Introduction to

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Thanks to the > 50 ABINIT contributors, and especially to GM Rignanese for contributions to the slides

ABINIT software project

Ideas (1997) :

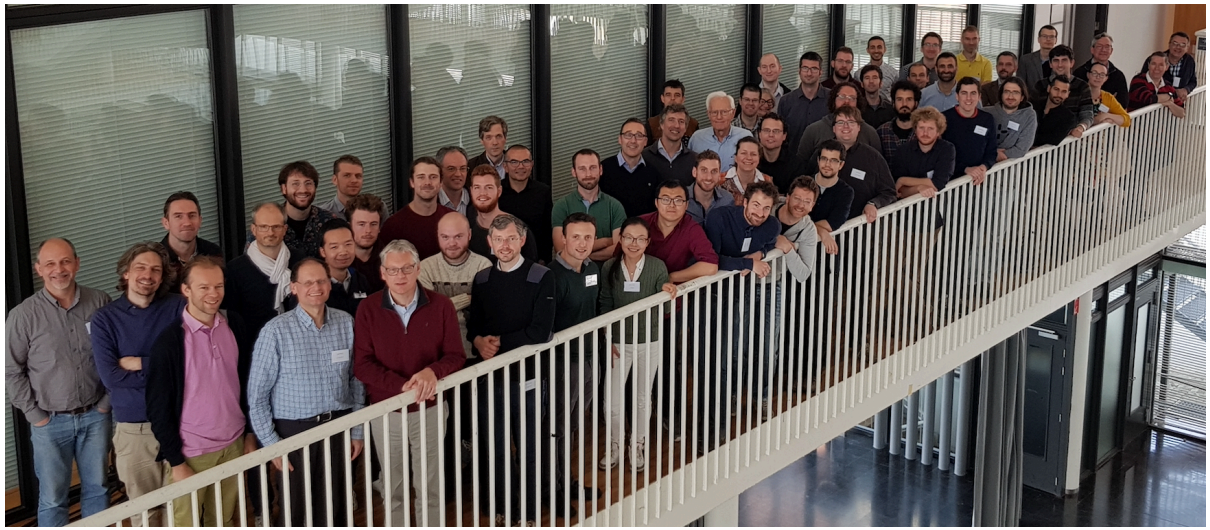
1) Software for first-principles simulations are more and more complex : needs a worldwide collaboration, of specialized, complementary, groups
2) Linux software development : ‘free software’ model

Now (2019) :

>2000 registered people on the forum
>800 kLines of Fortran90 + many python scripts (abipy)
about 50 contributors to ABINITv8

Last release v8.10.3,
used in this hands-on
http://www.abinit.org

Available freely
(GPL, like Linux).



The “Free” software concept

Free for freedom (also price ...)

- freedom 1 : unlimited use for any purpose
- freedom 2 : study and modify for your needs (need source access !)
- freedom 3 : copy
- freedom 4 : distribute modifications

From copyright to freedom (“copyleft”)

- copyright allows licensing
- licenses grants freedom

Terminology : Free software=Open source=Libre software

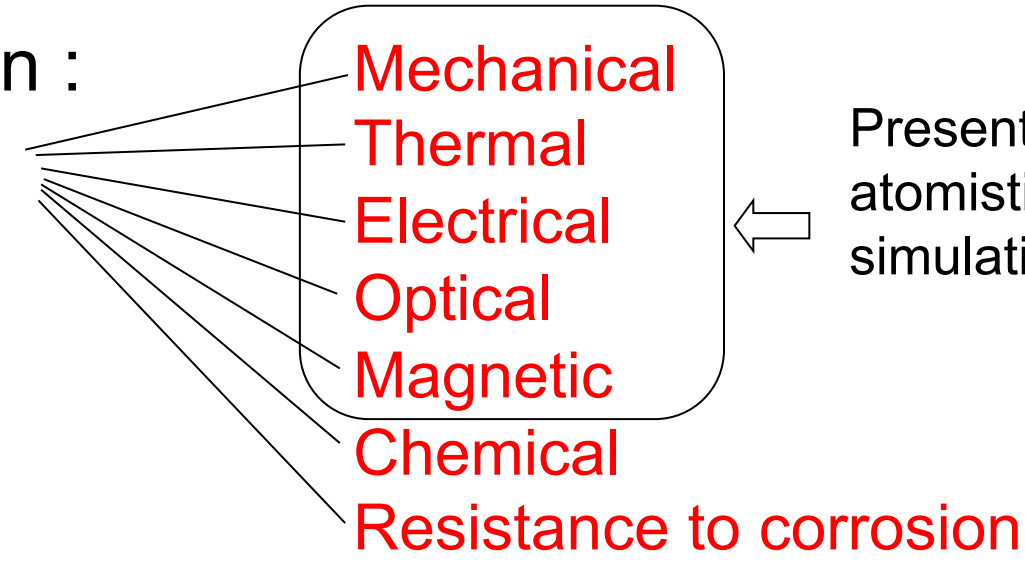
ABINIT pioneered the use of the GPL « Free software license » in the computational condensed matter community (2000)

http://www.abinit.org : download, documentation ...

Goals of materials research

Optimisation :

-Properties



Present impact of atomistic scale simulations

-Lifetime

-Synthesis

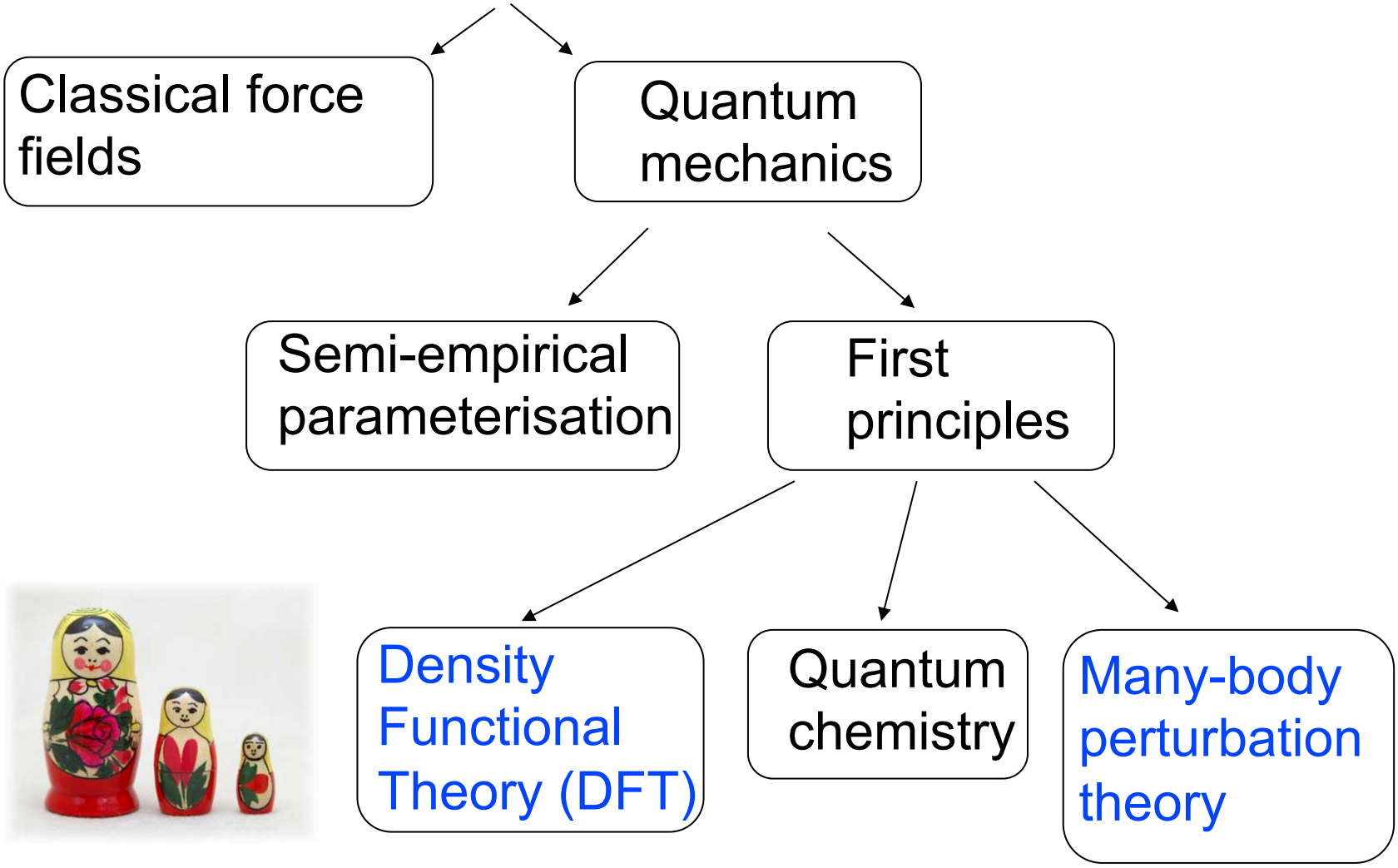
-Cost

-Ecologic/toxicologic caracteristics

Empirical approach ? (trial/error)

Semi-empirical approach ? (guided trials)

Theory levels



... incomplete overview !

Electronic many-body problem

After the Born-Oppenheimer approximation :

- decoupling of the nuclei and electron dynamics
- nuclei positions can be considered as fixed
- effective Born-Oppenheimer potential energy hypersurface

Born-Oppenheimer energy

$$E_n^{BO}\left(\{\mathbf{R}_I\}\right) = E_{II}\left(\{\mathbf{R}_I\}\right) + E_n^{el}\left(\{\mathbf{R}_I\}\right)$$

Potential created by nuclei, felt by the N electrons

$$V_{\text{ext}}(\mathbf{r}) = -\sum_I \frac{Z_I}{|\mathbf{r} - \mathbf{R}_I|}$$

$$\left[\sum_i \left(-\frac{1}{2}\nabla_i^2 + V_{ext}(\mathbf{r}_i)\right) + \sum_{i<j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}\right] \Psi_n(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E_n^{el}\, \Psi_n(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

Many-body Schrödinger equation,

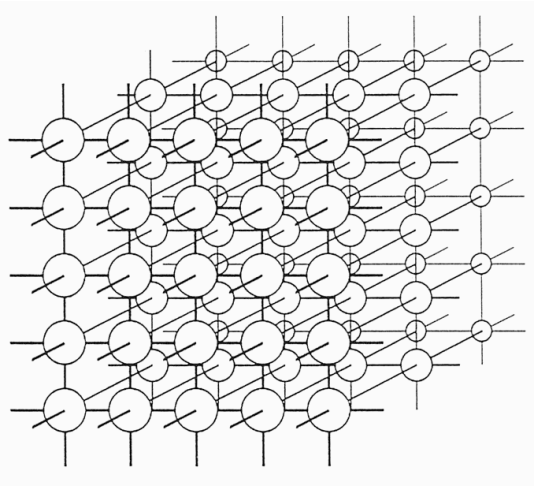
very difficult to address for more than 2 electrons

Basic difference between classical and quantum many-body systems

Classical objects : fields $p(\mathbf{r},t), V(\mathbf{r},t), T(\mathbf{r},t), \mathbf{E}(\mathbf{r},t), \ldots$

or trajectories $\mathbf{R}_1(t), \mathbf{R}_2(t), \mathbf{R}_3(t), \ldots \mathbf{R}_N(t)$

Quantum objects : wavefunctions for interacting particles $\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_N, t)$



Classical positions and velocities of 8 planets : 2x3x8=48 real numbers.

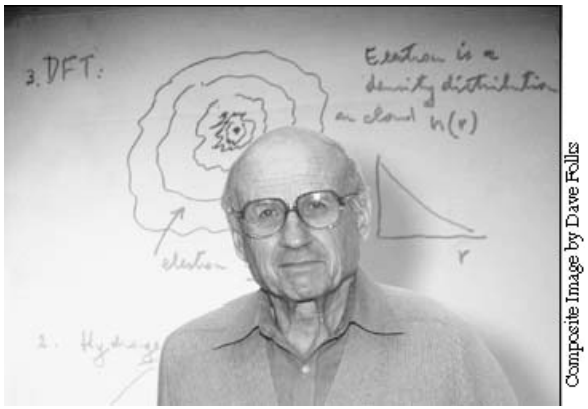
Suppose an oxygen atom : 8 electrons.
Quantum description at a particular time, on a discretized 10x10x10 real space mesh contained in a cube...
24-dimensional object 10^{24} real numbers

Density-functional theory (DFT)

Quantum objects : wavefunctions
for interacting particles $\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,...,\mathbf{r}_N,t)$

Hohenberg & Kohn (1964), Kohn & Sham (1965) :
Legendre transform between the density and potential
gives an effective potential for non-interacting particles

DFT : set of wavefunctions
for non-interacting particles $\psi_1(\mathbf{r},t),\psi_2(\mathbf{r},t),...\psi_N(\mathbf{r},t)$



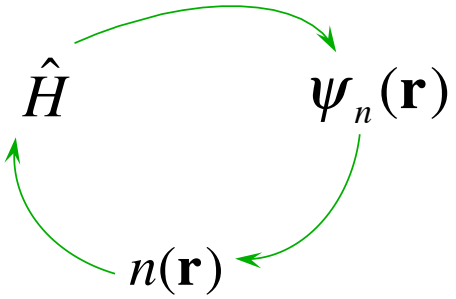
For the oxygen atom, back to
8x10x10x10 real numbers,
but with an approximate
treatment ...

W. Kohn, chemistry Nobel prize 1998

The Kohn-Sham orbitals and eigenvalues

Non-interacting electrons in the Kohn-Sham potential :

$$\left(-\frac{1}{2}\nabla^2 + V_{\mathrm{KS}}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \varepsilon_i\,\psi_i(\mathbf{r})$$



Density $\quad n(\mathbf{r}) = \sum_i \psi_i^*(\mathbf{r})\psi_i(\mathbf{r})$

$$V_{\mathrm{KS}}(\mathbf{r}) = V_{ext}(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r}' - \mathbf{r}|}\,\mathrm{d}\mathbf{r}' + \frac{\delta E_{\mathrm{xc}}[n]}{\delta n(\mathbf{r})}$$

Hartree potential Exchange-correlation potential

To be solved self-consistently !

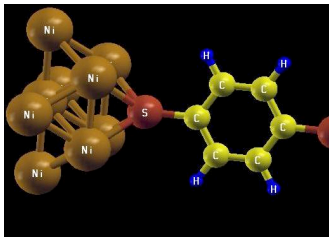
Note. At self-consistency, supposing XC functional to be exact :

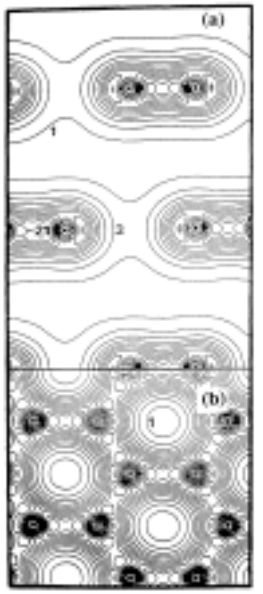
- the KS density = the exact density,
- the KS electronic energy = the exact electronic energy
- but KS wavefunctions and eigenenergies correspond to a fictitious set of independent electrons, so they do not correspond to any exact quantity.

Properties from DFT+MBPT+ ...

Computation of ...

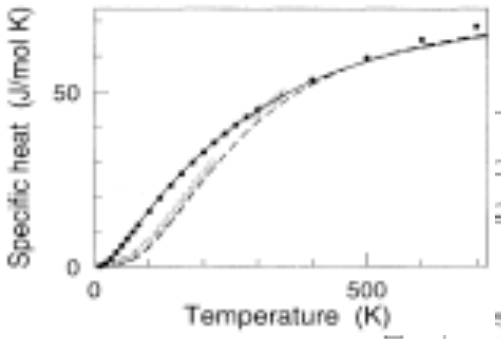
- interatomic distances, angles, total energies
- electronic charge densities, electronic energies

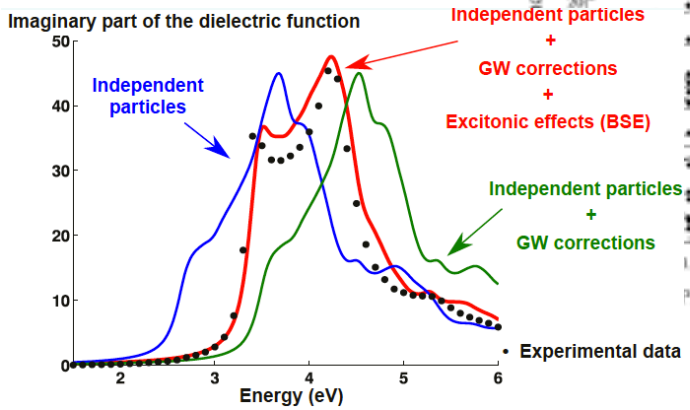


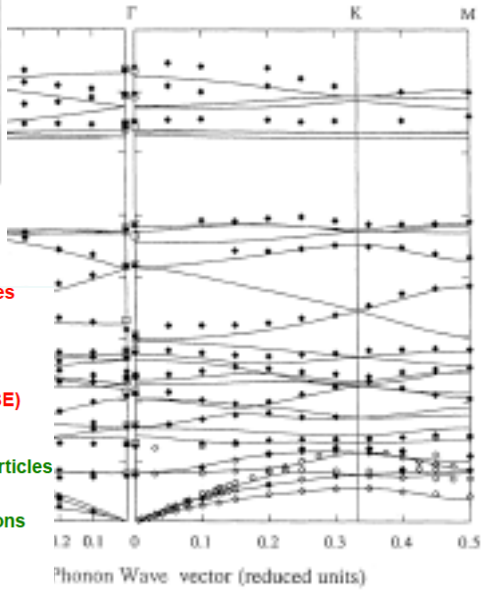


A basis for the computation of ...

- chemical reactions
- electronic transport
- vibrational properties
- thermal capacity
- dielectric behaviour
- optical response
- superconductivity
- surface properties
- spectroscopic responses
- ...







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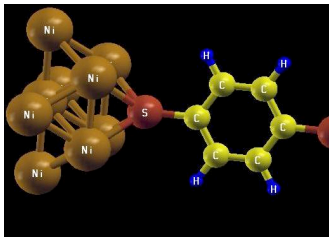
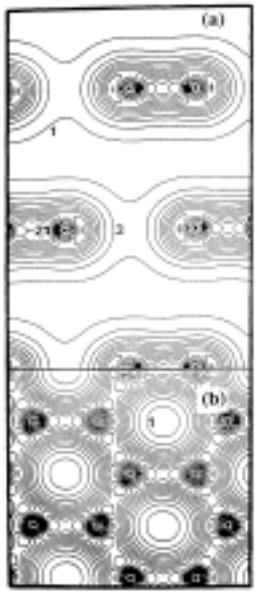




A basis for the computation of ...

chemical reactions

electronic transport

vibrational properties

thermal capacity

dielectric behaviour

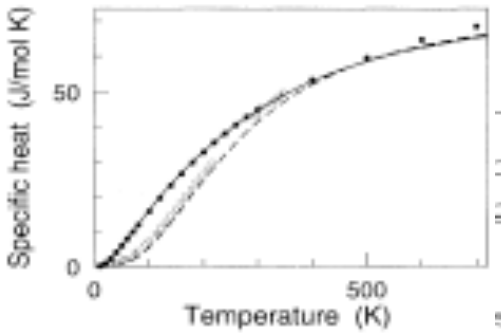
optical response

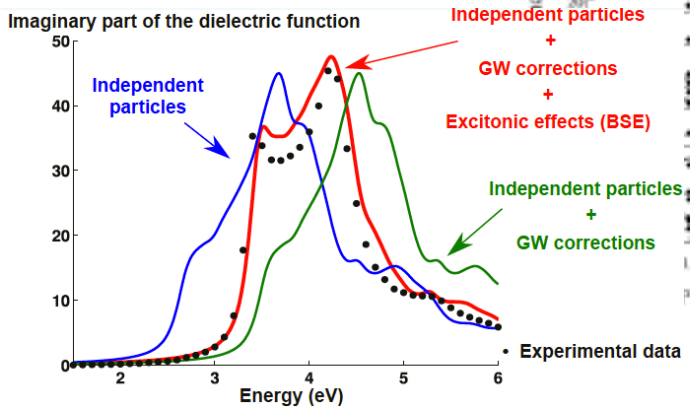
superconductivity

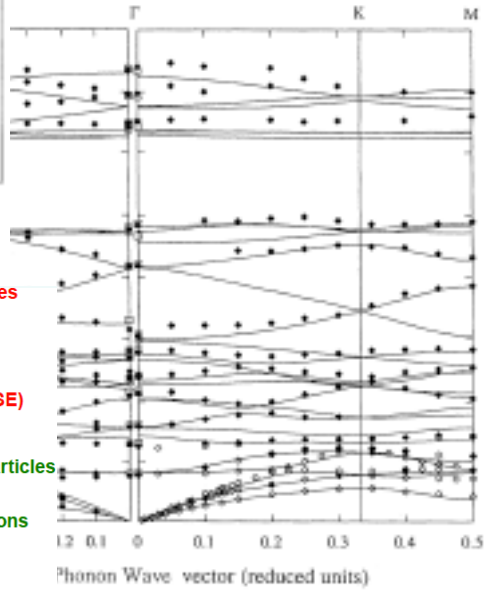
surface properties

spectroscopic responses

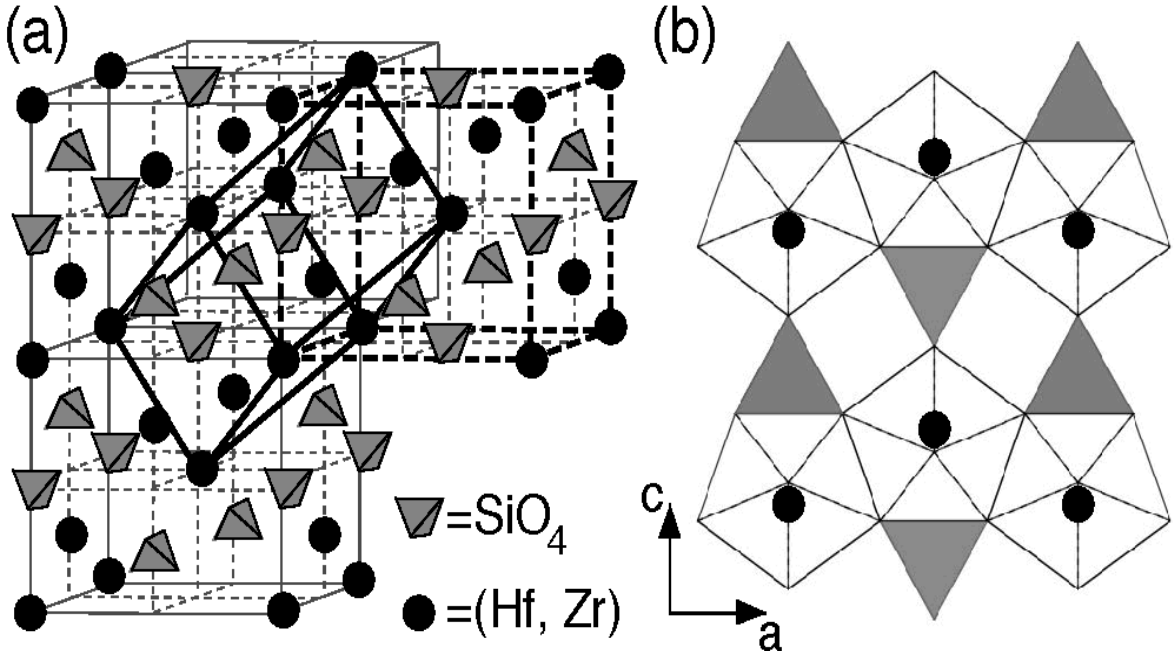
...







An example : Zircon / Hafnon



- body-centered tetragonal ($I4_1/amd$)
- primitive cell with 2 formula units of $MSiO_4$
- M atoms (0,3/4,1/8)
  Si atoms (0,1/4,3/8)
  O atoms (0,*u*,*v*)

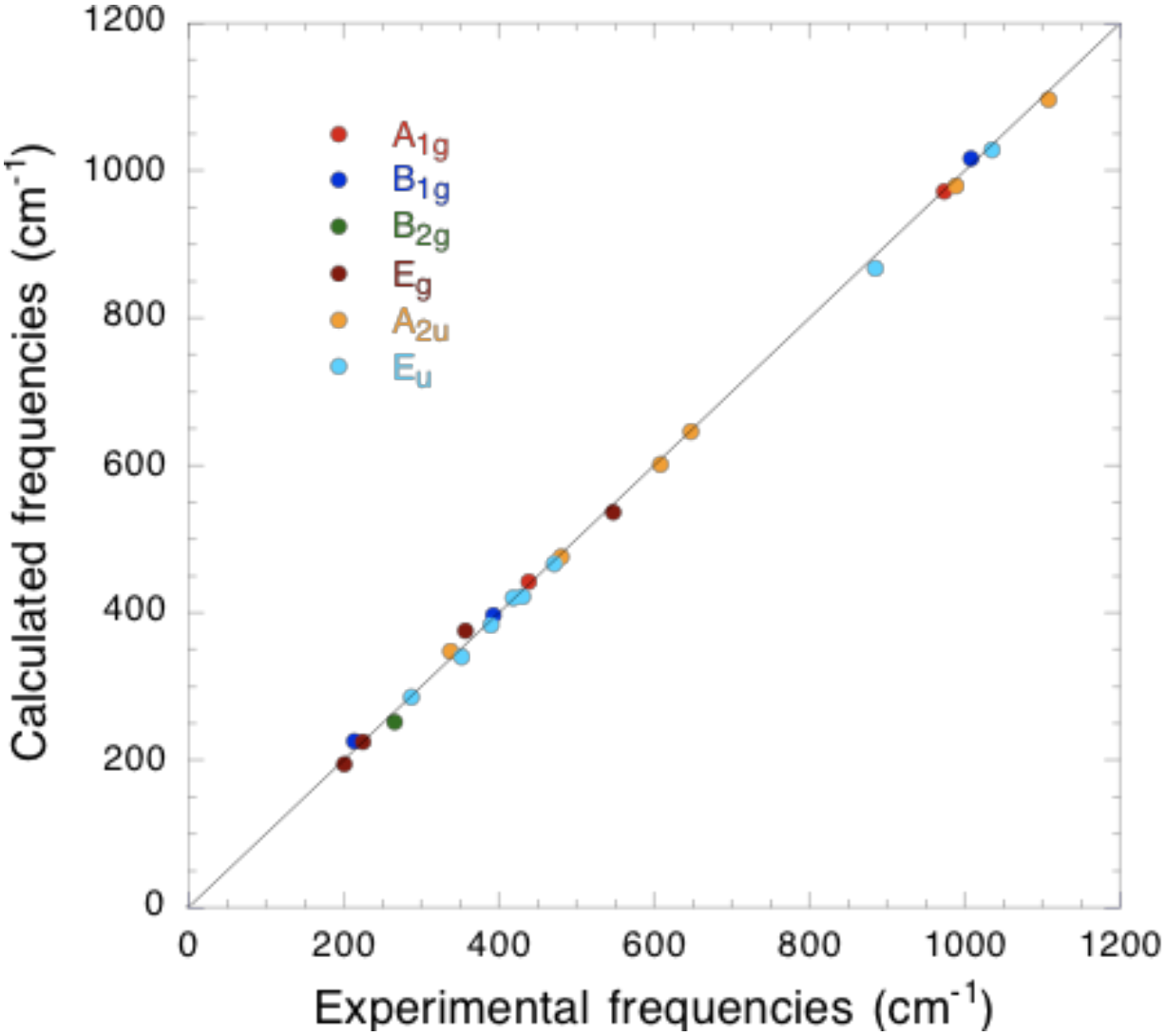
- $(SiO_4)^{4-}$ anions and M^{4+} cations
- alternating SiO_4 tetrahedra and MO_8 units, sharing edges to form chains parallel to [0 0 1]
- MO_8 units : 4 O atoms are closer to the Zr atoms than the 4 other ones
- O atoms are 3-fold coordinated

Structural parameters

	$HfSiO_4$		$ZrSiO_4$	
	Th.	Expt.	Th.	Expt.
a	6.61	6.57	6.54	6.61
c	5.97	5.96	5.92	6.00
u	0.0672	0.0655	0.0645	0.0646
v	0.1964	0.1948	0.1945	0.1967
Volume	130.42	128.63	126.60	131.08
d(Si-O)	1.62	1.61	1.61	1.62
d(M-O)	2.14	2.10	2.10	2.13
	2.27	2.24	2.24	2.27
$\angle$(O-Si-O)	97°	97°	97°	97°
	116°	117°	116°	116°

Interatomic distances and angles are within 1 or 2% of experimental values

Phonon frequencies at the zone center



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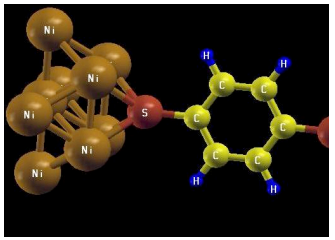

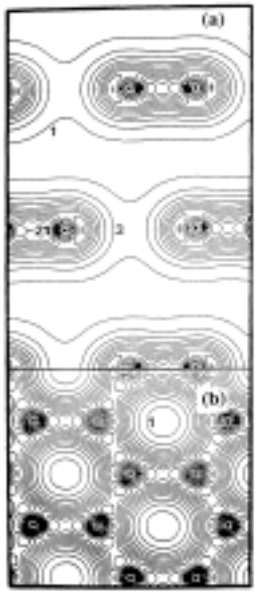

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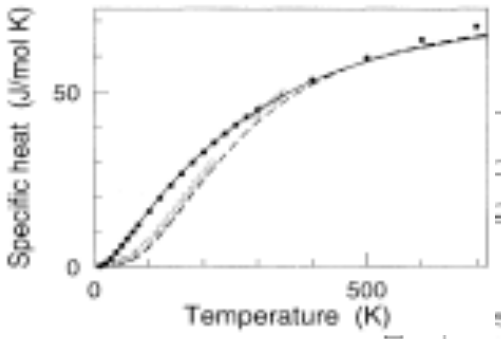
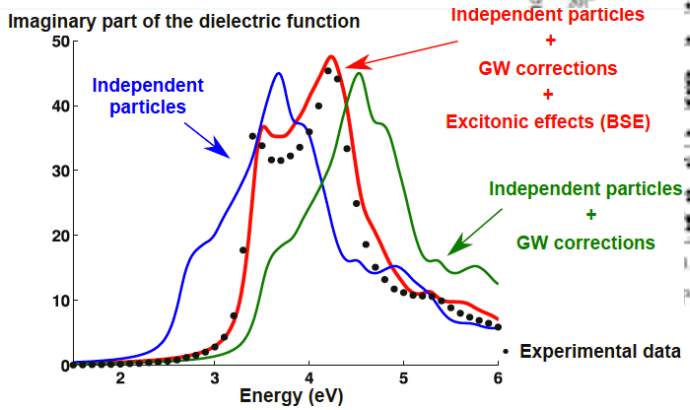
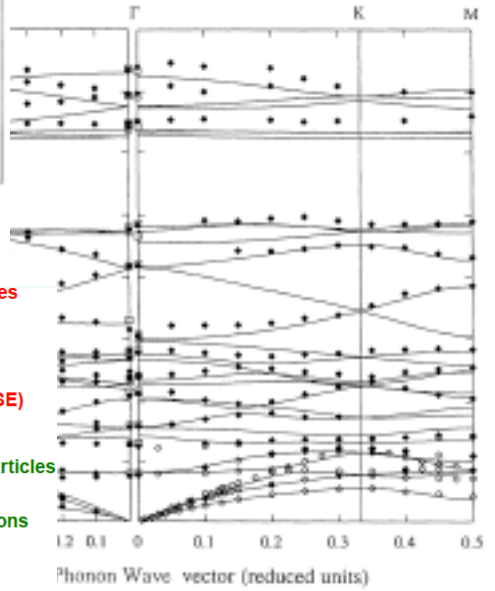






What can we do today ?

What can we do today ?

Don't give me a fish ...

... teach me how to fish ...

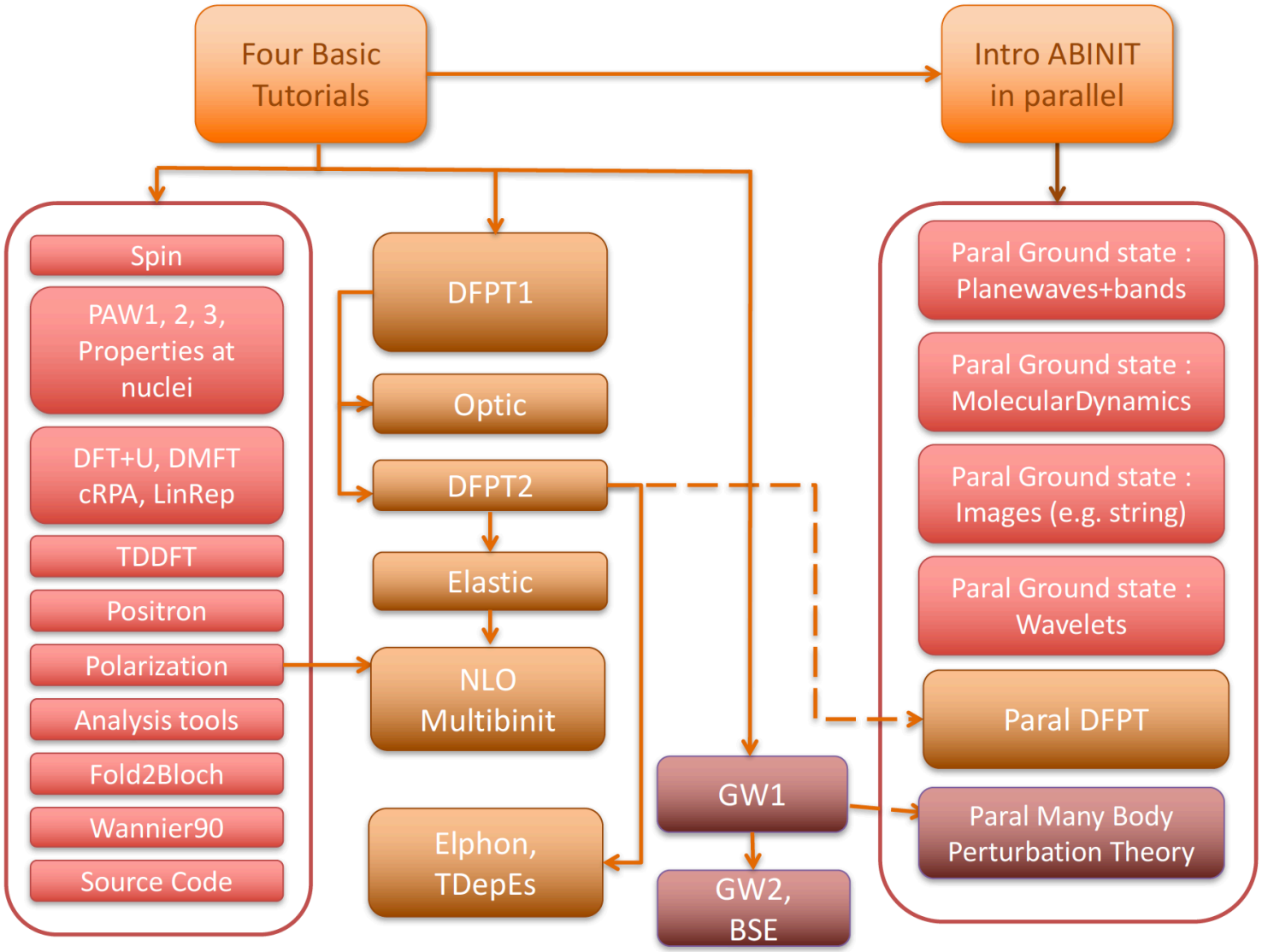
Basic Documentation

Web site http://www.abinit.org ; http://docs.abinit.org

- User's guides
- Installations notes
- List of input variables + description
- List of topics = a hub to input variables, files, tutorial, bibrefs
- over 800 example input files
- >30 tutorial lessons (each 1-2 hours)
  https://docs.abinit.org/tutorial

+ Forum Web site http://forum.abinit.org
+ Past ABINIT events (schools/workshops)
  https://www.abinit.org/events
  highly recommended:
  https://school2019.abinit.org/

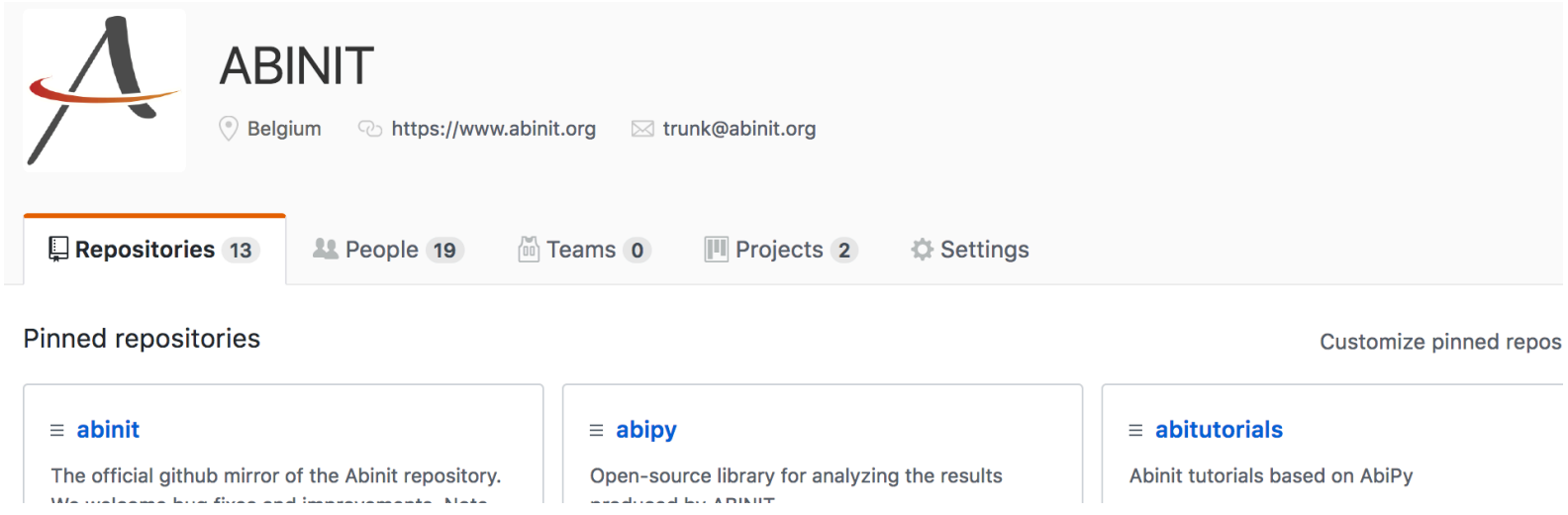
ABINIT tutorial : layout + dependencies



ABINIT + python : Abipy, Abitutorials …

ABINIT organization on GitHUB https://github.com/abinit

Abipy : python library for launching ABINIT jobs,
and analysing/plotting the results http://github.com/abinit/abipy
=> e.g. connecting ABINIT with tools for high-throughput calculations developed in the Materials Project context (e.g. Pymatgen, Fireworks) https://materialsproject.org/
Abitutorials : tutorial based on Jupyter notebooks ABINIT+python



ABINIT + python : Abipy, Abitutorials …

Abipy

Gallery of plotting scripts https://abinit.github.io/abipy/gallery/index.html
AbiPy workflows https://abinit.github.io/abipy/flow_gallery/index.html
Jupyter notebooks with interactive tutorials and examples results
https://nbviewer.jupyter.org/github/abinit/abitutorials/blob/master/abitutorials/index.ipynb

Introduction to AbiPy for newcomers
https://github.com/gmatteo/abipy_slides_aps_boston_2019

How to use the AbiPy command line interface
https://gmatteo.github.io/abipy_intro_aps_boston_abidev2019

Running ABINIT : basics

Density Functional Theory calculations

Representation of mathematical entities:

- wavefunctions
- density, potential ... ?

=> choice of a basis set ; entities are linear combination of the basis set functions

Treatment of periodic solid, molecules, surfaces, nanostructures, interfaces ... ?

=> treatment using adequate boundary conditions

Many different implementations ...

Here a few words about :

PseudoPotentials (or Projector Augmented Waves – PAW)

Periodic boundary conditions

Plane Wave basis set vs all-electron calculations with localized orbitals

Iterative algorithms

Core and valence electrons (I)

Core electrons occupy orbitals that are « the same » in the atomic environment or in the bonding environment

It depends on the accuracy of the calculation !

Separation between core and valence orbitals : the density...

$$n(\mathbf{r}) = \sum_{i}^{N} \psi_i^*(\mathbf{r})\psi_i(\mathbf{r})$$

$$= \sum_{i \in core}^{N_{core}} \psi_i^*(\mathbf{r})\psi_i(\mathbf{r}) + \sum_{i \in val}^{N_{val}} \psi_i^*(\mathbf{r})\psi_i(\mathbf{r}) = n_{core}(\mathbf{r}) + n_{val}(\mathbf{r})$$

« Frozen core » $\text{for i} \in \text{core} : \psi_i = \psi_i^{atom}$

Small core / Large core

It depends on the target accuracy of the calculation !

(remark also valid for pseudopotentials, with similar cores)

For some elements, the core/valence partitioning is obvious, for some others, it is not.

F atom : $\boxed{(1s)^2} + (2s)^2(2p)^5$

IP 1keV 10-100 eV

Ti atom : $\boxed{(1s)^2(2s)^2(2p)^6}(3s)^2(3p)^6(4s)^2(3d)^2$ small core

$\boxed{(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6}(4s)^2(3d)^2$ large core

IP 99.2 eV 43.3eV

Gd atom : small core with n=1,2,3 shells , might include 4s, 4p, and 4d in the core. 4f partially filled

Removing core electrons (I)

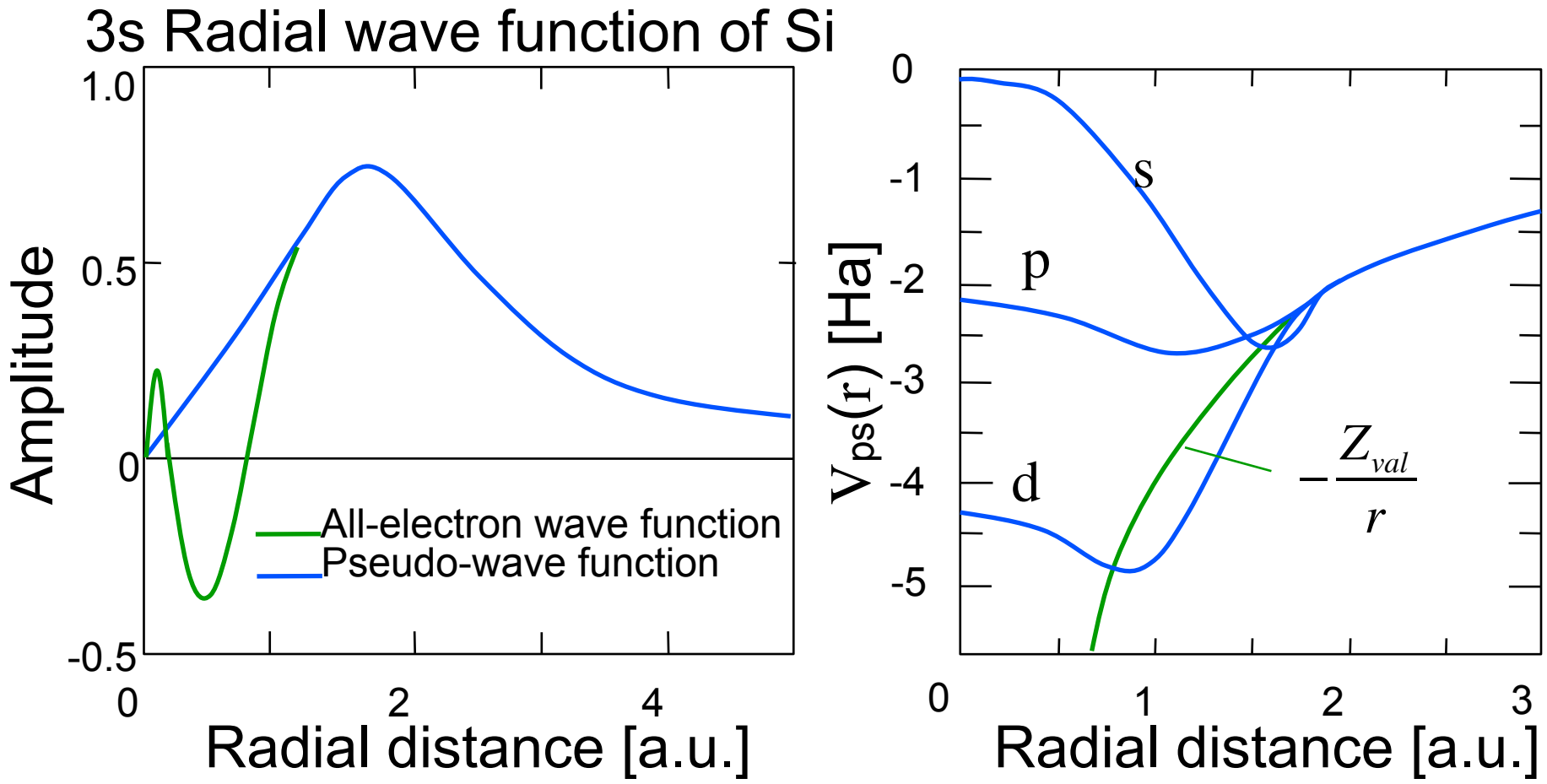
From the previous construction : valence orbitals must still be orthogonal to core orbitals
(=> oscillations, slope at the nucleus ...)

Pseudopotentials try to remove completely the core orbitals from the simulation

Problem with the number of nodes
This is a strong modification of the system ...

Pseudopotentials confine the strong changes within a « cut-off radius »

Example of pseudopotential

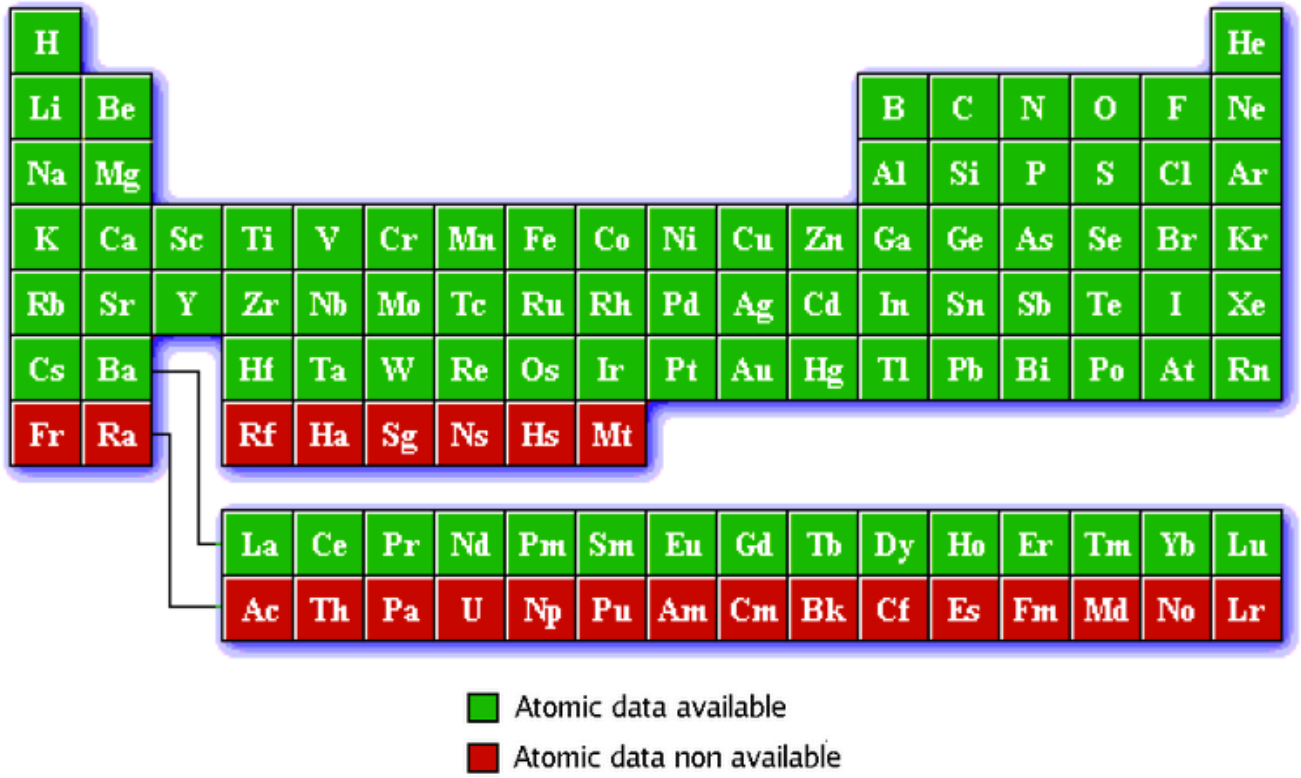


Pseudopotentials/PAW data in ABINIT

- Preferred PAW atomic dataset table : JTH

Jollet, Torrent, Holzwarth, Computer Physics Comm. 185, 1246 (2014)

https://www.abinit.org/psp-tables



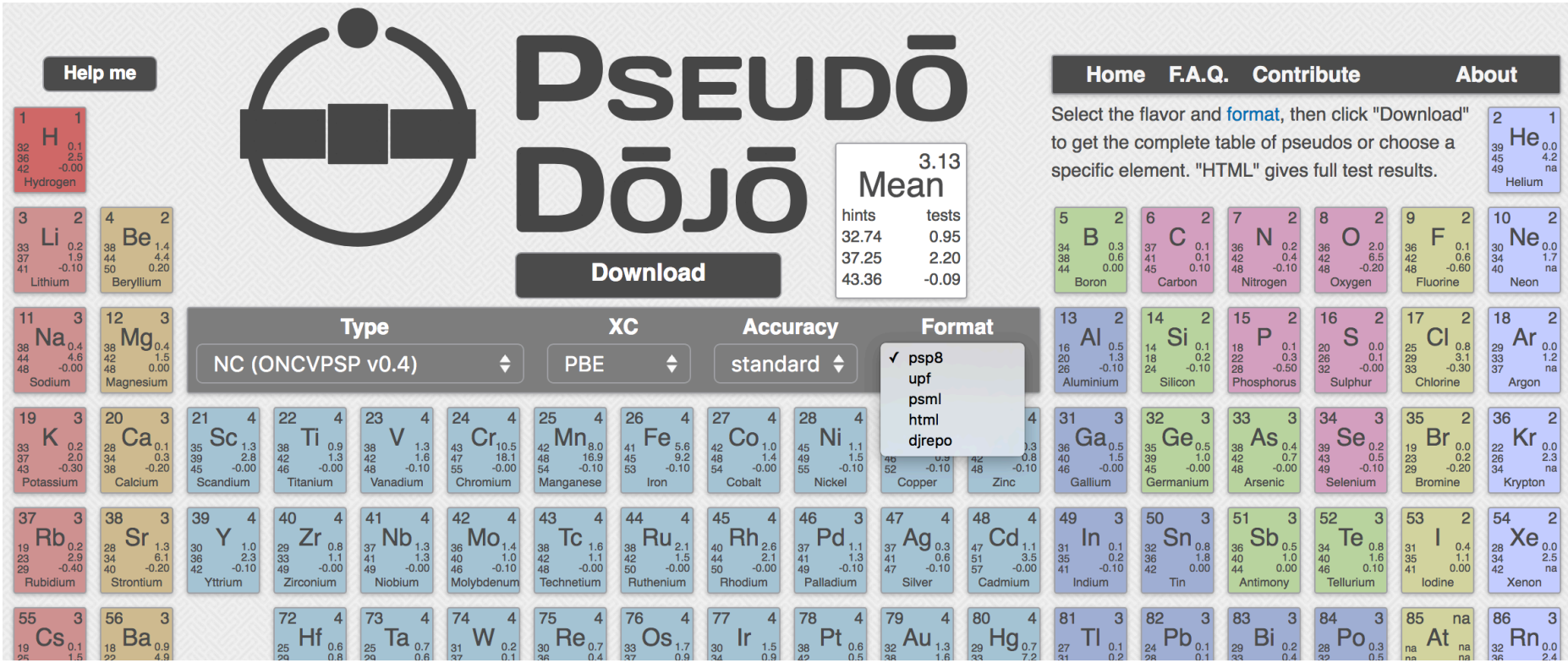
Also, possibility to use : GPAW table, GBRV v1.0 table, or norm-conserving pseudopotentials (e.g. ONCVPSP pseudo generator), or many others

Pseudopotentials/PAW data in ABINIT

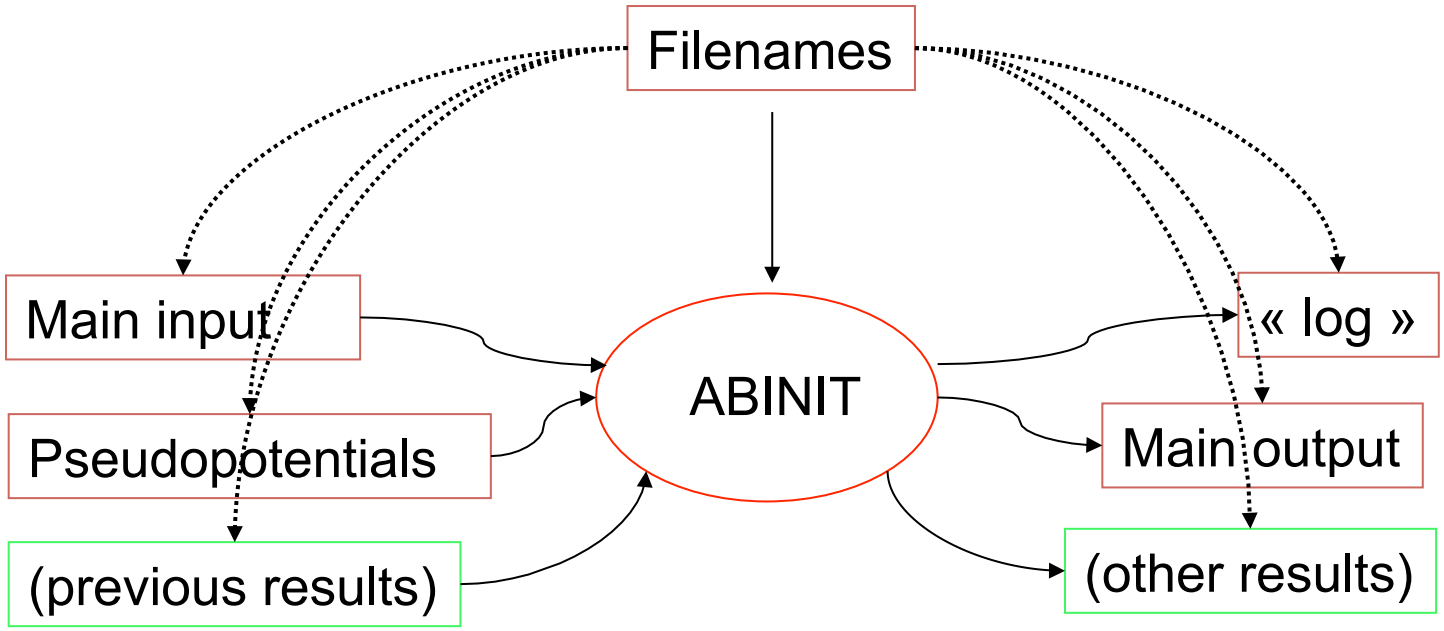
- Norm-conserving pseudos : pseudo-dojo approach

  Van Setten et al , Computer Physics Comm. 226, 39 (2018)

  https://www.pseudo-dojo.org



External files in a ABINIT run



Results :

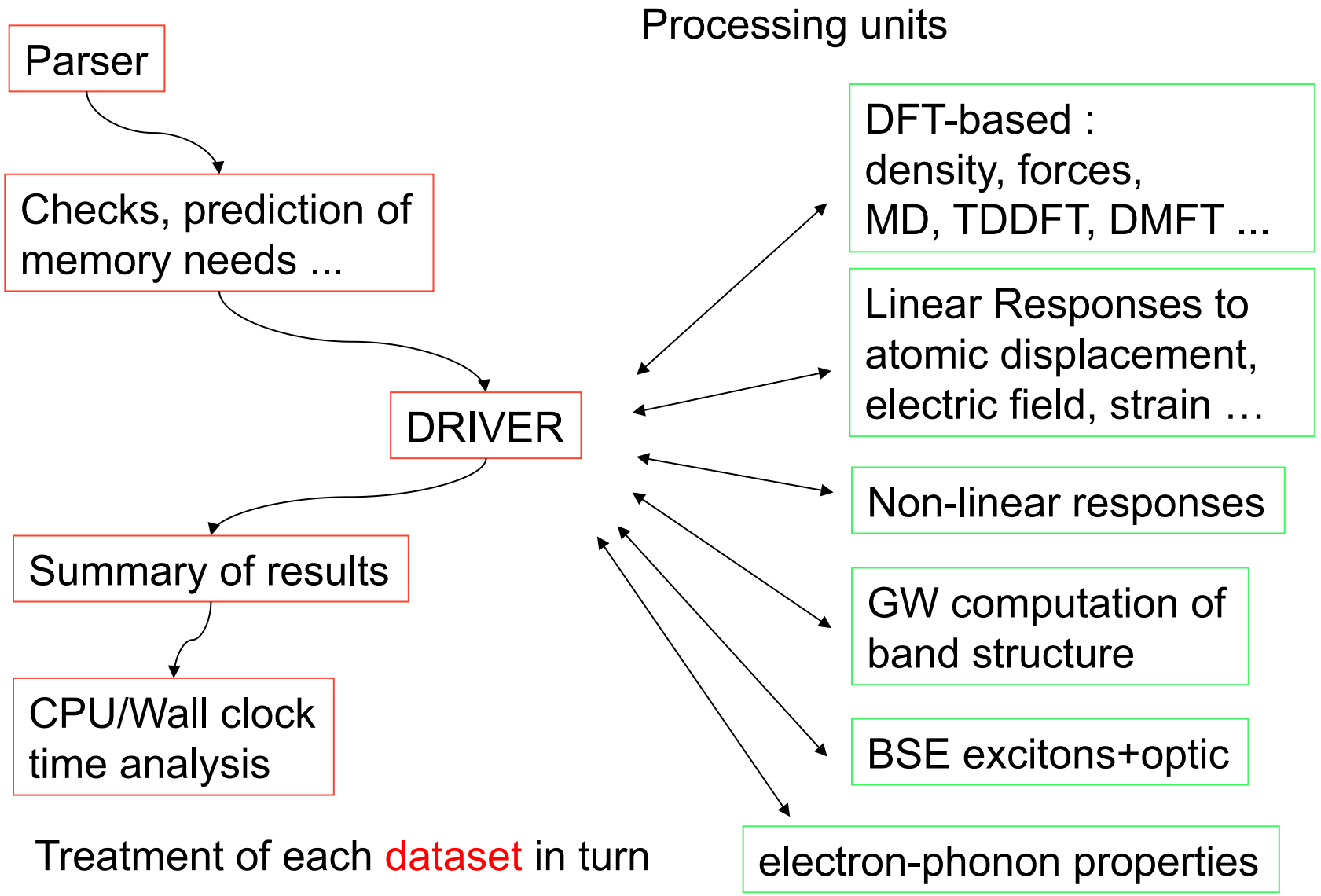
log, main output, energy derivatives (_DDB), ... – text files

density (_DEN), potential (_POT), wavefunctions (_WFK), ... – binary F90 files

or similar files in netCDF (_DEN.nc, _POT.nc, _WFK.nc)

Advantage of netCDF : portable, addressed by content, extensible, Python-friendly

ABINIT : the pipeline and the driver



Basic ‘files’ file : delivers filenames

h2.in	Name of input file
h2.out	Name of main output file
h2i	‘Root’ name for possibly other input files
h2o	‘Root’ name for possibly other output files
h2	‘Root’ name for temporary files
hydrogen.hgh	Name for the pseudopotential file for atoms of type 1
[oxygen.pspnc	Name for the pseudopotential file for atoms of type 2]
[92u.psp	Name for the pseudopotential file for atoms of type 3]

Made of at least 6 lines (more if > 1 type of atoms) with one name/address specified on each of these lines.

A basic ‘input’ file : dihydrogen (I)

```
# H2 molecule in big cubic box
# Characters after  ’#’ or after ‘!’ are comments, will be ignored.
# Keywords followed by values. Order of keywords in file is not important.

# Definition of the unit cell
acell 10 10 10          # Keyword "acell" refers to
                        #  lengths of primitive vectors (default in Bohr)
# Definition of the atom types
ntypat 1                # Only one type of atom
znucl 1                 # Keyword "znucl" refers to atomic number of
                        # possible type(s) of atom. Pseudopotential(s)
                        # mentioned in "filenames" file must correspond
                        # to type(s) of atom. Here, the only type is Hydrogen.
# Definition of the atoms
natom 2                 # Two atoms
typat 1 1               # Both are of type 1, that is, Hydrogen
xcart                   # This keyword indicate that location of the atoms
                        # will follow, one triplet of number for each atom
  -0.7 0.0 0.0          # Triplet giving cartesian coordinates of atom 1, in Bohr
   0.7 0.0 0.0          # Triplet giving cartesian coordinates of atom 2, in Bohr
```

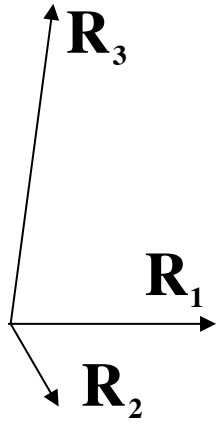
A basic input file : dihydrogen (II)

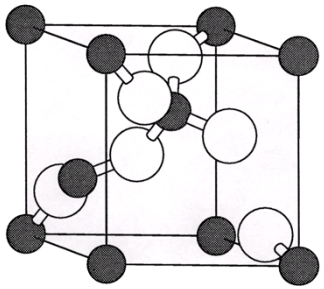
```
# Definition of planewave basis set
ecut 10.0          # Maximal plane-wave kinetic energy cut-off, in Hartree

# Definition of k-point grid
kptopt 0           # Enter k points manually
nkpt 1             # Only one k point is needed for isolated system,
                   # taken by default to be 0.0 0.0 0.0

#Definition of SCF (self-consistent field) procedure
nstep 10           # Maximal number of SCF cycles
toldfe 1.0d-6      # Will stop when, twice in a row, the difference
                   # between two consecutive evaluations of total energy
                   # differs by less than toldfe (default in Hartree)
diemac 2.0         # Although this is not mandatory, it is worth to precondition the
                   # SCF cycle. A model dielectric function, used as standard
                   # preconditioner, is described in "dielng" input variable section.
                   # Here, we follow prescriptions for molecules in a big box
## After modifying the following section, one might need to …
#%%<BEGIN TEST_INFO>          Metadata … to be ignored in the tutorial !
```

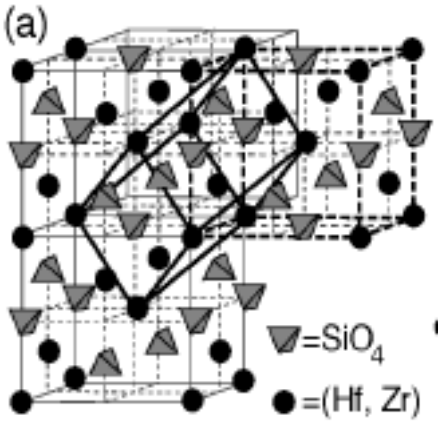
ABINIT : periodic codes + PWs

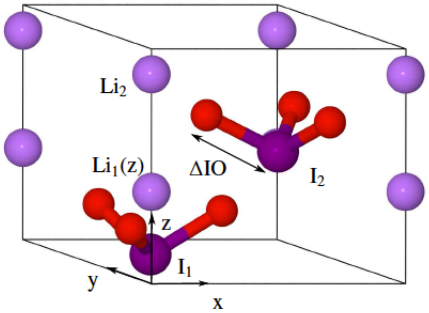
Plane waves e^{iKr} : particularly simple and efficient (when used with pseudopotentials), but infinite spatial extent.

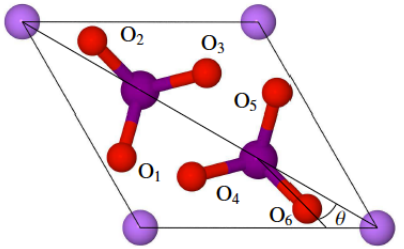
Cannot use a finite set of planewaves for finite systems !
Need periodic boundary conditions.
Primitive vectors $\mathbf{R}_j$, primitive cell volume Ω_0





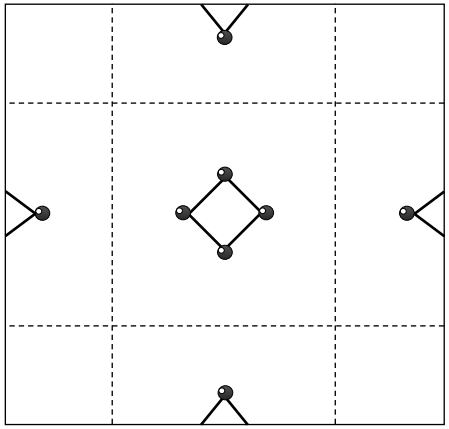




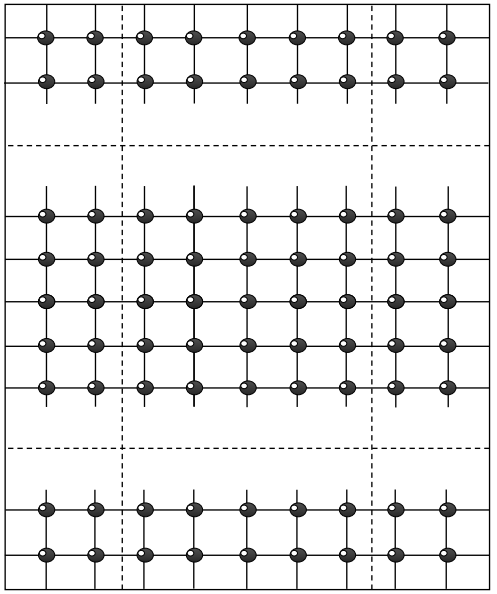


OK for crystalline solids
But : finite systems, surfaces, defects, polymers, nanosystems ... ?

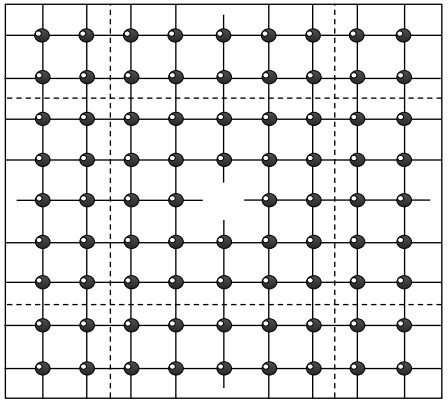
Solution : the supercell technique



Molecule,
cluster



Surface : treatment
of a slab
Interface

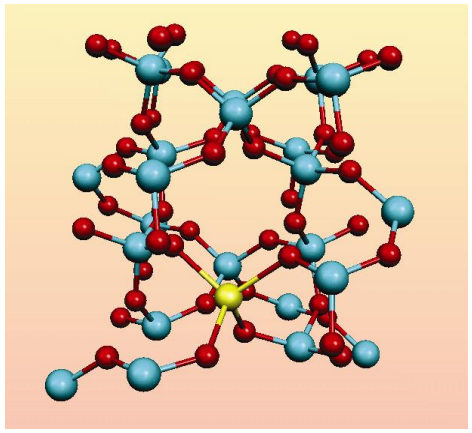


Point defect in a bulk solid

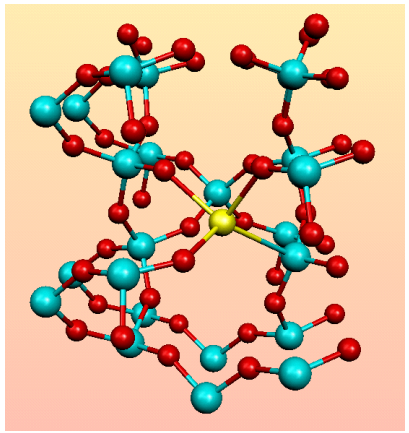
The supercell must be sufficiently big : convergence study

Examples of defects SiO_2-quartz : Pb

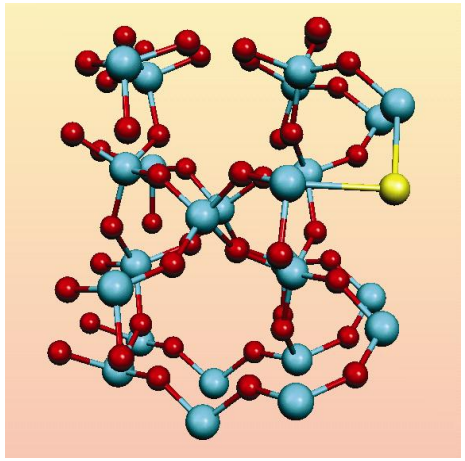
72-atom supercell of quartz



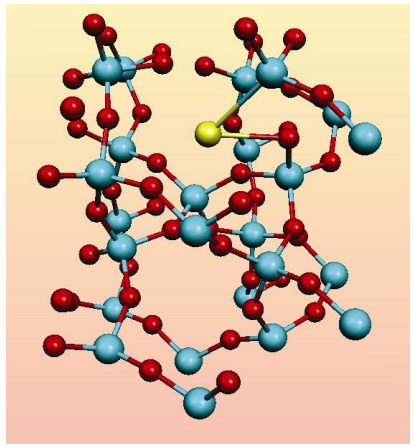
Pb^{Si}



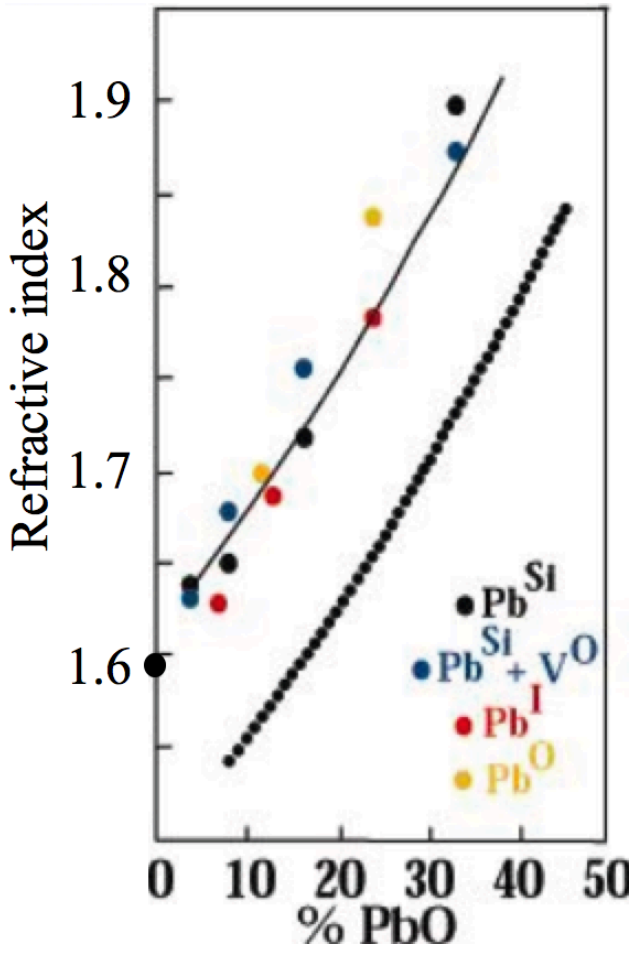
$Pb^{Si} + V^{O}$



Pb^{O}



Pb^{I}



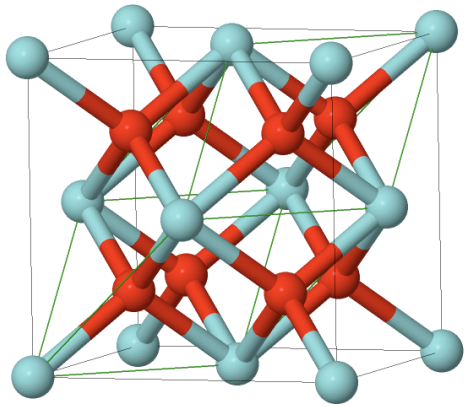
Comparison with amorphous SiO_2

Main input file : input variable flexibility

- cell primitive vectors → rprim
  … or angle (degrees) between primitive vectors → angdeg
  + scale cell vector lengths → acell
  + scale cartesian coordinates → scalecart
- number of atoms → natom
- reduced coordinates → xred (initial guess …)
  … or cartesian coordinates → xcart (in Bohr) / xangst (in Å)
- types of atoms → ntypat , typat
- space group → spgroup + natrd
  … or number of symmetries → nsym
  + symmetry operations → symrel + tnons

Example : cubic zirconium dioxide

Face-centered cubic, with three atoms per primitive cell



```
natom 3
acell 3*5.01 Angst      NOTE "*" is a repeater
rprim  0.0 0.5 0.5
       0.5 0.0 0.5
       0.5 0.5 0.0
typat 1 2 2
xred 3*0.0  3*0.25 3*0.75
=> symmetries are found automatically
```

OR

```
natom 3
acell 3*5.01 Angst
rprim  0.0 0.5 0.5
       0.5 0.0 0.5
       0.5 0.5 0.0
typat 1 2 2
spgroup 225      natrd 2
xred 3*0.0  3*0.25        => the set of atoms is completed automatically
```

Periodic system : wavevectors

For a periodic Hamiltonian : wavefunctions characterized by a wavevector $\mathbf{k}$ (crystal momentum) in Brillouin Zone

Bloch theorem $\psi_{m,\mathbf{k}}(\mathbf{r}+\mathbf{R}_j) = e^{i\mathbf{k}.\mathbf{R}_j}\psi_{m,\mathbf{k}}(\mathbf{r})$

$\psi_{m,\mathbf{k}}(\mathbf{r}) = \left(N\Omega_0\right)^{-1/2} e^{i\mathbf{k}.\mathbf{r}} u_{m,\mathbf{k}}(\mathbf{r})$ $\quad$ $u_{m,\mathbf{k}}(\mathbf{r}+\mathbf{R}_j)=u_{m,\mathbf{k}}(\mathbf{r})$

Normalization ?

Born-von Karman supercell $\quad$ supercell vectors $N_j\mathbf{R}_j$ with $N=N_1N_2N_3$

$\psi_{m,\mathbf{k}}(\mathbf{r}+N_j\mathbf{R}_j) = \psi_{m,\mathbf{k}}(\mathbf{r})$

Planewave basis set

Reciprocal lattice : set of $\mathbf{G}$ vectors such that $e^{iGR_j} = 1$

e^{iGr} has the periodicity of the real lattice

$$u_k(\mathbf{r}) = \sum_{\mathbf{G}} u_k(\mathbf{G})\, e^{iGr}$$

$$\psi_k(\mathbf{r}) = \left(N\Omega_0\right)^{-1/2} \sum_{\mathbf{G}} u_k(\mathbf{G})\, e^{i(k+G)r}$$

$$u_k(\mathbf{G}) = \frac{1}{\Omega_o} \int_{\Omega_o} e^{-iGr}\, u_k(\mathbf{r})\, d\mathbf{r}$$ (Fourier transform)

Kinetic energy of a plane wave $-\frac{\nabla^2}{2} \rightarrow \frac{(\mathbf{k}+\mathbf{G})^2}{2}$

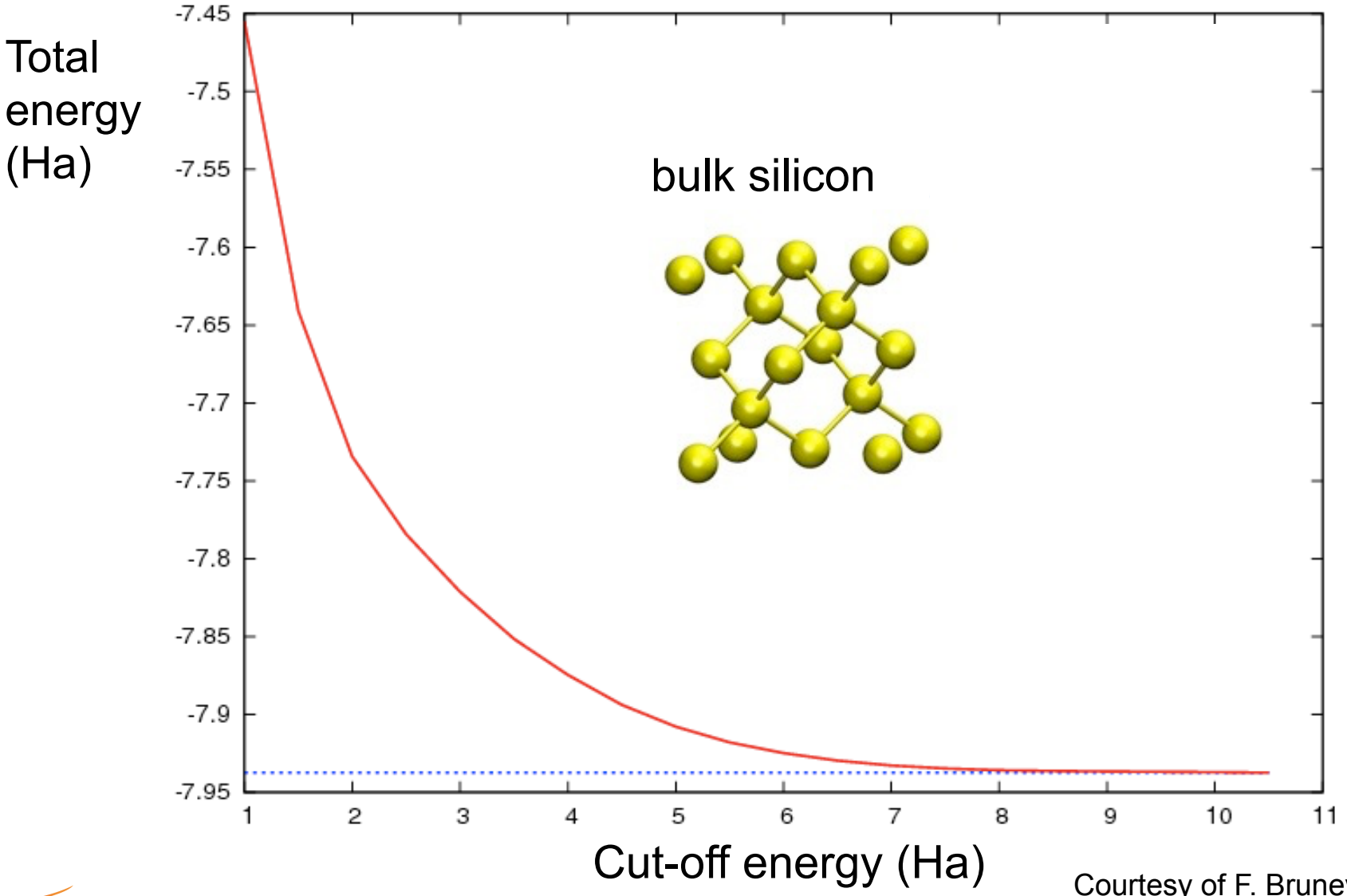
The coefficients $u_k(\mathbf{G})$ for the lowest eigenvectors decrease exponentially with the kinetic energy $\frac{(\mathbf{k}+\mathbf{G})^2}{2}$

Selection of plane waves determined by a cut-off energy E_{cut}

$$\frac{(\mathbf{k}+\mathbf{G})^2}{2} < E_{cut}$$ Plane wave sphere

ecut

Convergence wrt to kinetic energy cutoff



Courtesy of F. Bruneval

From discrete states to Brillouin zone

Discrete summations over states :

Total kinetic energy $\sum_n \langle \psi_n | -\frac{1}{2}\nabla^2 | \psi_n \rangle$

Density $n(\mathbf{r}) = \sum_n \psi_n^*(\mathbf{r})\psi_n(\mathbf{r})$

In the periodic case : summation over energy bands + integration over the Brillouin zone

Total kinetic energy $\sum_n \frac{1}{\Omega_{0\mathbf{k}}} \int_{\Omega_{0\mathbf{k}}} f(\varepsilon_F - \varepsilon_{n\mathbf{k}}) \langle \psi_{n\mathbf{k}} | -\frac{1}{2}\nabla^2 | \psi_{n\mathbf{k}} \rangle d\mathbf{k}$

Density $n(\mathbf{r}) = \sum_n \frac{1}{\Omega_{0\mathbf{k}}} \int_{\Omega_{0\mathbf{k}}} f(\varepsilon_F - \varepsilon_{n\mathbf{k}}) \psi_{n\mathbf{k}}^*(\mathbf{r})\psi_{n\mathbf{k}}(\mathbf{r}) d\mathbf{k}$

How to treat $\frac{1}{\Omega_{o\mathbf{k}}} \int_{\Omega_{o\mathbf{k}}} X_{\mathbf{k}} \, d\mathbf{k}$?

Brillouin zone integration

$$\frac{1}{\Omega_{o\mathbf{k}}} \int_{\Omega_{o\mathbf{k}}} X_{\mathbf{k}} \, d\mathbf{k} \Rightarrow \sum_{\{\mathbf{k}\}} w_{\mathbf{k}} X_{\mathbf{k}} \qquad [\text{ with } \sum_{\{\mathbf{k}\}} w_{\mathbf{k}} = 1 \,]$$

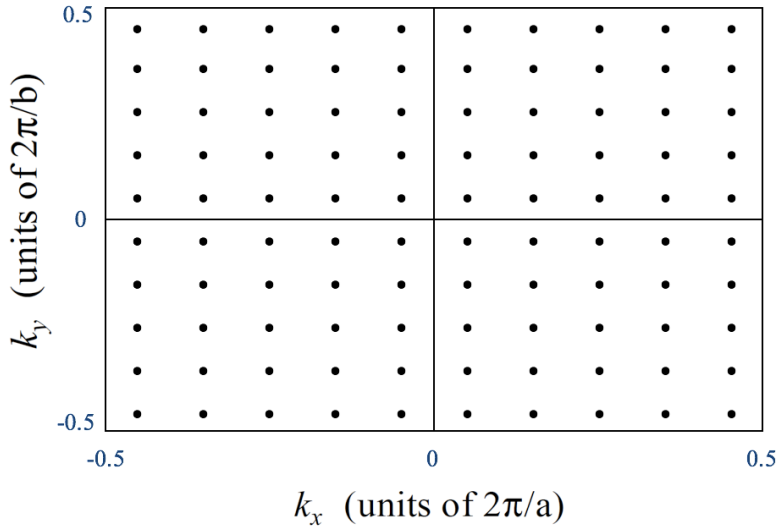
How to chose $\{\mathbf{k}\}$ and $\{w_{\mathbf{k}}\}$?

Special points

Weights

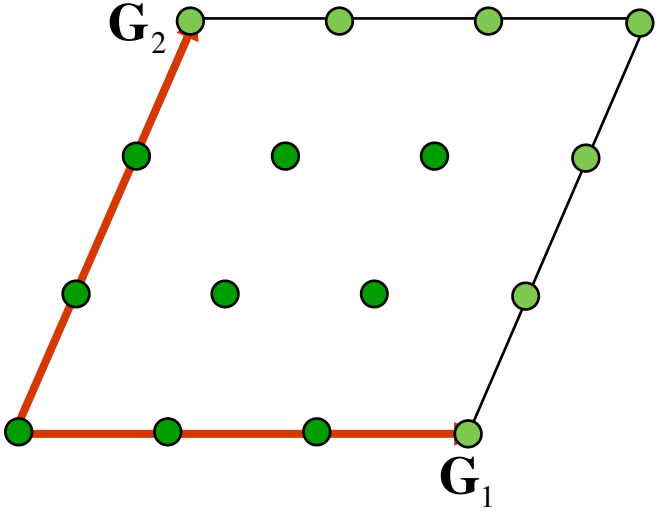
Simple answer : Homogeneous grid (1D - 2D - 3D) and equal weights

Homogeneous sampling of the Brillouin zone

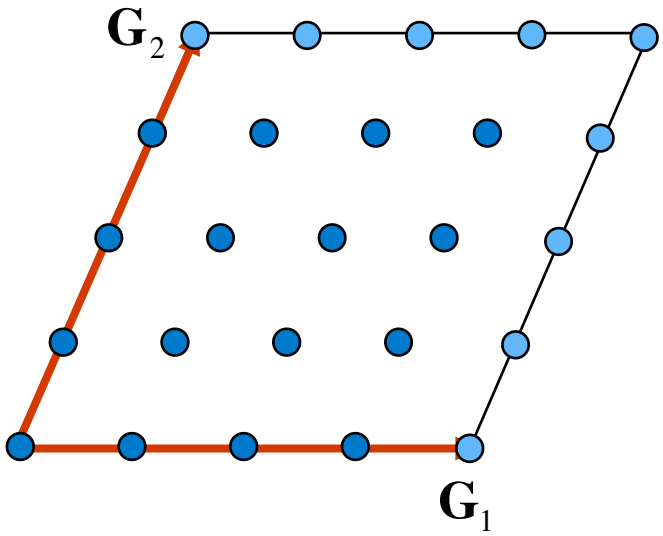


BZ integration : Monkhorst-Pack grid

- Uniformly spaced grid of $n_{k1} \times n_{k2} \times n_{k3}$ points in the first Brillouin Zone [Monkhorst & Pack, Phys. Rev. B 13, 5188 (1976)]



$n_{k1} = n_{k2} = 3$

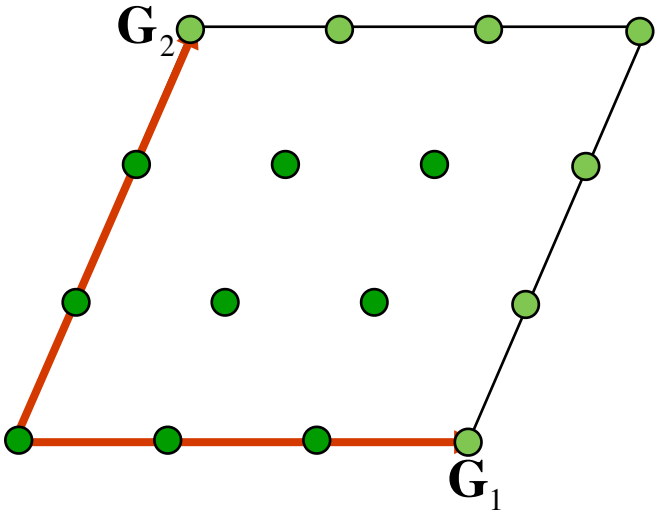


$n_{k1} = n_{k2} = 4$

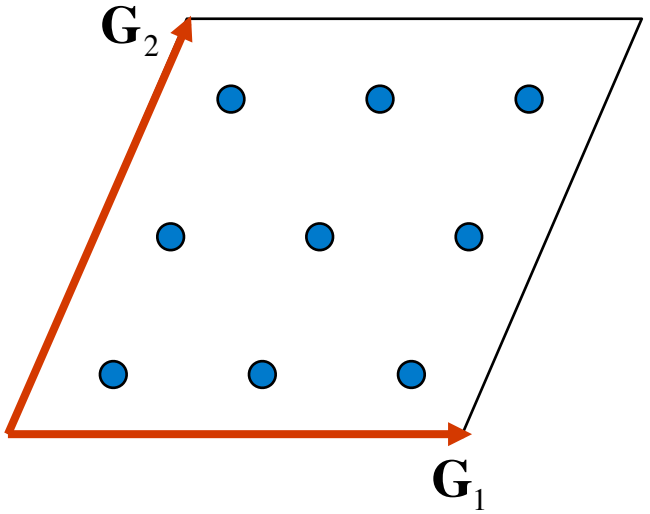
`ngkpt nk1 nk2 nk3`

Unshifted and shifted grids

- k-points grid can be chosen to be shifted : not centered at Γ.
- Advantage : comparable accuracy can be obtained with fewer k-points in IBZ (especially for highly symmetric cases)



$n_{k1} = n_{k2} = 3$
unshifted



$n_{k1} = n_{k2} = 3$
shifted by (1/2,1/2)

```
ngkpt nk1 nk2 nk3
shiftk sk1 sk2 sk3   (default: 0.5 0.5 0.5)
```

Algorithmics : problems to be solved

(1) Kohn - Sham equation

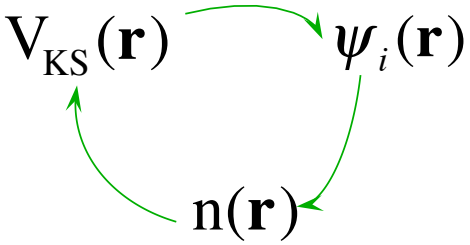
$$\underline{\underline{A}}\ \underline{x}_i = \lambda_i \underline{x}_i$$

$$\left[-\frac{1}{2}\nabla^2 + V_{KS}(\mathbf{r})\right]\psi_i(\mathbf{r}) = \varepsilon_i\,\psi_i(\mathbf{r})$$

$\{\mathbf{G}_j\}$ $\{\mathbf{r}_j\}$

Size of the system	[2 atoms…	600 atoms…] + vacuum ?
Dimension of the vectors $\underline{x}_i$	300…	100 000… (if planewaves)
# of (occupied) eigenvectors	4…	1200…

(2) Self-consistency

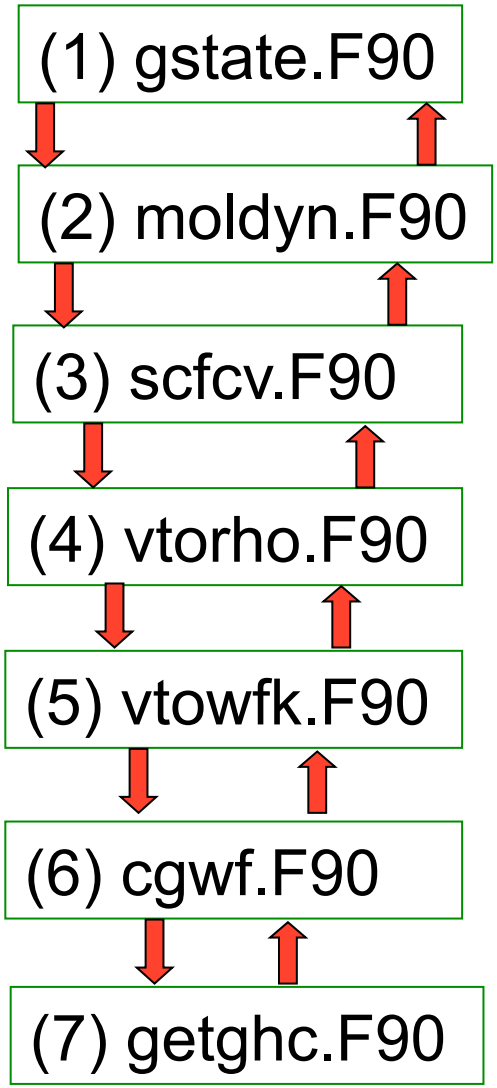


(3) Geometry optimization

Find the positions $\{\mathbf{R}_\kappa\}$ of ions such that the forces $\{\mathbf{F}_\kappa\}$ vanish
[= Minimization of energy]

Current practice : iterative approaches

Stages in the main processing unit



Ground-state

Molecular dynamics

Self-consistent field convergence

From a potential (v) to a density (rho)

From a potential (v) to
a wavefunction at some k-point

Conjugate-gradient on one wavefunction

Get the application of the Hamiltonian

A basic ‘input’ file : dihydrogen (I)

```
# H2 molecule in big cubic box
# Characters after  ’#’ or after ‘!’ are comments, will be ignored.
# Keywords followed by values. Order of keywords in file is not important.

# Definition of the unit cell
acell 10 10 10          # Keyword "acell" refers to
                        #  lengths of primitive vectors (default in Bohr)
# Definition of the atom types
ntypat 1                # Only one type of atom
znucl 1                 # Keyword "znucl" refers to atomic number of
                        # possible type(s) of atom. Pseudopotential(s)
                        # mentioned in "filenames" file must correspond
                        # to type(s) of atom. Here, the only type is Hydrogen.
# Definition of the atoms
natom 2                 # Two atoms
typat 1 1               # Both are of type 1, that is, Hydrogen
xcart                   # This keyword indicate that location of the atoms
                        # will follow, one triplet of number for each atom
  -0.7 0.0 0.0          # Triplet giving cartesian coordinates of atom 1, in Bohr
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```

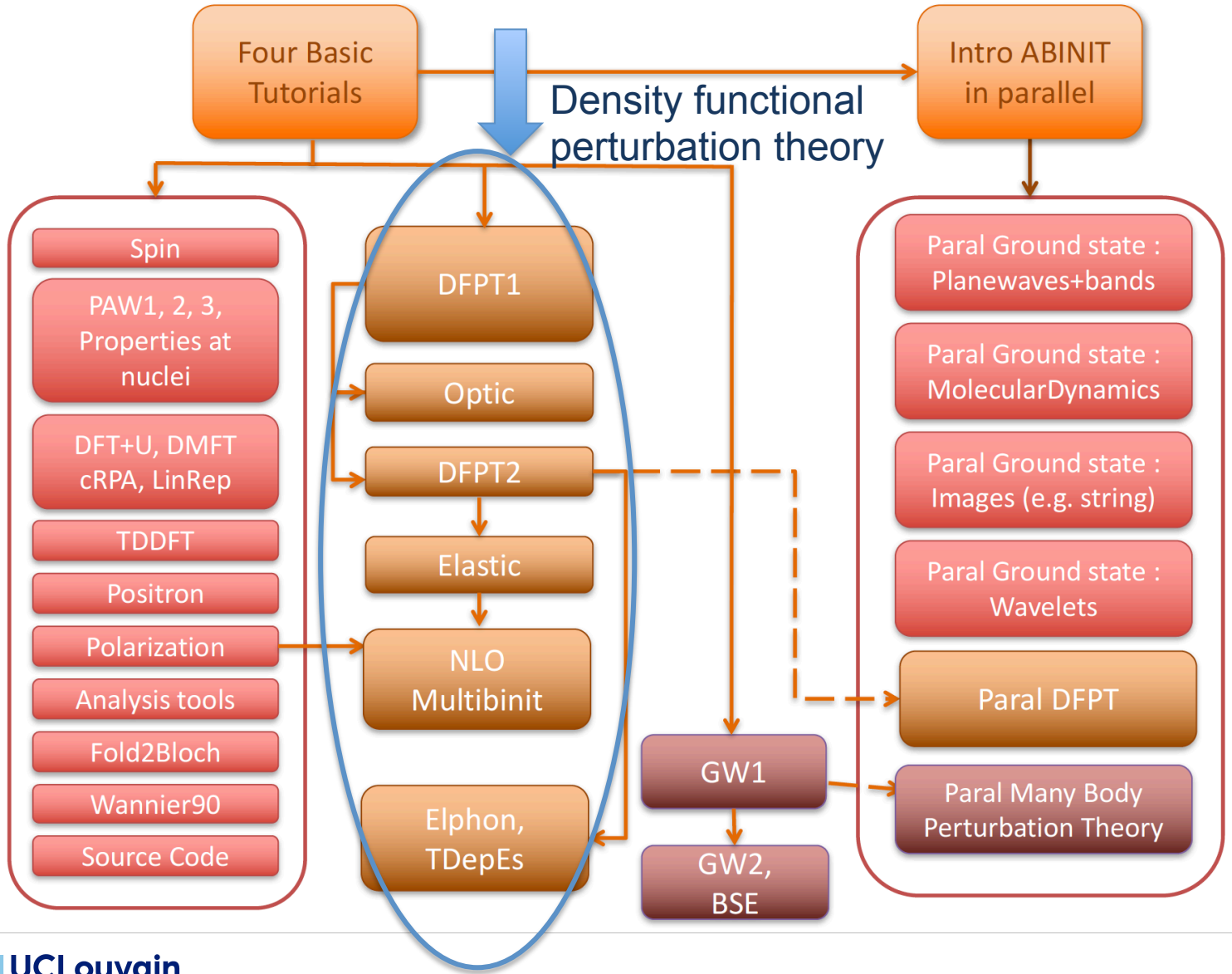
A basic input file : dihydrogen (II)

```
# Definition of planewave basis set
ecut 10.0          # Maximal plane-wave kinetic energy cut-off, in Hartree

# Definition of k-point grid
kptopt 0           # Enter k points manually
nkpt 1             # Only one k point is needed for isolated system,
                   # taken by default to be 0.0 0.0 0.0

#Definition of SCF (self-consistent field) procedure
nstep 10           # Maximal number of SCF cycles
toldfe 1.0d-6      # Will stop when, twice in a row, the difference
                   # between two consecutive evaluations of total energy
                   # differs by less than toldfe (default in Hartree)
diemac 2.0         # Although this is not mandatory, it is worth to precondition the
                   # SCF cycle. A model dielectric function, used as standard
                   # preconditioner, is described in "dielng" input variable section.
                   # Here, we follow prescriptions for molecules in a big box
## After modifying the following section, one might need to …
#%%<BEGIN TEST_INFO>          Metadata … to be ignored in the tutorial !
```

ABINIT tutorial : layout + dependencies



Density Functional Perturbation Theory

Many physical properties = derivatives of total energy
(or suitable thermodynamic potential) with respect to perturbations.

Consider :

- atomic displacements (phonons)
- dilatation/contraction of primitive cell
- homogeneous external field (electric field, magnetic field ...)

Derivatives of total energy (electronic part + nuclei-nuclei interaction) :

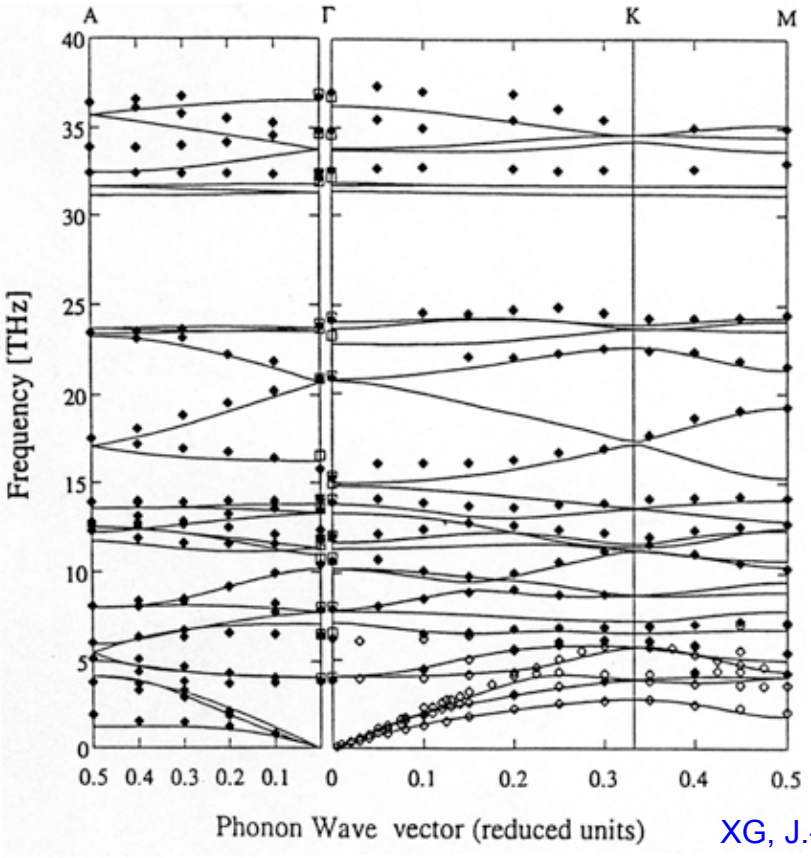
1st order derivatives : forces, stresses, dipole moment ...

2nd order derivatives : dynamical matrix, elastic constants, dielectric susceptibility
atomic polar tensors or Born effective charge tensors
piezoelectricity, internal strains ...

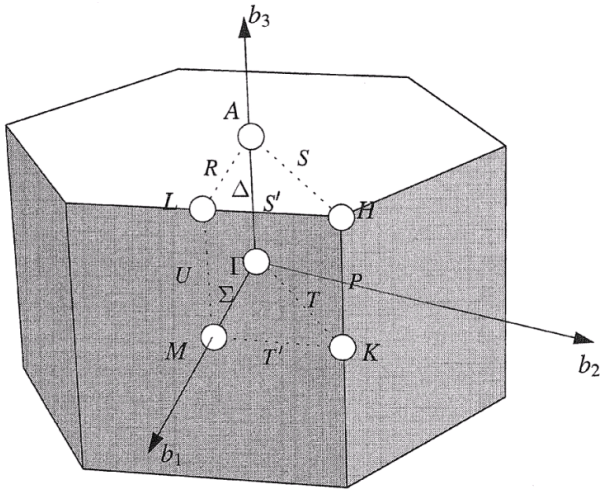
3rd order derivatives : non-linear dielectric susceptibility, Raman susceptibilities
electro-optic effect, phonon - phonon interaction, Grüneisen parameters, ...

Further properties obtained by integration over phononic degrees of freedom :
entropy, thermal expansion, phonon-limited thermal conductivity ...

Phonon band structure



SiO_2 alpha-quartz



XG, J.-C.Charlier, D.C.Allan, M.P.Teter, *Phys. Rev. B* 50, 13055 (1994)

Analysis of instabilities

$MgSiO_3$

CUBIC

(5at/cell)

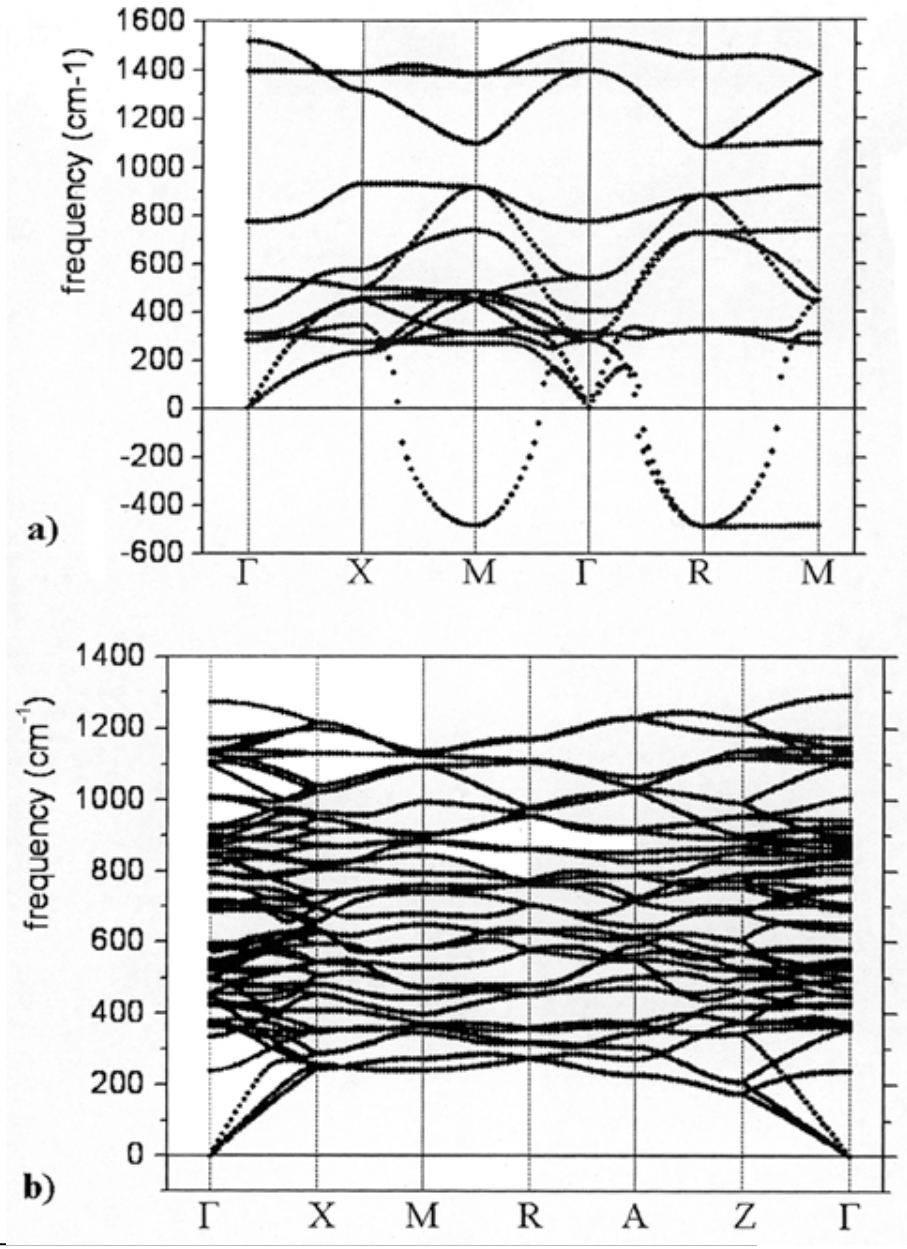
Phonon dispersion relations.

(a) Ideal cubic phase : unstable.

(b) Condensations of the unstable phonon modes generate
a (meta) stable orthorhombic phase

ORTHORHOMBIC

(20at/cell)



Helmoltz free energy and specific heat

$$F = U - TS$$

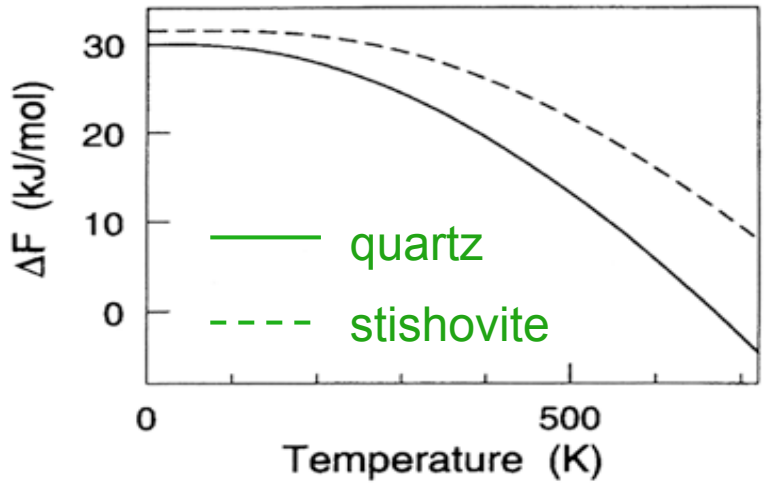
$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = T\left(\frac{\partial S}{\partial T}\right)_V = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_V$$

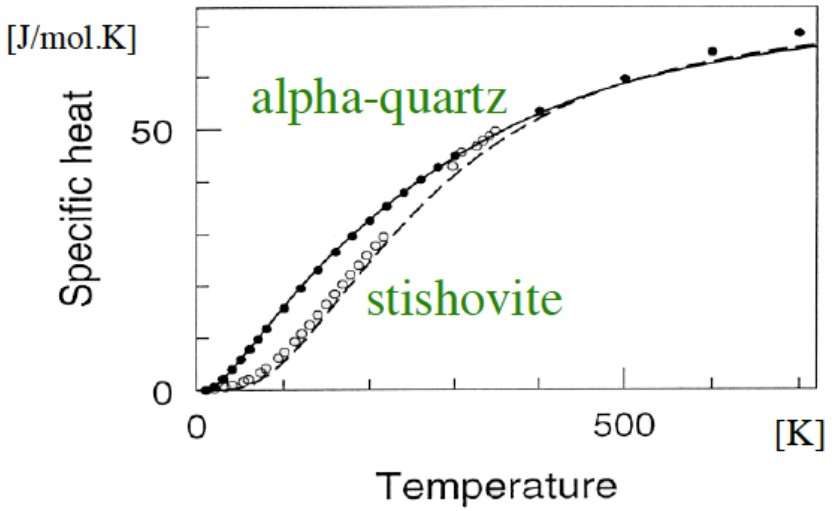
Vibrational contribution to F :

$$\Delta F = 3n_{at}N\ k_B T \int_0^{\omega_{max}} \ln\left\{2\sinh\left(\frac{\omega}{2k_B T}\right)\right\} g(\omega)d\omega$$

Vibrational contribution to Cv :

$$C_V = 3n_{at}N\ k_B \int_0^{\omega_{max}} \left(\frac{\omega}{2k_B T}\right)^2 \mathrm{csch}^2\left(\frac{\omega}{2k_B T}\right) g(\omega)d\omega$$



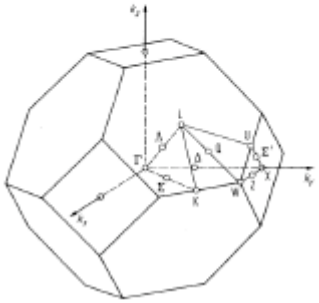


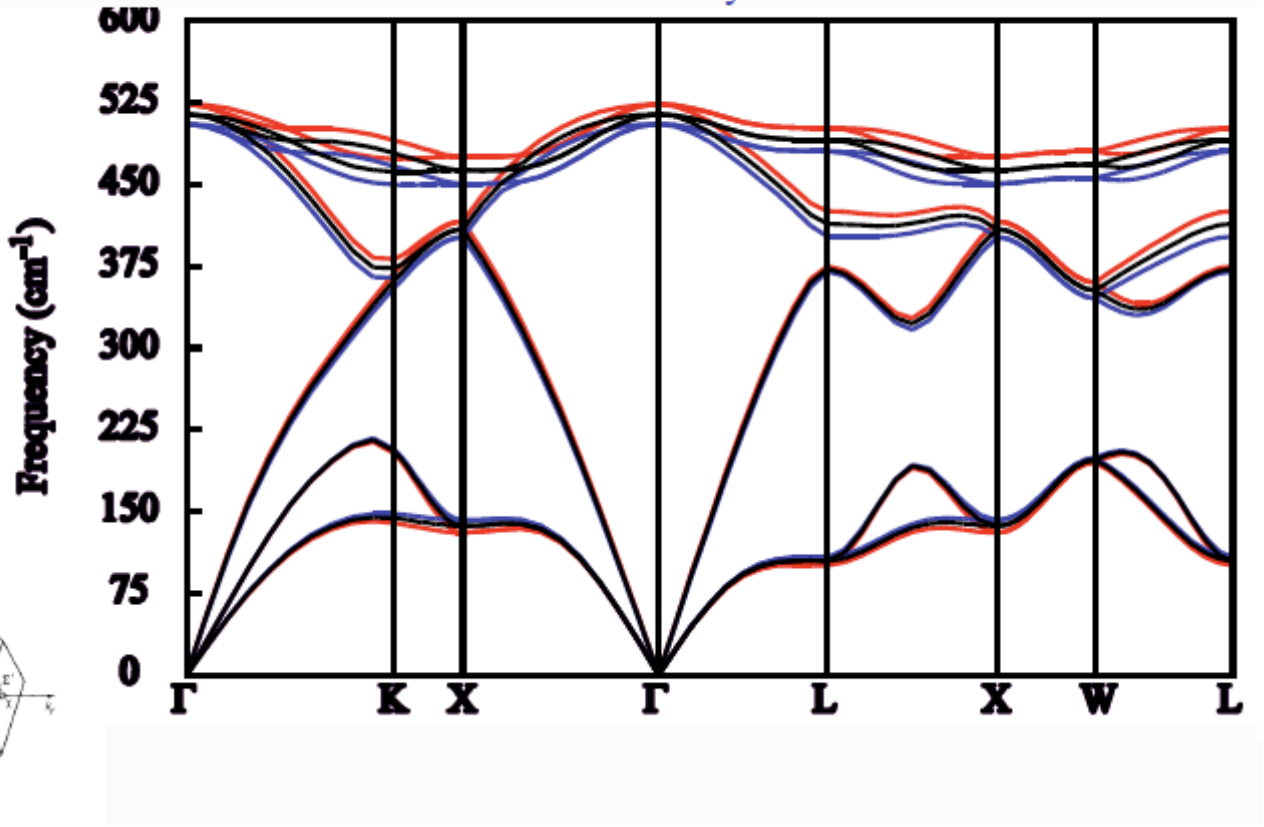
Ab initio thermal expansion

$$\alpha(T) = \frac{V}{3B} \sum_{\vec{q},m} \frac{1}{\hbar \omega_{\vec{q},m}} \gamma_{\vec{q},m} \frac{\partial n(\omega_{\vec{q},m})}{\partial T}$$

$$\gamma_{m,\vec{q}} = -\frac{\partial(\ln \omega_{m,\vec{q}})}{\partial(\ln V)}$$

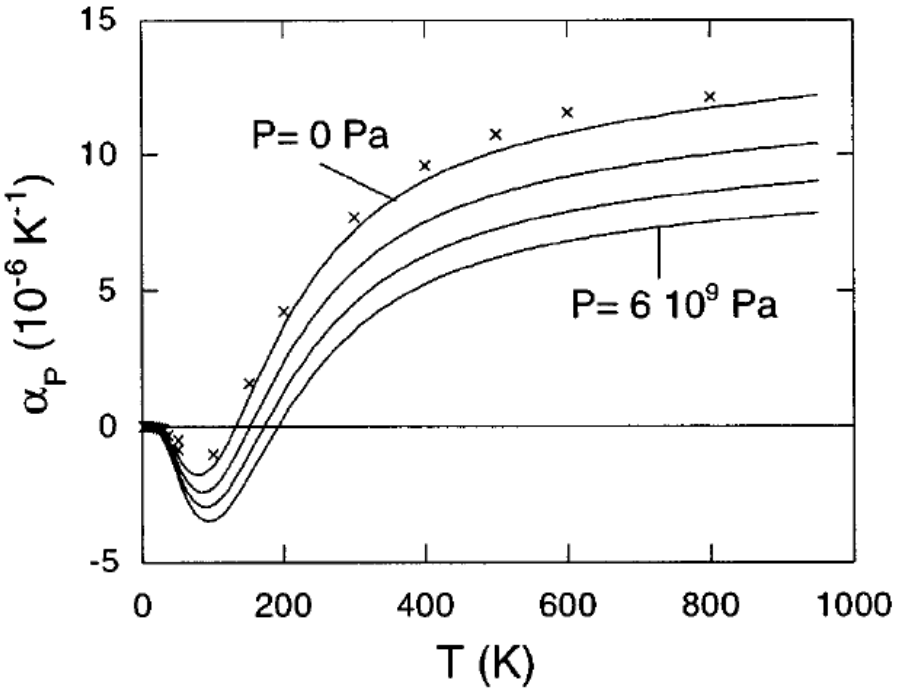
Alternative path : minimisation of free energy

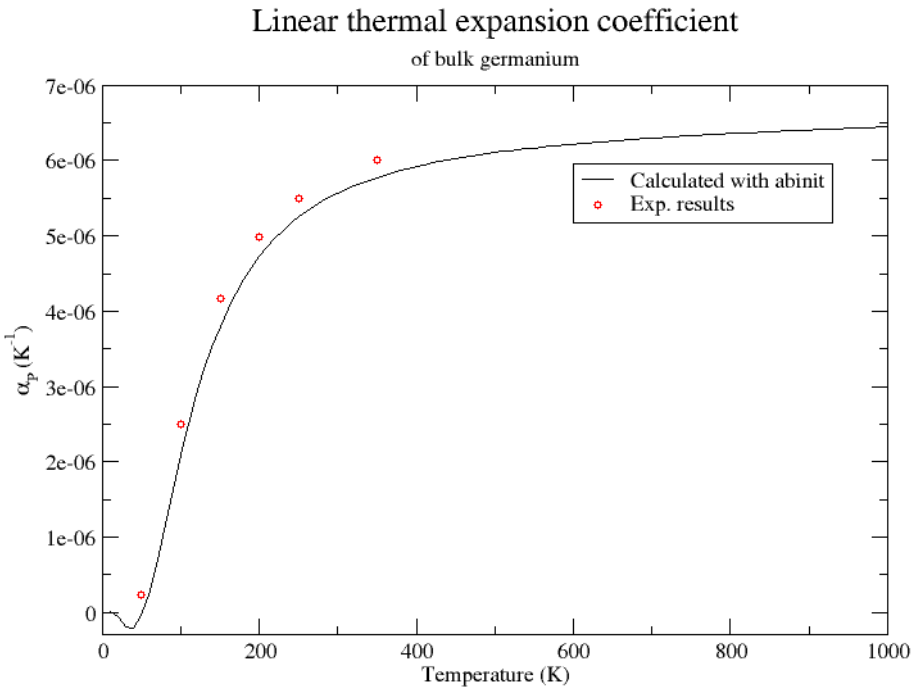




Ab initio thermal expansion

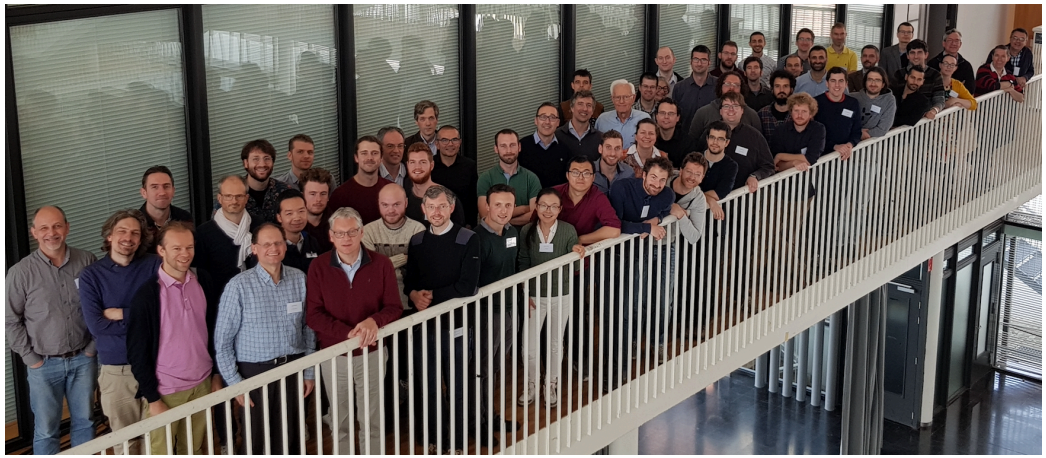
Linear thermal expansion coefficient of bulk silicon





G.-M. Rignanese, J.-P. Michenaud and XG
Phys. Rev. B 53, 4488 (1996)

Wrap-up



Free software (open source)

Excellent documentation

Implementation of density-functional theory (DFT), many body-perturbation theory (MBPT - GW or BSE), density-functional perturbation theory (DFPT), dynamical mean-field theory (DMFT), ...

Versatile (many properties of materials)
Especially good at vibrational, dielectric, thermodynamic, spectroscopic, optical properties

Interested to contribute ?

There is a postdoc position open at Skoltech !
Contact X.Gonze@skoltech.ru
https://join.skoltech.ru/postdoc-positions/

Postdoctoral research position in Computational Materials Science
(still open ...)

Developer's corner on ABINIT Wiki
https://wiki.abinit.org

Developer's corner on ABINIT Web site
https://docs.abinit.org/developers