



## Summer Workshop 2023 @ HUST, Hanoi

# Introduction to Density-Functional Theory with Quantum ESPRESSO

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<https://nguyen-group.github.io/>

# Self-Introduction



- 10/2014 - 09/2016: M.Sc. in Physics, Tohoku University
- 10/2016 - 03/2019: Ph.D. in Physics (JSPS DC), Tohoku University
- 04/2019 - now: Assistant Professor, FRIS, Tohoku University
- 07/2021 - now: Prominent Research Fellow, Tohoku University
- 2018: Visiting Scholar, IMR, CAS, China
- 2023-2024: Visiting Scholar, QMG, MIT, USA

Our office



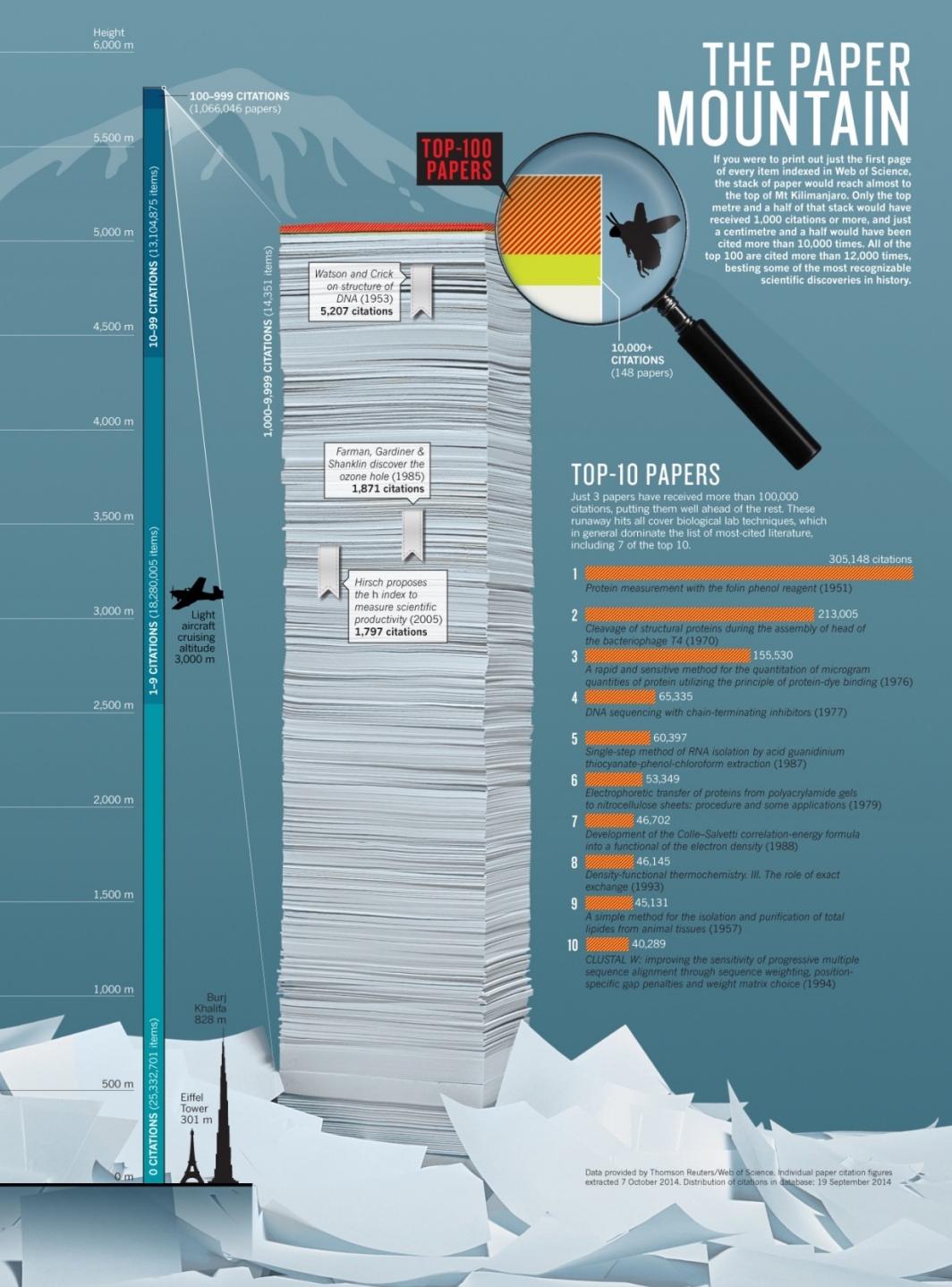
Aoba-ku  
station



# Content

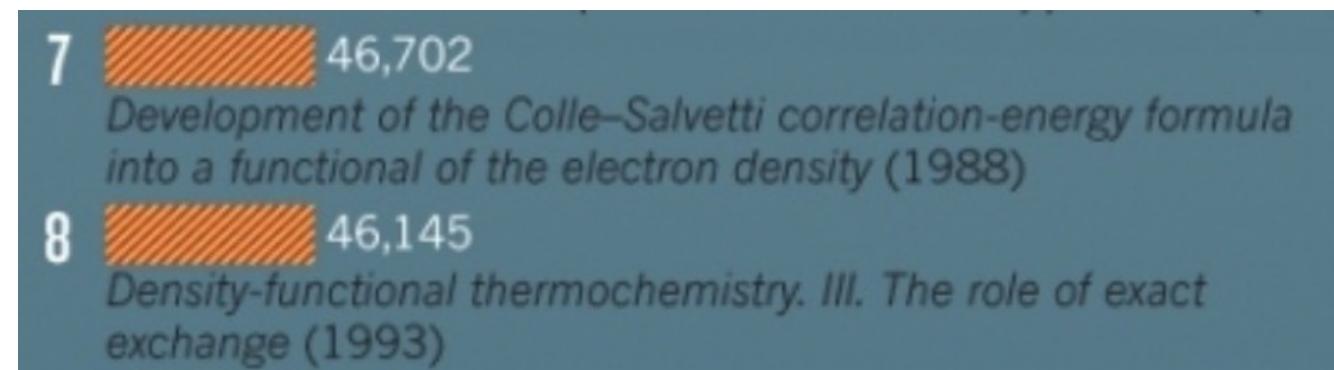
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- What is density-functional theory (DFT)?
- How to run an example by using DFT?
- Some applications of the DFT from my research
- Challenge and future of the DFT



# 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**

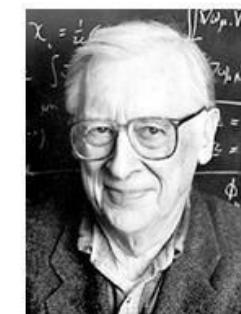


## The Nobel Prize in Chemistry 1998



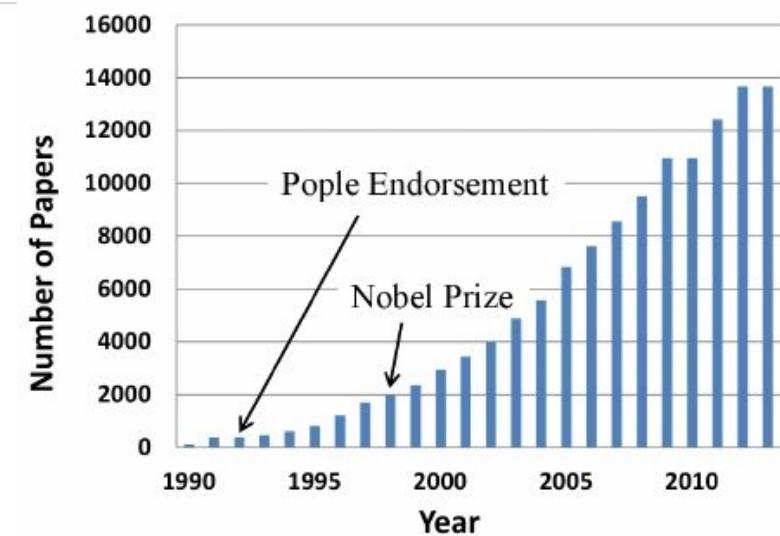
Walter Kohn

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](#)

130,981 citations (2023)

GGA made the DFT possible for practice.

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](#)

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 \(38,993\)](#)

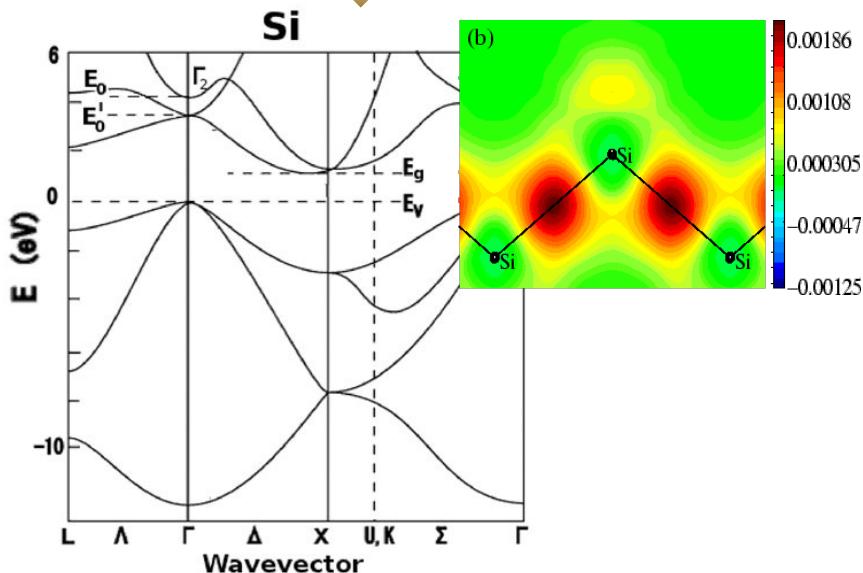
Hohenberg–Kohn theorems

Starting point of the concepts of DFT

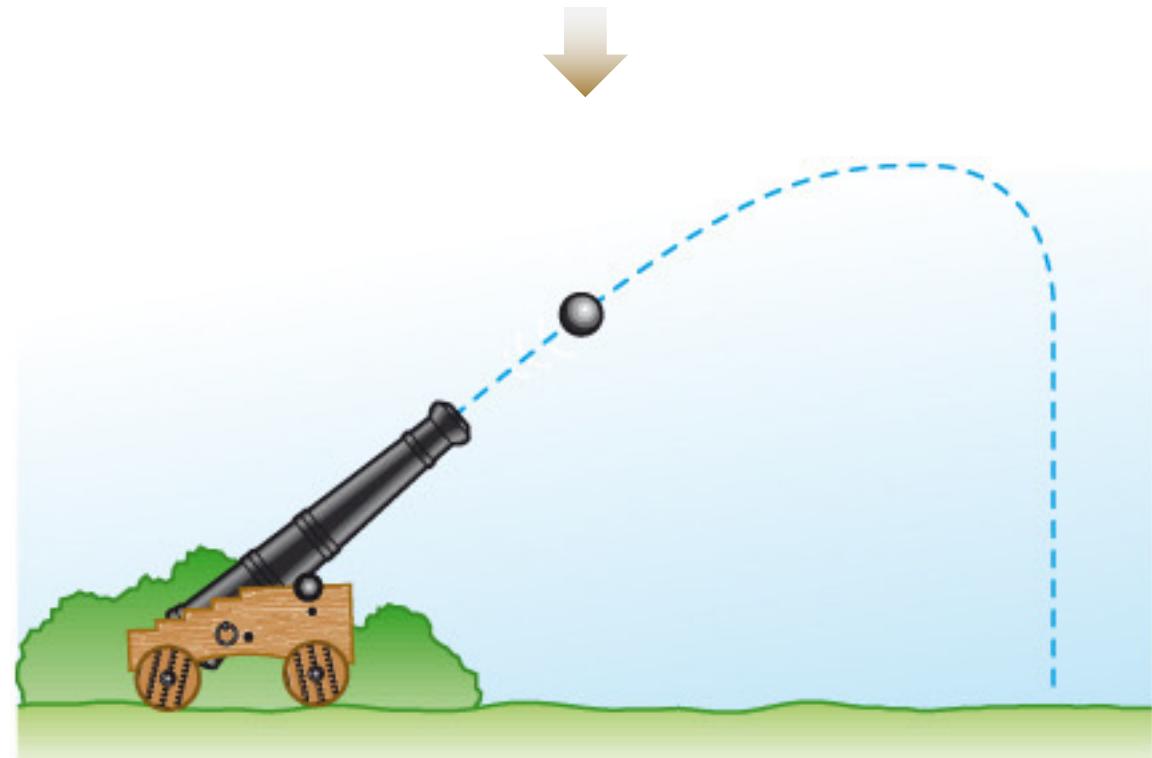
# What is DFT?

DFT is a method for solving the Schrödinger equation

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



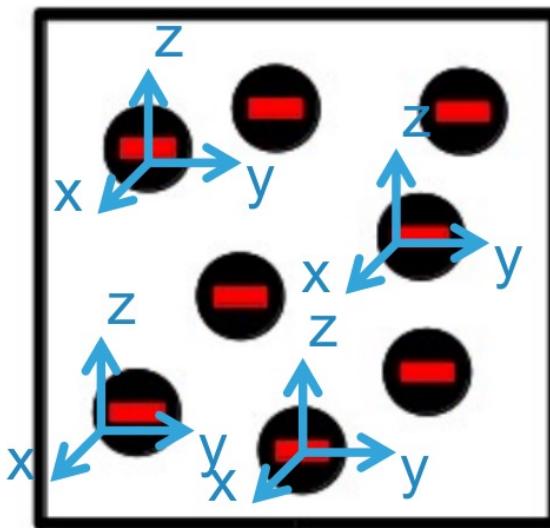
The Newton equation  
 $F = ma$



# The Idea of DFT - Electron Density

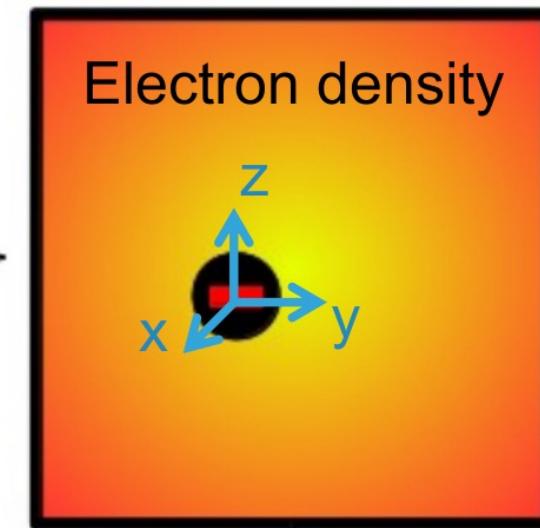


Just store data  
for Si case:  
 $5000^{84}$  numbers



3N-dimensional  
partial differential equation (PDE)

Reduction of dimensionality!



3-dimensional PDE



$5000^3$  numbers



The idea can work with only the case that two models are equivalent

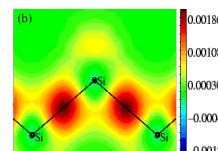
# The Hohenberg-Kohn (H-K) Theorems

## The H-K existence 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 H-K variational 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.



$n(r)$

Electron density

Inhomogeneous Electron Gas

P. Hohenberg and W. Kohn

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

Physics

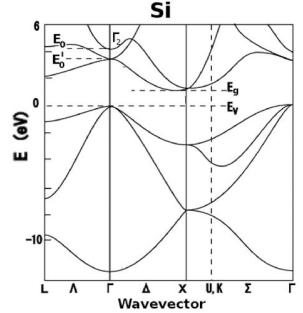
Article

References

Citing Articles (38,993)

Density-functional theory

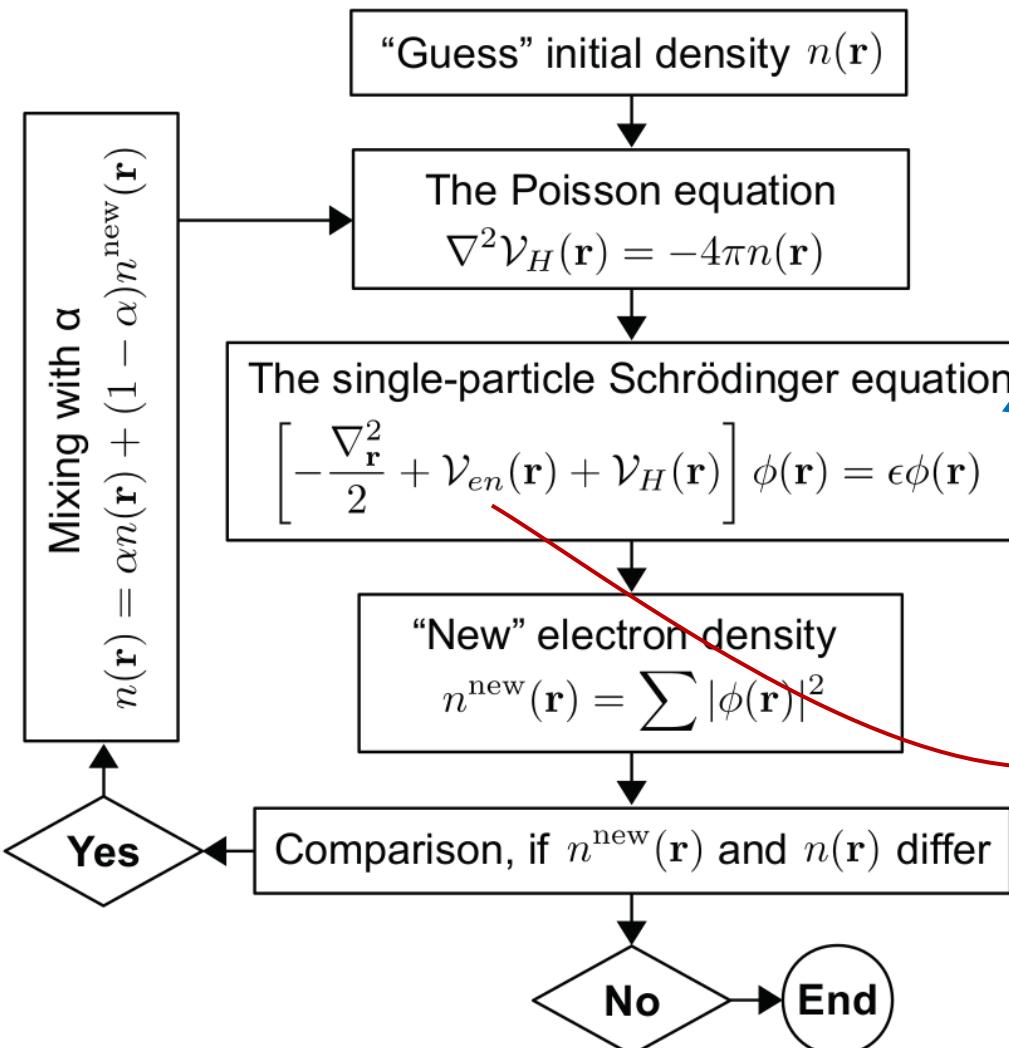
$E[n(r)]$



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

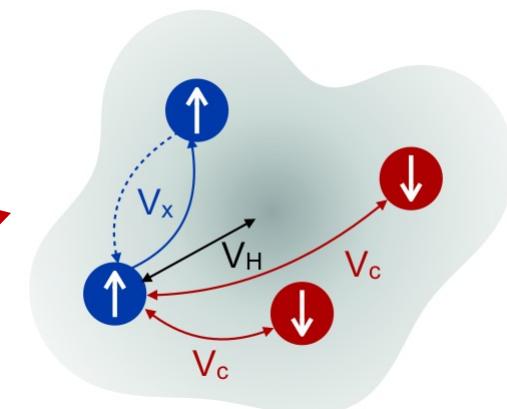
References

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 -  $V_c$ )

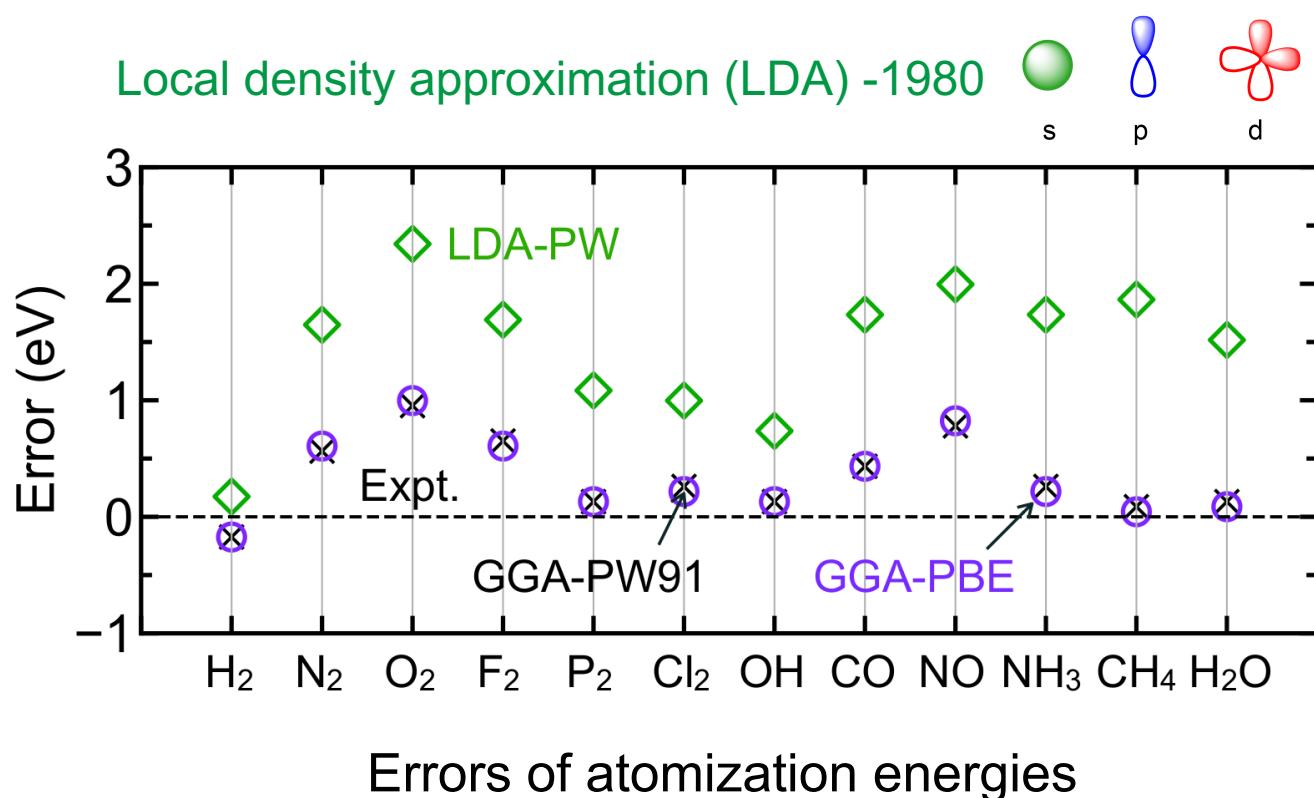
Exchange-correlation potential  
(Unknown functional)

# How to Deal with Unknown Functional?

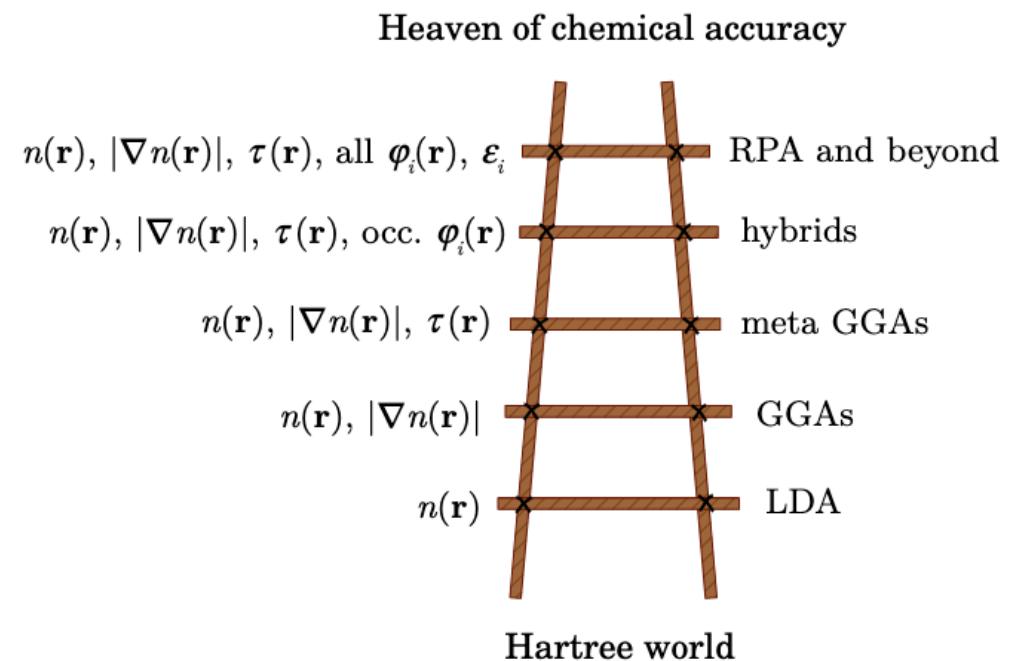
Generalized Gradient Approximation Made Simple

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	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)

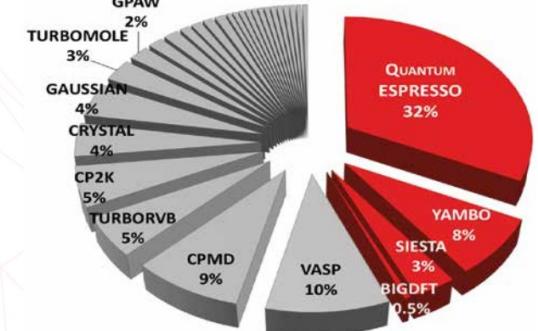
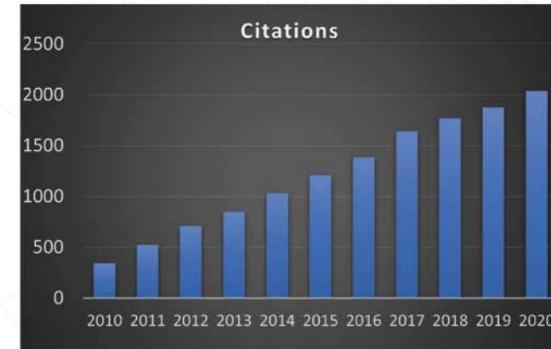


Fig1a

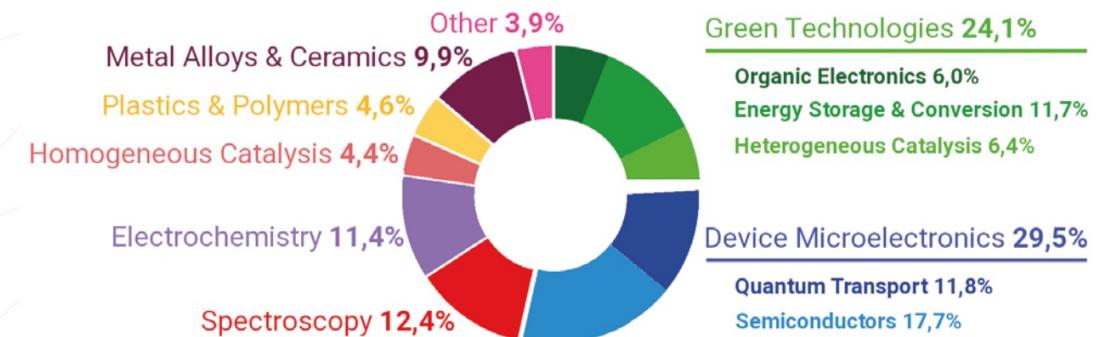


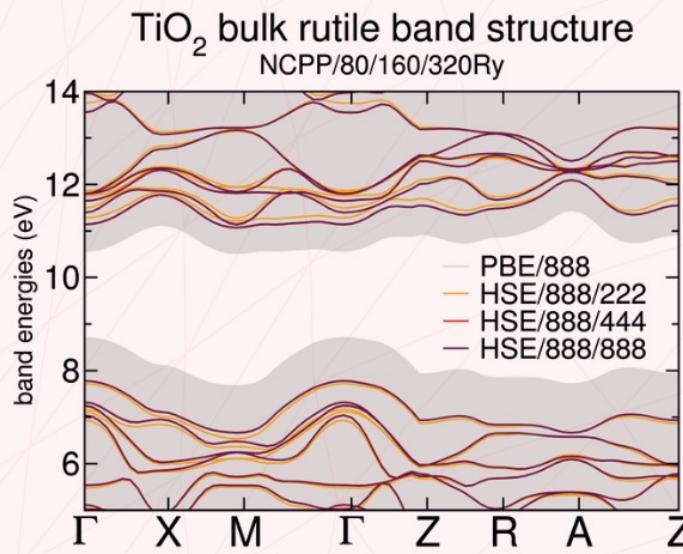
Fig1b

# Some Features of QE

Quantum ESPRESSO is a bundle of codes (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

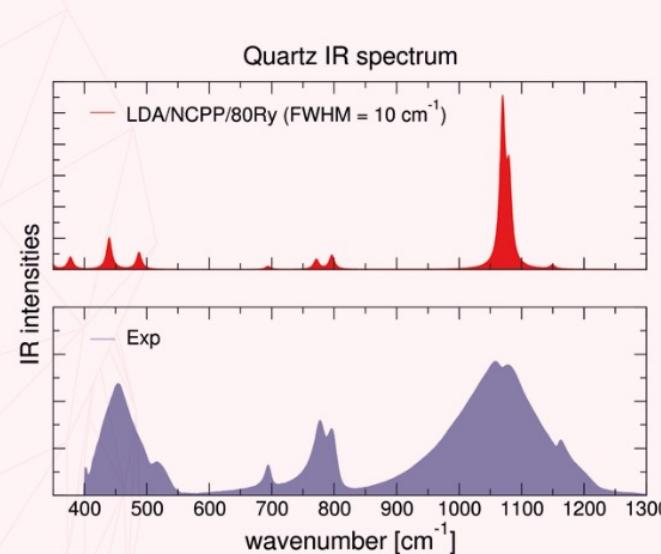


## CP:

- ◆ Car-Parrinello molecular dynamics

## Phonon:

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

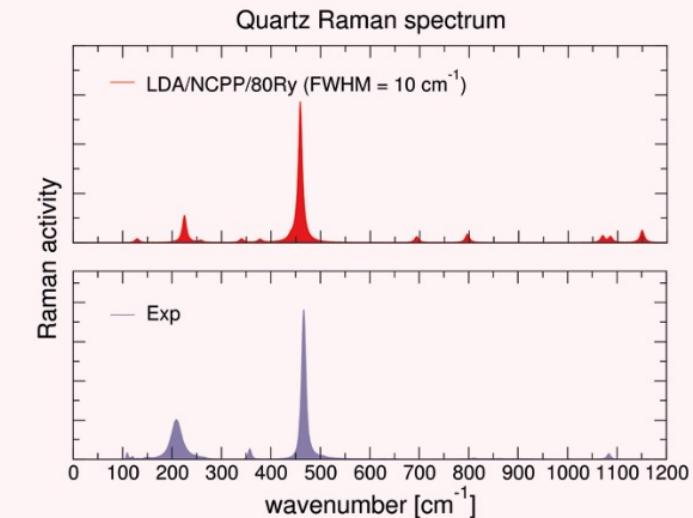


## TDDFPT:

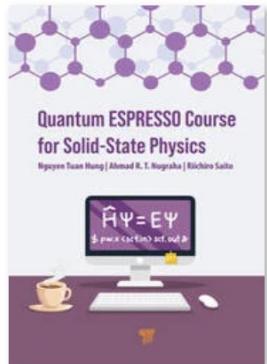
- ◆ UV-Vis absorption
- ◆ Electron energy loss spectroscopy
- ◆ Spin wave spectroscopy

## NEB:

- ◆ Reaction paths



# Is It Easy 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



Share



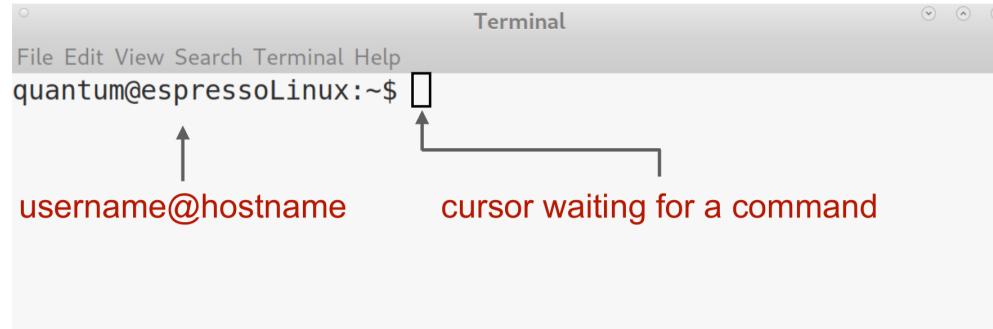
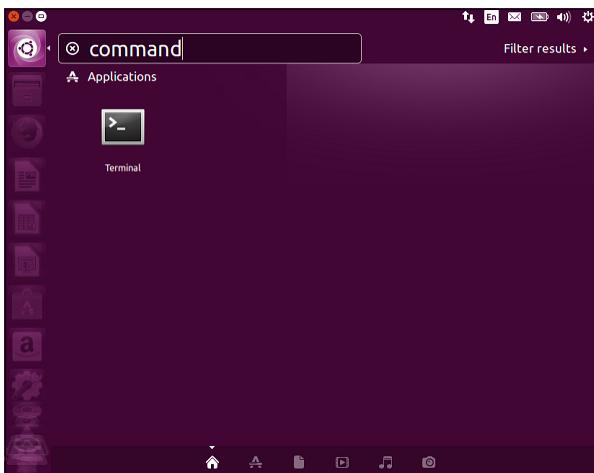
Citation

- ❑ How to **install & run** softwares in a personal PC.
- ❑ **23 tutorials** for many physical properties: electron, phonon, optic, superconductivity, Raman, .... (can download free at GitHub: <https://github.com/nguyen-group/QE-SSP>)
- ❑ Theory for DFT & solid-state physics for Quantum ESPRESSO

Many workshops about Quantum-ESPRESSO are organized by us.

- 2016: Tohoku University (Japan)
- 2019: Zhejiang University (China)
- 2019: Vietnam School of Physics (Vietnam)
- 2022: HUST (Vietnam), Tokyo Metropolitan University (Japan)

# How to Install QE



## Quick installation of Quantum Espresso:

Step 1: Update system:

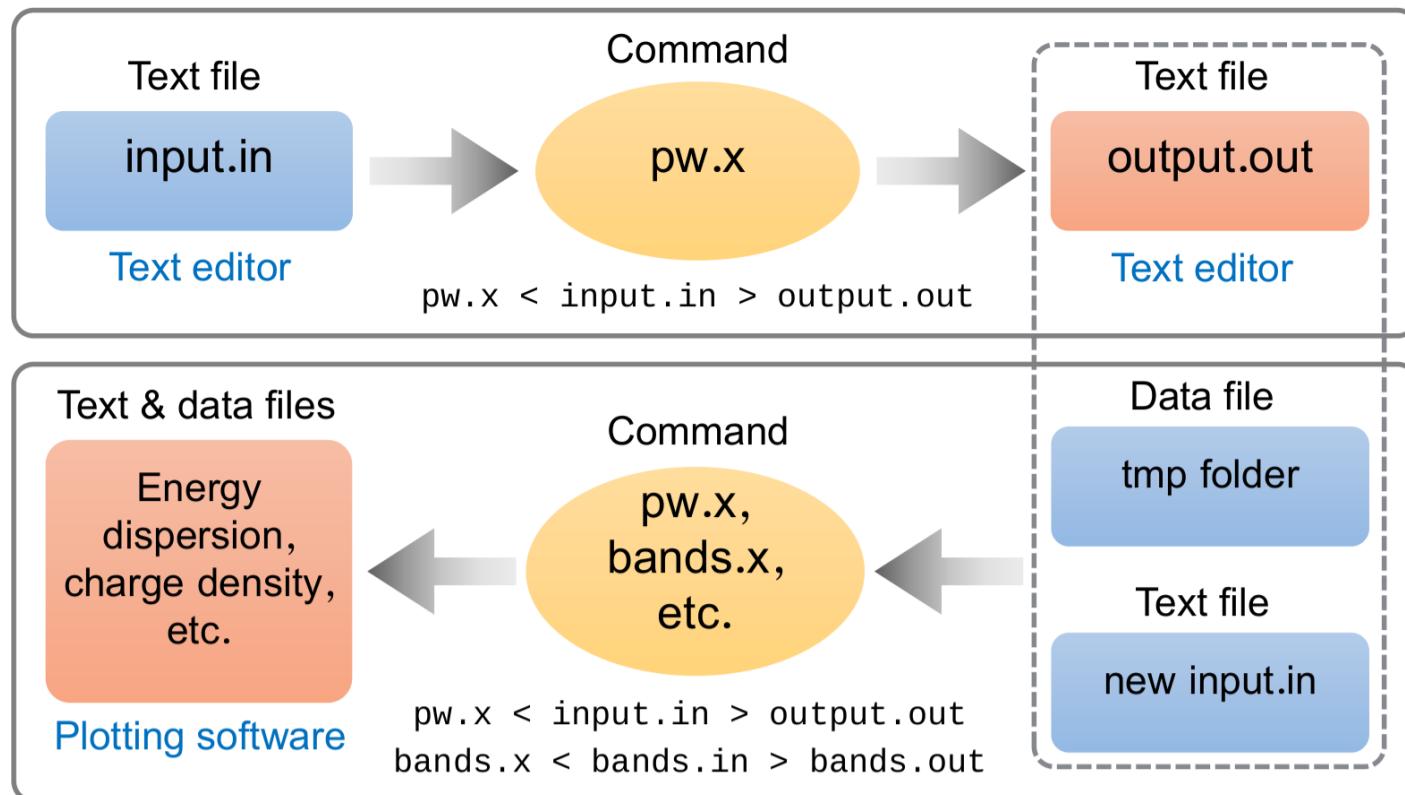
```
$ sudo apt-get update
```

Step 2: Install: quantum-espresso

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

You also can install easy in MacOS or Window

# Quantum ESPRESSO Workflow



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

Download input files for examples

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

# Let's Do An Example without Knowing Everything

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

## 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
```

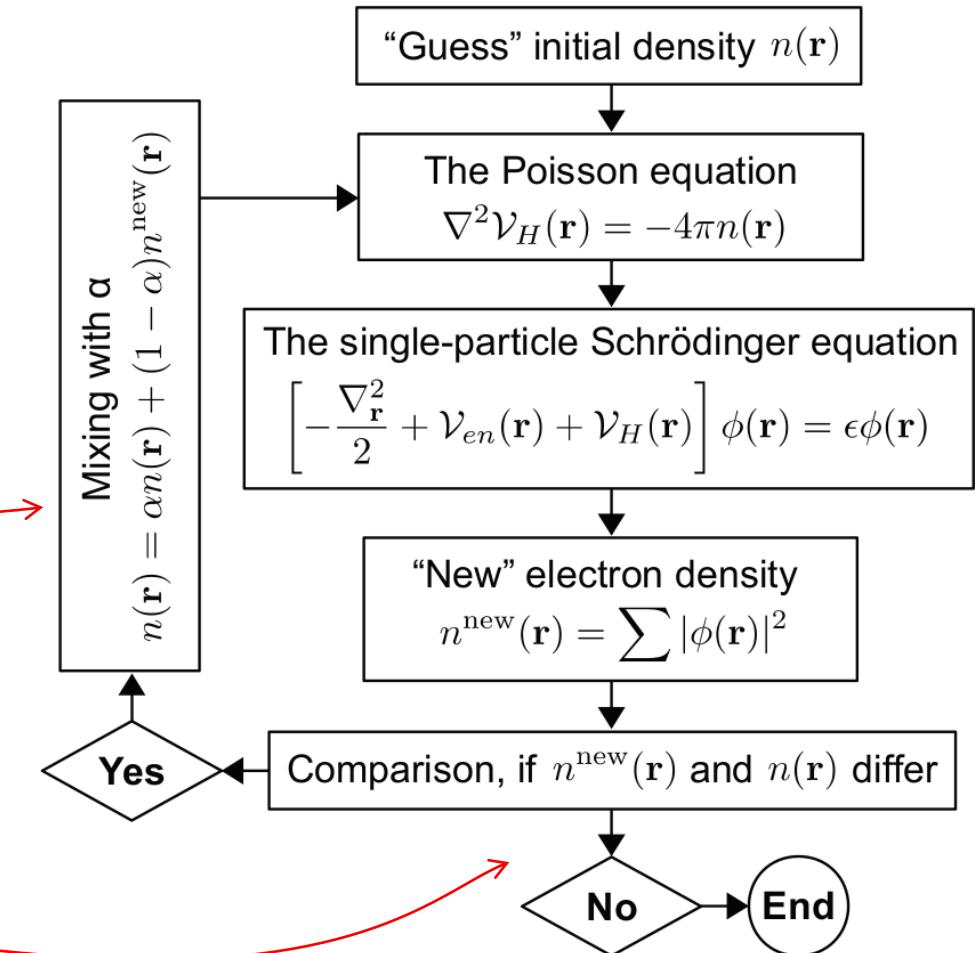
# QE-SSP/gr/scf/scf.in

```

1 &CONTROL
2 calculation = 'scf' ←
3 pseudo_dir = '../pseudo/'
4 outdir = '../tmp/'
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26 C 0.666666666 0.333333333 0.500000000
27 K_POINTS (automatic)
28 12 12 1 0 0 0

```

## Self-consistent field method



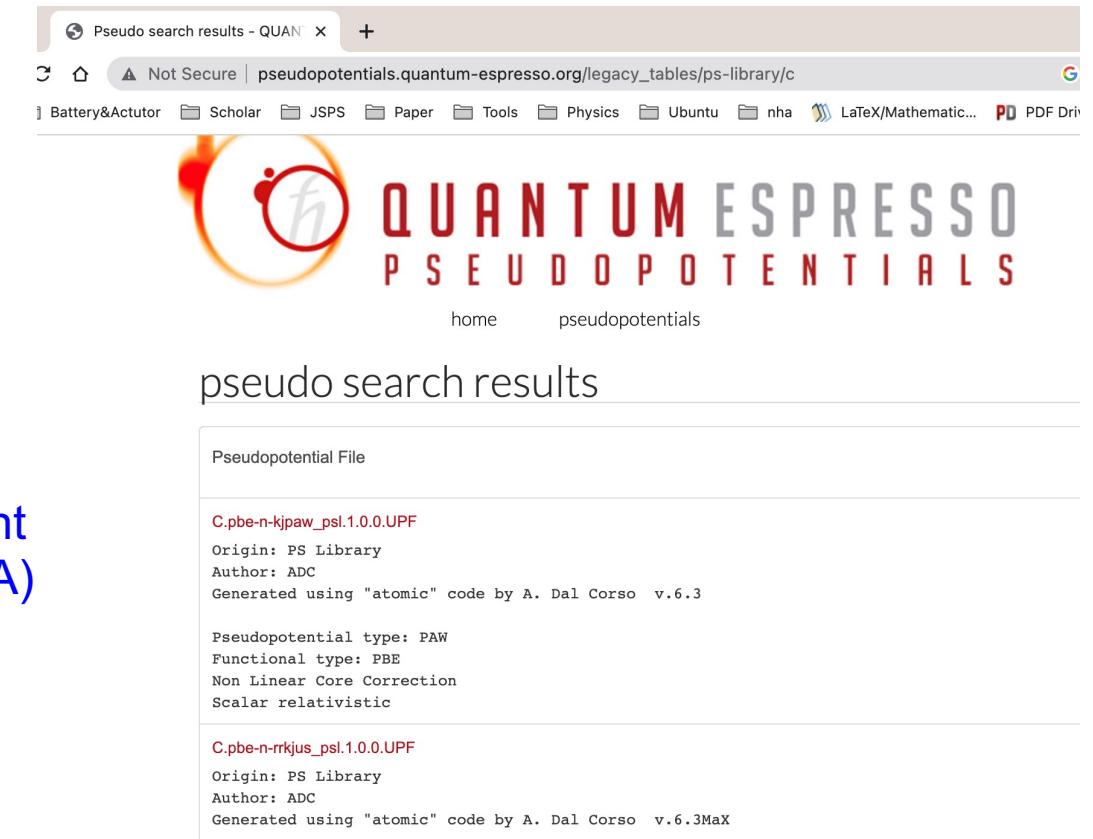
## QE-SSP/gr/scf/scf.in

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1 &CONTROL
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4 outdir = '../tmp/'
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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



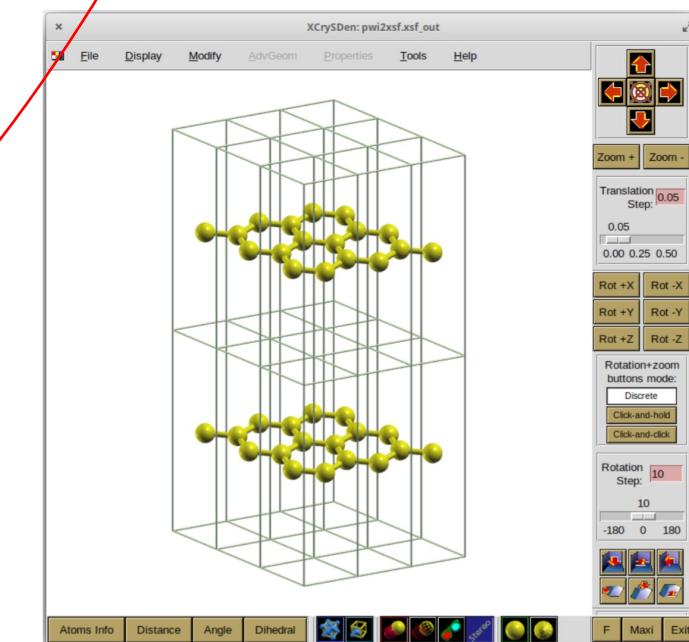
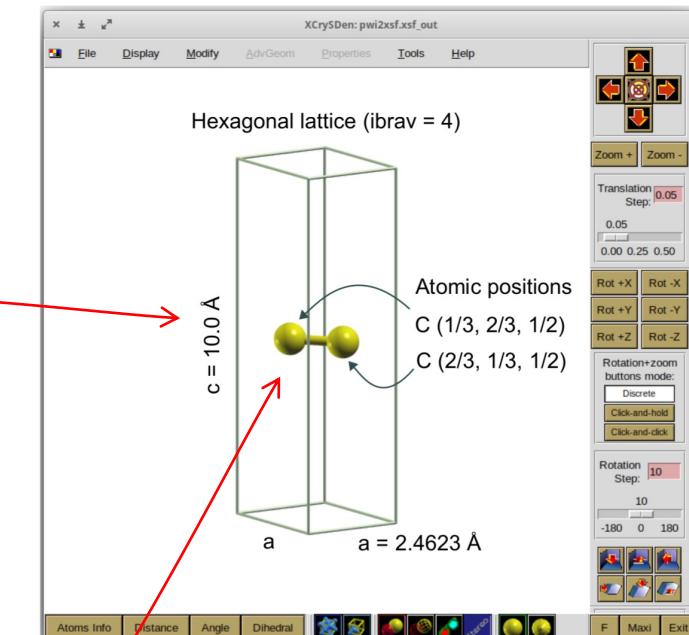
The screenshot shows a web browser window titled "Pseudo search results - QUAN". The URL is "pseudopotentials.quantum-espresso.org/legacy\_tables/ps-library/c". The page features the Quantum Espresso logo and navigation links for home and pseudopotentials. Below this, a section titled "pseudo search results" displays two entries:

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
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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



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

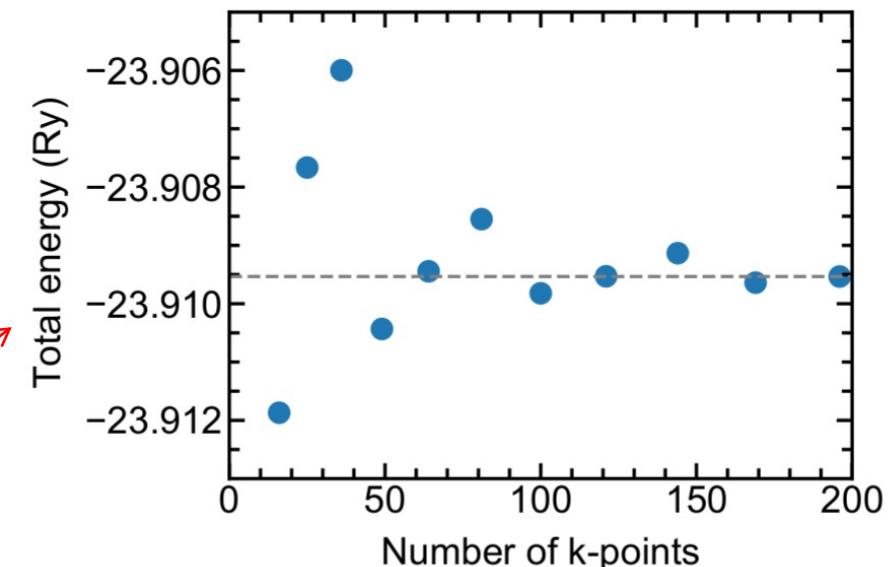
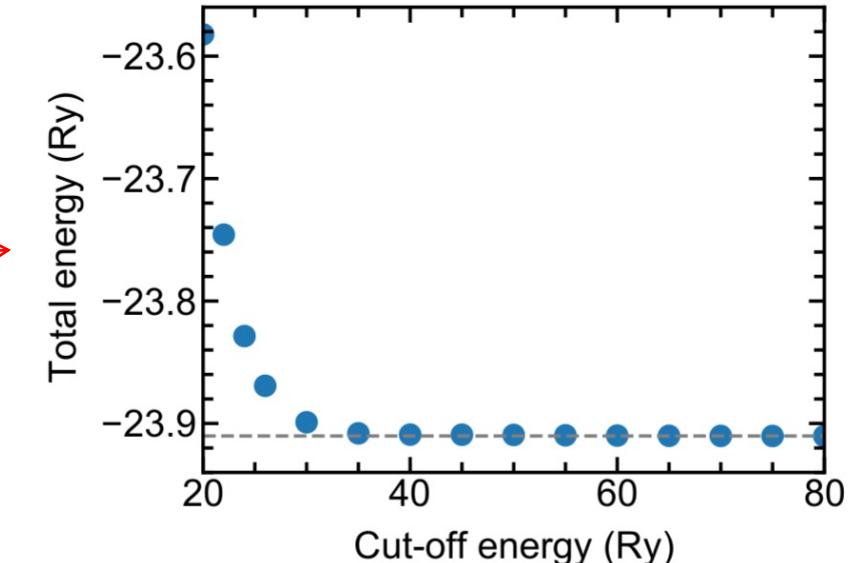
```

1 &CONTROL
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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 checking



# You can ask ChatGPT

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:

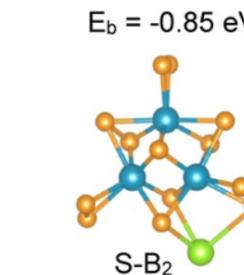
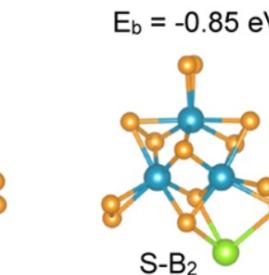
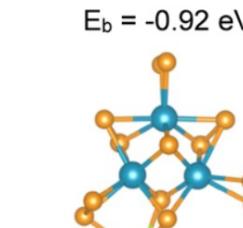
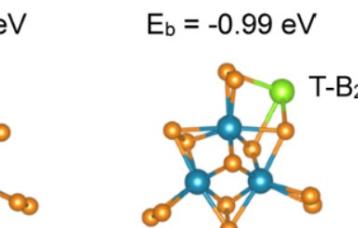
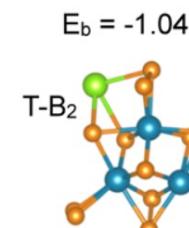
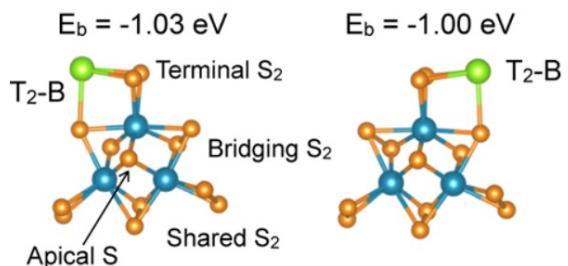
```
java
&inputph
  prefix = 'graphene_phonon'
  tr2_ph = 1.0e-14
  fildyn = 'graphene.dyn'
  amass(1) = 12.011
  outdir = './tmp'
/
&input
  asr = 'simple'
  fildyn = 'graphene.dyn'
  nat = 2
  ntyp = 1
  ecutwfc = 40
/
CELL_PARAMETERS {angstrom}
  2.462000 0.000000 0.000000
  0.000000 2.462000 0.000000
  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
```



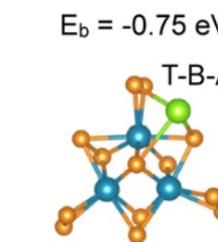
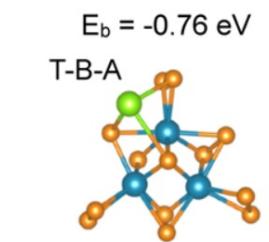
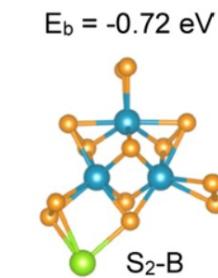
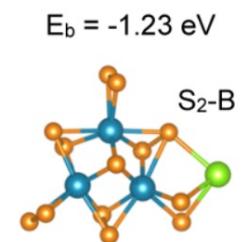
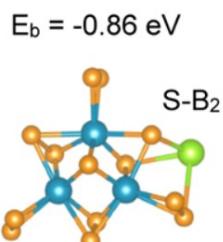
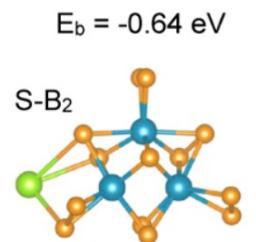
# Applications: Battery

Binding energy:

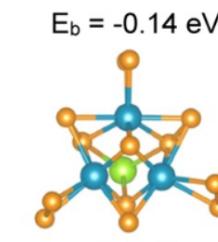
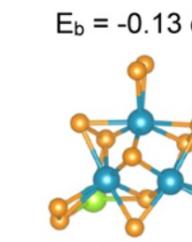
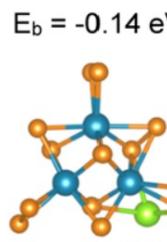
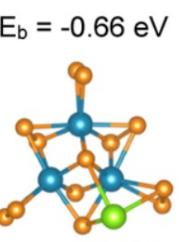
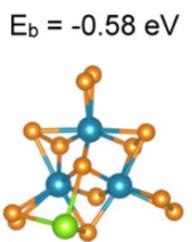
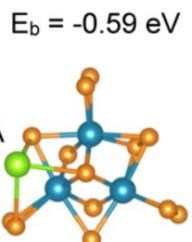
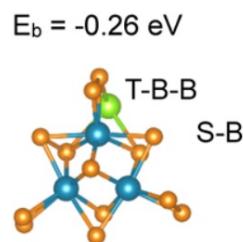
$$E_b = E(\text{Na} + \text{Mo}_3\text{S}_{11}) - E(\text{Na}) - E(\text{Mo}_3\text{S}_{11})$$



$E_b < 0$ : Binding

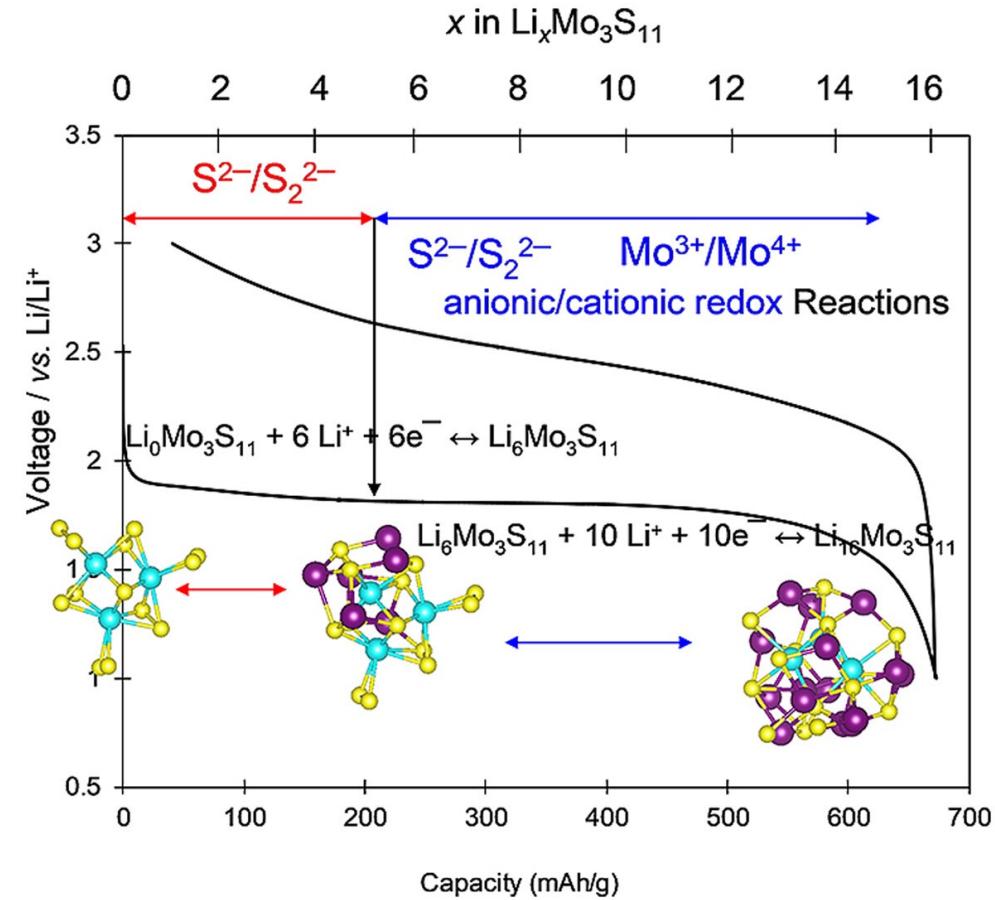
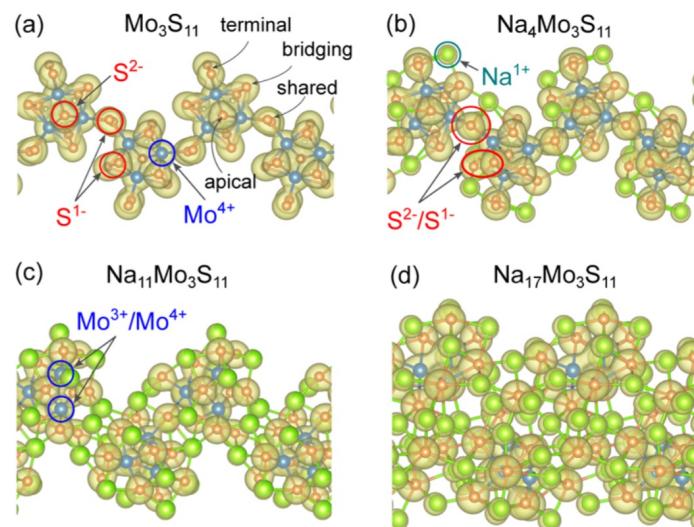
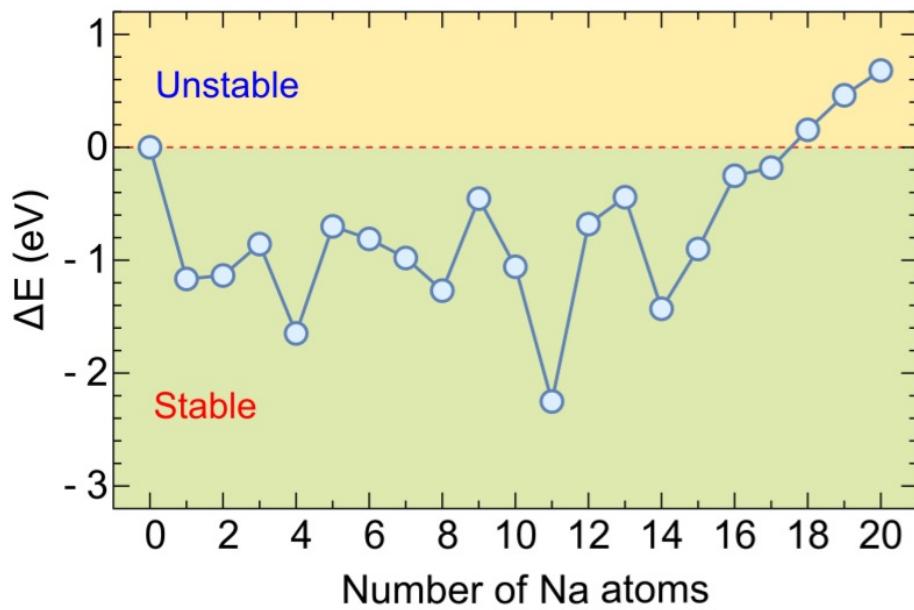


$E_b > 0$ : No binding



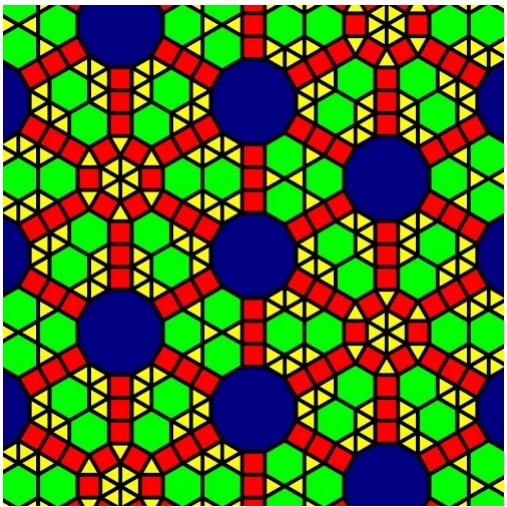
N. T. Hung et al., *J. Phys. Chem. C* 123, 30856 (2019)

# Applications: Battery



Q. D. Truong, L. C. Yin, N. T. Hung, et al., *Electrochim. Acta* 332, 135218 (2020).

# Applications: Designing New Materials



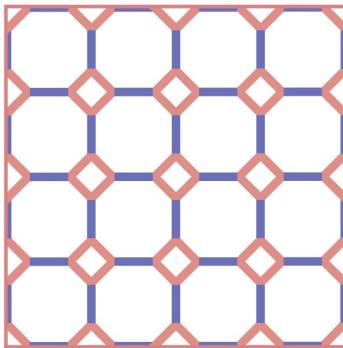
Archimedean lattice



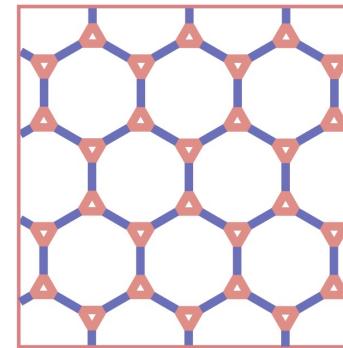
New 3D Carbon networks

N. T. Hung, et al., *Carbon*  
125, 472-479 (2017).

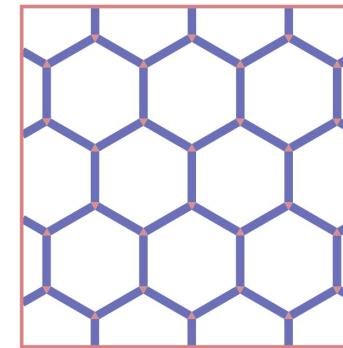
(a)  $(4,8^2)$  3D Carbon



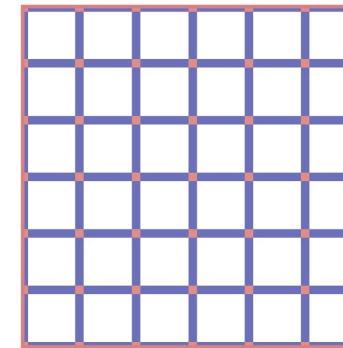
$(3,12^2)$  3D Carbon



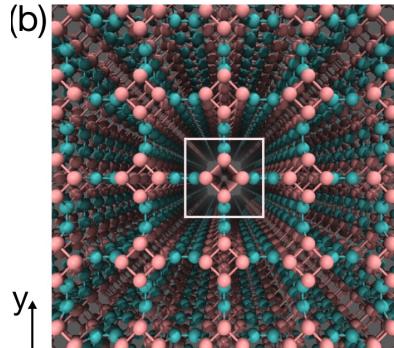
$(6^3)$  3D Carbon



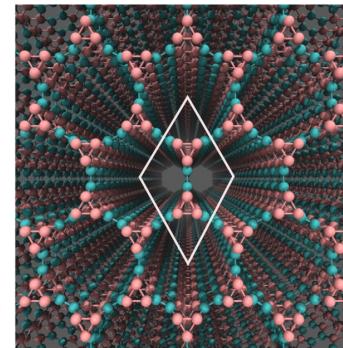
$(4^4)$  3D Carbon



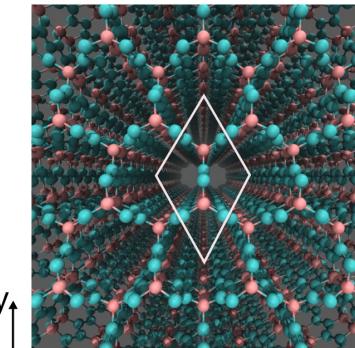
(b)



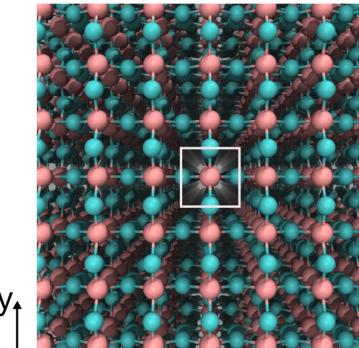
(b)



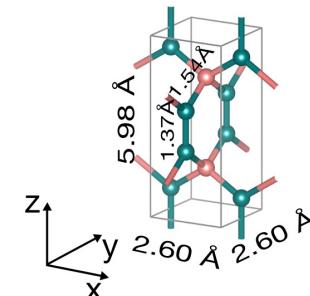
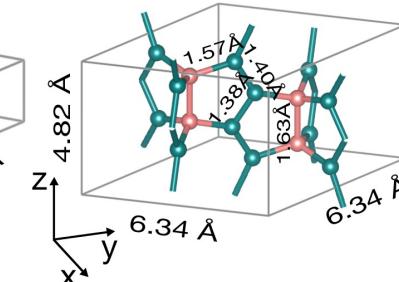
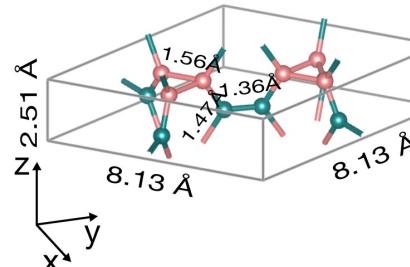
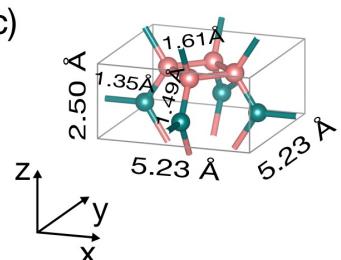
(b)



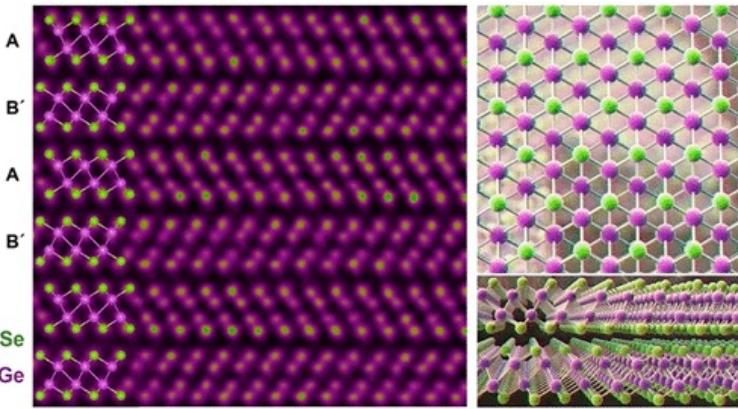
(b)



(c)

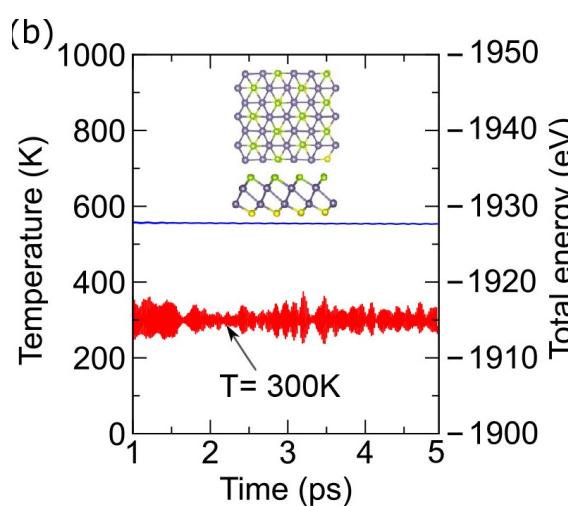


# Applications: Designing New Materials

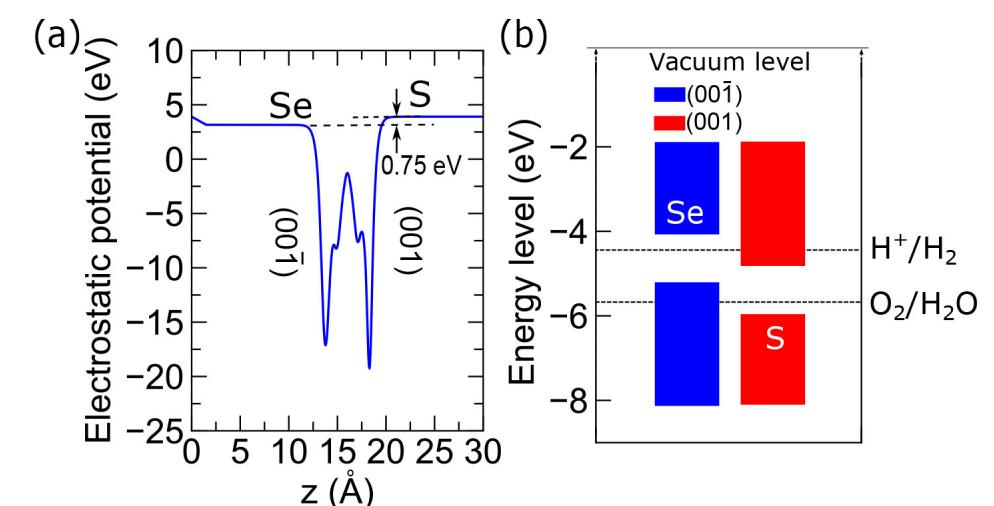
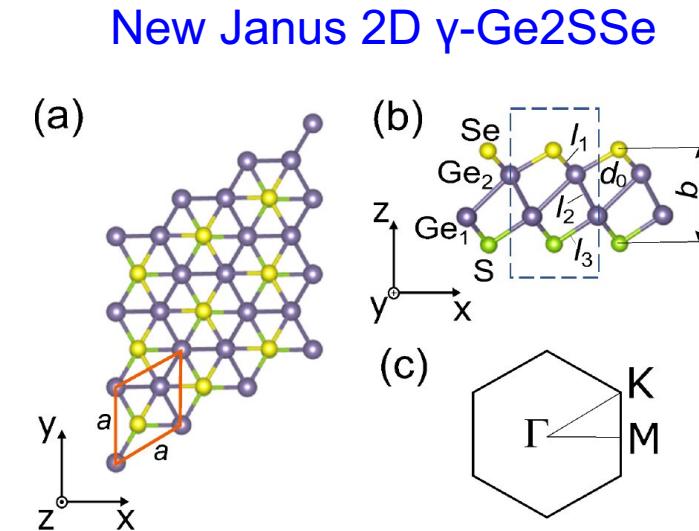


Successful synthesis of  $\gamma$ -GeSe  
(*Nano Lett.* 21, 4305, 2021)

V. V. Thanh, D. V. Truong  
and N. T. Hung, *ACS Appl.  
Energy Mater.* 6, 910-919  
(2023).



Replace Se atom  
to S atom

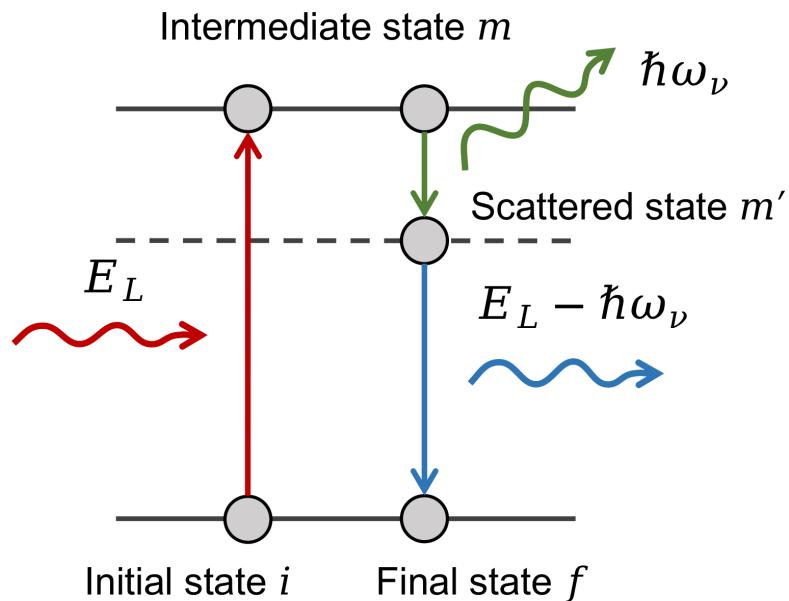


High-performance material for photocatalysis and thermoelectricity

# Applications: Understanding Raman spectra

The Raman calculation is not easy in the theory

Resonant Raman scattering



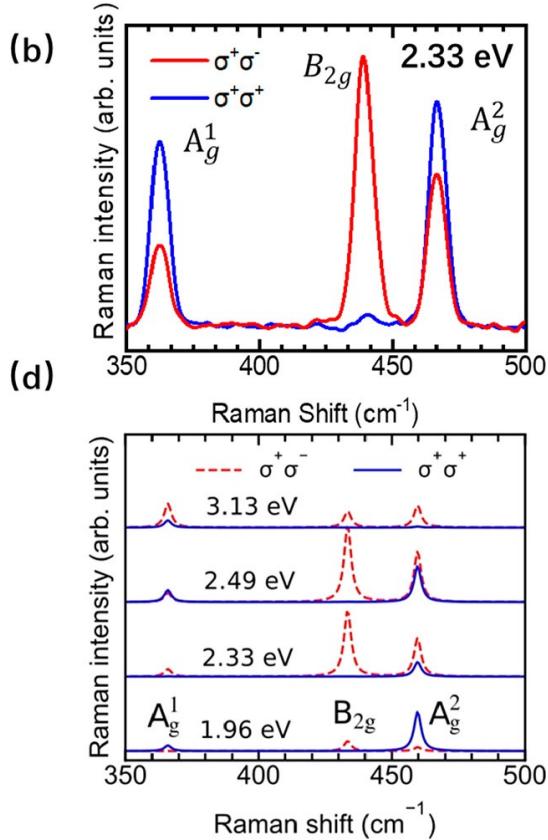
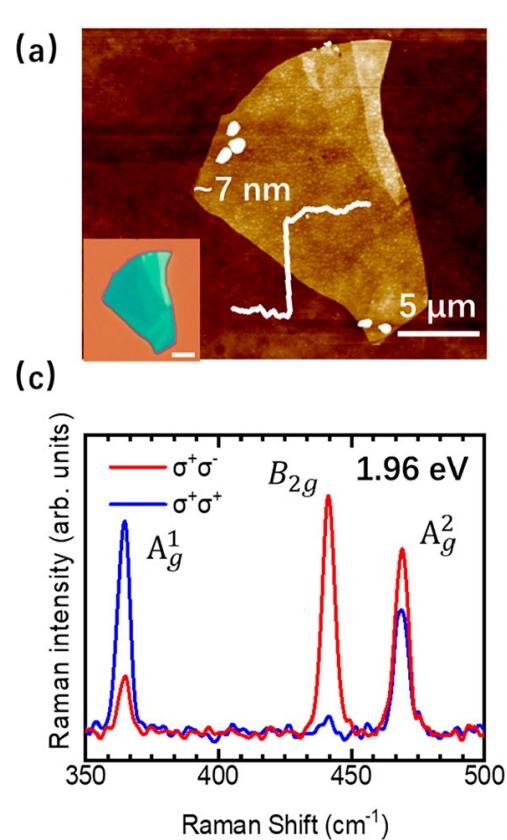
Raman intensity is given by the third-order perturbation:

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

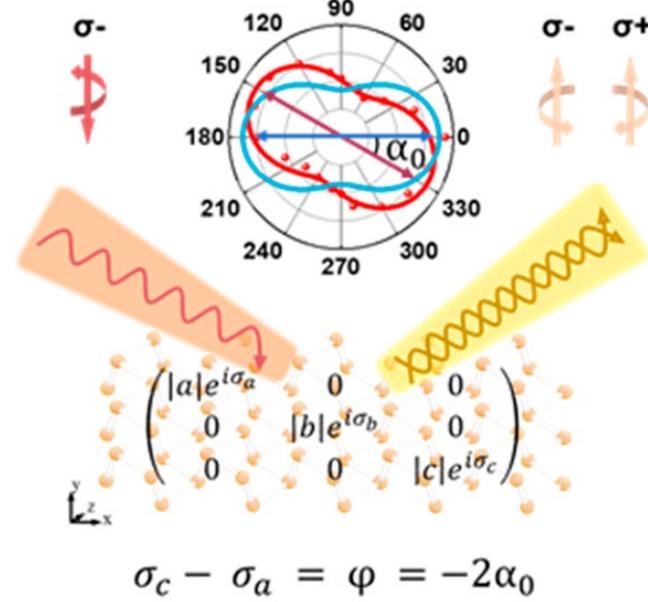
electron-photon    electron-phonon

# Applications: Understanding Raman spectra

Helicity-changing Raman spectra of black phosphorus under **circularly polarized light**



Experiment

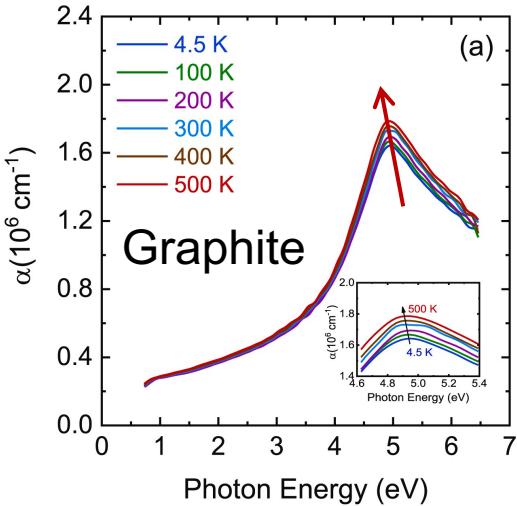


Theory

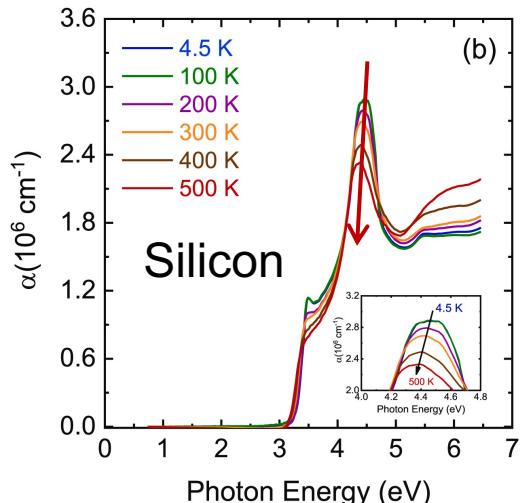
**Complex Raman tensor**  
(Experiment can not observe)

# Applications: Understanding optical spectra

Question from experimentalist: WHY?



Can not explain why optical absorption is higher with higher T?



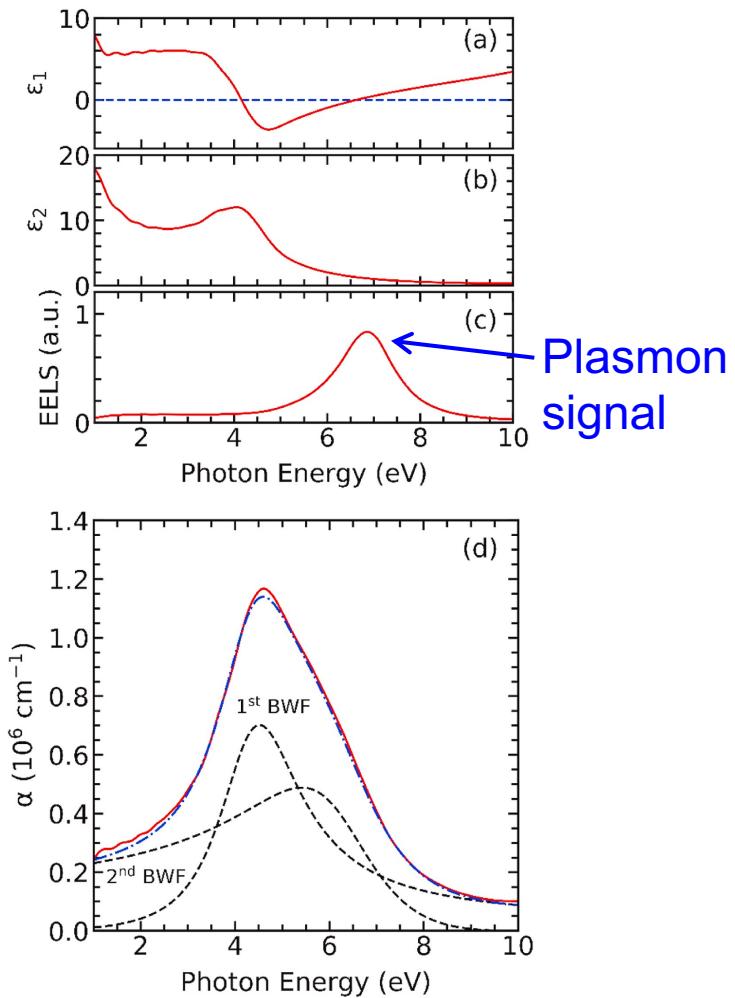
The limit of experiment is not easy to increase photon energy.

Can explain by standard theory:  
Higher T  $\rightarrow$  higher lifetime of electron

$$\text{EELS} = \text{Im} \left[ \frac{-1}{\varepsilon(\omega)} \right] = \frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}$$

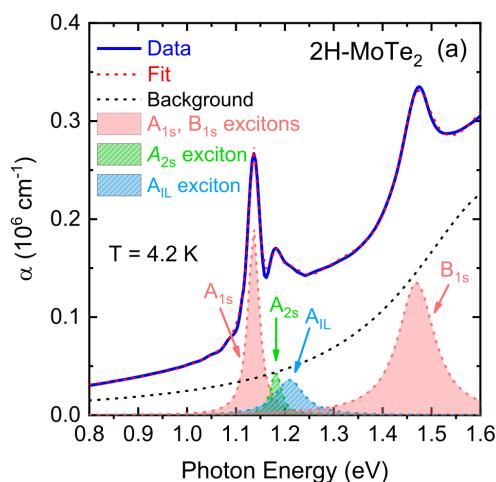
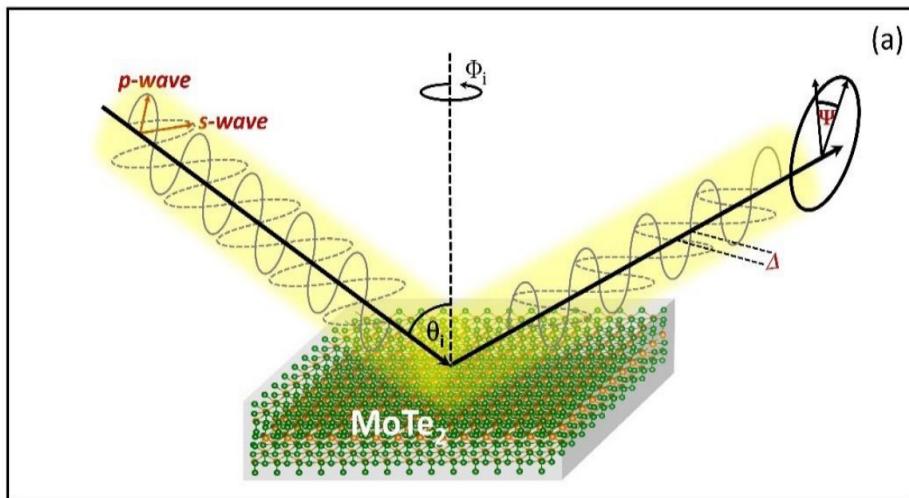
But easy in DFT

$$\alpha = \frac{\sqrt{2}\omega}{c} \sqrt{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)}$$

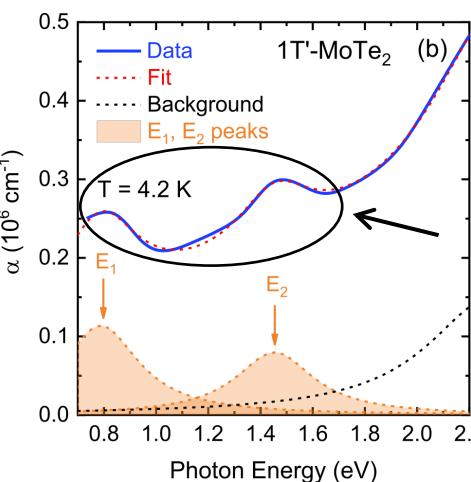


Answer: Plasmon-assisted optical absorption

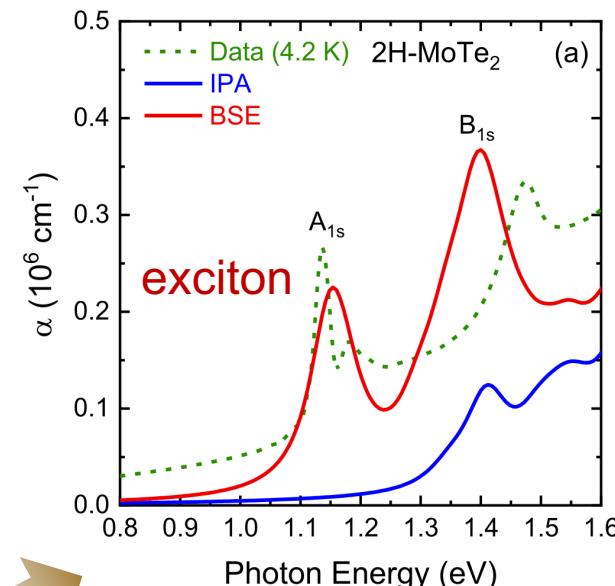
# Applications: Understanding exciton effect



Well-known from previous works

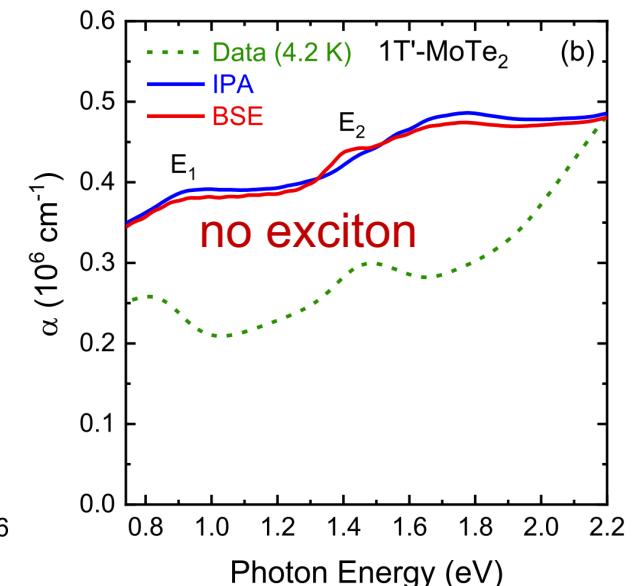


New phase (semimetal)



Origin of peaks come from excitation or not?

D. P. Gulo, N. T. Hung, et al., *Phys. Rev. Mater.* 7, 044001-1-13 (2023)

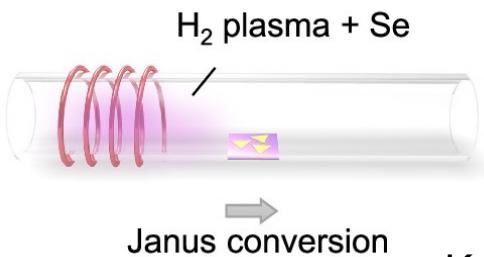
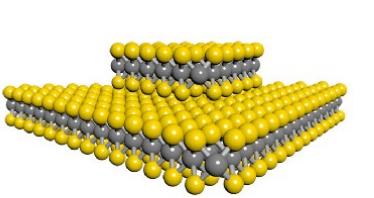


- IPA: independent particle approximation (not considering exciton effect or electron-hole interaction)
- BSE: Bethe-Salpeter equation (including exciton effect)

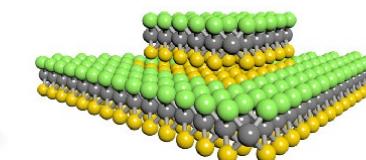
Experiment is not easy to distinguish physical phenomena, but in DFT, we can do that.

# Applications: Can DFT be first?

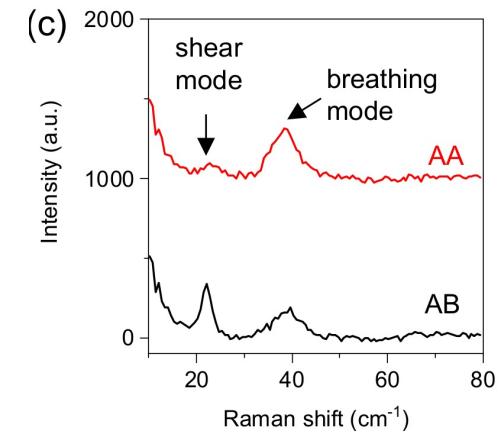
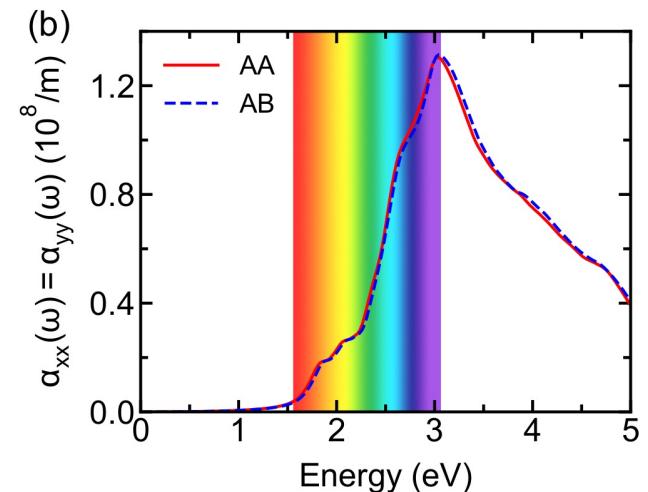
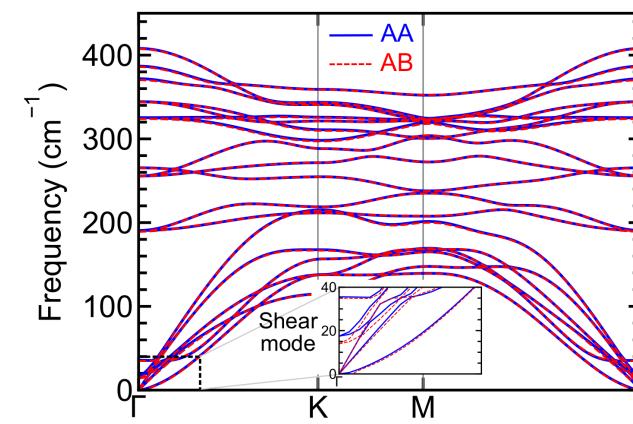
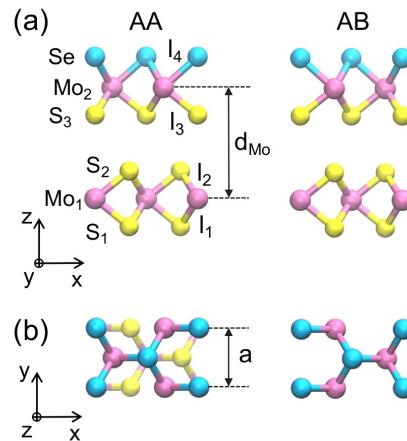
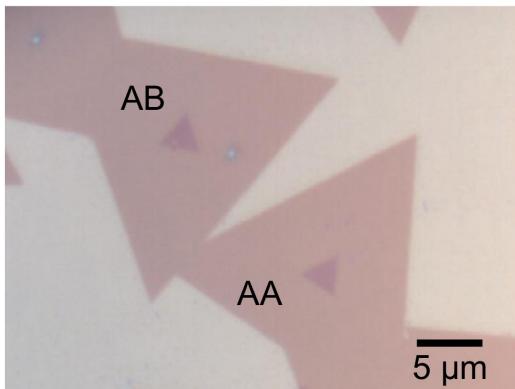
MoS<sub>2</sub> bilayer



MoS<sub>2</sub>/MoSSe heterostructure



K. Zhang et al., JACS 142, 17499 (2020)



Both AA and AB stakings exist BUT electronic, phonon, liner optical properites are almost similar expect the Raman of shear mode at low frequency (not easy to observe)  
→ How to distinguish the AA and AB structure of heterostructure by other way?

# Applications: Can DFT be first?

## Non-linear optic with second harmonic generation (SHG)

Polarization:  $\mathbf{P}_i(t) = \epsilon_0(\chi_{ij}^{(1)}\mathbf{E}_j(t) + \chi_{ijk}^{(2)}\mathbf{E}_j(t)\mathbf{E}_k(t) + \dots)$

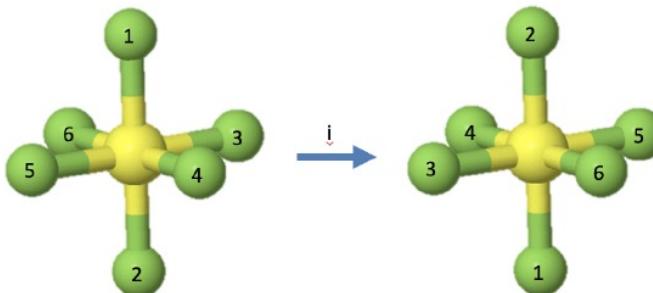
optical linear response

optical non-linear response

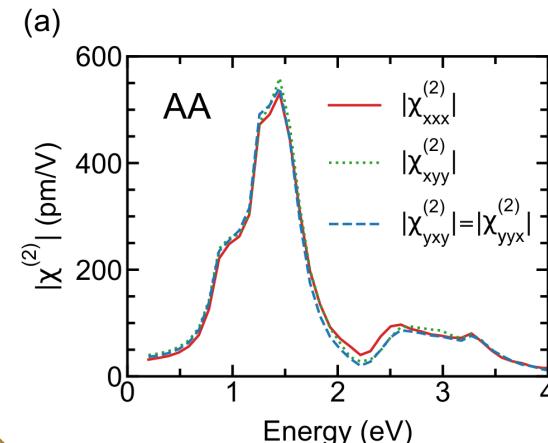
For inversion symmetry:  $\mathbf{P} \rightarrow -\mathbf{P}$  and  $\mathbf{E} \rightarrow -\mathbf{E}$   
 $\rightarrow \chi^{(2)}$  must be zero

For broken inversion symmetry  $\rightarrow \chi^{(2)} \neq \text{zero}$

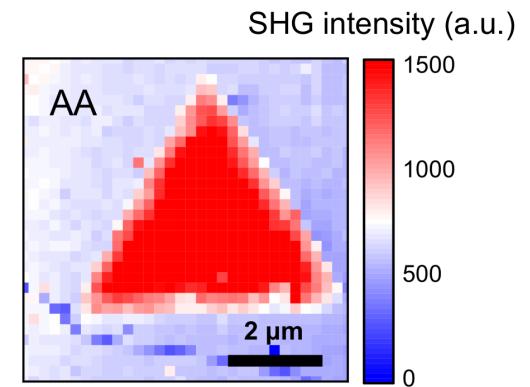
Inversion symmetry:  $(x, y, z) \rightarrow (-x, -y, -z)$



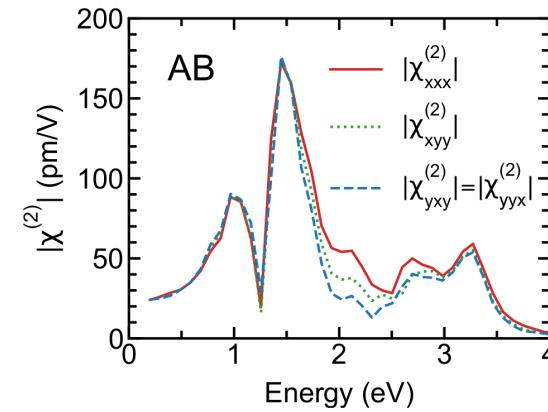
Theory



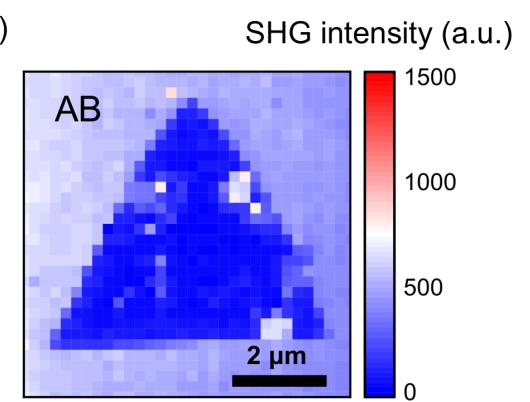
Experiment



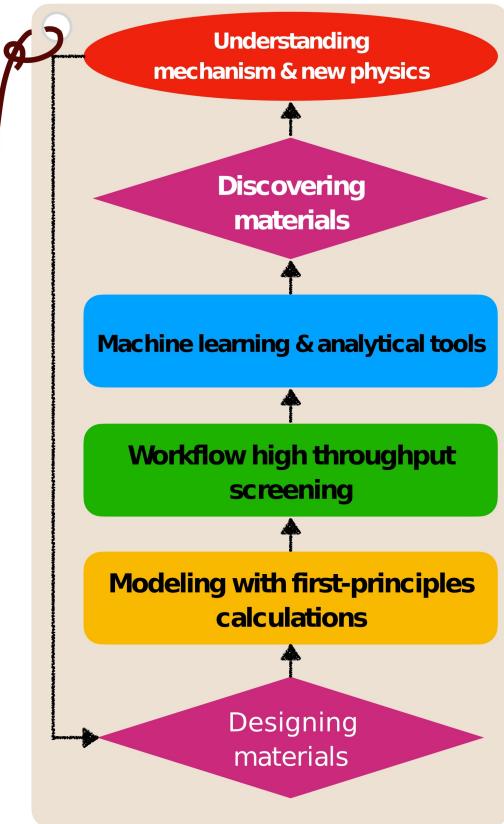
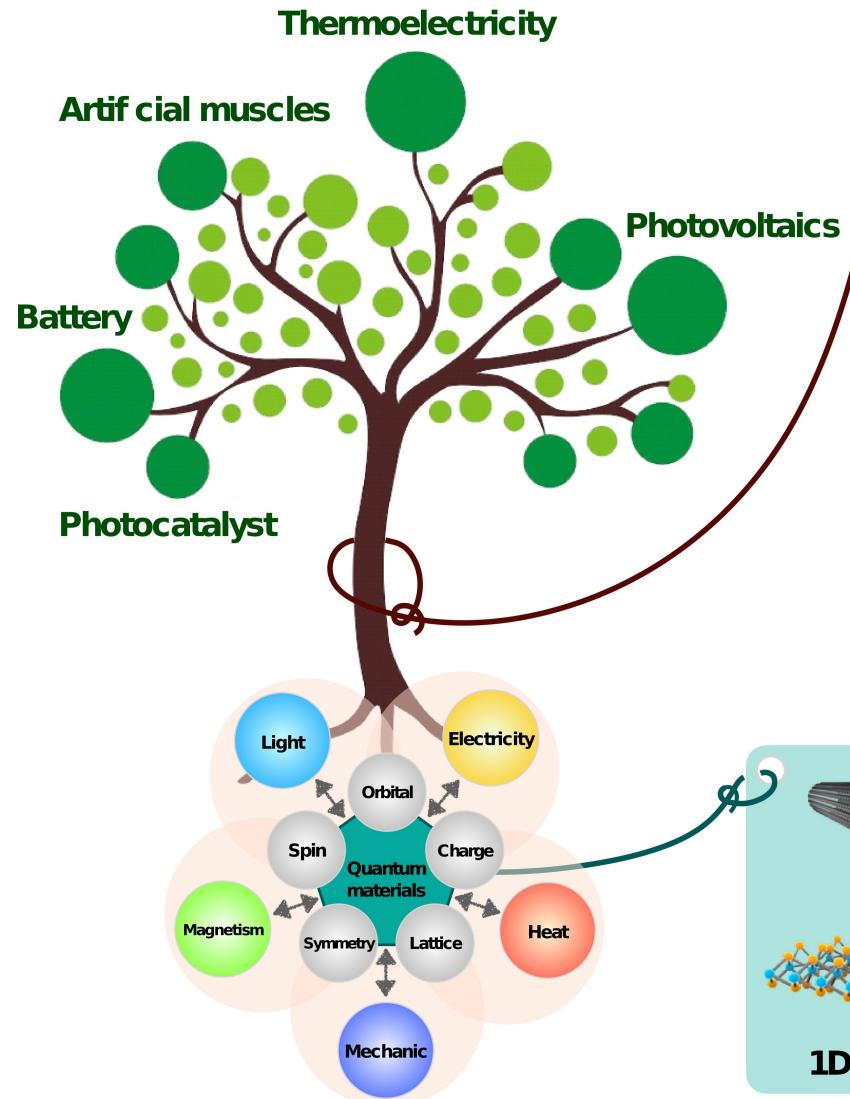
(c)



(d)

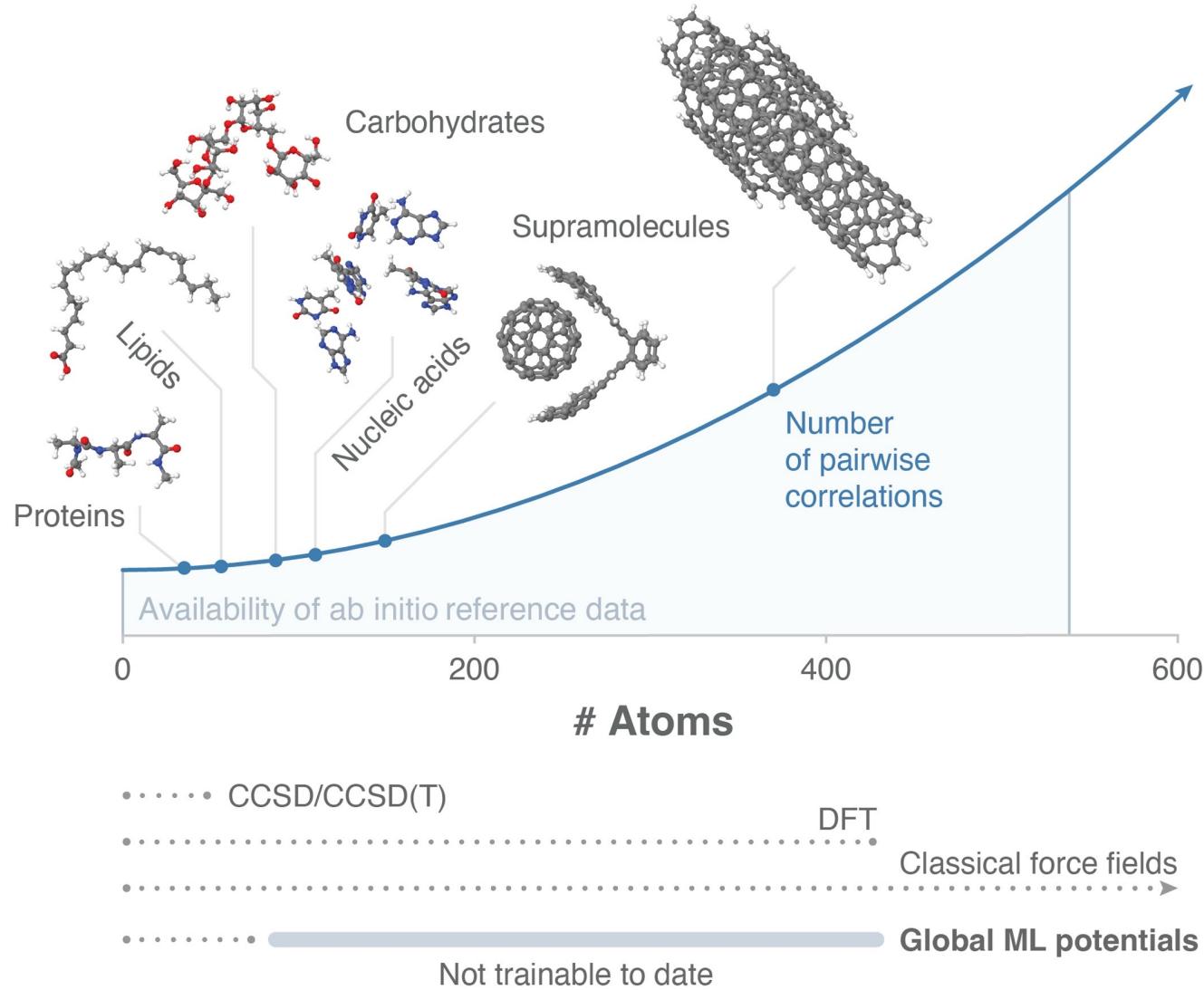


# Energy tree



For detail: <https://nguyen-group.github.io>

# Large-scale DFT Calculations and Moving to GPUs



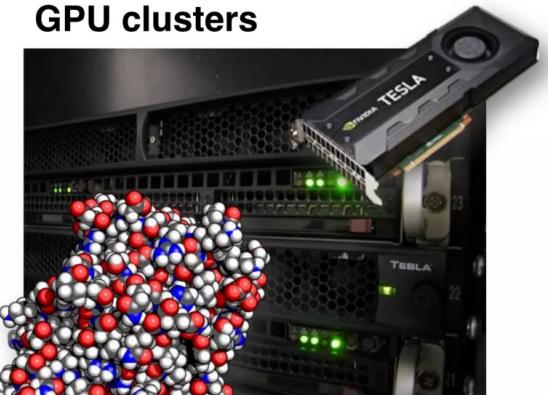
Chmiela et al., Sci. Adv. 9, eadf0873 (2023)

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



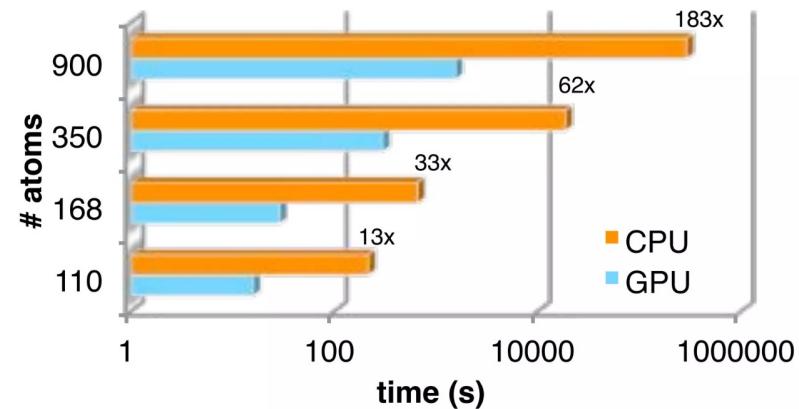
DFT on a **handful of atoms** (three to ~100)

**now:**  
GPU clusters

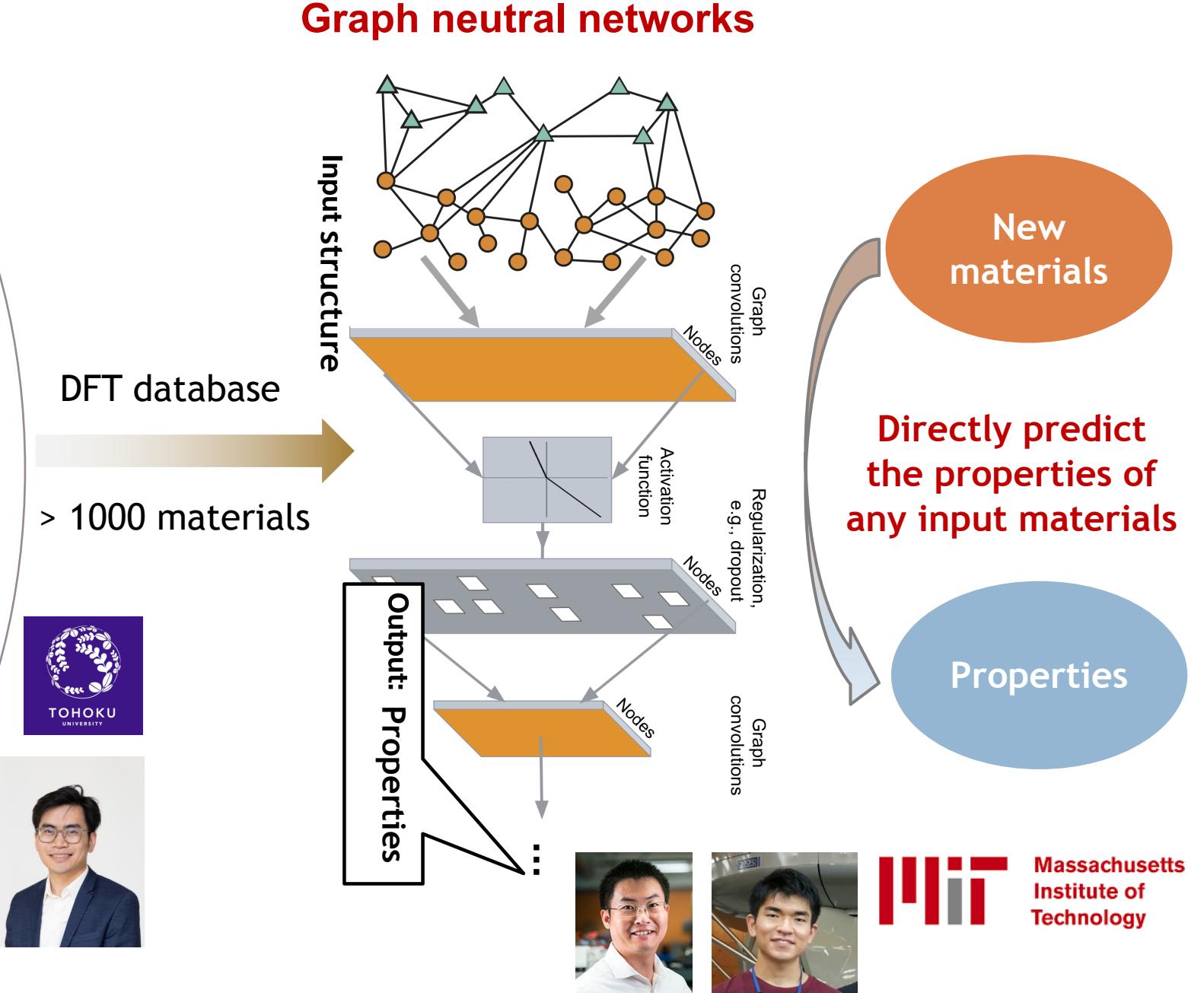
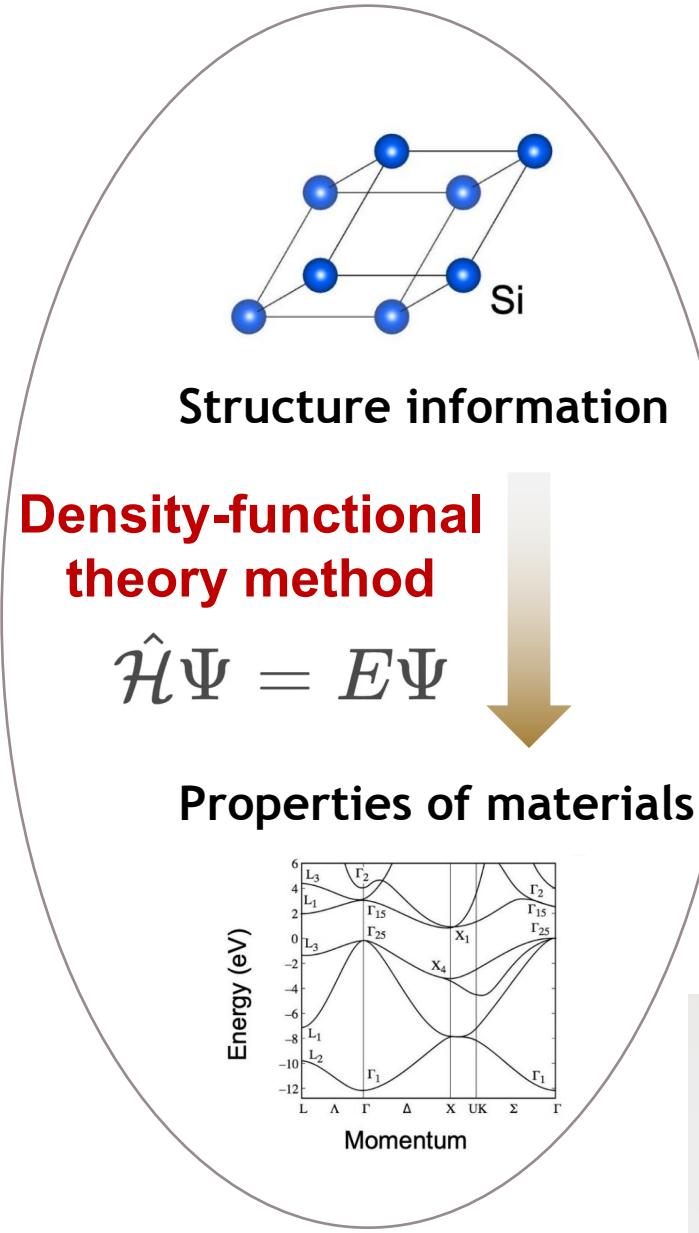


DFT or better on **three thousand atoms!**

Novel architecture & GPU-optimized algorithms:



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





Please enjoy running Quantum ESPRESSO!

# Many Other Examples

