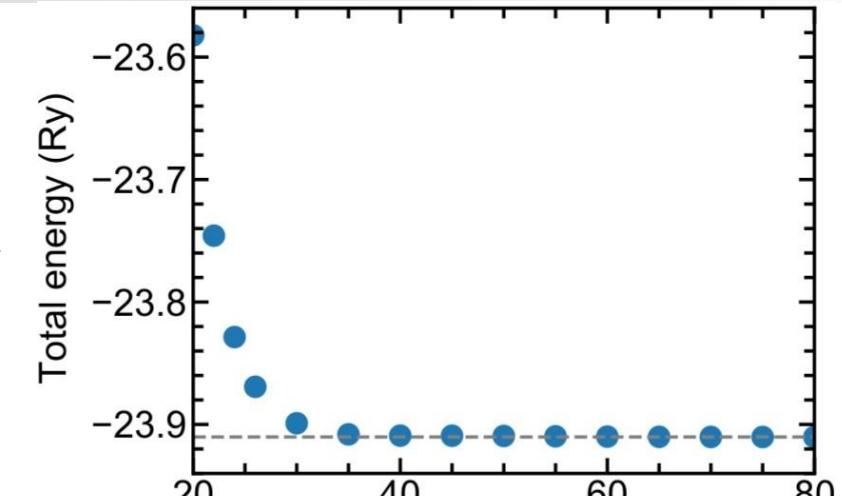
```

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

```

We need to test!!!

## Convergence test



# Intermezzo: You can ask ChatGPT (but some codes might be wrong)

TU

Can you write a Quantum ESPRESSO code for calculating the total energy of graphene?



Certainly! Here's an example of a Quantum ESPRESSO input file for calculating the total energy of graphene:

```
java
&control
  calculation = 'scf'
  prefix = 'graphene_energy'
  pseudo_dir = '/path/to/pseudopotentials'
 outdir = './tmp'
/
&system
  ibrav = 4
  celldm(1) = 2.462
  nat = 2
  ntyp = 1
  ecutwfc = 40
/
&electrons
/
ATOMIC_SPECIES
  C 12.011 C.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS {angstrom}
  C 0.000000 0.000000 0.000000
  C 1.230986 0.711000 0.000000
K_POINTS automatic
  10 10 1 0 0 0
```

TU

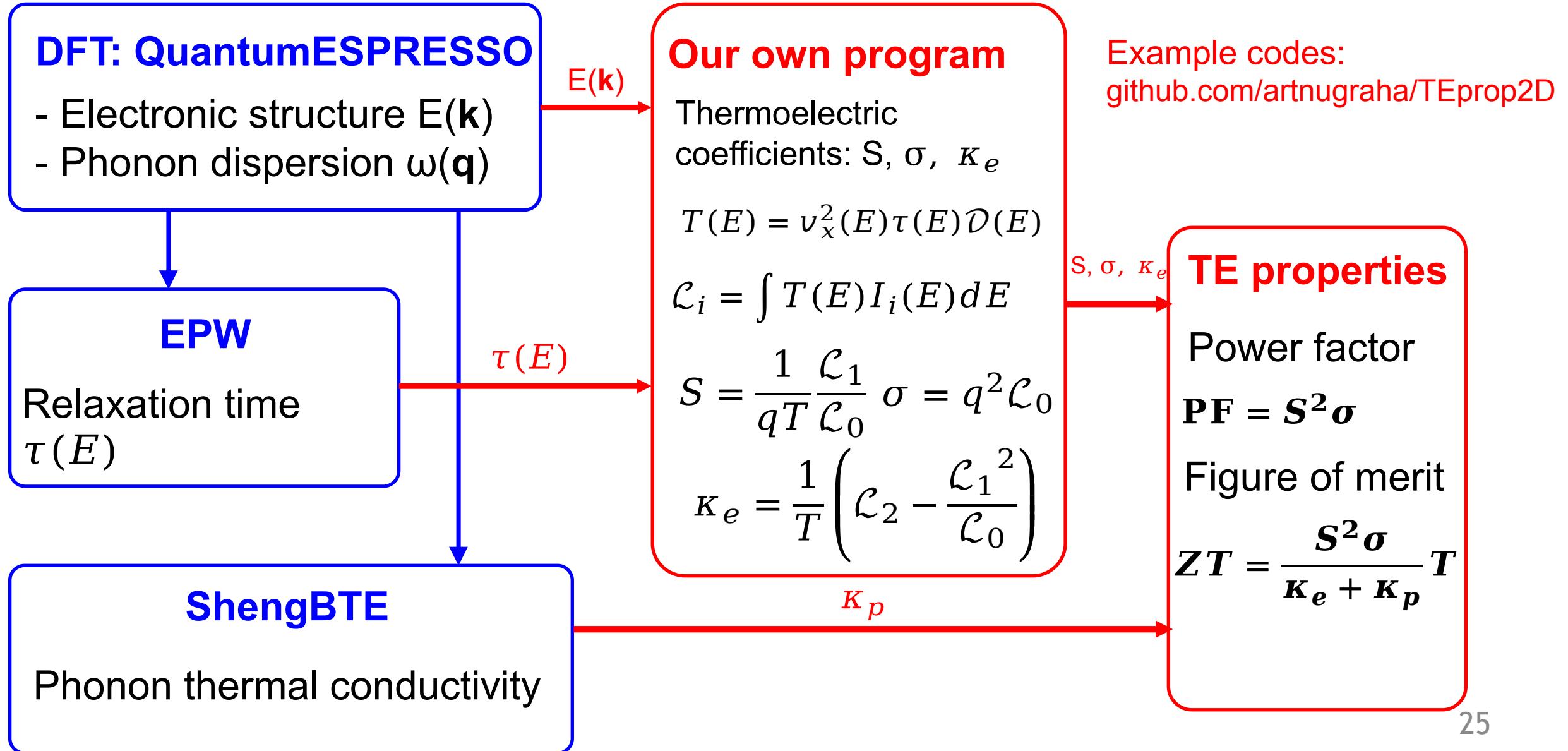
Can you write a Quantum ESPRESSO code for calculating the phonon of graphene?



Certainly! Here's an example of a Quantum ESPRESSO input file for calculating the phonon dispersion of graphene:

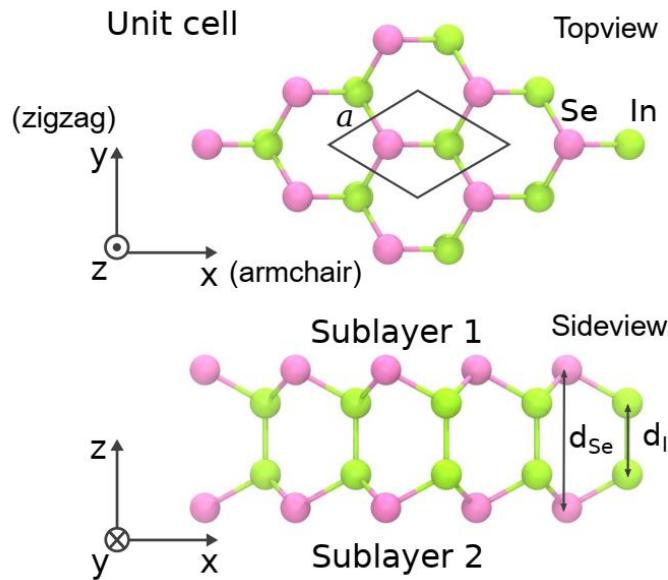
```
java
&inputph
  prefix = 'graphene_phonon'
  tr2_ph = 1.0e-14
  fildyn = 'graphene.dyn'
  amass(1) = 12.011
  outdir = './tmp'
/
&input
  asr = 'simple'
  fildyn = 'graphene.dyn'
  nat = 2
  ntyp = 1
  ecutwfc = 40
/
CELL_PARAMETERS {angstrom}
  2.462000 0.000000 0.000000
  0.000000 2.462000 0.000000
  0.000000 0.000000 20.0
ATOMIC_SPECIES
  C 12.011 C.pbe-n-kjpaw_psl.1.0.0.UPF
ATOMIC_POSITIONS {angstrom}
  C 0.000000 0.000000 0.000000
  C 1.230986 0.711000 0.000000
K_POINTS {automatic}
  12 12 1 0 0 0
```

# Applications: Thermoelectrics Simulation

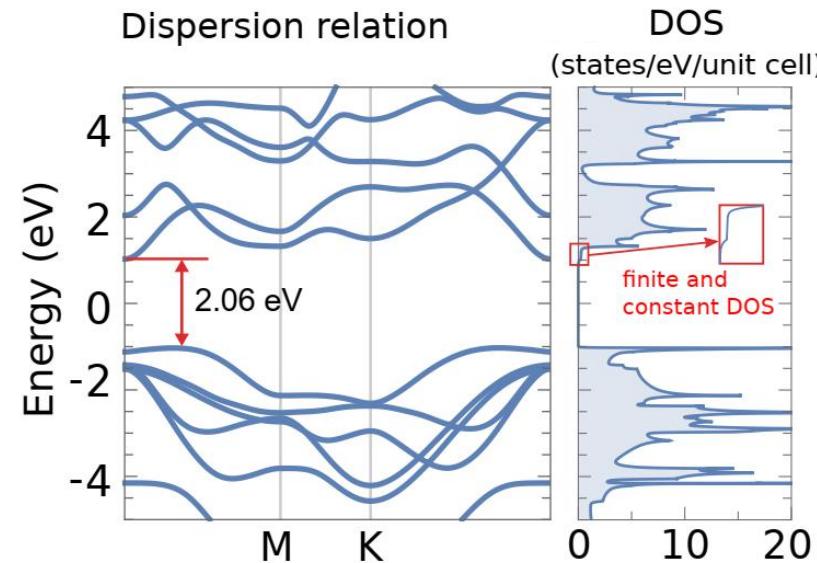


# Applications: Thermoelectrics of monolayer InSe

Hung, Nugraha, Saito, Appl. Phys. Lett. 111, 092107 (2017)

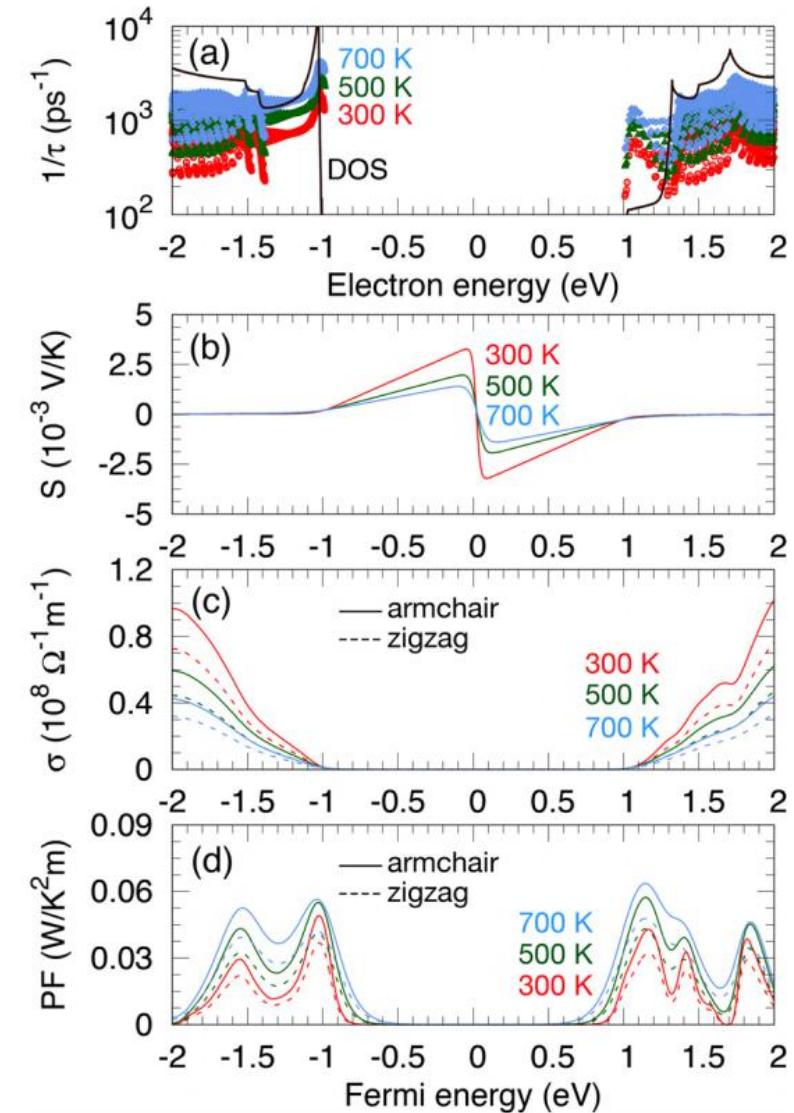


$\text{PF} \sim 10 \times \text{PF}$  (bulk  $\text{Bi}_2\text{Te}_3$ )  
 $\text{ZT} \sim 0.1\text{-}0.2$

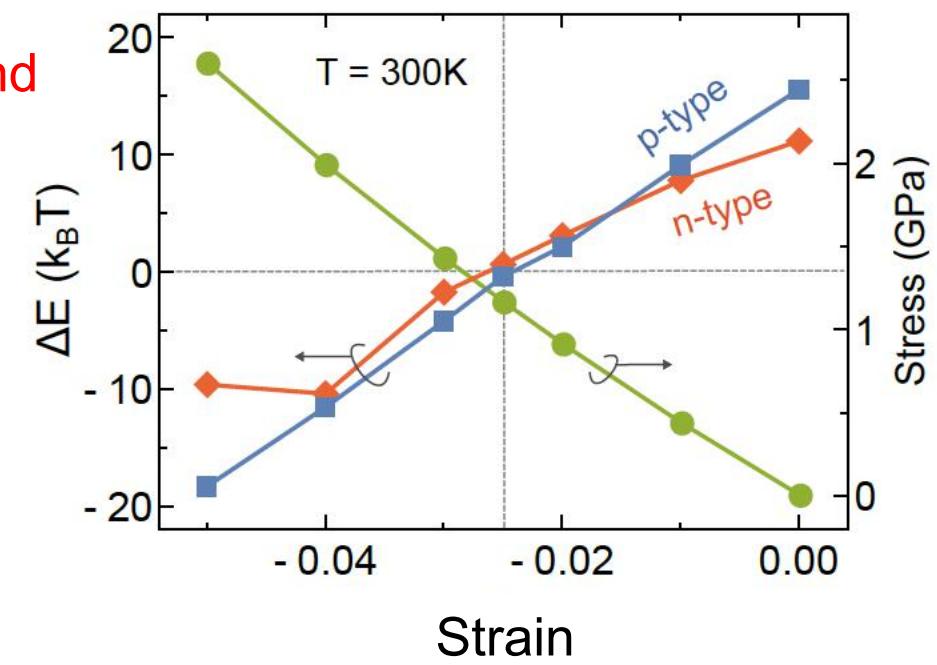
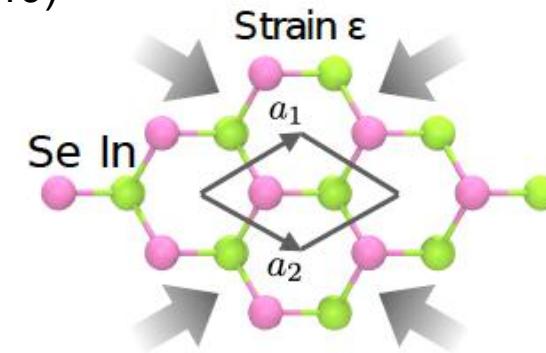
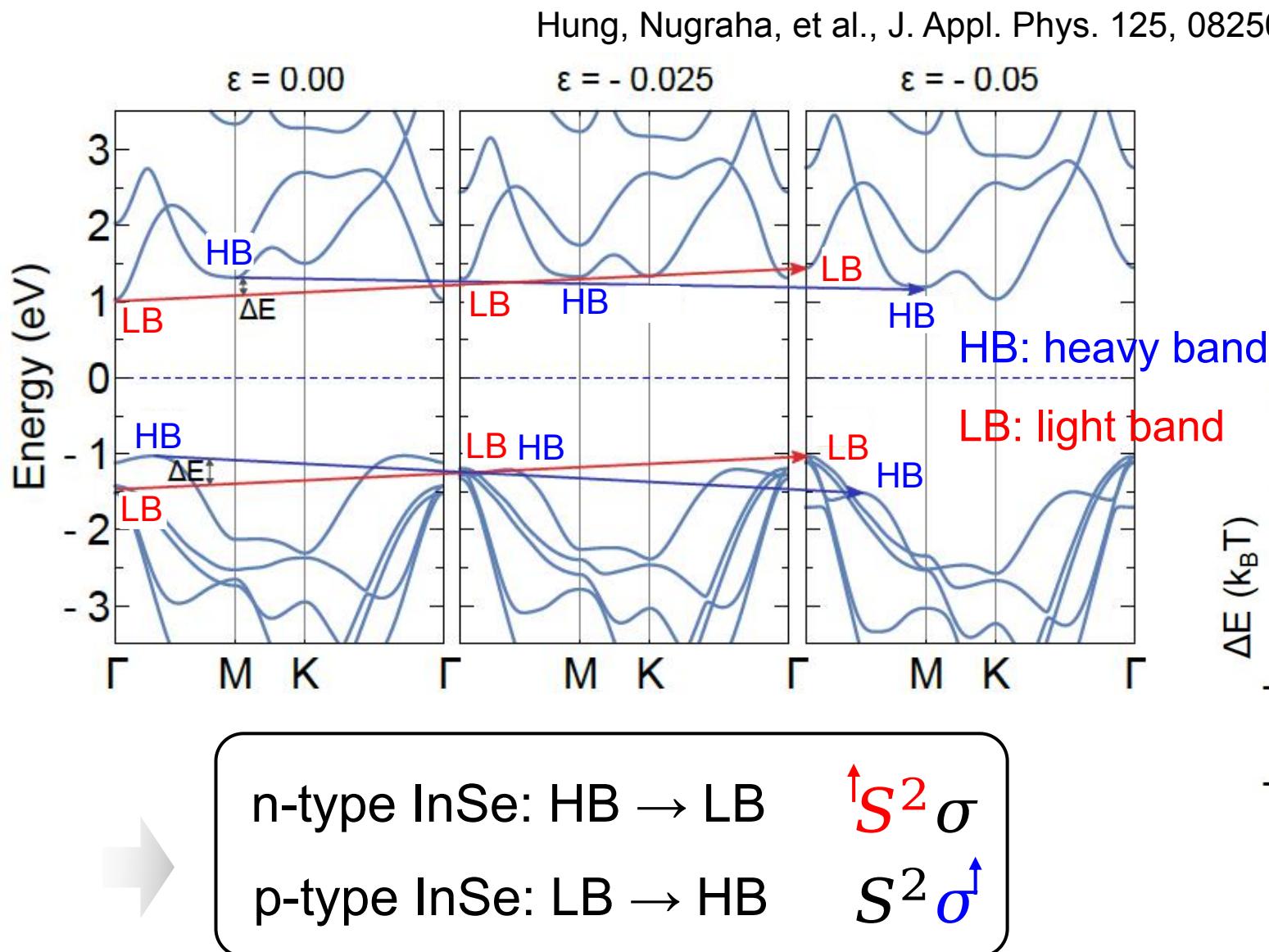


Anisotropic TE properties  
TE armchair > TE zigzag

- Both n-type and p-type InSe have good PF
- ZT improvement is still needed

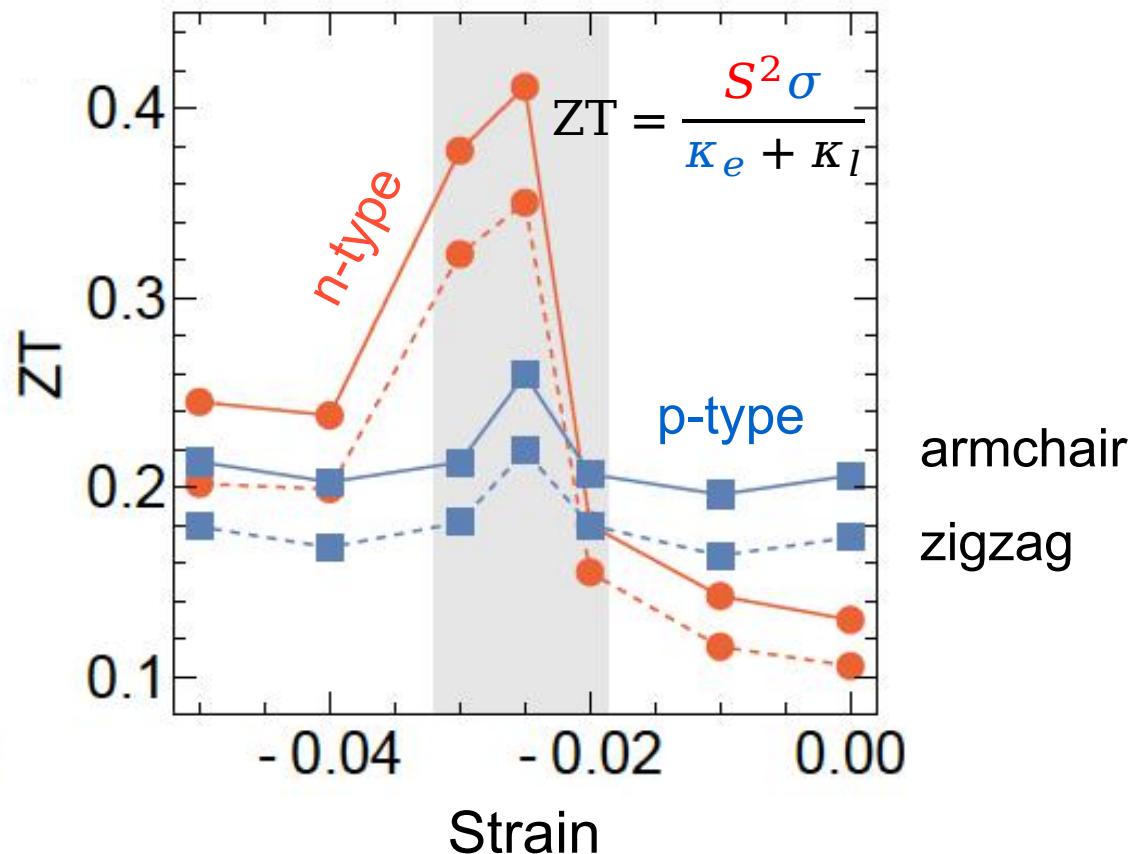
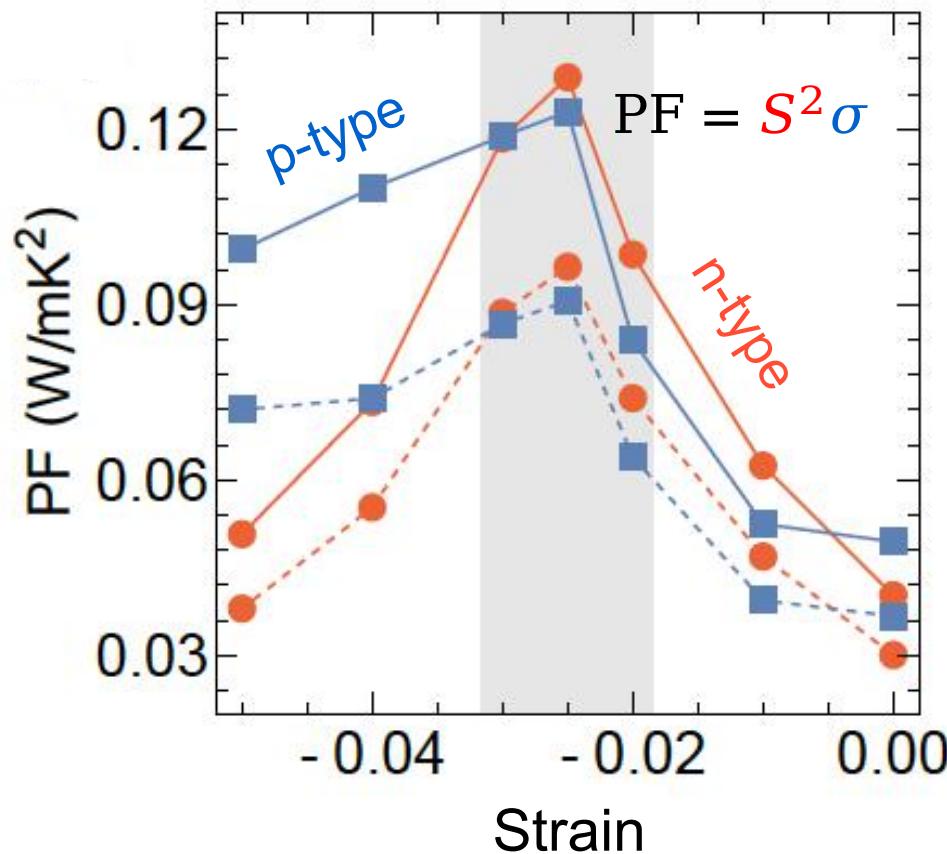


# Applications: Band Convergence for Thermoelectrics



# Applications: Band Convergence for Thermoelectrics

Hung, Nugraha, et al., J. Appl. Phys. 125, 082502 (2019)

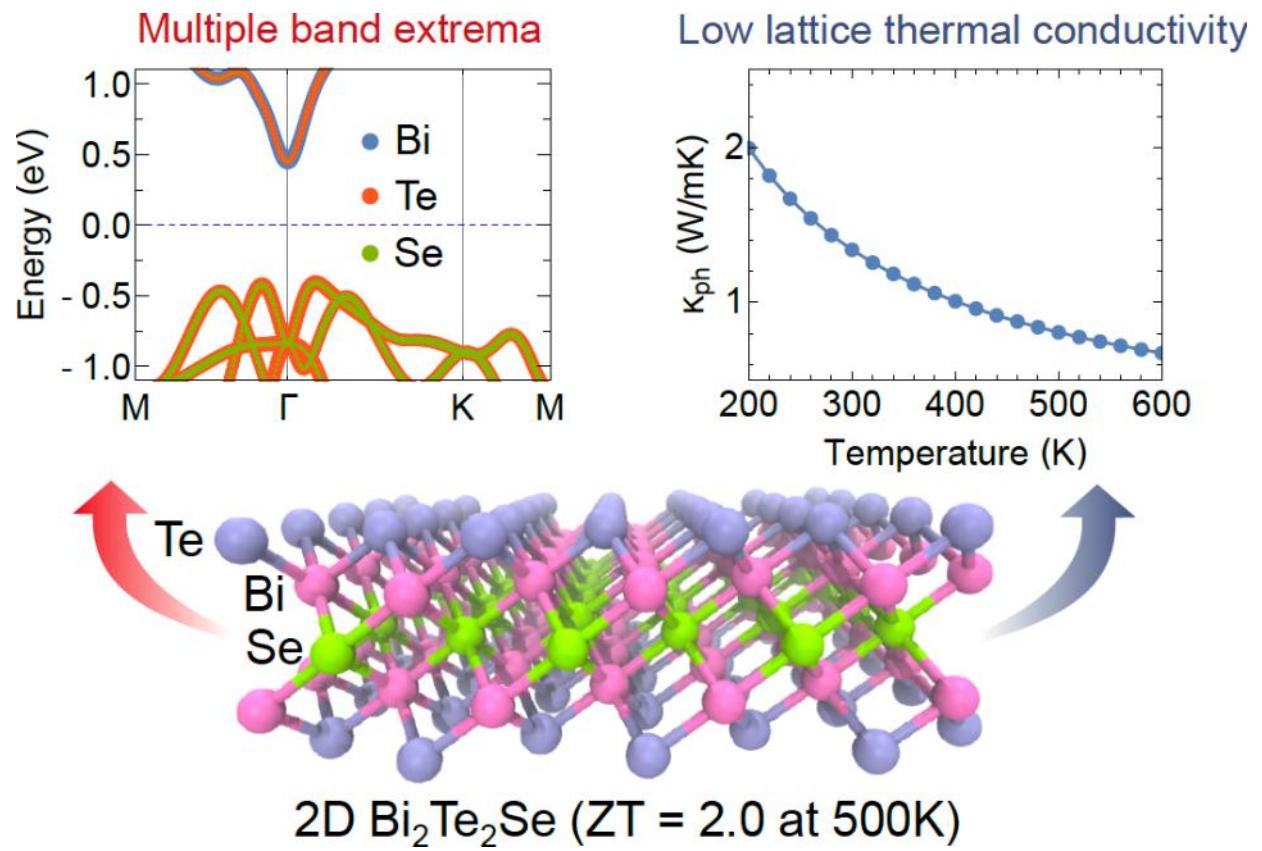
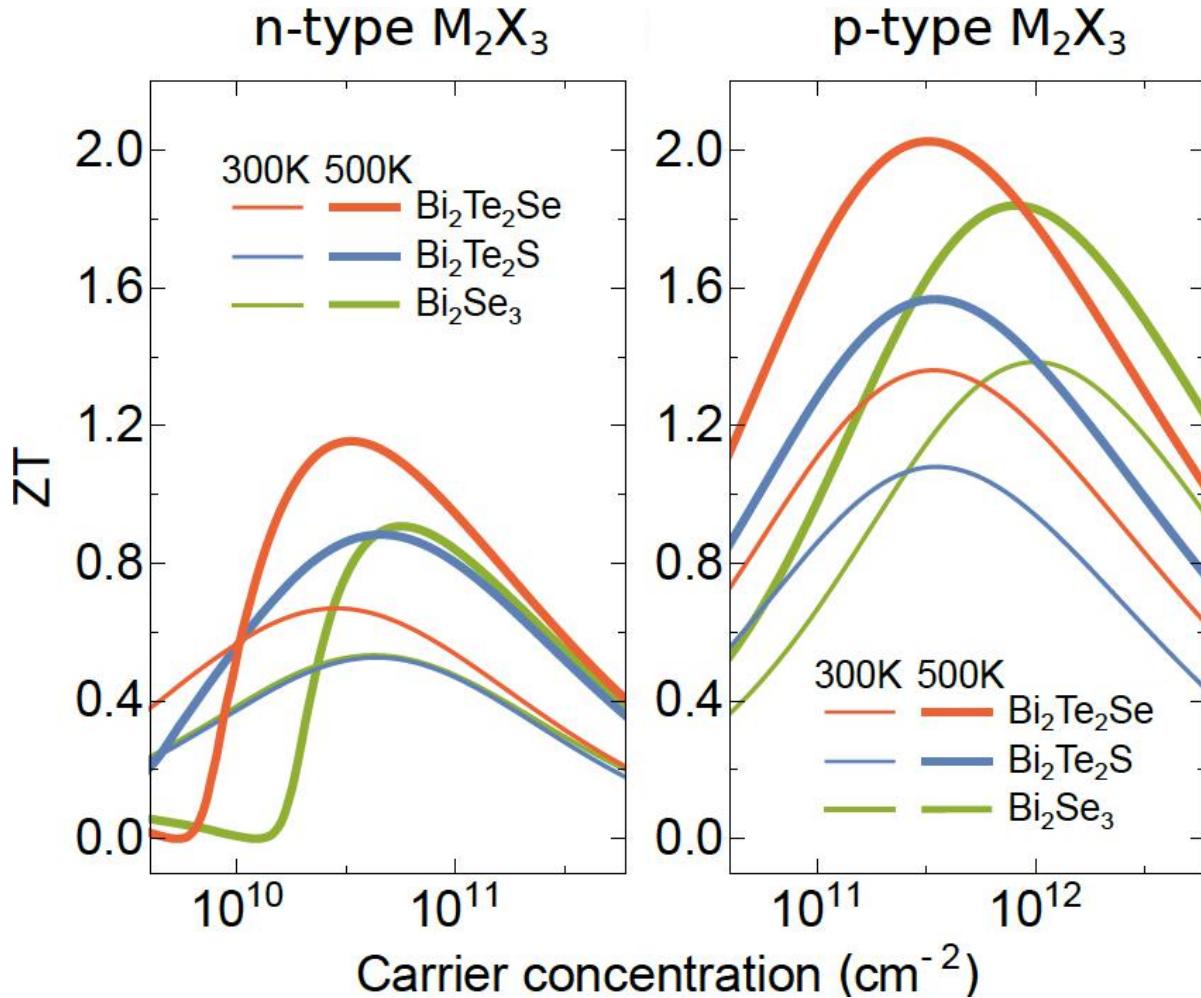


- Both PF and ZT are enhanced by band convergence
- $\text{HB} \rightarrow \text{LB}$  is better than  $\text{LB} \rightarrow \text{HB}$  for ZT

but  $ZT \sim 0.4$  is not really satisfying

# Applications: Finding the best 2D thermoelectrics

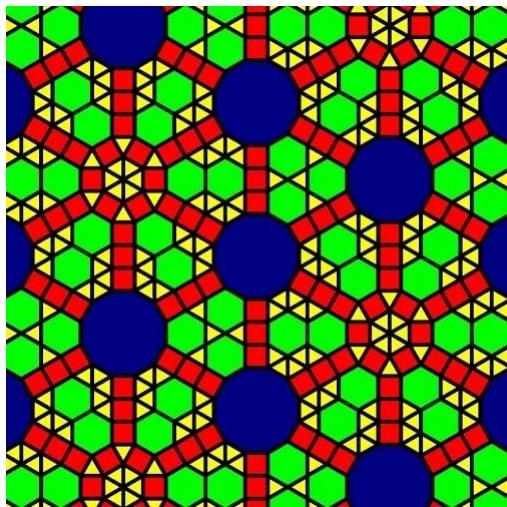
Hung, Nugraha, Saito, Nano Energy 58, 743 (2019)



Can we achieve  $ZT = 2$  for 2D tetradymite?

YES

# Applications: Designing New Materials

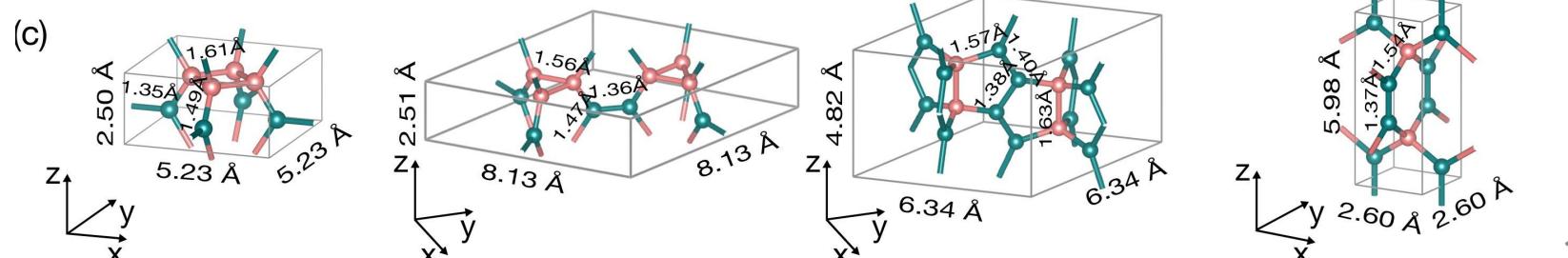
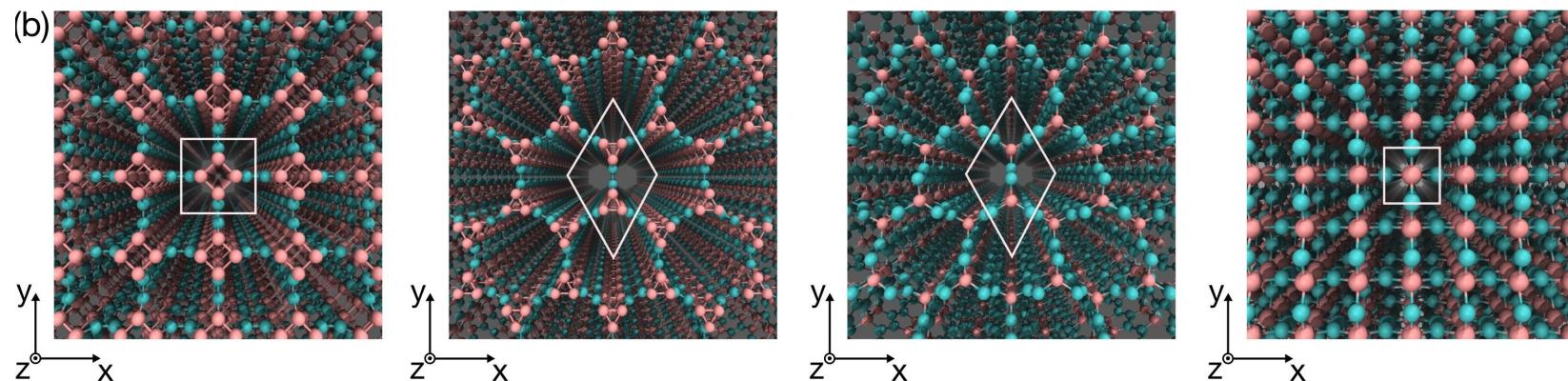
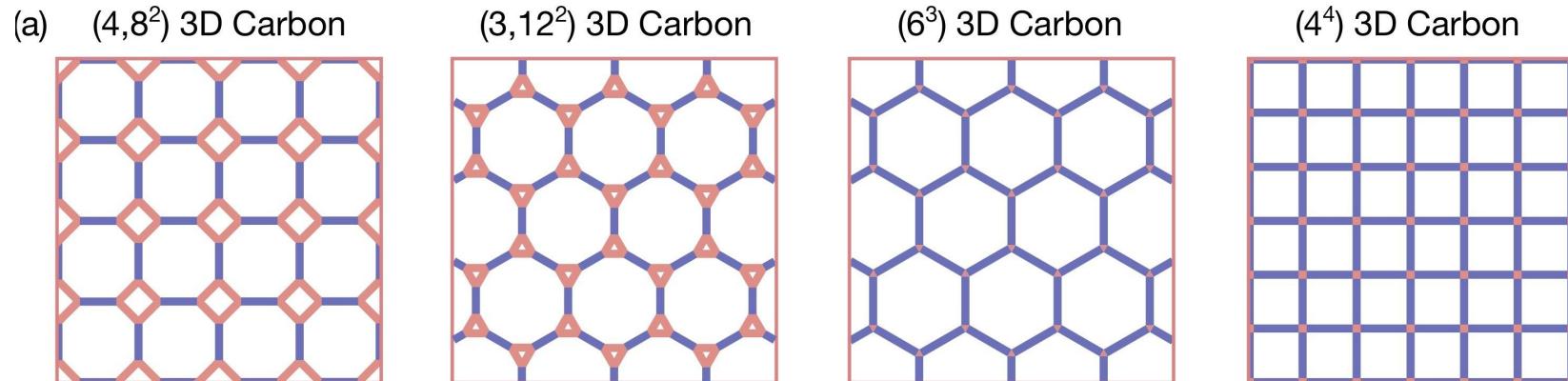


Archimedean lattice



New 3D Carbon networks

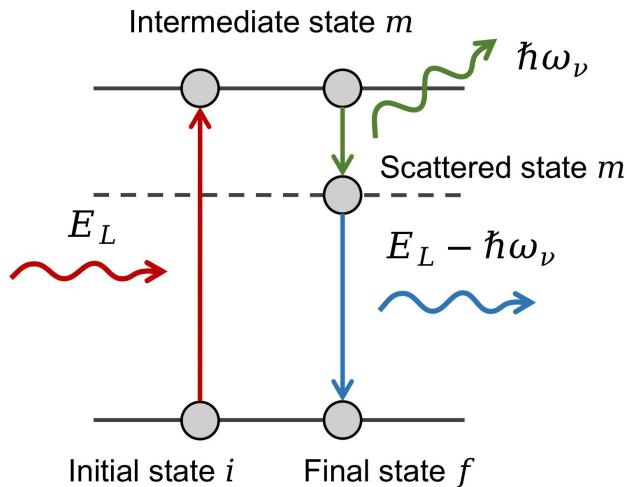
Hung, Nugraha, Saito,  
*Carbon* 125, 472-479 (2017)



# Applications: Light-Matter Interactions (Raman)

The Raman calculation **is not easy**  
**but QE calculation can match experimental data**

Resonant Raman scattering



NANO  
LETTERS

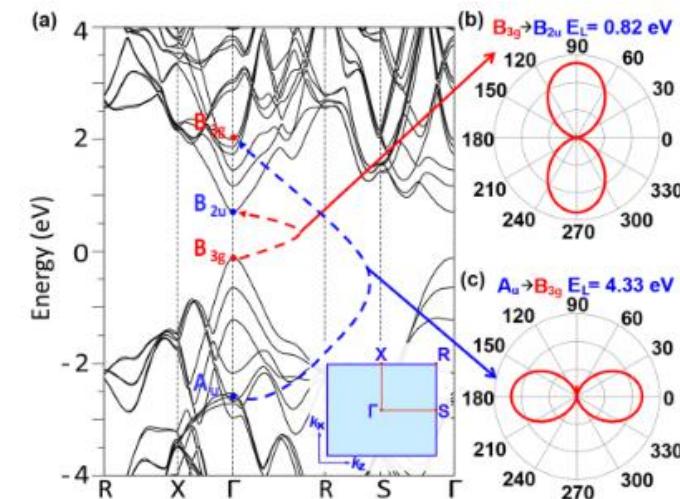
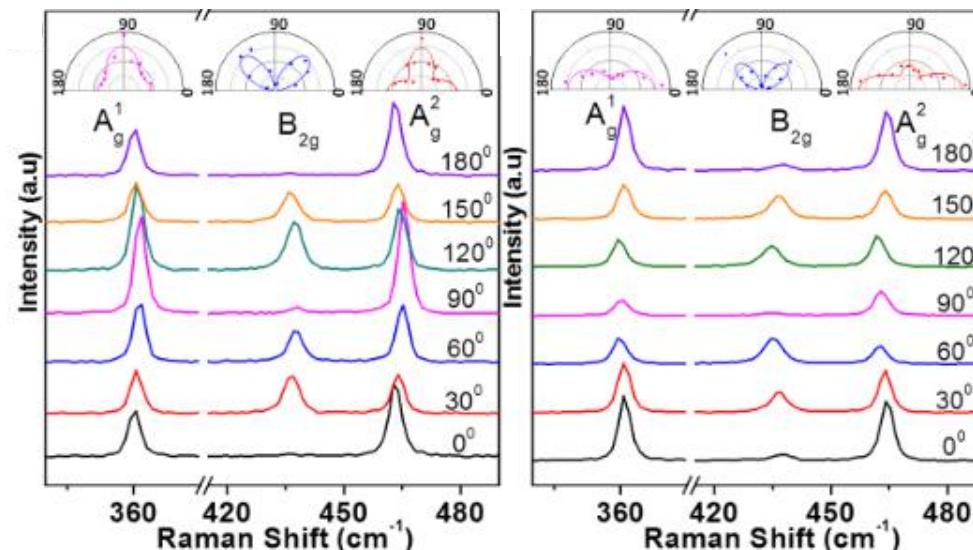
pubs.acs.org/NanoLett  
Anisotropic Electron-Photon and Electron-Phonon Interactions in Black Phosphorus

Xi Ling,<sup>\*†</sup> Shengxi Huang,<sup>†</sup> Eddwi H. Hasdeo,<sup>‡</sup> Liangbo Liang,<sup>§,⊥</sup> William M. Parkin,<sup>||</sup> Yuki Tatsumi,<sup>‡</sup> Ahmad R. T. Nugraha,<sup>‡</sup> Alexander A. Puretzky,<sup>†</sup> Paul Masih Das,<sup>||</sup> Bobby G. Sumpter,<sup>†</sup> David B. Geohegan,<sup>†</sup> Jing Kong,<sup>†</sup> Riichiro Saito,<sup>\*</sup> Marija Drndic,<sup>||</sup> Vincent Meunier,<sup>§</sup> and Mildred S. Dresselhaus<sup>\*†</sup>

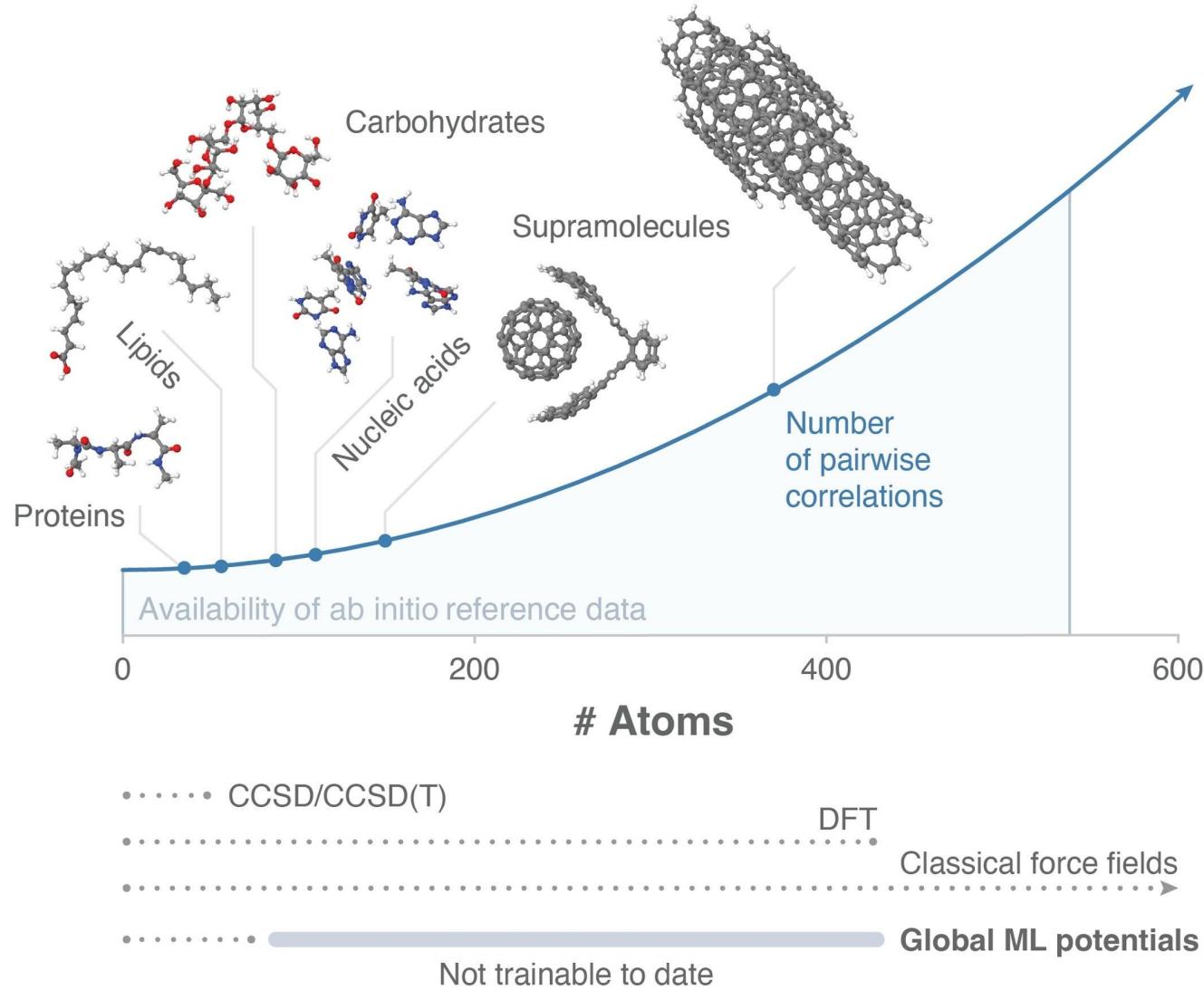
Ling et al., Nano Lett. (2016)

Raman intensity from perturbation theory:

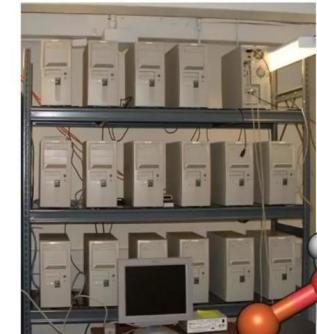
$$I(E_L, E_{RS}) = \sum_{\nu} \left| \sum_{\mathbf{k}} \sum_{i,m,m'} \frac{\mathcal{M}_{\text{opt}}^{m' \rightarrow i}(\mathbf{k}) \mathcal{M}_{\text{ep}}^{m \rightarrow m'}(\mathbf{k}, \nu) \mathcal{M}_{\text{opt}}^{i \rightarrow m}(\mathbf{k})}{[E_L - \Delta E_{mi}(\mathbf{k})][E_L - \Delta E_{m'i}(\mathbf{k}) - \hbar\omega_\nu]} \right|^2 \times \delta(E_{RS} - \hbar\omega_\nu),$$



# Large-scale DFT Calculations and Moving to GPUs

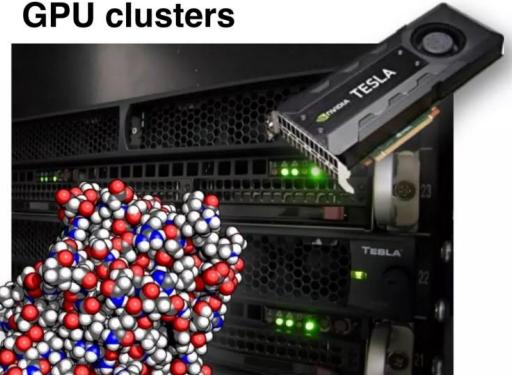


**then (mid-2000s):**  
Beowulf clusters



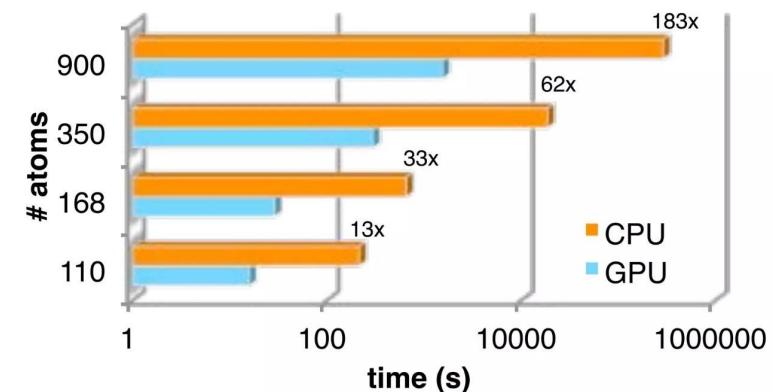
DFT on a **handful of atoms** (three to ~100)

**now:**  
GPU clusters



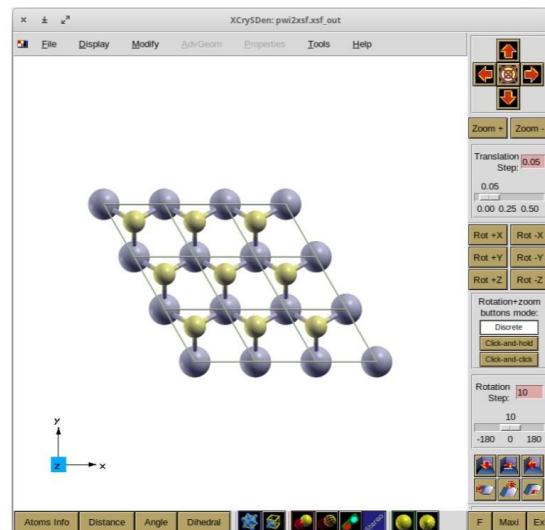
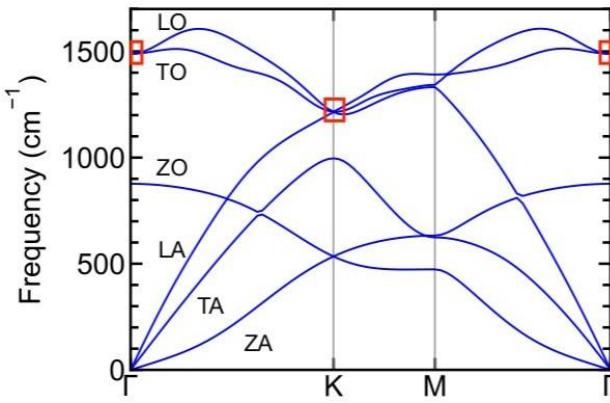
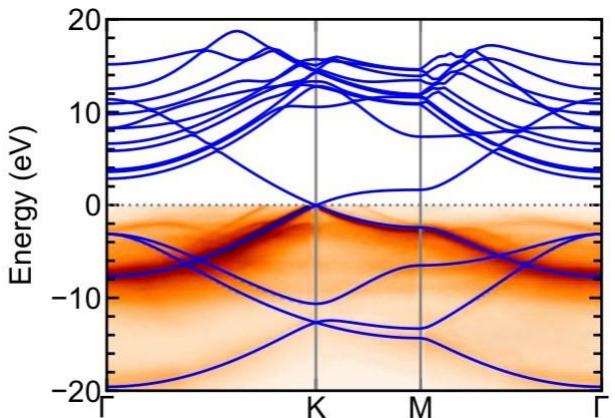
DFT or better on **three thousand atoms!**

Novel architecture & GPU-optimized algorithms:

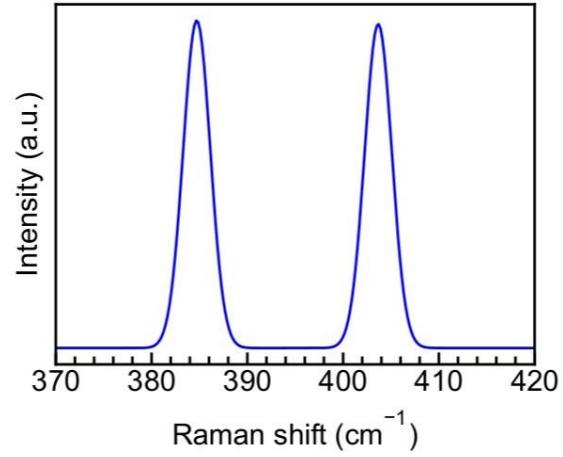
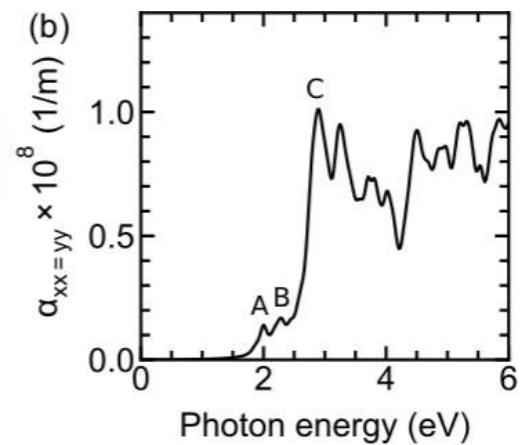
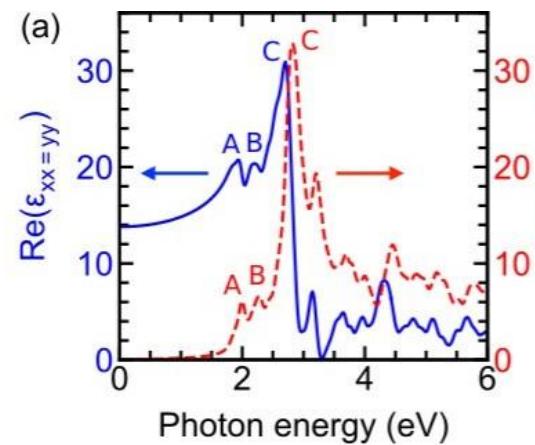


I.S. Ufimtsev and T. J. Martinez *J. Chem. Theory Comput.* 5, 1004 (2009).

# Many Other Examples in Chap. 3 of Textbook (incl. Wannier90)



Please enjoy running Quantum ESPRESSO!



Unpublished, preprint  
version for Chap. 3