



Summer Workshop 2023 @ HUST, Hanoi

Introduction to Density-Functional Theory with Quantum ESPRESSO

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Department of Physics, Tohoku University



<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

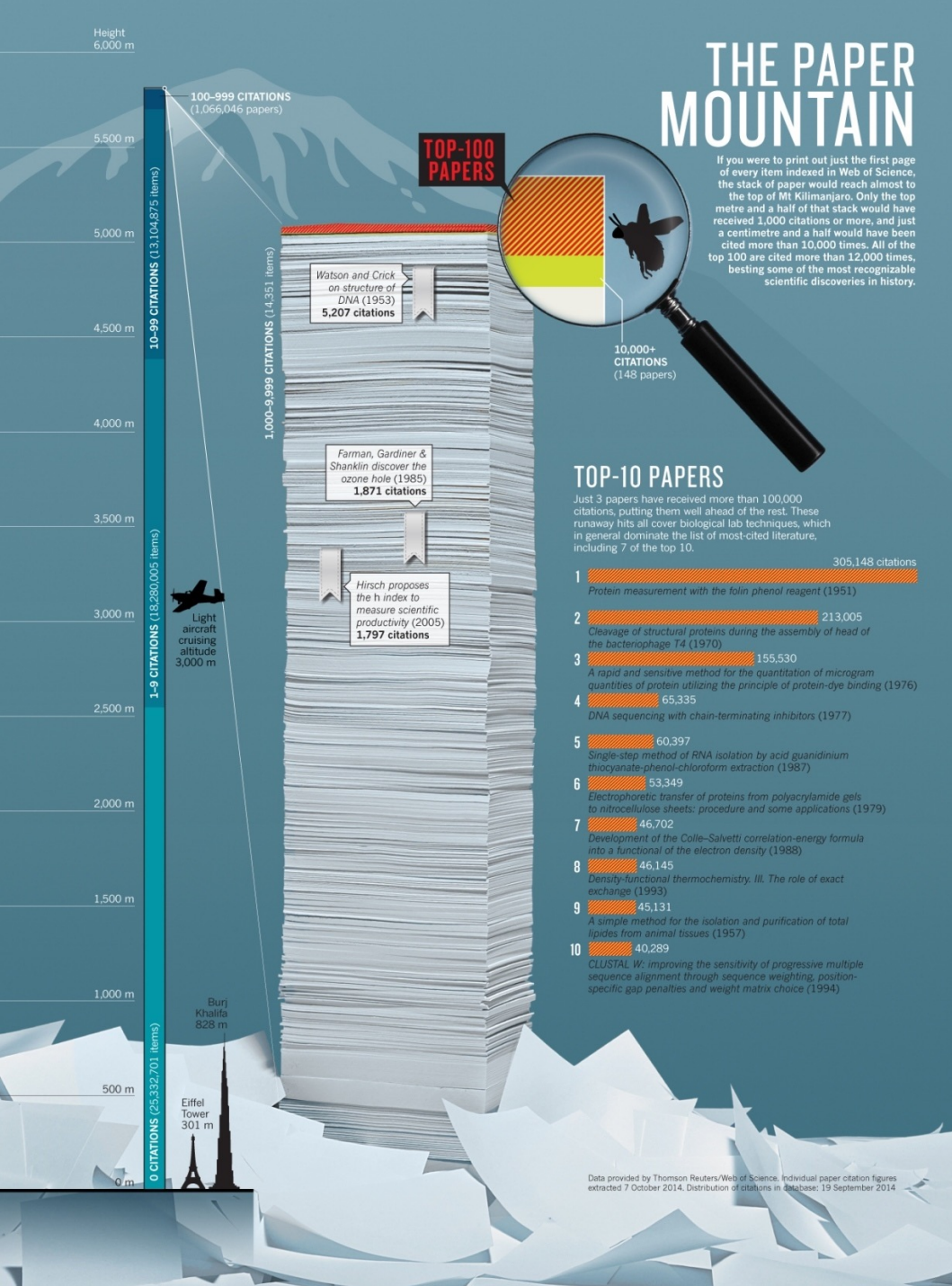
Our office

Aoba-ku
station



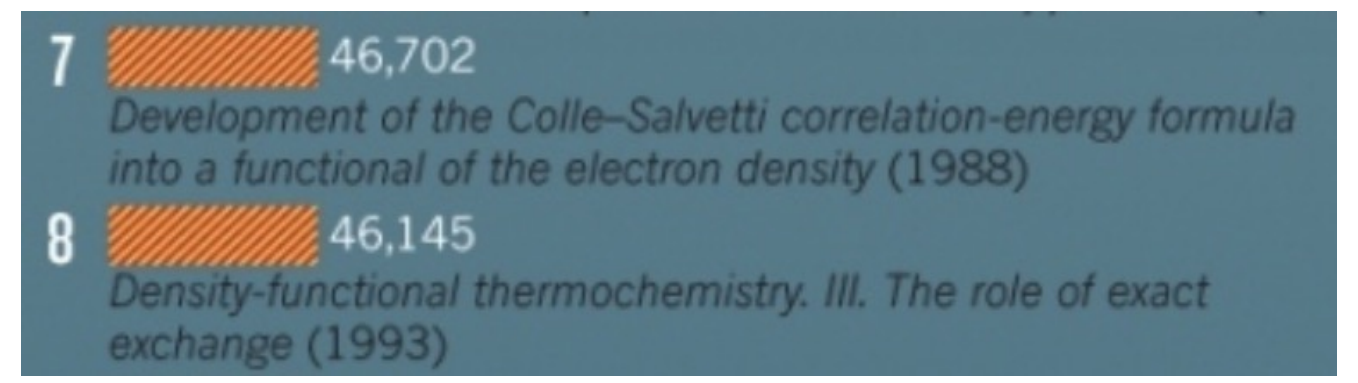
Content

- 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

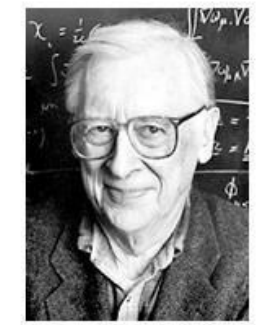
THE TOP 10 PAPERS: 2 papers on density-functional theory (DFT) in the top 10 most cited papers in the entire scientific literature, ever. **NATURE, OCT 2014**



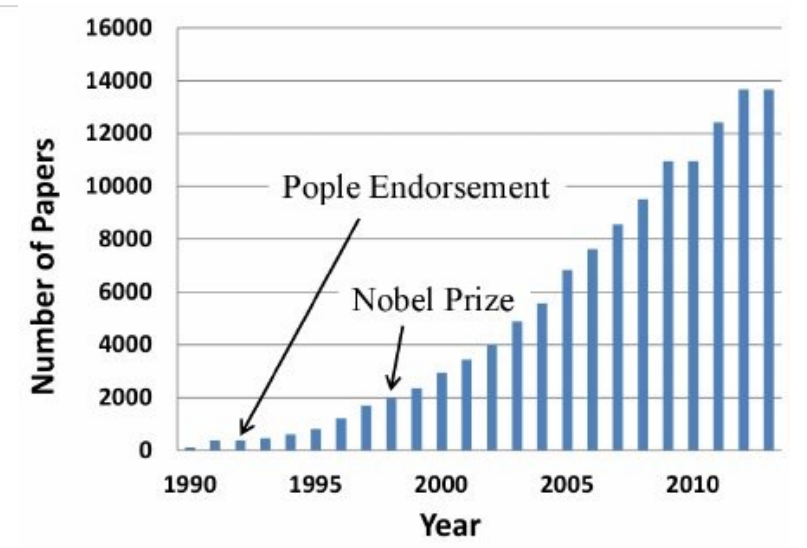
The Nobel Prize in Chemistry 1998



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	BlochI
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)

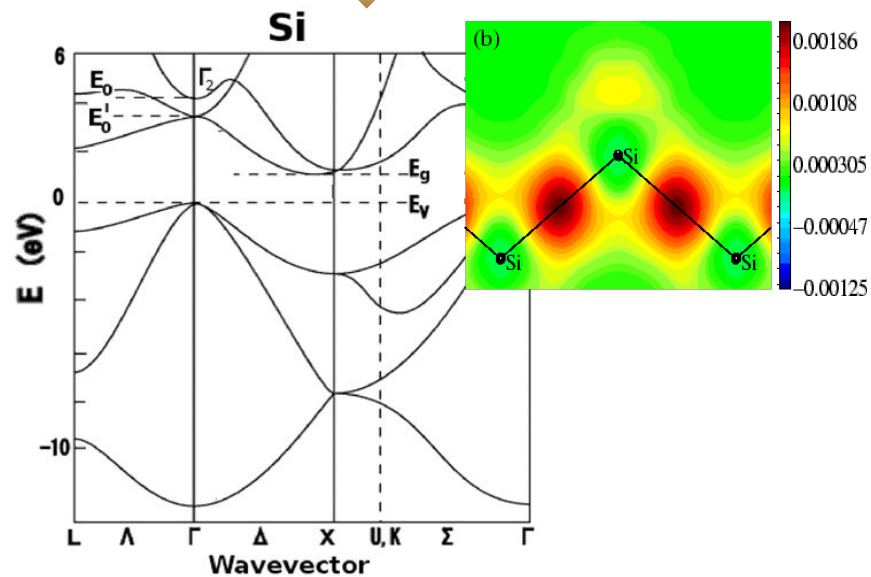
Hohenberg–Kohn theorems

Starting point of the concepts of DFT

What is DFT?

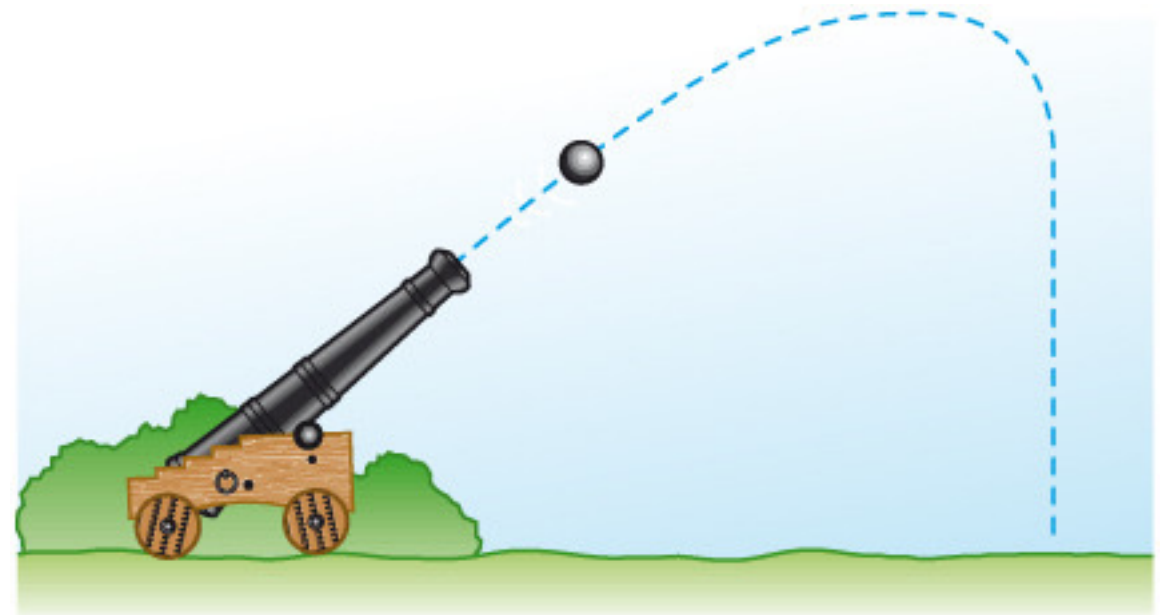
DFT is a method for solving the Schrödinger equation

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



The Newton equation

$$F = ma$$



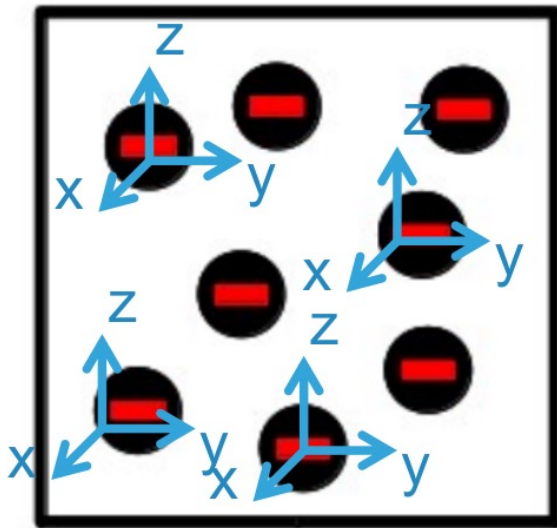
The Idea of DFT - Electron Density



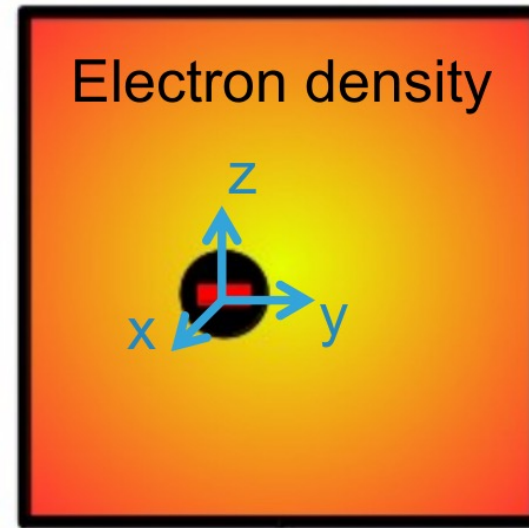
Reduction of dimensionality!



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



3N-dimensional
partial differential equation (PDE)



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 $E[n(\mathbf{r})]$ 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

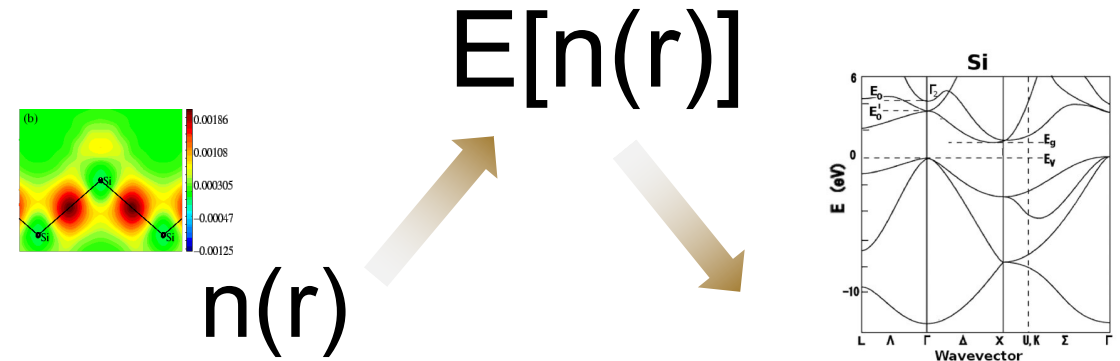
Physics

Article

References

Citing Articles (38,993)

Density-functional theory

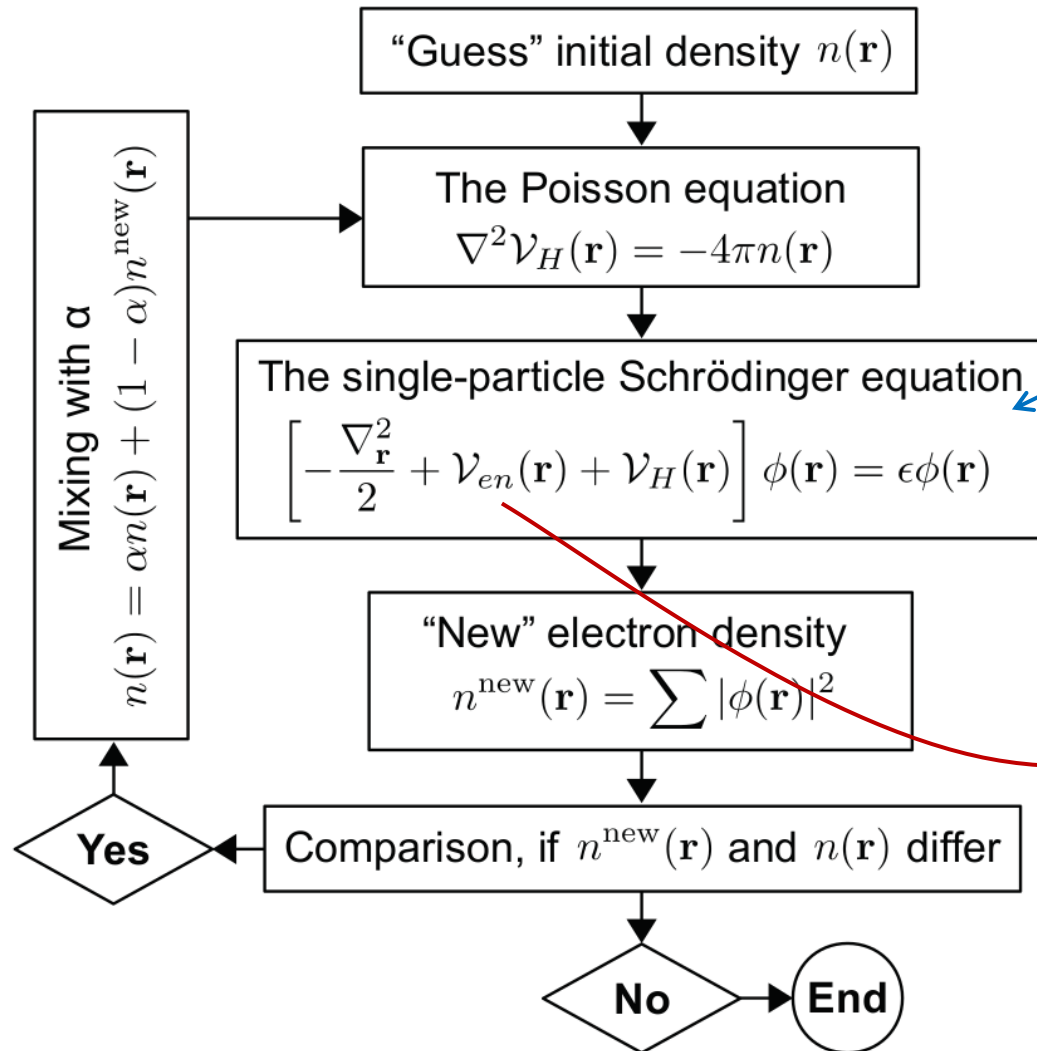


Electron density

Properties

How to Know $n(\mathbf{r})$?

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

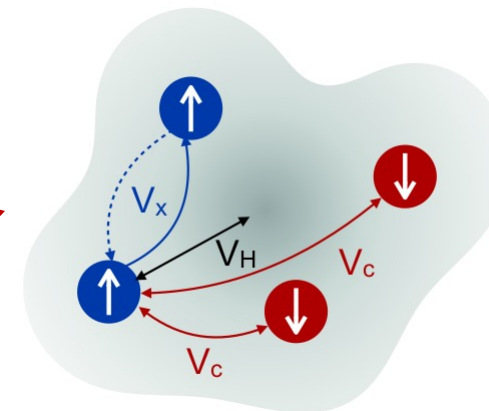
References

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)

Article

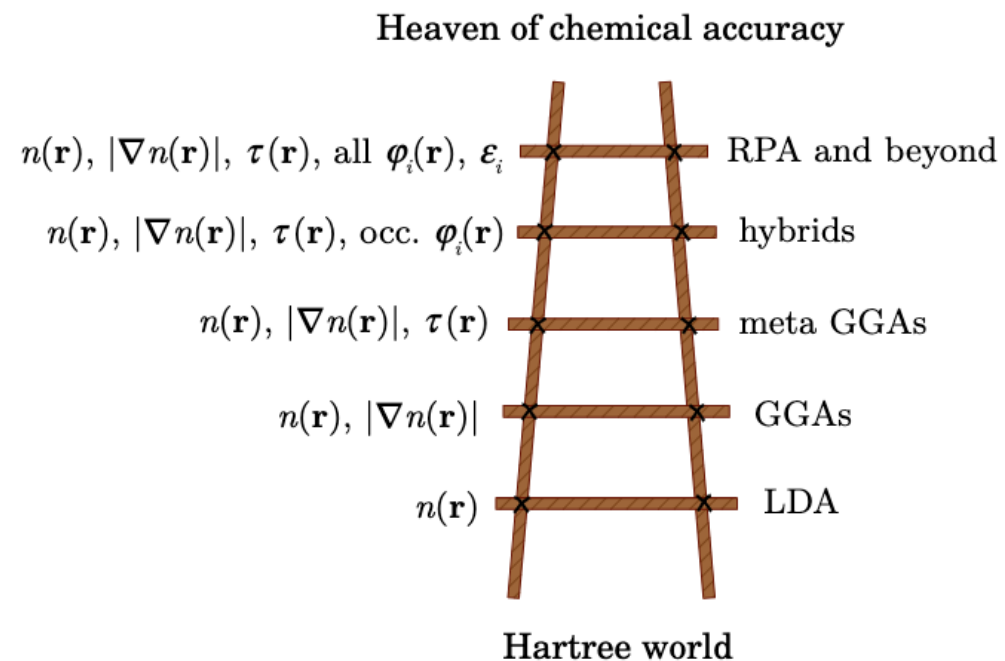
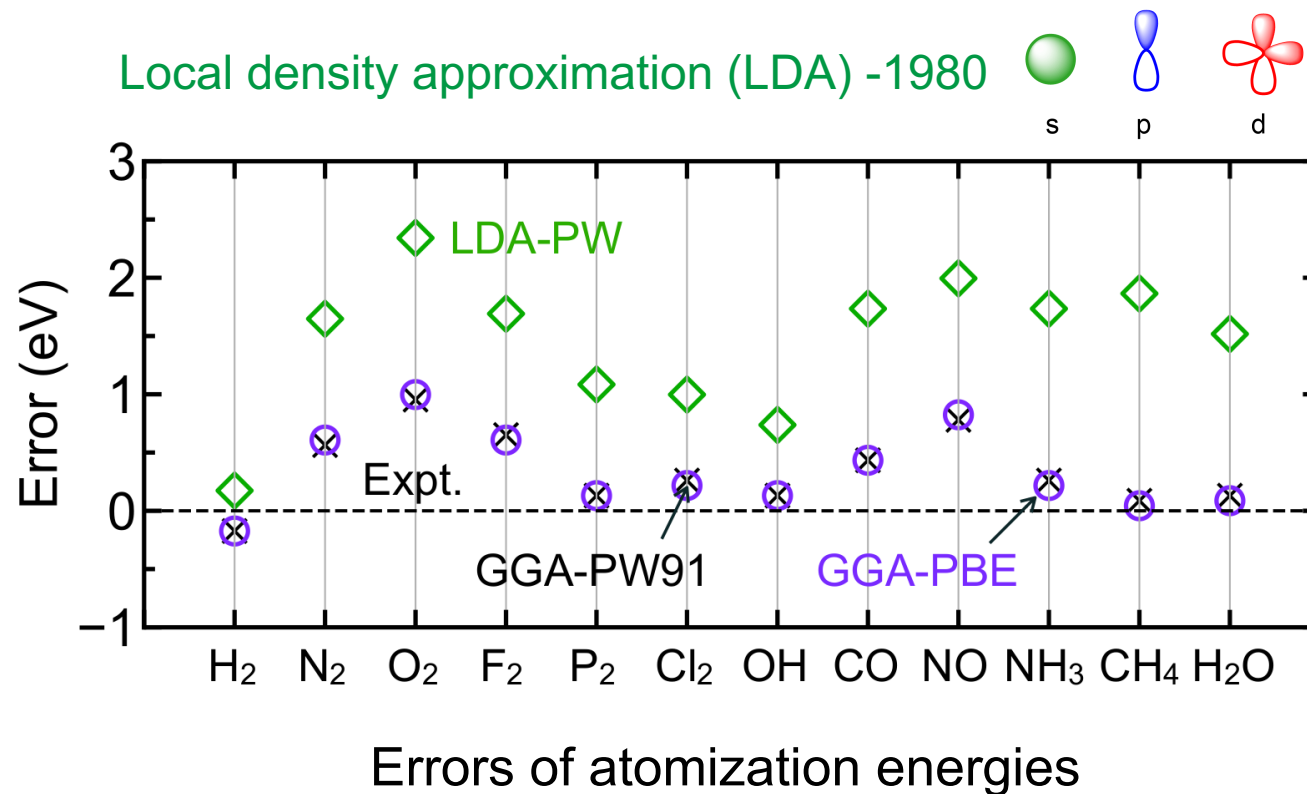
References

Citing Articles (130,981)

PDF

Export Citation

It takes 30 years to introduce a good approximation functional



Which Codes for DFT?

Trends in atomistic simulation engines

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 \$	PBC PP PW	Source NGC conda DNF Macports APT SingularityHub AUR Nix Spack EasyBuild Yum	Free	🔒	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	↗

Easy to install

Free

Chemical Sciences and Materials @ 2022 (PRACE)

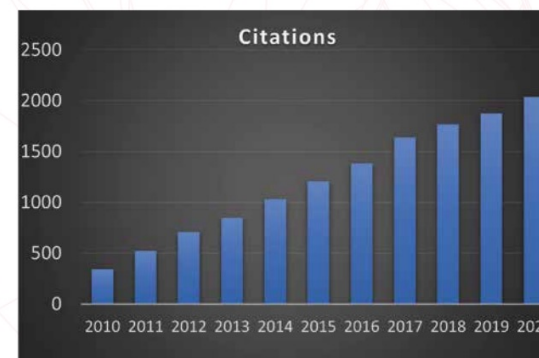


Fig1a

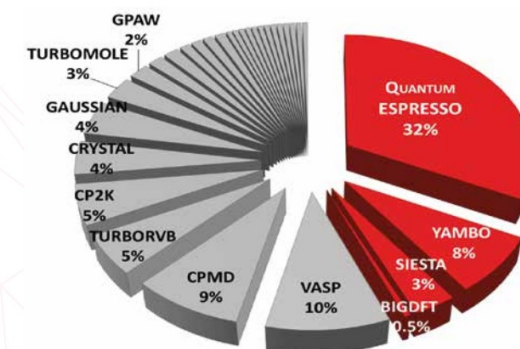
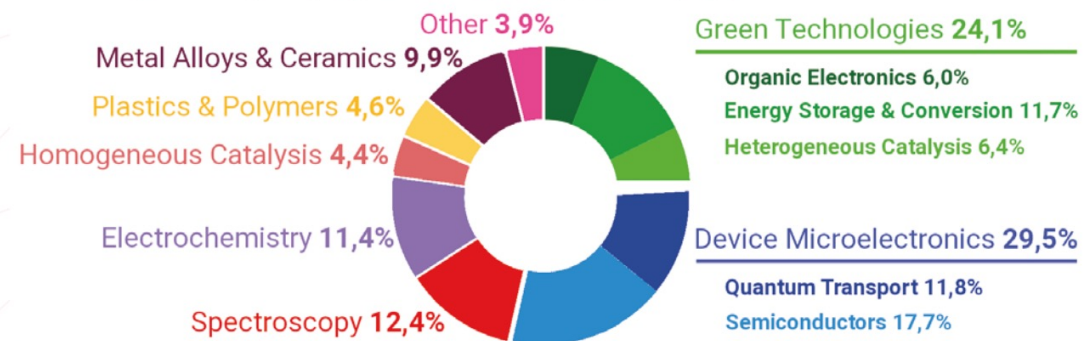


Fig1b



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:

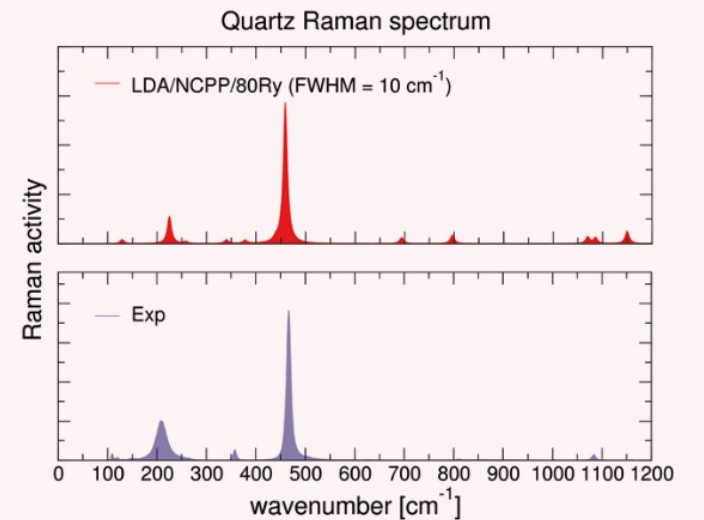
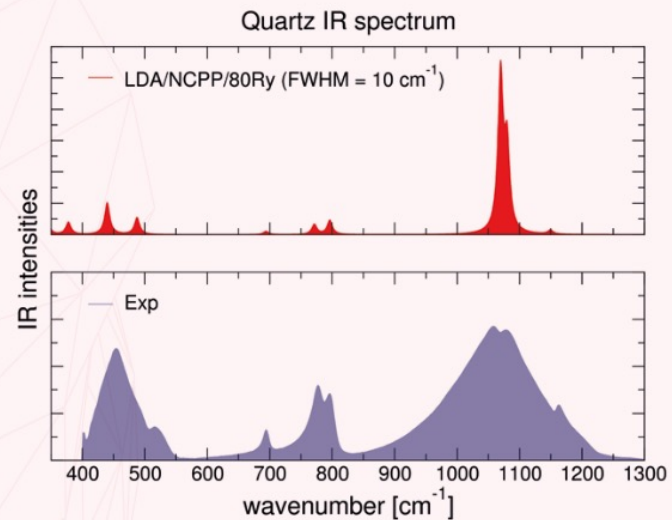
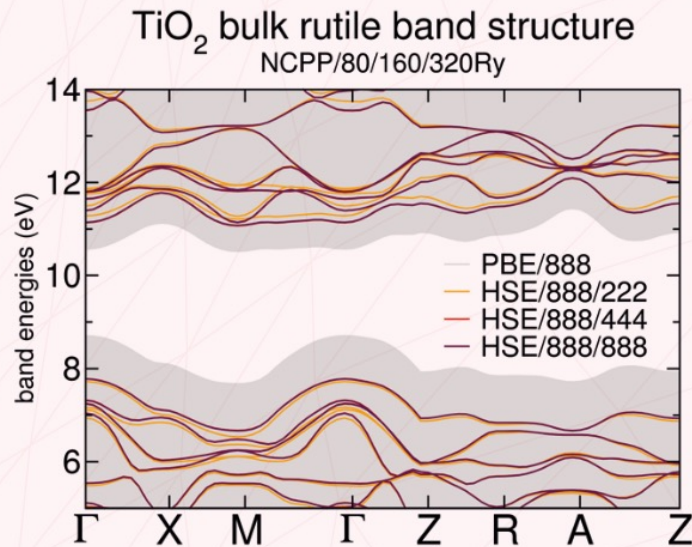
- ◆ Phonon frequencies
- ◆ IR and Raman spectra (e.g. Fig2b, Fig2c)
- ◆ Dielectric properties

TDDFPT:

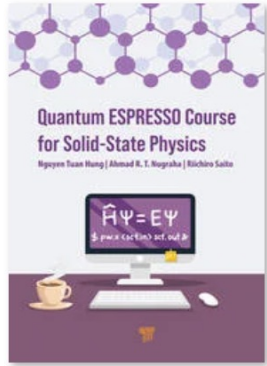
- ◆ UV-Vis absorption
- ◆ Electron energy loss spectroscopy
- ◆ Spin wave spectroscopy

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

- ❑ 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>)
- ❑ Thoery for DFT & solid-state physics for Quantum ESPRESSO



Share



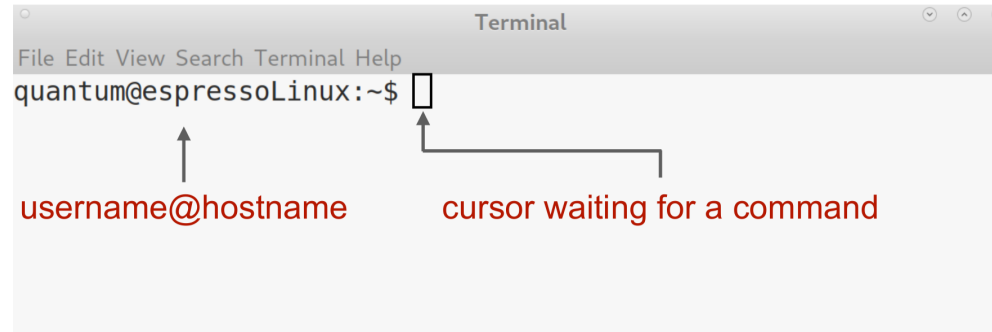
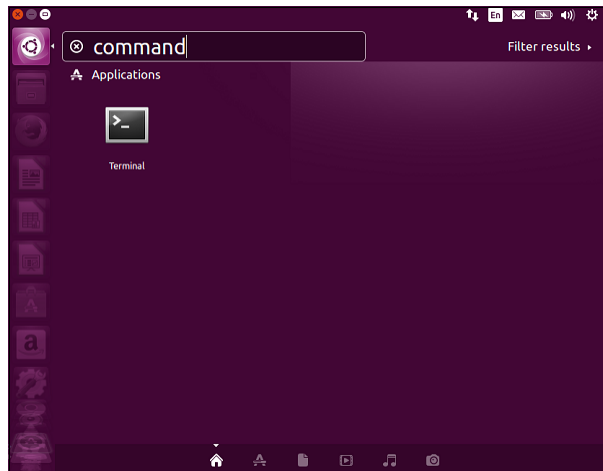
Citation



Many workshops about Quantum-ESPRESSO are organized by us.

- 2016: Tohoku Univerisity (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:

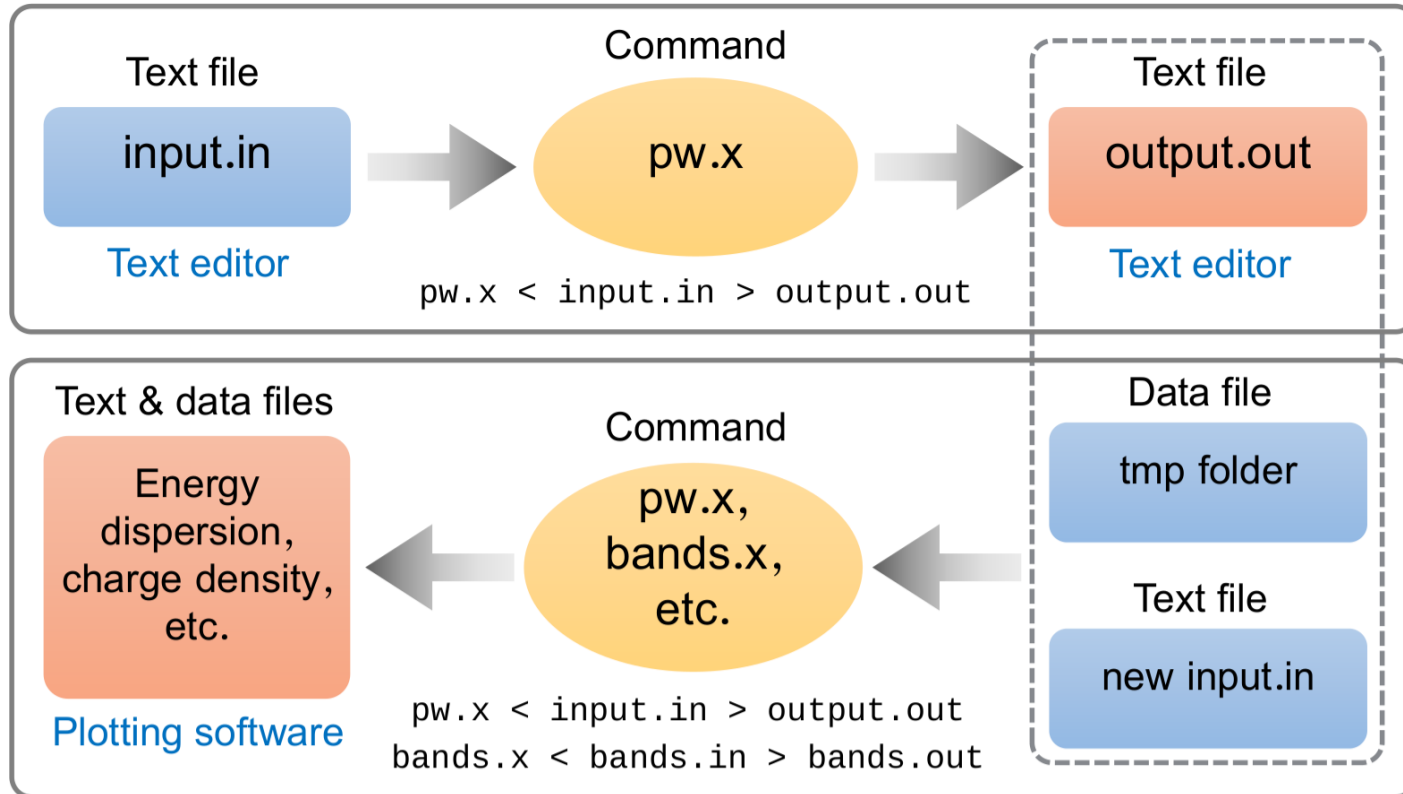
```
$ sudo apt-get update
```

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
```

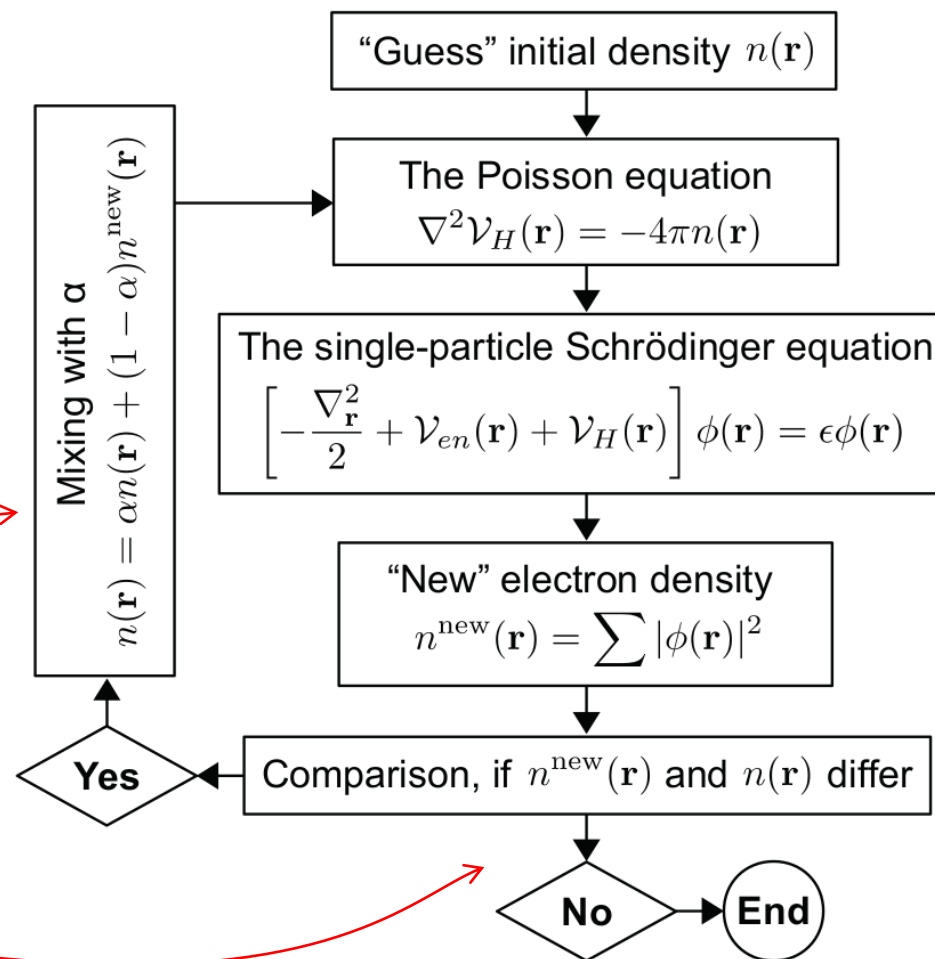
QE-SSP/gr/scf/scf.in

```

1 &CONTROL
2 calculation = 'scf'
3 pseudo_dir = '../pseudo/'
4 outdir      = '../tmp/'
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'
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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



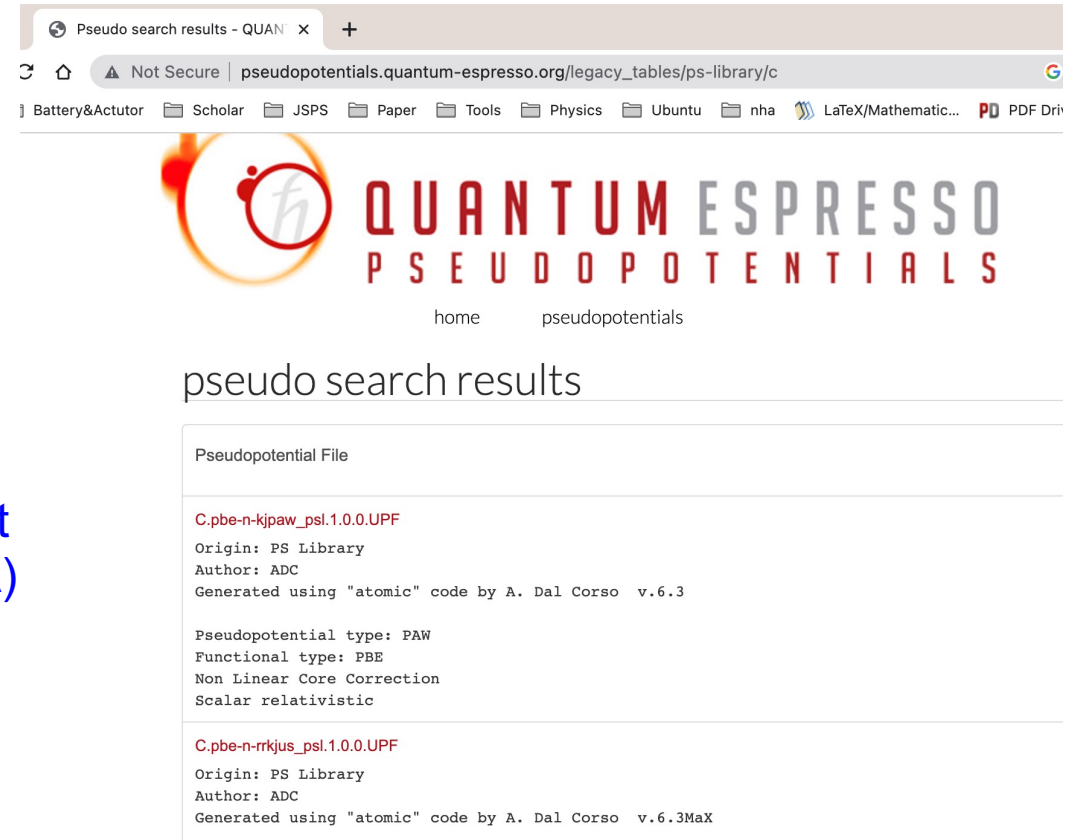
QE-SSP/gr/scf/scf.in

```
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
```

output data
(charge density, etc.)

name of project

Generalized gradient
approximation (GGA)



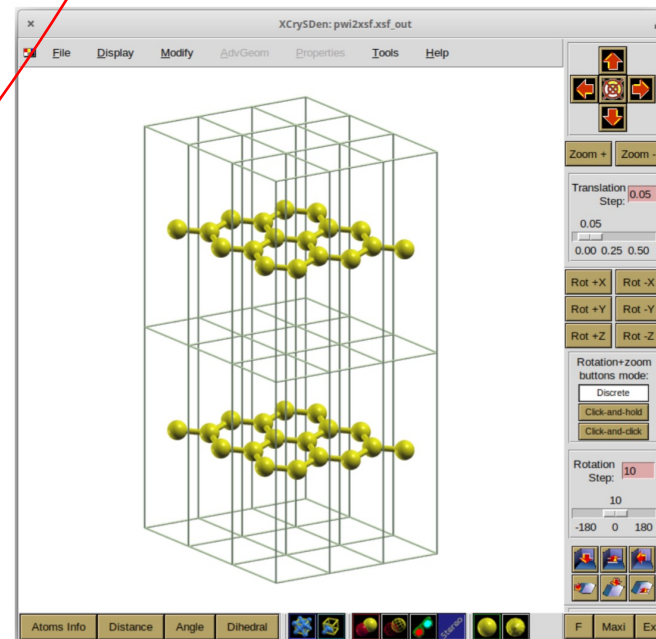
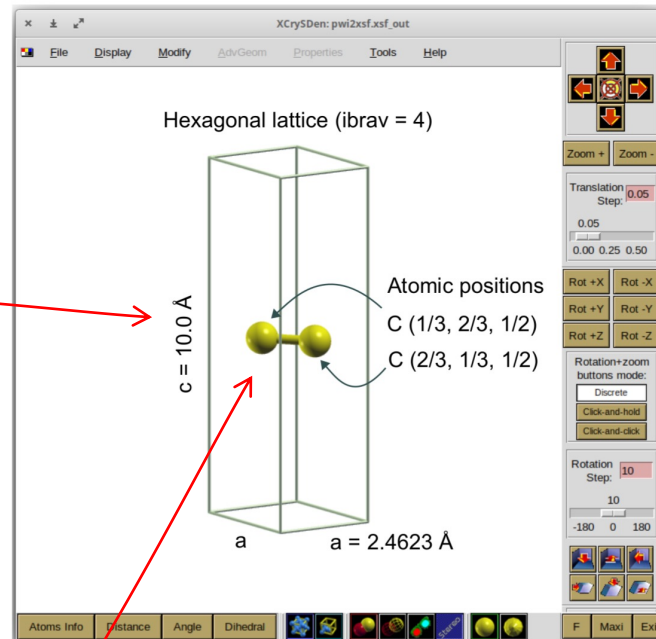
The screenshot shows a web browser window with the address bar displaying "pseudopotentials.quantum-espresso.org/legacy_tables/ps-library/c". The page features the Quantum Espresso logo and the text "QUANTUM ESPRESSO PSEUDOPOTENTIALS". Below the logo, there are navigation links for "home" and "pseudopotentials". The main content area is titled "pseudo search results" and lists two pseudopotential files:

- 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

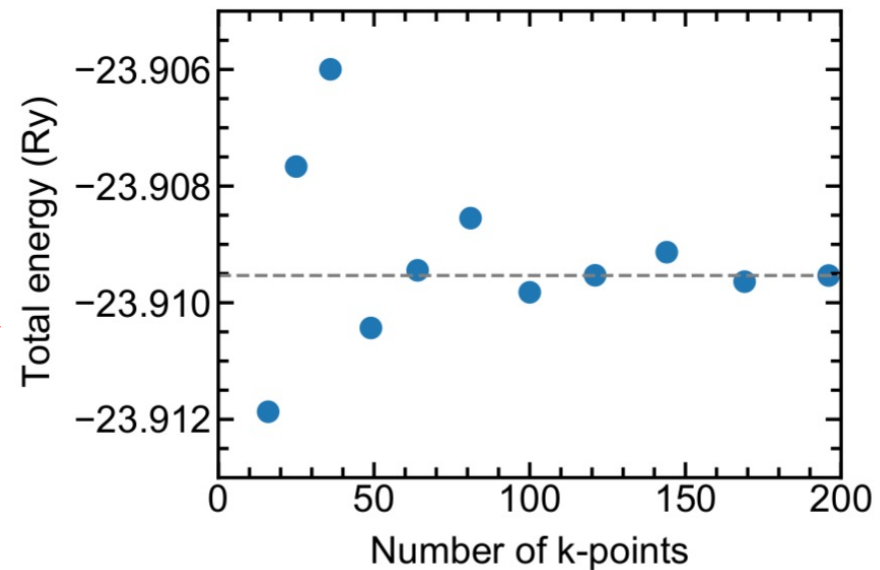
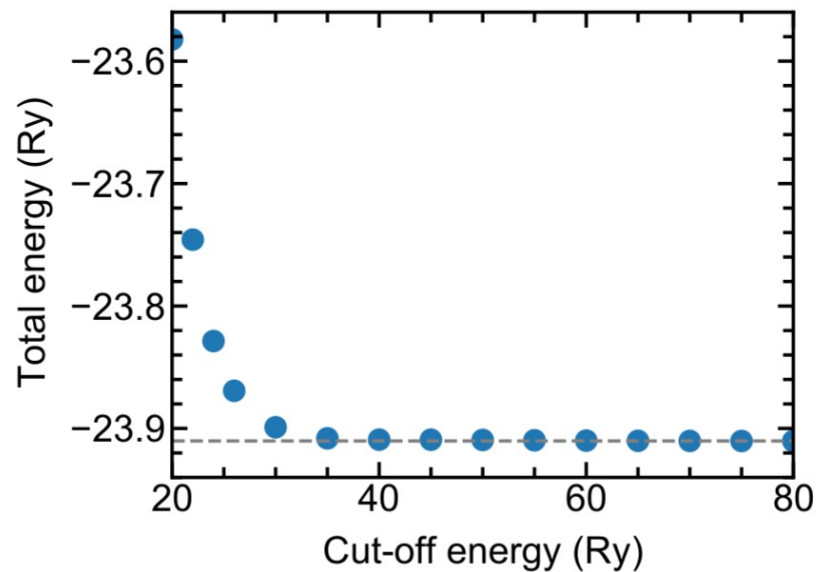


QE-SSP/gr/scf/scf.in

```
1 &CONTROL
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3 pseudo_dir = '../pseudo/'
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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
```

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 Copy code
&control
  calculation = 'scf'
  prefix = 'graphene_energy'
  pseudo_dir = '/path/to/pseudopotentials'
  outdir = './tmp'
/
&system
 ibrav = 4
  cellldm(1) = 2.462
  nat = 2
  ntyp = 1
  ecutwfc = 40
/
&electrons
/
ATOMIC_SPECIES
  C 12.011 C.pbe-n-kjpaw_ps1.1.0.0.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:

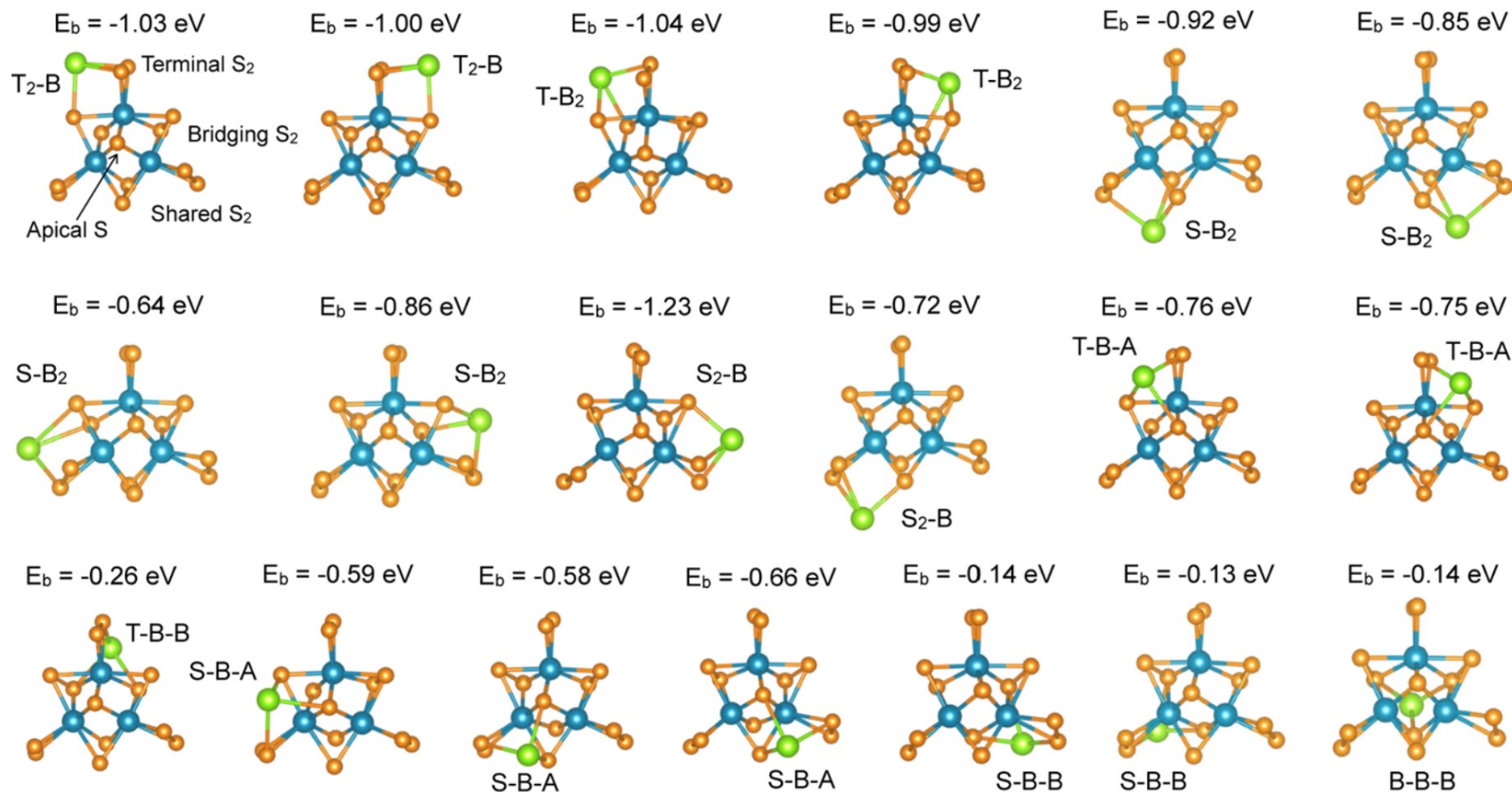


```
java Copy code
&inputph
  prefix = 'graphene_phonon'
  tr2_ph = 1.0e-14
  fildyn = 'graphene.dyn'
  amass(1) = 12.011
  outdir = './tmp'
/
&input
  asr = 'simple'
  fildyn = 'graphene.dyn'
  nat = 2
  ntyp = 1
  ecutwfc = 40
/
CELL_PARAMETERS {angstrom}
  2.462000 0.000000 0.000000
  0.000000 2.462000 0.000000
  0.000000 0.000000 20.0
ATOMIC_SPECIES
  C 12.011 C.pbe-n-kjpaw_ps1.1.0.0.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:

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

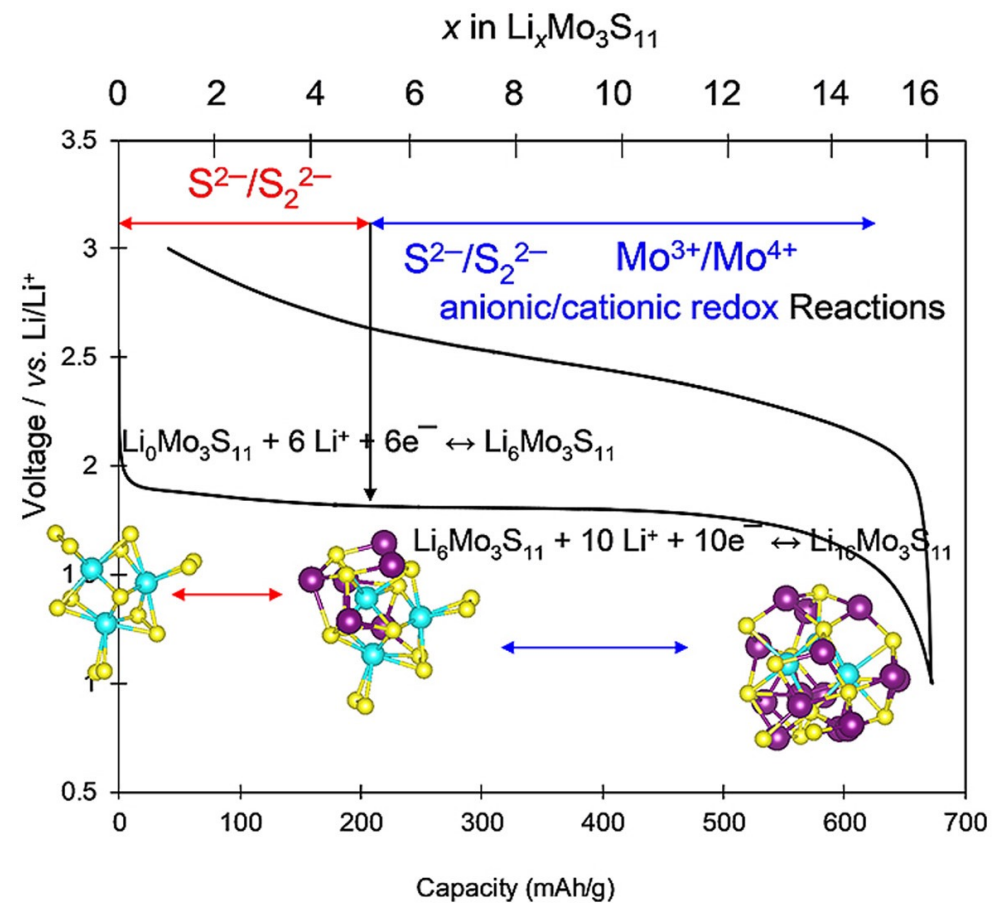
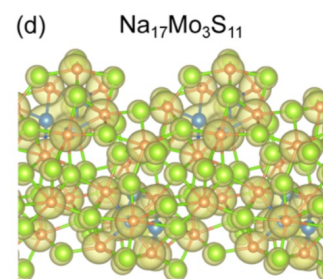
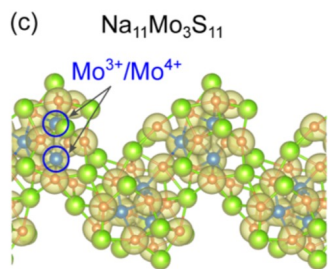
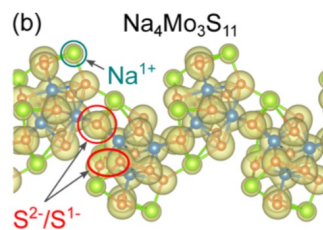
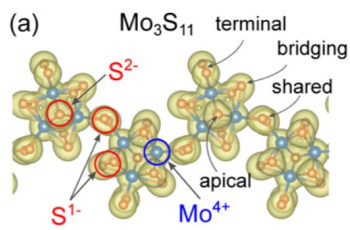
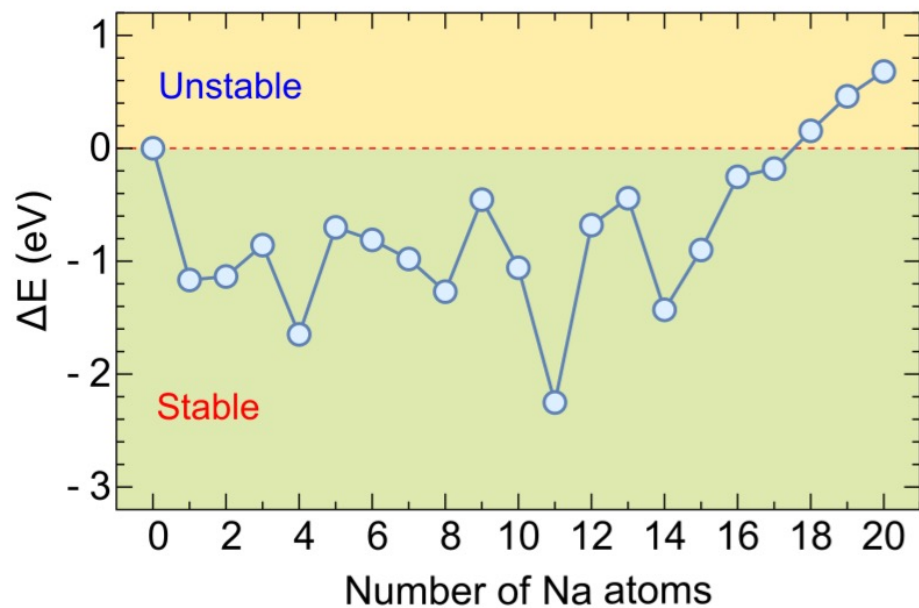


$E_b < 0$: Binding

$E_b > 0$: No
binding

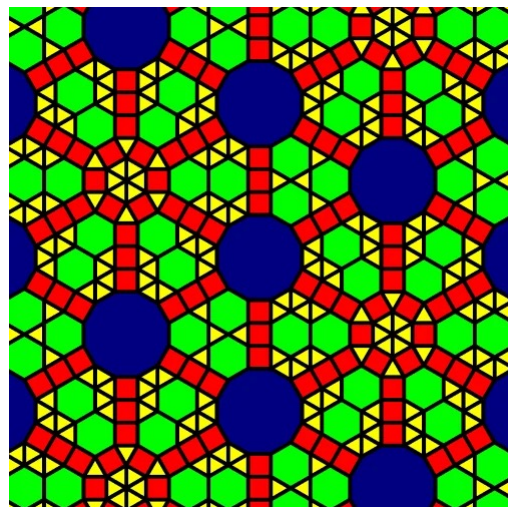
N. T. Hung et al., *J. Phys. Chem. C* 123, 30856 (2019)

Applications: Battery



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

Applications: Designing New Materials

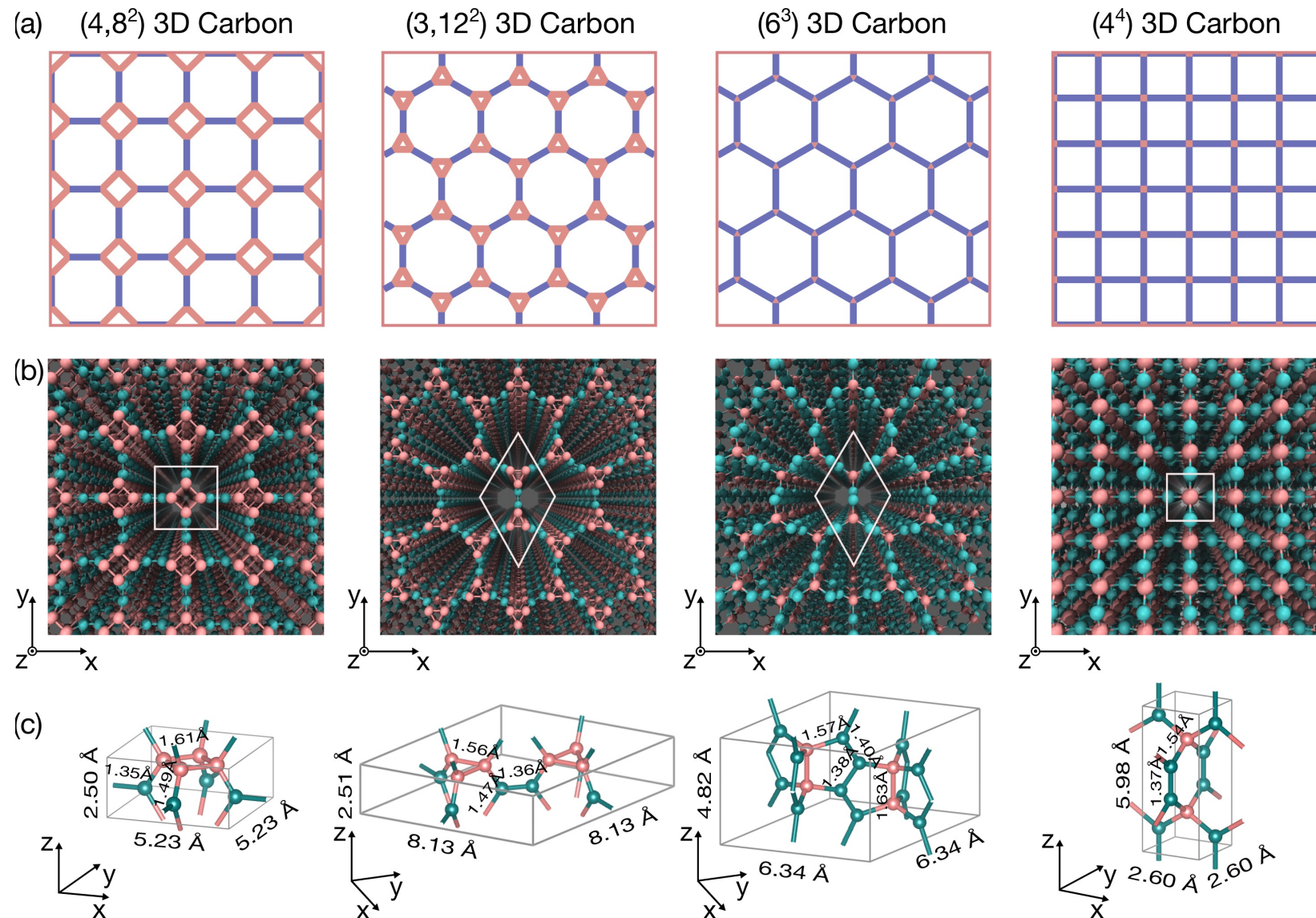


Archimedean lattice

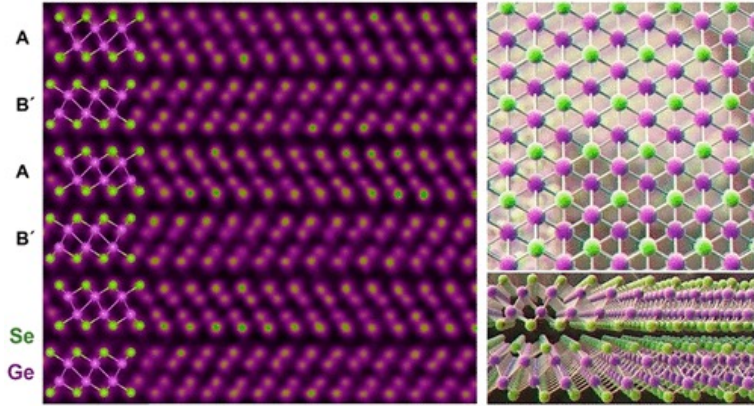


New 3D Carbon networks

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



Applications: Designing New Materials



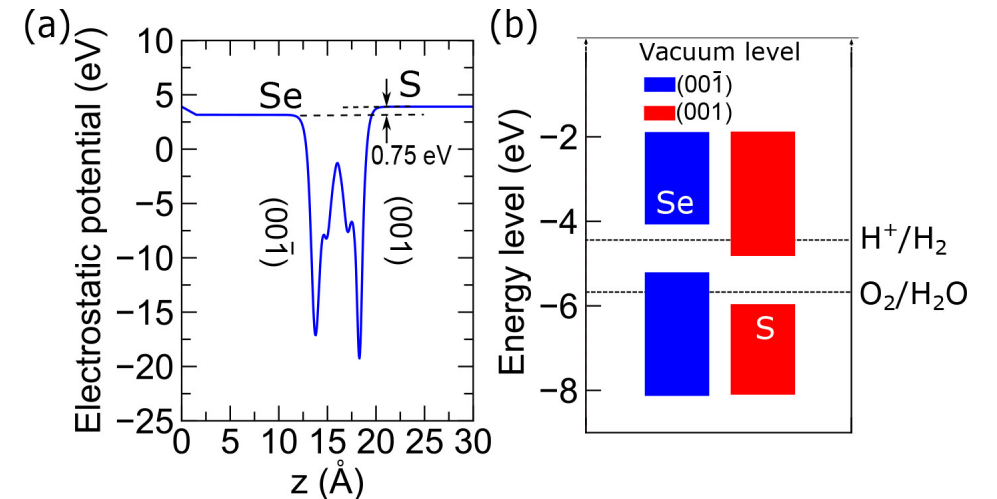
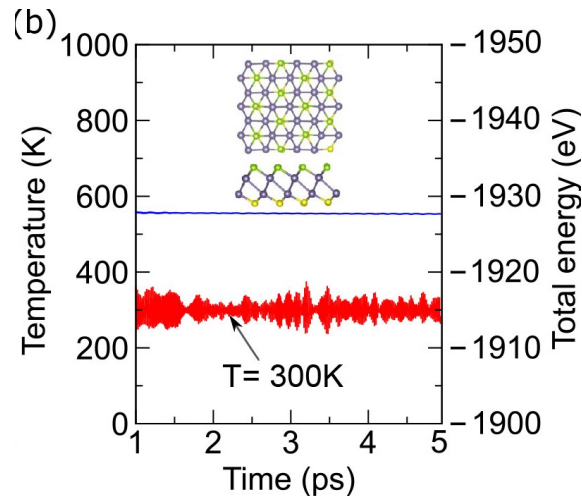
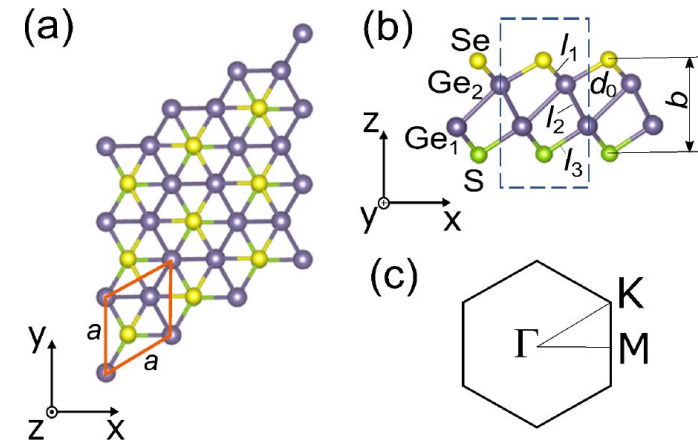
Successful synthesis of γ -GeSe
(Nano Lett. 21, 4305, 2021)

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

Replace Se atom
to S atom



New Janus 2D γ -Ge₂SSe

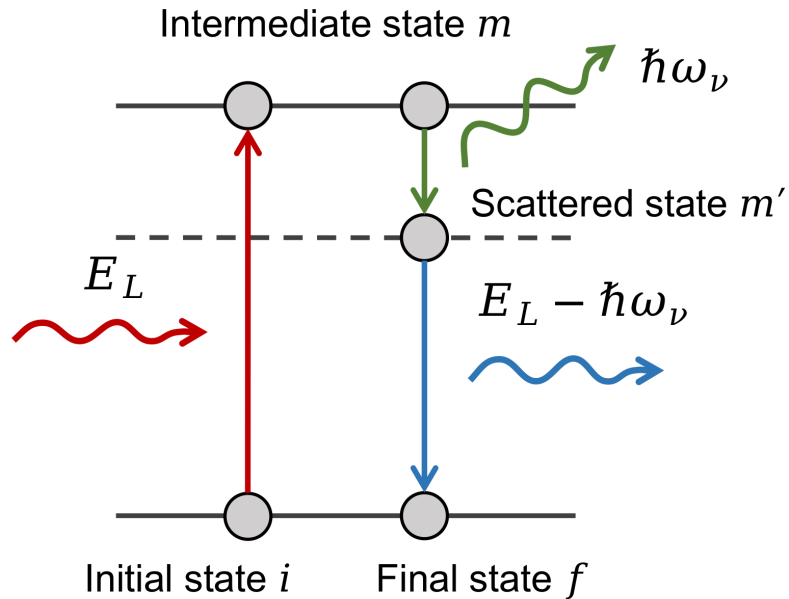


High-performance material for photocatalysis and thermoelectricity

Applications: Understanding Raman spectra

The Raman calculation is not easy in the theory

Resonant Raman scattering

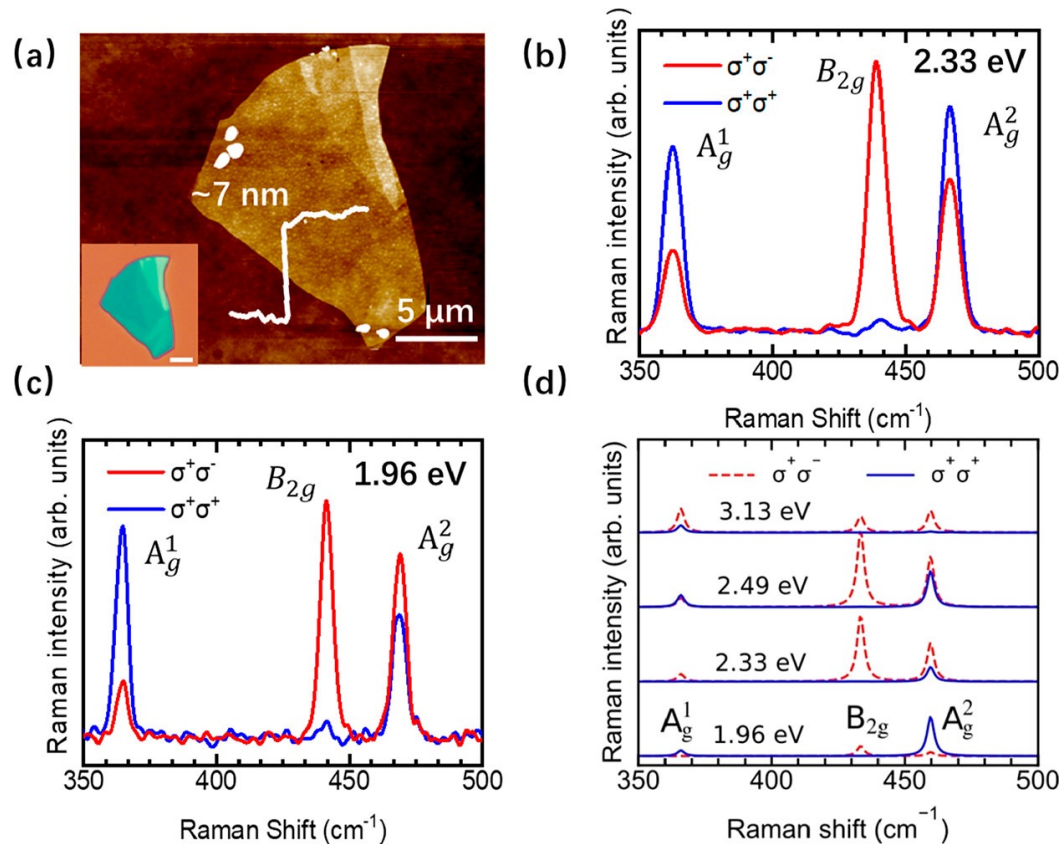


Raman intensity is given by the third-order perturbation:

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

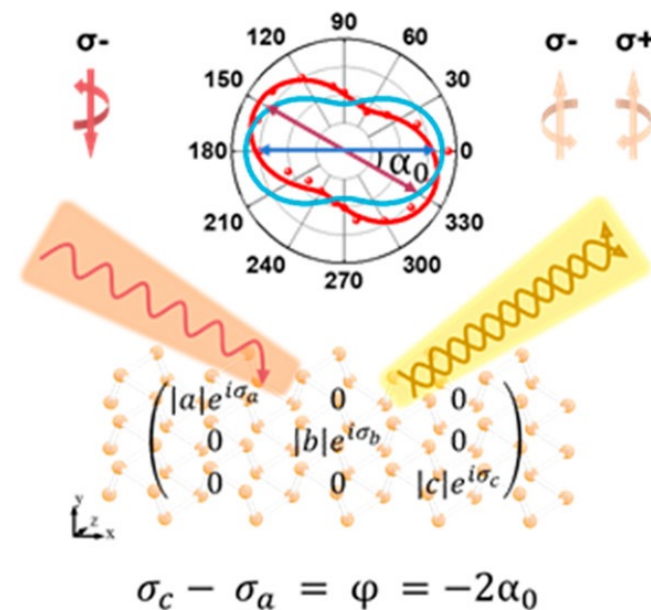
Applications: Understanding Raman spectra

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



Experiment

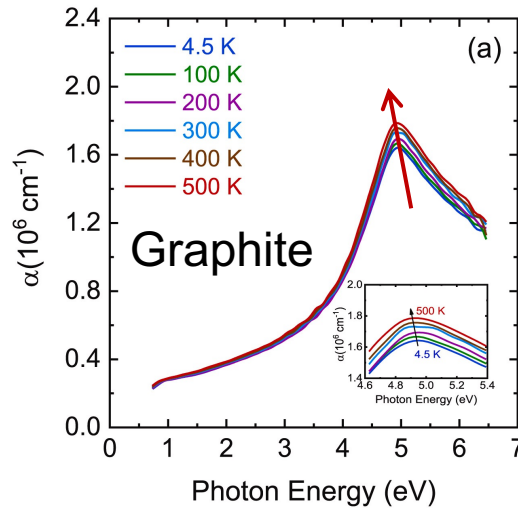
Theory



Complex Raman tensor
(Experiment can not observe)

Applications: Understanding optical spectra

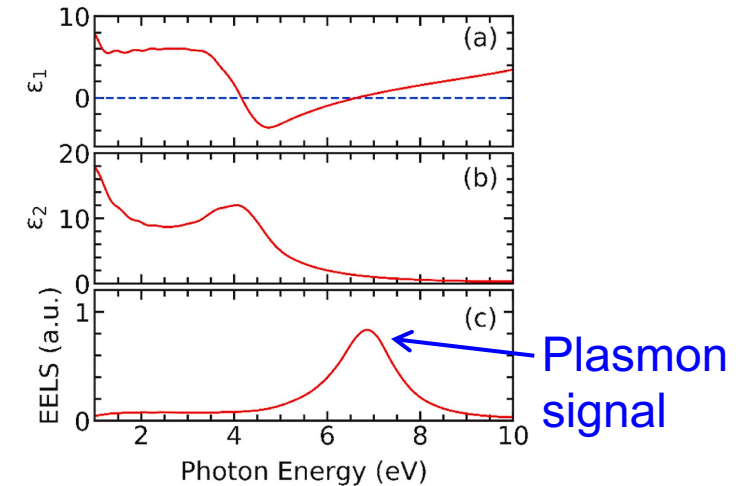
Question from experimentalist: WHY?



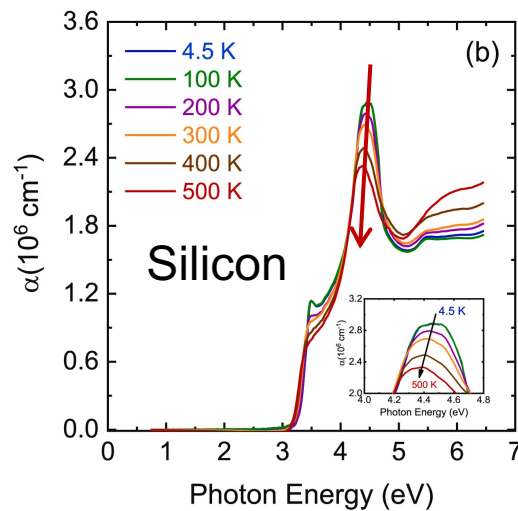
Can not explain why optical absorption is higher with higher T?

$$\text{EELS} = \text{Im} \left[\frac{-1}{\epsilon(\omega)} \right] = \frac{\epsilon_2(\omega)}{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)}$$

But easy in DFT

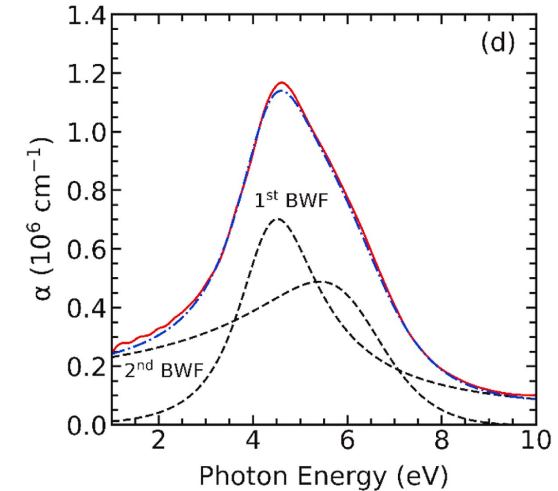


The limit of experiment is not easy to increase photon energy.



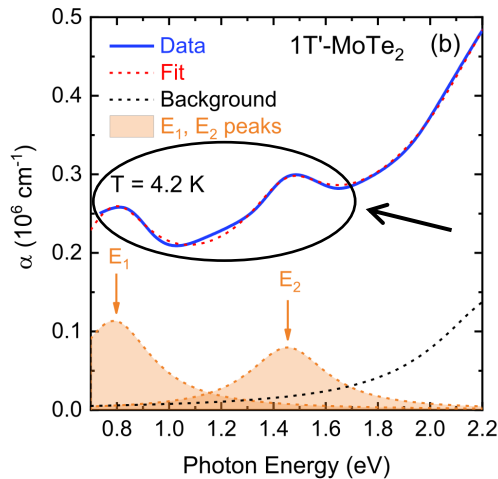
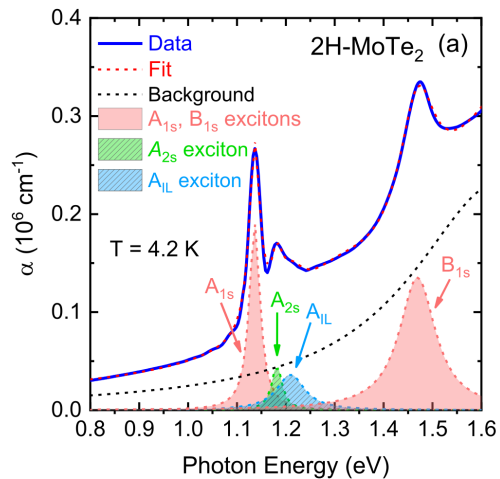
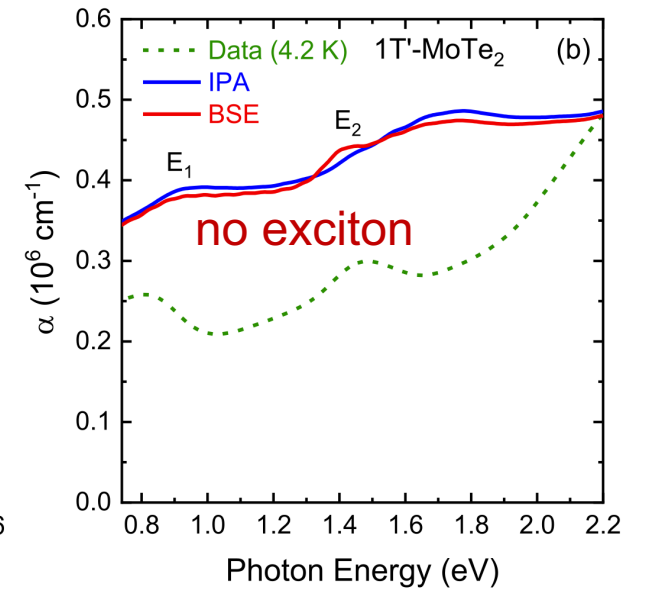
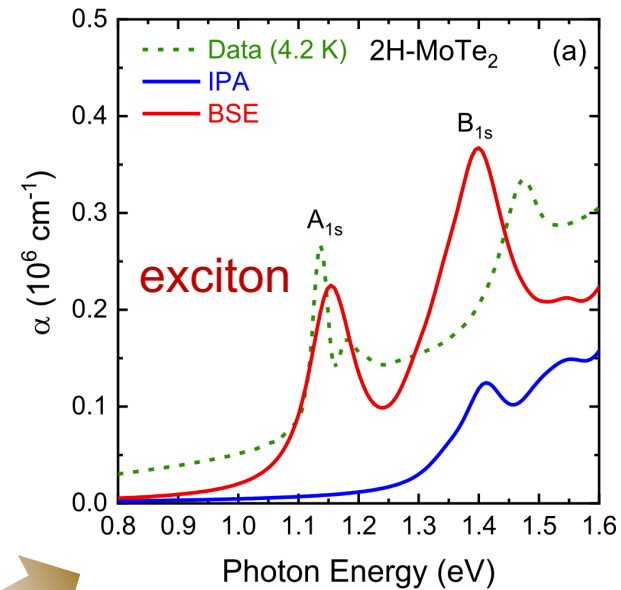
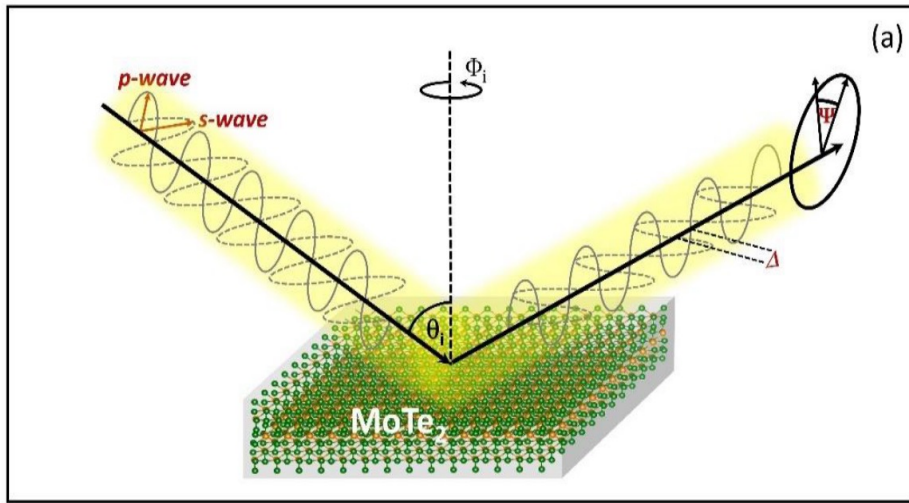
Can explain by standard theory: Higher T --> higher lifetime of electron

$$\alpha = \frac{\sqrt{2}\omega}{c} \sqrt{\sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} - \epsilon_1(\omega)}$$



Answer: Plasmon-assisted optical absorption

Applications: Understanding exciton effect



Origin of peaks
come from
exciton or not?

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

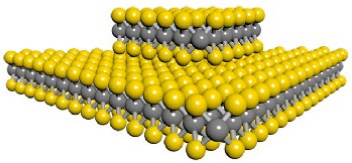
Experiment is not easy to distinguish physical phenomena, but in DFT, we can do that.

Well-known from
previous works

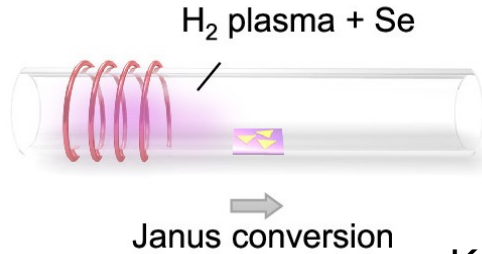
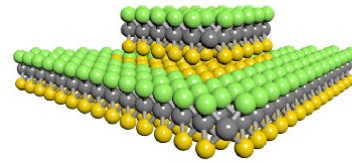
New phase
(semimetal)

Applications: Can DFT be first?

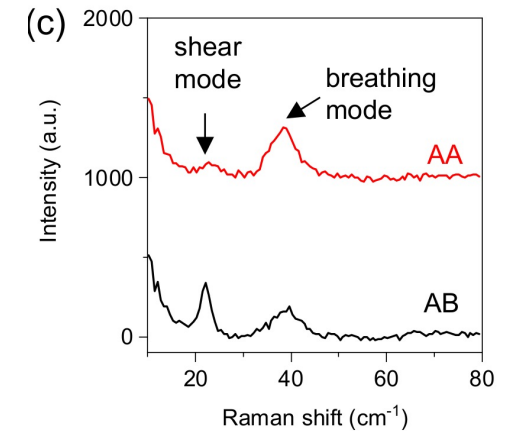
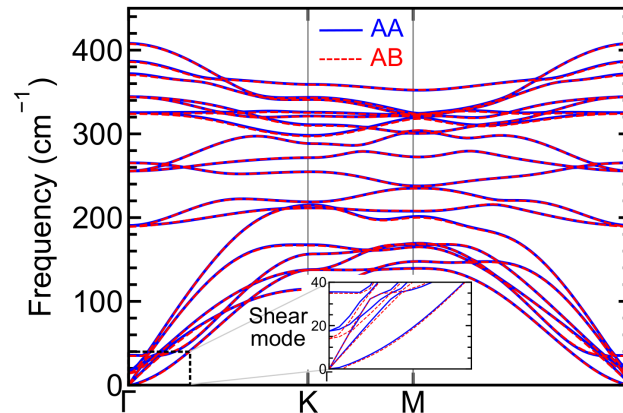
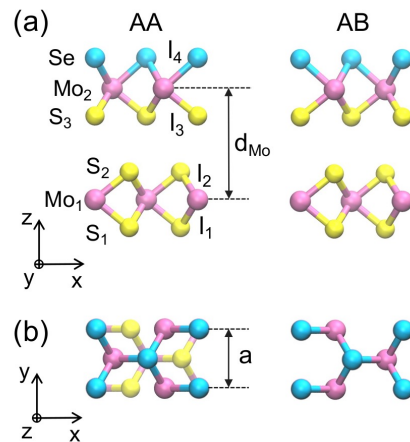
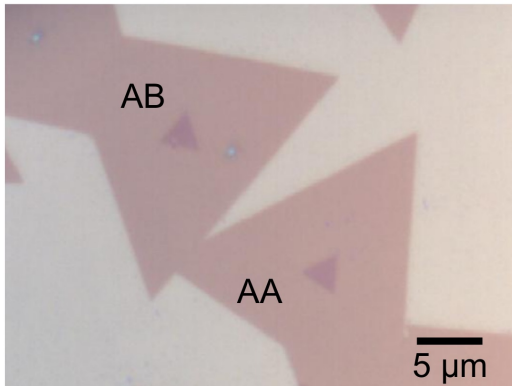
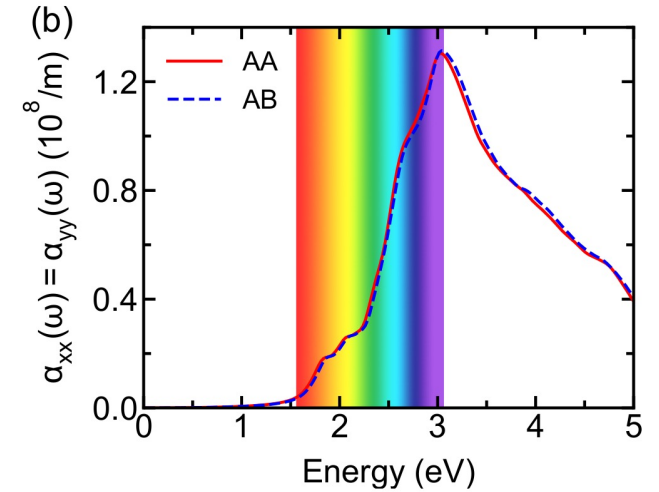
MoS₂ bilayer



MoS₂/MoSse heterostructure



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



Both AA and AB stackings exist BUT electronic, phonon, linear optical properties 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)

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

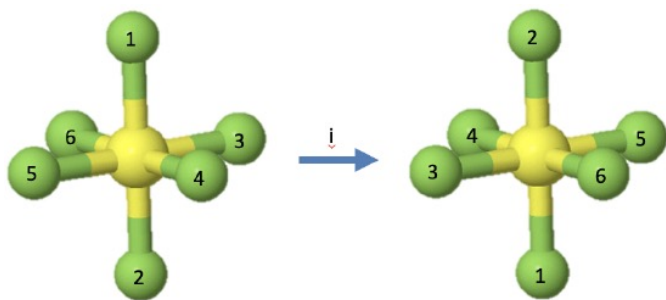
optical linear
response

optical non-linear
response

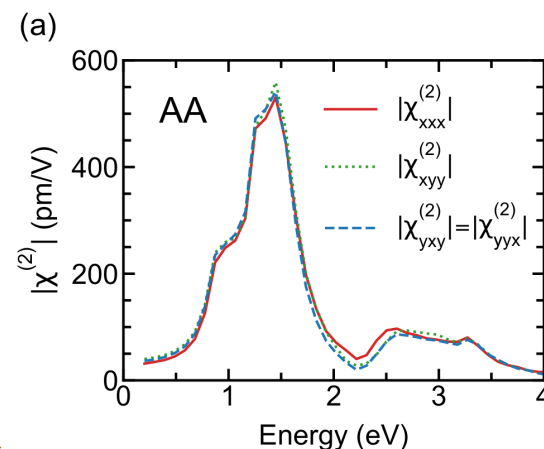
For inversion symmetry: $\mathbf{P} \rightarrow -\mathbf{P}$ and $\mathbf{E} \rightarrow -\mathbf{E}$
 $\rightarrow \chi^{(2)}$ must be zero

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

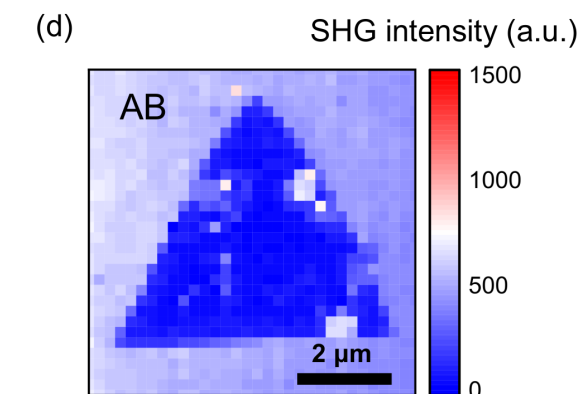
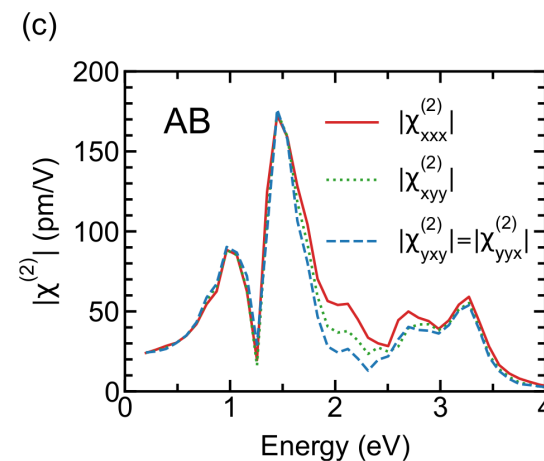
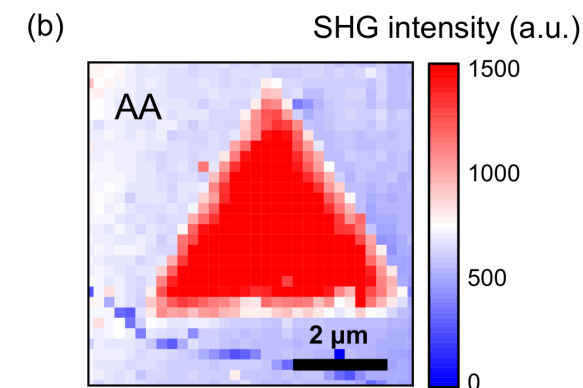
Inversion symmetry: $(x, y, z) \rightarrow (-x, -y, -z)$



Theory



Experiment



N. T. Hung, K. Zhang et al., *submitted* (2023)

Energy tree

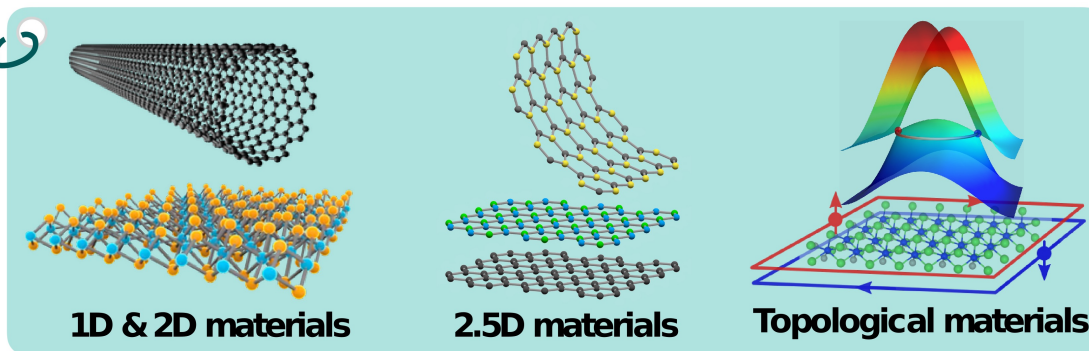
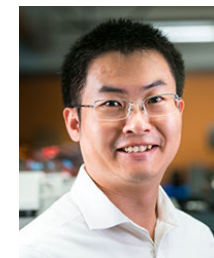
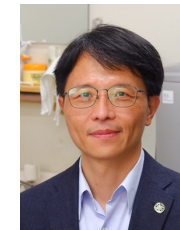
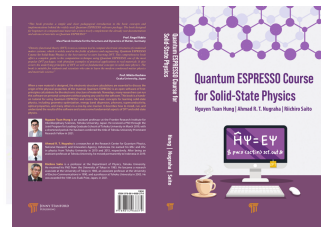
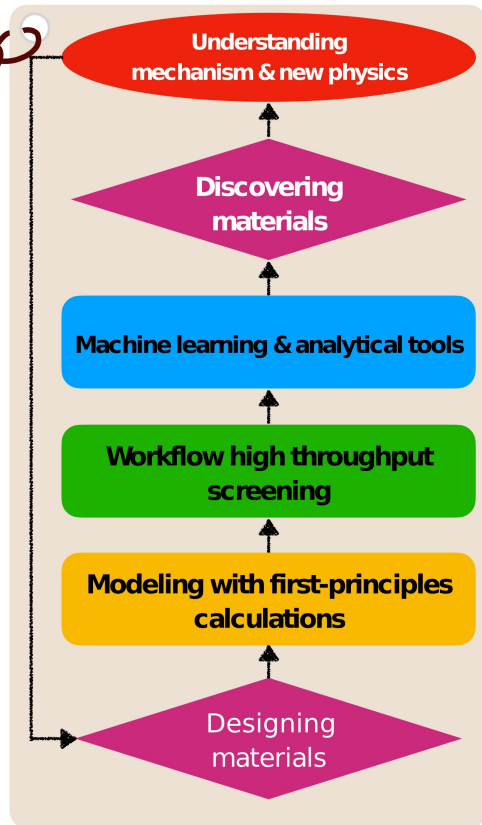
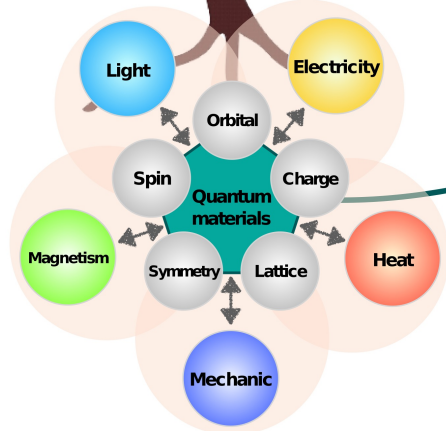
Thermoelectricity

Artificial muscles

Photovoltaics

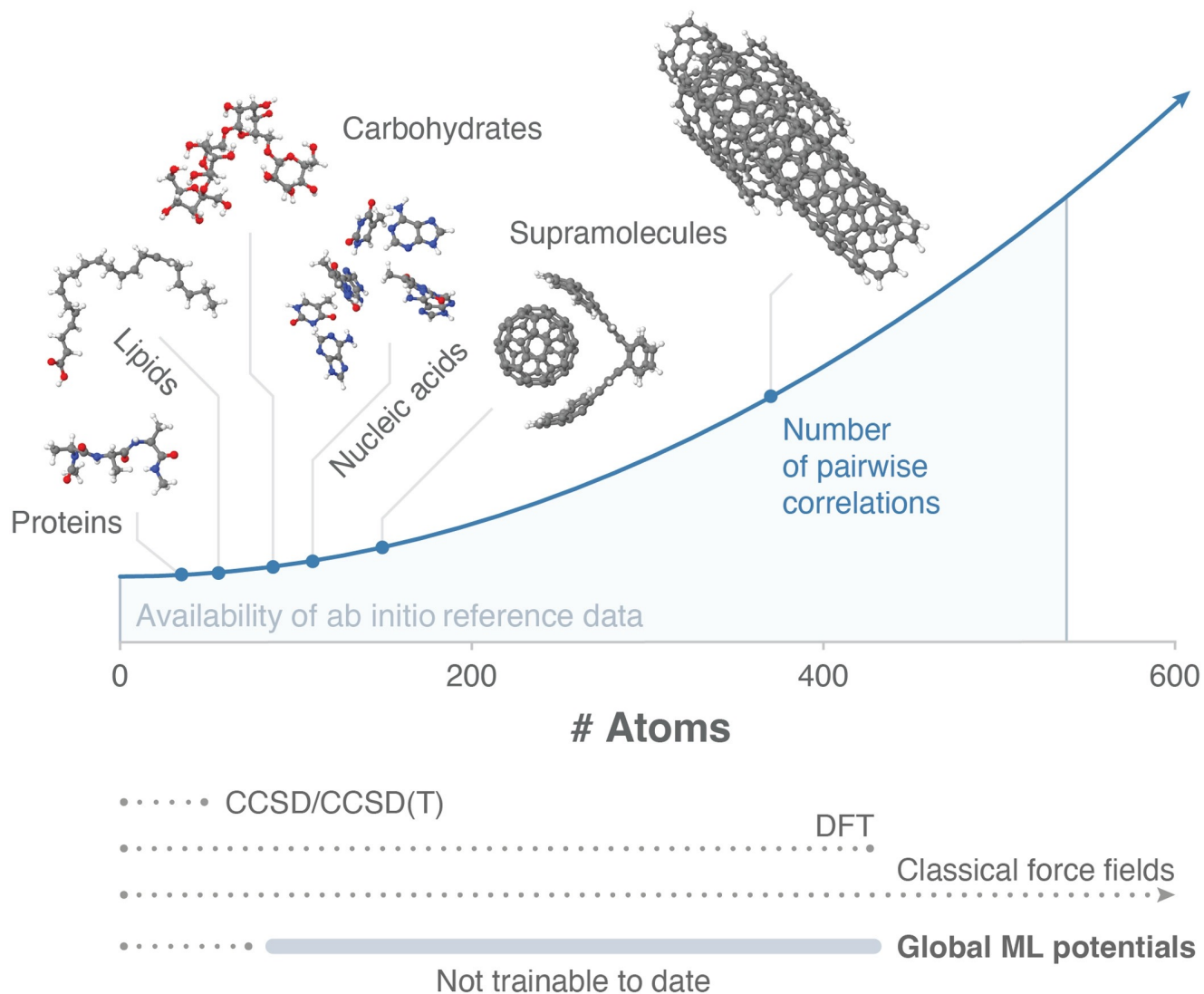
Battery

Photocatalyst



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

Large-scale DFT Calculations and Moving to GPUs



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

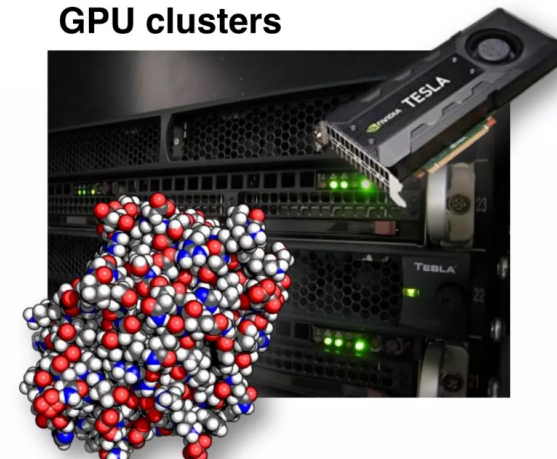
then (mid-2000s):
Beowulf clusters



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

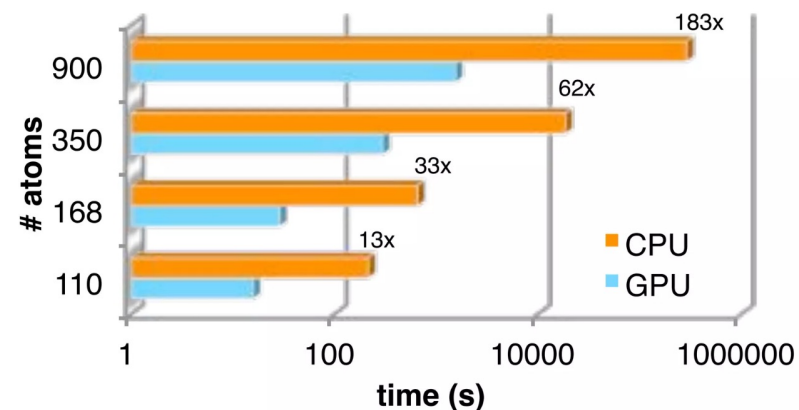
now:
GPU clusters

TeraChem: see <http://petachem.com>

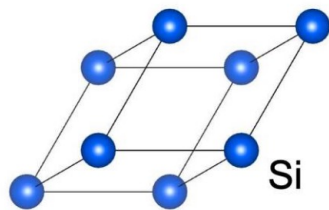


DFT or *better* on **three thousand atoms!**

Novel architecture & GPU-optimized algorithms:



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

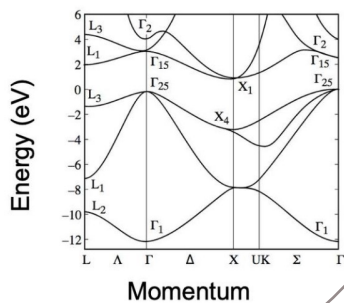


Structure information

Density-functional theory method

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

Properties of materials

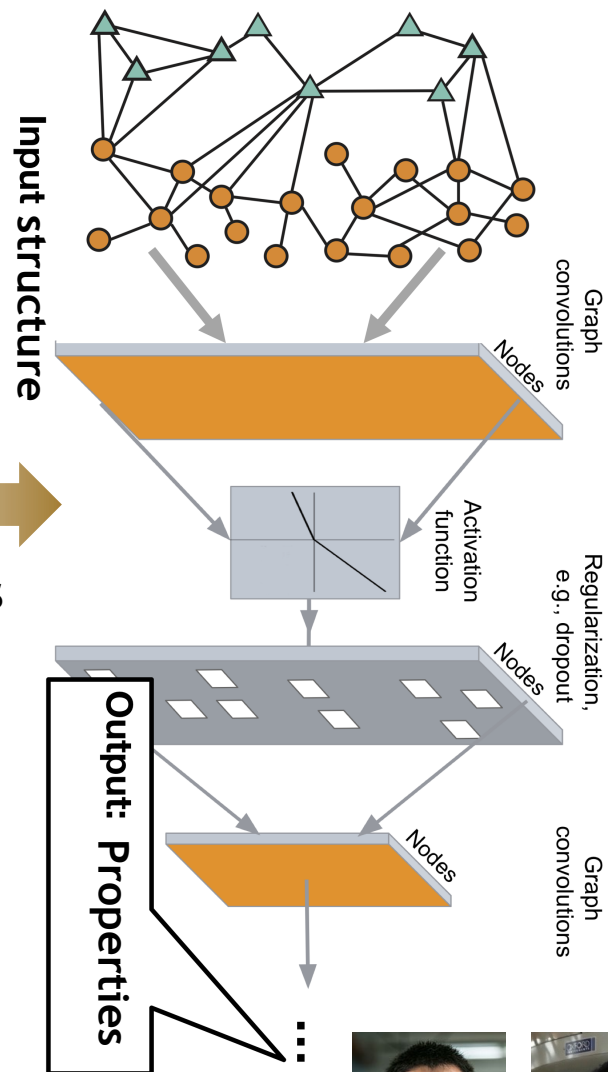


DFT database

> 1000 materials



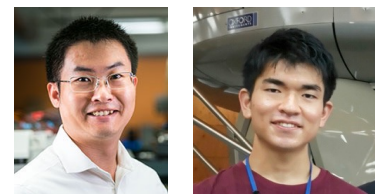
Graph neutral networks



New materials

Directly predict the properties of any input materials

Properties





Please enjoy running Quantum ESPRESSO!

Many Other Examples

