In the name of allah

Introduction to **ABINIT**

Under Supervision of Dr. Mozaffari

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Outline

- Capabilities of ABINIT
- Introducing the files file
- Format of the input file
- How to run the code?
- The main output file

Codes

siesta

QUANTUM ESPRESSO

Å abinit

VASP

Yambo©

ABINIT: an ab initio computational package for ground and excited calculations.

History

Software project started in 1997.
The first version was released in 2000.

Theory

Ground state: DFT
Excited state:
MBPT+GW
TDDFT

abinit

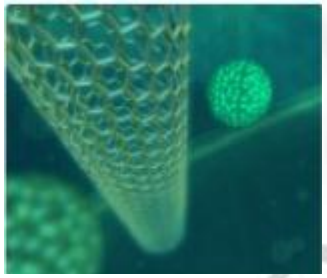
Method

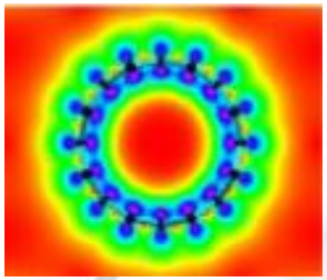
Pseudopotentials
and
Planewave basis set.

Support

ABINIT site.
Help files
and Tutorials online.
Users Forum.

http://www.abinit.org



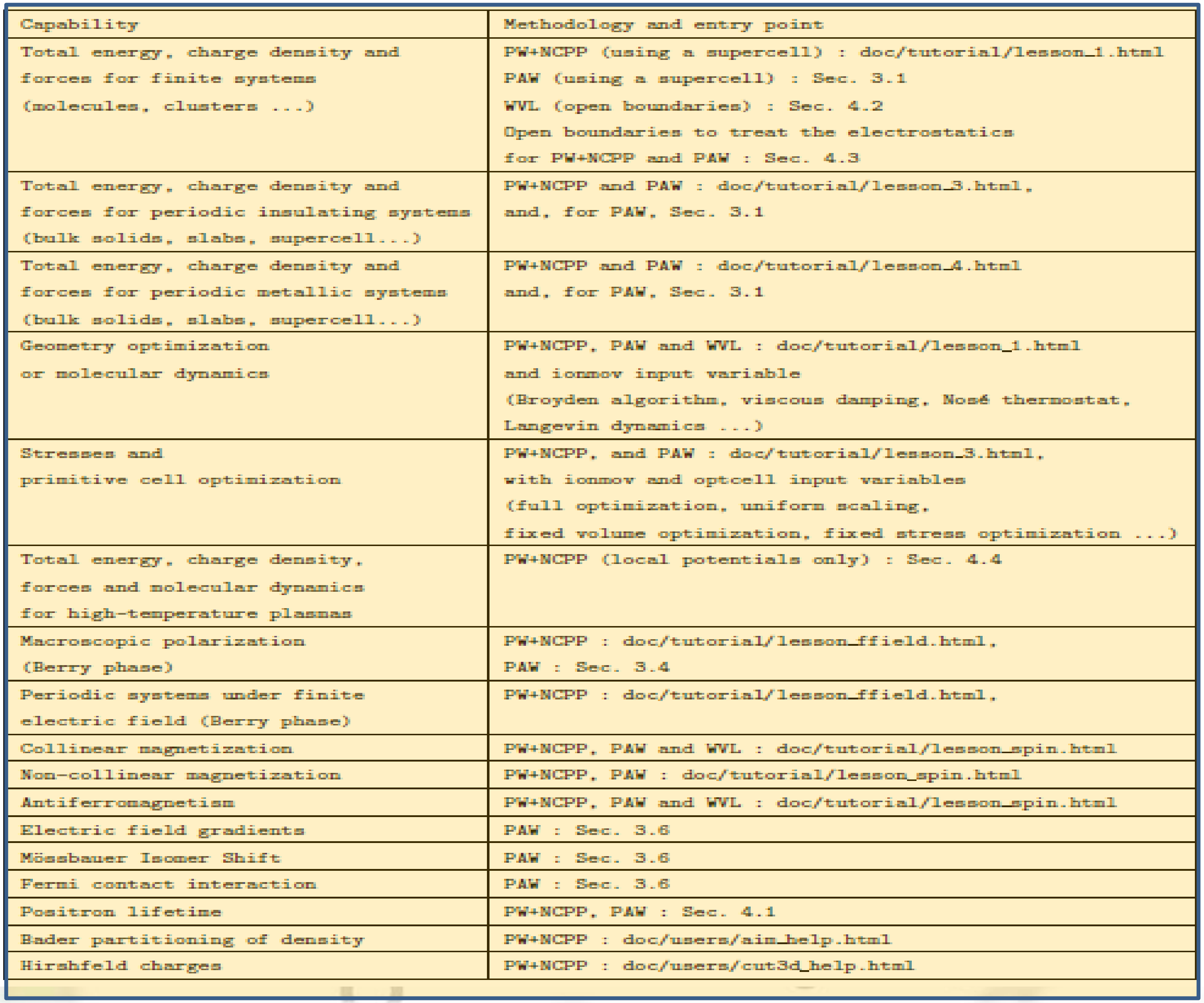


Capabilities of ABINIT

This package has the purpose of computing accurately material and nanostructure properties :

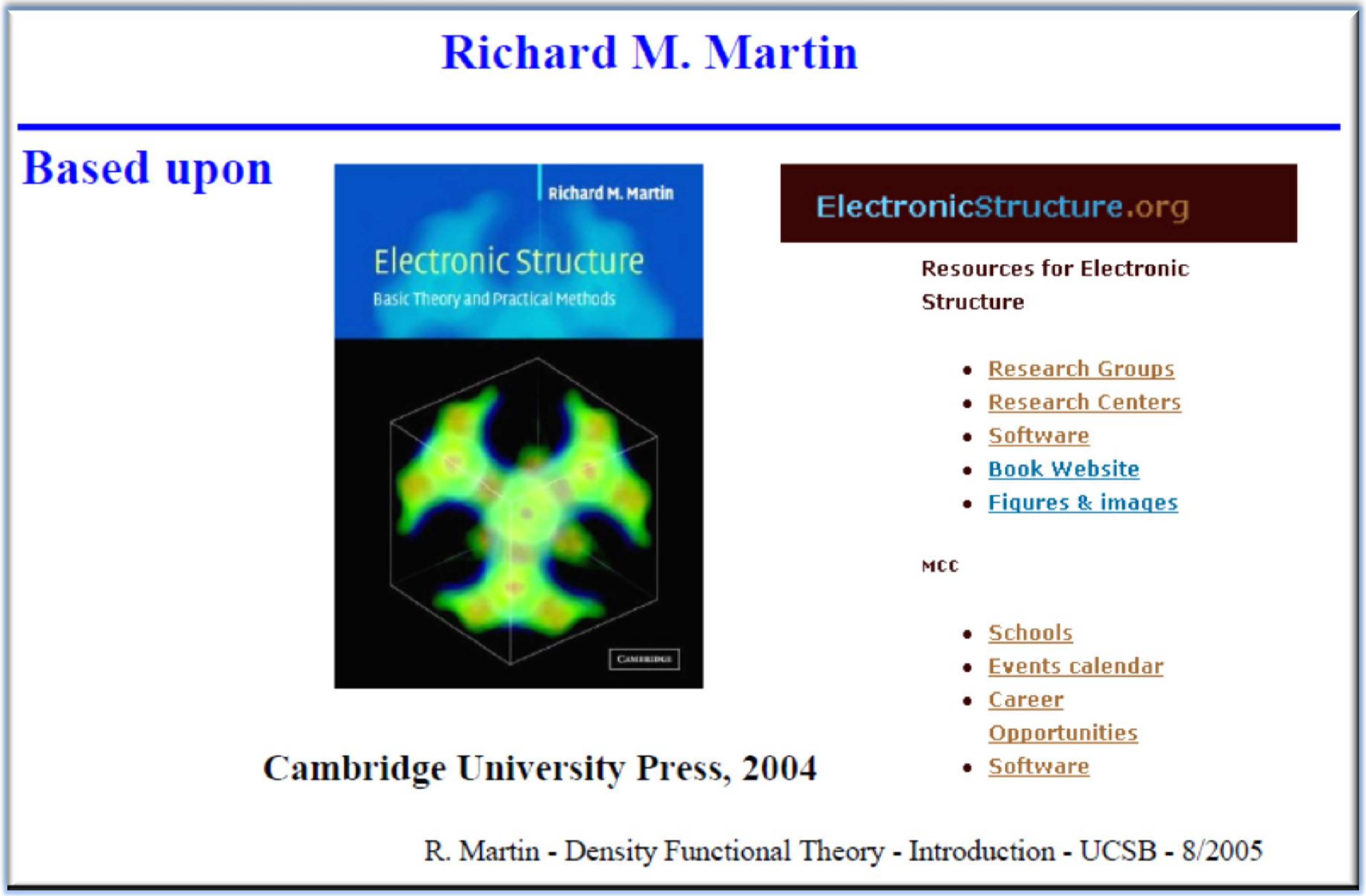
Beyond the computation of the total energy, charge density and electronic structure of such systems, ABINIT also implements many dynamical, dielectric, thermodynamical, mechanical, optical and magnetic *properties.*

Main Reference: X. Gonze et al. ***"ABINIT: First-principles approach to material and nanosystem properties"***, **Comput. Phys. Comm. 180**, (2009)



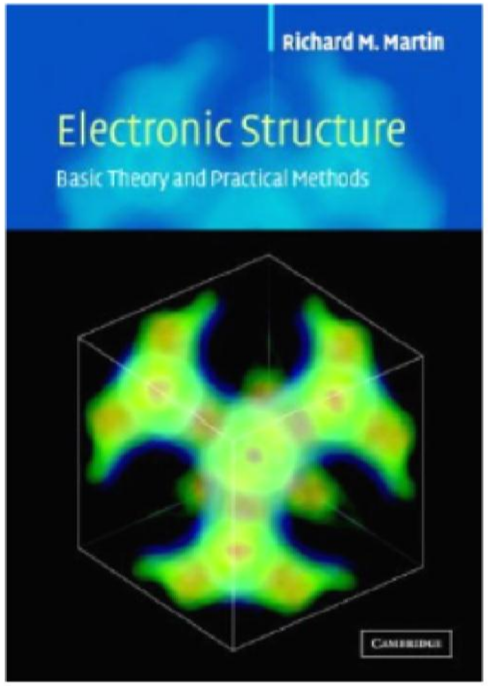
Capability	Methodology and entry point
Total energy, charge density and forces for finite systems (molecules, clusters ...)	PW+NCPP (using a supercell) : doc/tutorial/lesson_1.html PAW (using a supercell) : Sec. 3.1 WVL (open boundaries) : Sec. 4.2 Open boundaries to treat the electrostatics for PW+NCPP and PAW : Sec. 4.3
Total energy, charge density and forces for periodic insulating systems (bulk solids, slabs, supercell...)	PW+NCPP and PAW : doc/tutorial/lesson_3.html, and, for PAW, Sec. 3.1
Total energy, charge density and forces for periodic metallic systems (bulk solids, slabs, supercell...)	PW+NCPP and PAW : doc/tutorial/lesson_4.html and, for PAW, Sec. 3.1
Geometry optimization or molecular dynamics	PW+NCPP, PAW and WVL : doc/tutorial/lesson_1.html and ionmov input variable (Broyden algorithm, viscous damping, Nosé thermostat, Langevin dynamics ...)
Stresses and primitive cell optimization	PW+NCPP, and PAW : doc/tutorial/lesson_3.html, with ionmov and optcell input variables (full optimization, uniform scaling, fixed volume optimization, fixed stress optimization ...)
Total energy, charge density, forces and molecular dynamics for high-temperature plasmas	PW+NCPP (local potentials only) : Sec. 4.4
Macroscopic polarization (Berry phase)	PW+NCPP : doc/tutorial/lesson_ffield.html, PAW : Sec. 3.4
Periodic systems under finite electric field (Berry phase)	PW+NCPP : doc/tutorial/lesson_ffield.html,
Collinear magnetization	PW+NCPP, PAW and WVL : doc/tutorial/lesson_spin.html
Non-collinear magnetization	PW+NCPP, PAW : doc/tutorial/lesson_spin.html
Antiferromagnetism	PW+NCPP, PAW and WVL : doc/tutorial/lesson_spin.html
Electric field gradients	PAW : Sec. 3.6
Mössbauer Isomer Shift	PAW : Sec. 3.6
Fermi contact interaction	PAW : Sec. 3.6
Positron lifetime	PW+NCPP, PAW : Sec. 4.1
Bader partitioning of density	PW+NCPP : doc/users/aim_help.html
Hirshfeld charges	PW+NCPP : doc/users/cut3d_help.html

- If you have never used another electronic structure code, you should browse through the Chaps. 1 to 13 of the book *Electronic Structure.*



Richard M. Martin

Based upon



Cambridge University Press, 2004

ElectronicStructure.org

Resources for Electronic Structure

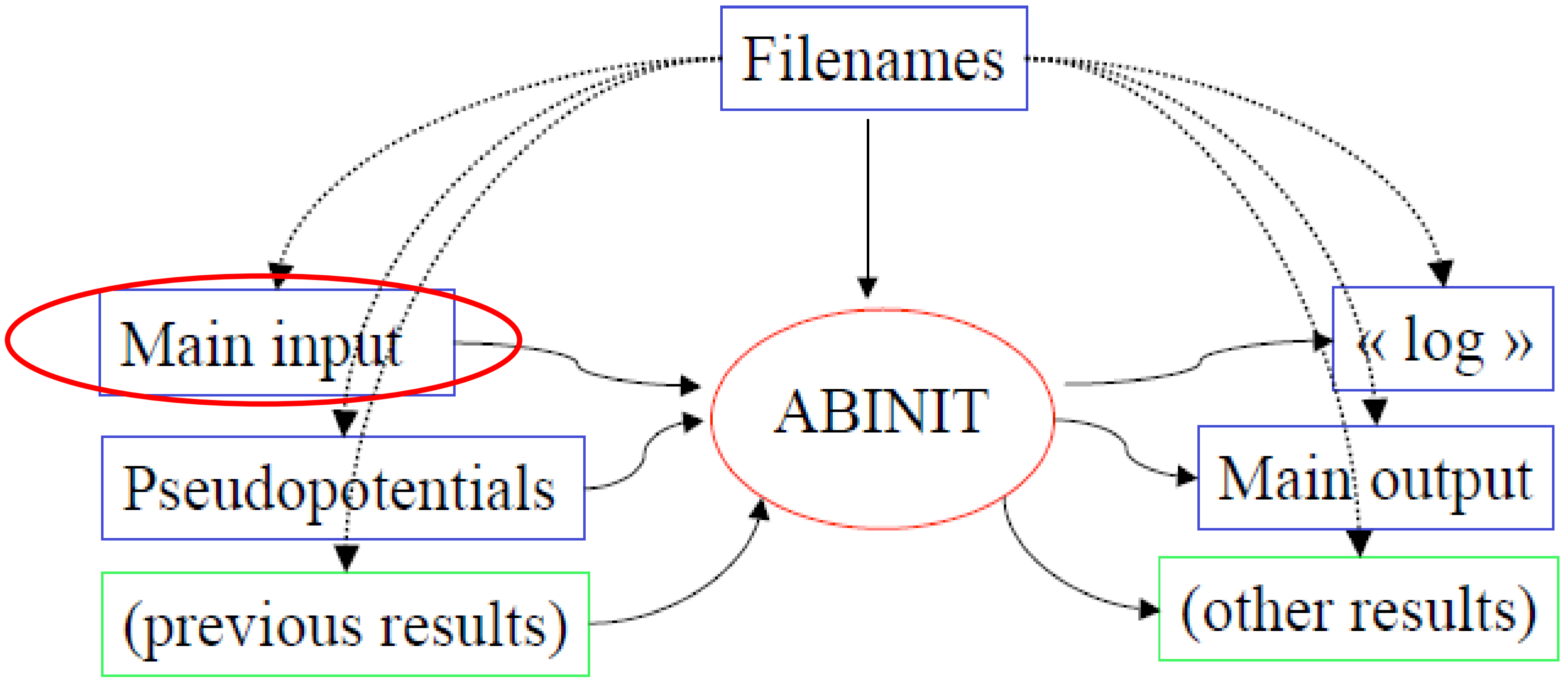
- Research Groups
- Research Centers
- Software
- Book Website
- Figures & images

MCC

- Schools
- Events calendar
- Career Opportunities
- Software

R. Martin - Density Functional Theory - Introduction - UCSB - 8/2005

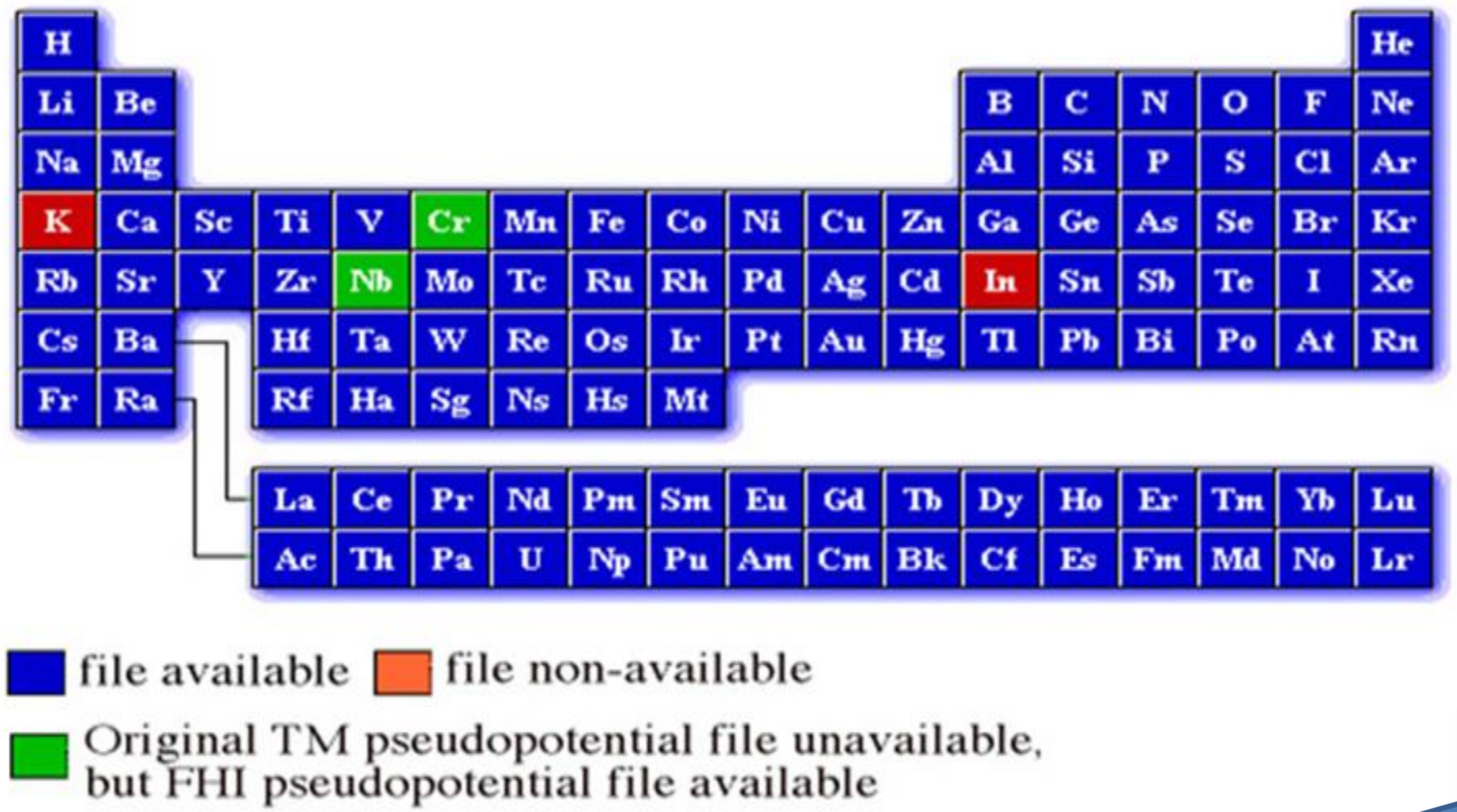
schematic picture of the different files in ABINIT □□■□□□□□□□□□□



Results : density (_DEN), potential (_POT), wavefunctions (_WFK), ...

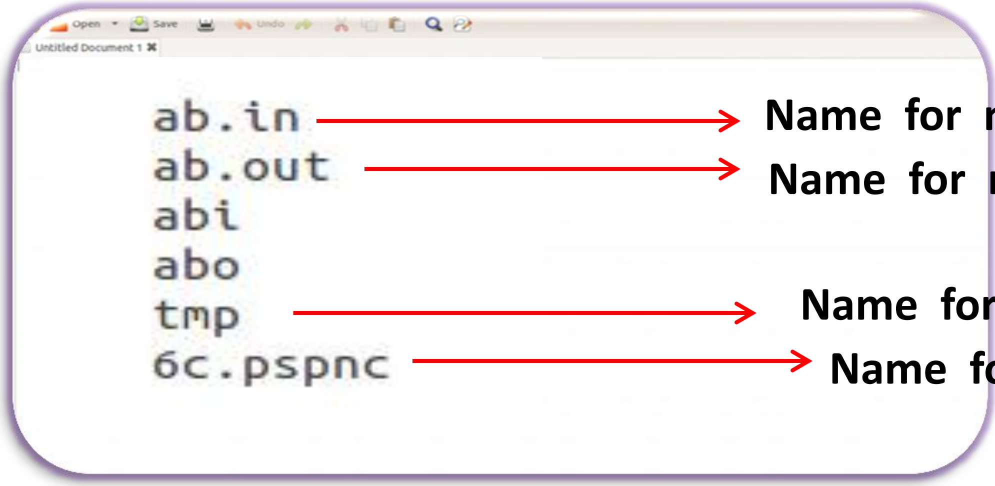
http://www.abinit.org/downloads/psp-links/psp-links/lda_tm

The pseudopotential files



The files file

- Open a text editor and type below lines:



```
ab.in
ab.out
abi
abo
tmp
6c.pspnc
```

Name for main input file
Name for main output file
Name for temporary file
Name for pseudopotential file

- Save it as: ab.files

Main input file

- The parameters are input to the code from a single input file.
- The names of all the parameters can be found in the input variables file.

acell bdgw bs_algorithm bs_ferq_mesh ecut ecuteps enunit ixc

iscf nsppol nstep nsym soenergy symsigma xred zcut

znucl gwcalctype gwmem kptopt ngfft ngkpt npwkss

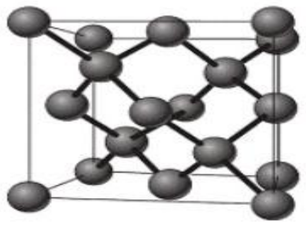
Definition of the crystal structure

```
acell    11.954  11.954  4.263  angstrom  # cell lattice vector scaling

rprim         1.0    0.0    0.0   # primitive translations in real space
              0.0    1.0    0.0
              0.0    0.0    1.0
```

- anything to the right of a "#" on any line is ignored by the code.
- the code choose (by default) atomic units:
  - the Hartree for energy
  - the Bohr for lengths

Other units:

- **'Ry ' => Rydberg (for energies)**
- **'eV ' => electron-volts (for energies)**
- **'angstr...' => Angstrom (for lengths)**



#Definition of the atom types

```
ntypat    3           # number of types of atoms
znucl    29 49 8      # nuclear charge
```

#Definition of the atoms

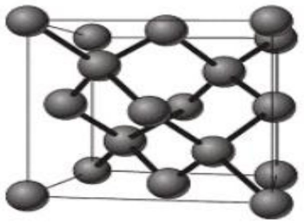
```
natom    4          # total number of atoms in the unit cell
typat    1 2 3 3    # an integer label to every atom in the unit cell

xred
      0.0000   0.0000   0.0000
      0.5000   0.5000   0.5000
      0.1061   0.1061   0.1061
     -0.1061  -0.1061  -0.1061
```

Example:CuInO2

There are three options for atom positions:

xcart: vectors (X) of atom positions in CARTesian coordinates -length in Bohr-

xangst: vectors (X) of atom positions in cartesian coordinates -length in ANGSTrom-



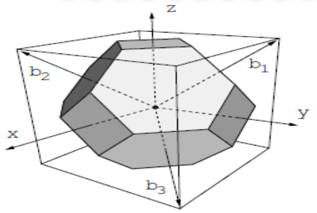
xred: vectors (X) of atom positions in REDuced coordinates

The choice of the k-point mesh

$$n(r) = \frac{\Omega_{cell}}{(2\pi)^3} \sum_n \int_{BZ} d^3k \left|\phi_{n,k}(r)\right|^2 \longrightarrow n(r) = \sum_n \sum_{i=1}^{N_k} w_i \left|\phi_{n,k_i}(r)\right|^2$$

```
kptopt   1        # option for the automatic generation of k points,

ngkpt    4 4 4    # number of grid points for kpoints generation
```

```
kptopt   0        # option for the manually generation of k points,

nkpt     40       # number of kpoints

kpt        0.00000000E+00  0.00000000E+00  0.00000000E+00
           0.00000000E+00  0.00000000E+00  2.50000000E-02
           0.00000000E+00  0.00000000E+00  5.00000000E-02
                           …
```



The cutoff of the plane wave basis

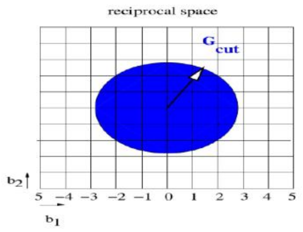
- ABINIT decomposes the Kohn-Sham wave function into an infinite sum of plane waves:

$$\varphi_{n,k}(r) = \frac{1}{\sqrt{\Omega_{cell}}} \sum_{G} c_{n,k}(G) e^{i(k+G).r}$$

- a parameter ecut has to be set that limits the summation to be executed only over:

$$\frac{1}{2}|k+G|^2 \le E_{cutoff} \quad , \quad N_{pw} \propto \Omega_{cell} (E_{cutoff})^{3/2}$$

```
ecut   30          #Hartree

#other option        60   Ry
#other option        816  eV
```



• Kohn-Sham equations

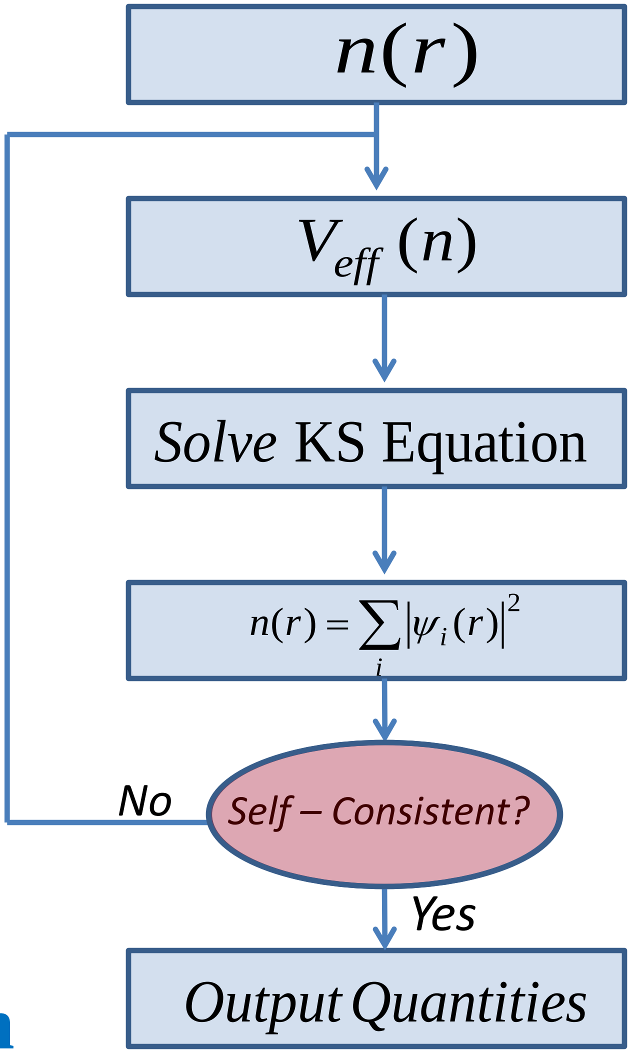
$$(-\frac{\nabla^2}{2}+V_{eff}[n])\psi_i(r)=\varepsilon_i\psi_i(r)$$

$$V_{eff}[n]=V_{ext}(r)+V_{Hartree}[n]+V_{xc}[n]$$

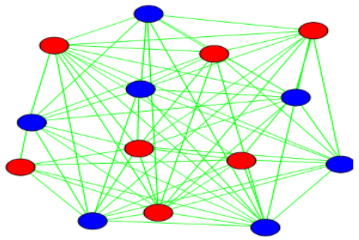
✓ exchange-correlation energy

$$V_{xc}(r)=\frac{\partial E_{xc}[n(r)]}{\partial n(r)}$$

Local density approximation



✓LDA: Teter Pade parametrization



R. M. Martin, *Electronic Structure*, page 173

the choice of the exchange-correlation potential

- **ixc** #Integer for eXchange-Correlation choice

1=> LDA or LSD, Teter Pade parametrization (4/93, published in S. Goedecker, M. Teter, J. Huetter, Phys.Rev.B54, 1703 (1996)), which reproduces Perdew-Wang (which reproduces Ceperley-Alder!).

2=> LDA, Perdew-Zunger-Ceperley-Alder (no spin-polarization)

3=> LDA, old Teter rational polynomial parametrization (4/91) fit to Ceperley-Alder data

…

11=> GGA, Perdew-Burke-Ernzerhof GGA functional

12=> GGA, x-only part of Perdew-Burke-Ernzerhof GGA functional

13=> GGA potential of van Leeuwen-Baerends, while for energy, Perdew-Wang 92 functional

…

27=> GGA, HTCH407 of A.D. Boese, and N.C. Handy, J. Chem. Phys 114, 5497 (2001).

Self-Consistent Field

- ❑ In order to find a **good solution for KS equation**, **ABINIT does self-consistent iterations.**

```
iscf      5          # integer for self-consistent-field cycles

toldfe    1.0d-6     # tolerance on the difference of total energy

nstep     50         # maximal number of scf cycles
```

- ❑ **This procedure is repeated until the total energy does not change any more.**

- **iscf** # Integer for Self-Consistent-Field cycles

1 => get the largest eigenvalue of the SCF cycle

2 => SCF cycle, simple mixing of the potential

3 => SCF cycle, Anderson mixing of the potential

…

17 => SCF cycle, Pulay mixing of the density based on the npulyit previous iterations .

- **toldfe** # TOLerance on the DiFference of total Energy

- **toldff** # TOLerance on the DiFference of Forces

Other input variables

nband	128	# Number of BANDs
enunit	1	# print eigenvalues in eV
prtden	1	# provide output of electron density

How to run the code?

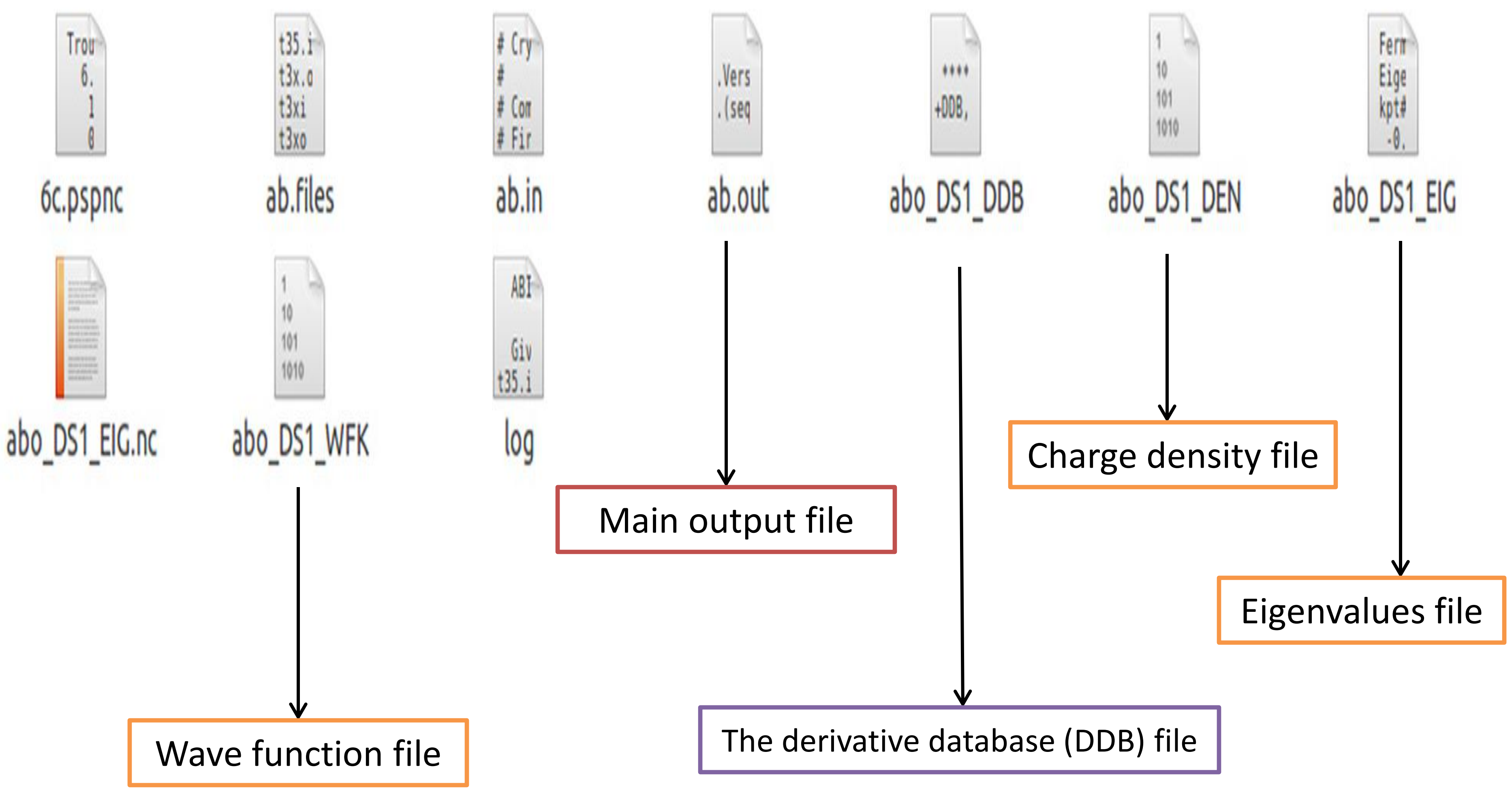
6c.pspnc
ab.files
ab.in

- ABINIT is run interactively (in Unix) with the command:

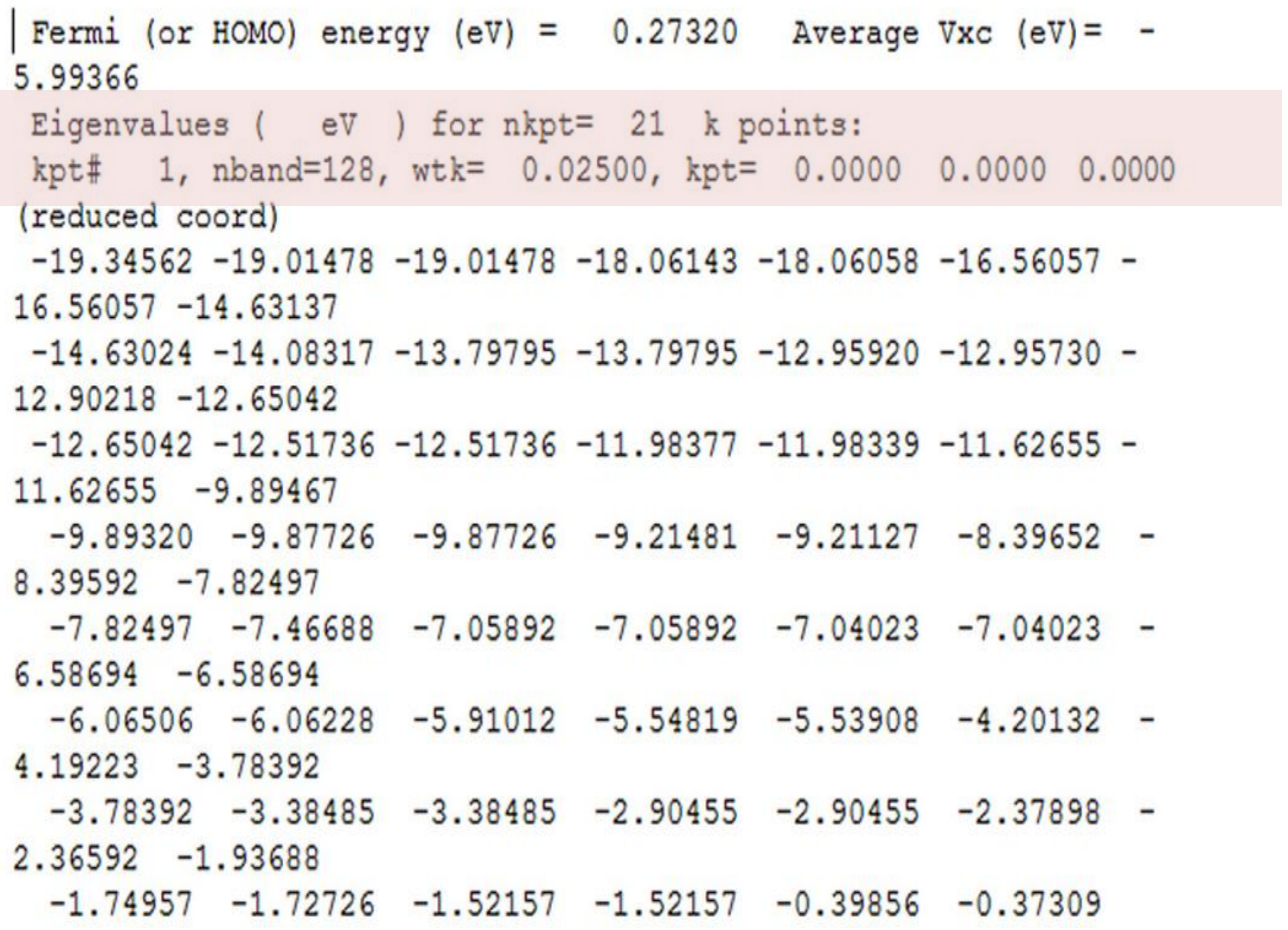
abinit<ab.files>& log

- where standard out and standard error are piped to the the log file called "log”.

The output files □□□□□□□□□■□□

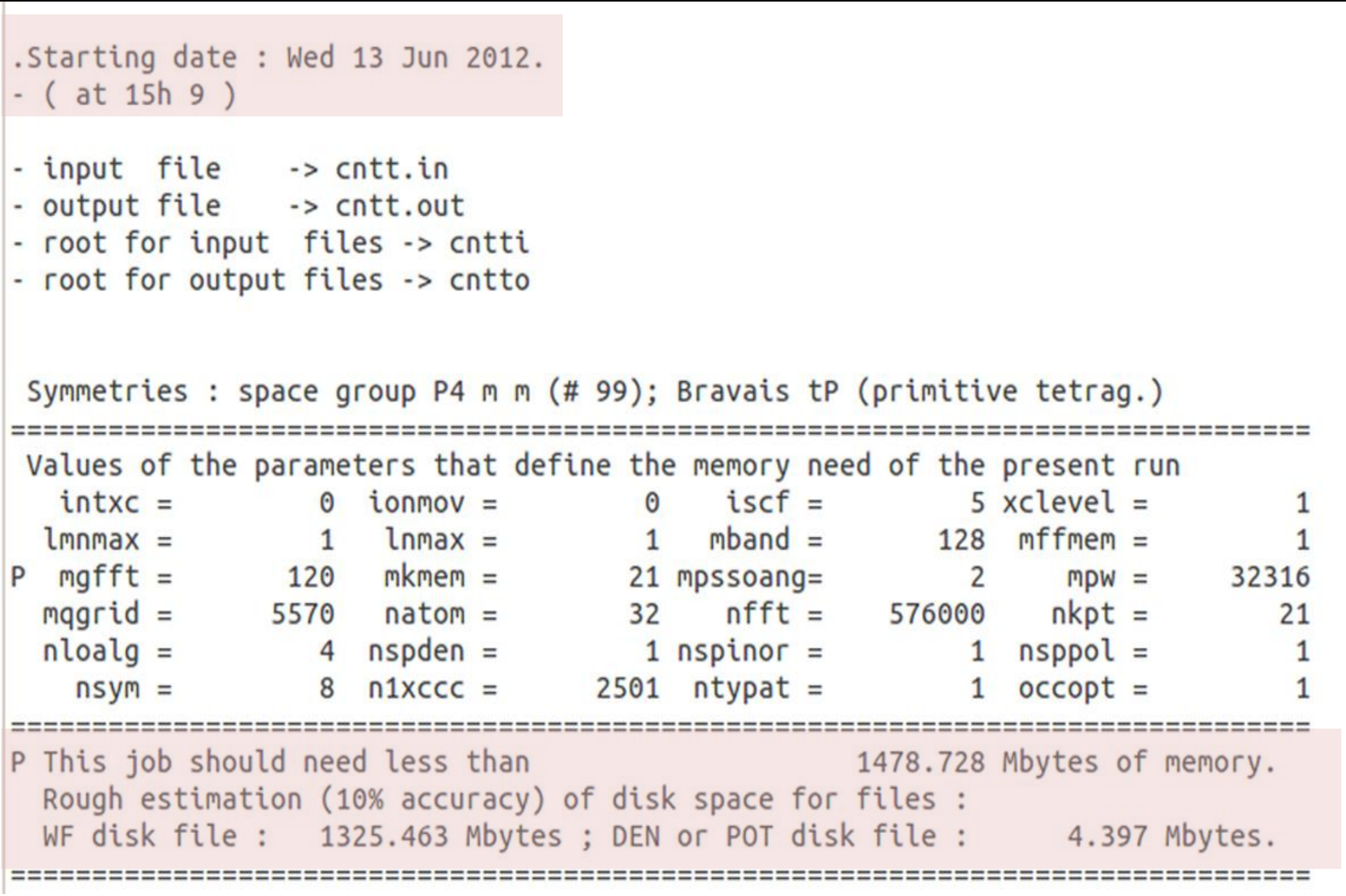


The eigenvalues file □□□□□□□□■□□



```
Fermi (or HOMO) energy (eV) =   0.27320   Average Vxc (eV)=  -
5.99366
 Eigenvalues (   eV  ) for nkpt=  21  k points:
 kpt#   1, nband=128, wtk=  0.02500, kpt=  0.0000  0.0000  0.0000
(reduced coord)
 -19.34562 -19.01478 -19.01478 -18.06143 -18.06058 -16.56057 -
16.56057 -14.63137
 -14.63024 -14.08317 -13.79795 -13.79795 -12.95920 -12.95730 -
12.90218 -12.65042
 -12.65042 -12.51736 -12.51736 -11.98377 -11.98339 -11.62655 -
11.62655  -9.89467
  -9.89320  -9.87726  -9.87726  -9.21481  -9.21127  -8.39652  -
8.39592  -7.82497
  -7.82497  -7.46688  -7.05892  -7.05892  -7.04023  -7.04023  -
6.58694  -6.58694
  -6.06506  -6.06228  -5.91012  -5.54819  -5.53908  -4.20132  -
4.19223  -3.78392
  -3.78392  -3.38485  -3.38485  -2.90455  -2.90455  -2.37898  -
2.36592  -1.93688
  -1.74957  -1.72726  -1.52157  -1.52157  -0.39856  -0.37309
```

The main output files □□□□□□□□□□■□



```
.Starting date : Wed 13 Jun 2012.
- ( at 15h 9 )

- input  file     -> cntt.in
- output file     -> cntt.out
- root for input  files -> cntti
- root for output files -> cntto


 Symmetries : space group P4 m m (# 99); Bravais tP (primitive tetrag.)
================================================================================
 Values of the parameters that define the memory need of the present run
   intxc =         0   ionmov =         0     iscf =         5 xclevel =         1
  lmnmax =         1    lnmax =         1    mband =       128  mffmem =         1
P  mgfft =       120    mkmem =        21 mpssoang=         2     mpw =     32316
  mqgrid =      5570    natom =        32     nfft =    576000    nkpt =        21
  nloalg =         4   nspden =         1  nspinor =         1  nsppol =         1
    nsym =         8   n1xccc =      2501   ntypat =         1  occopt =         1
================================================================================
P This job should need less than                    1478.728 Mbytes of memory.
  Rough estimation (10% accuracy) of disk space for files :
  WF disk file :   1325.463 Mbytes ; DEN or POT disk file :      4.397 Mbytes.
================================================================================
```

The main output files

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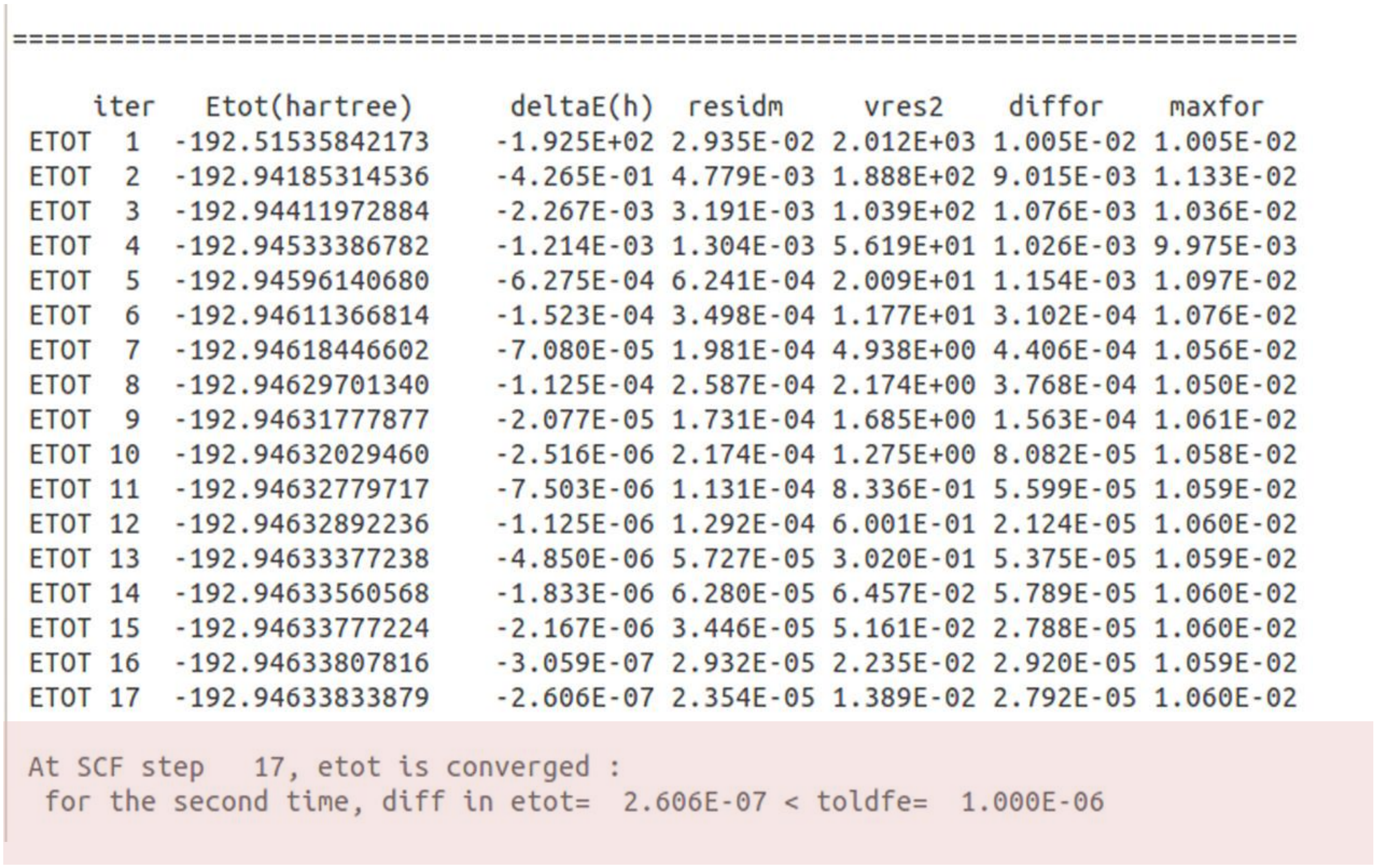
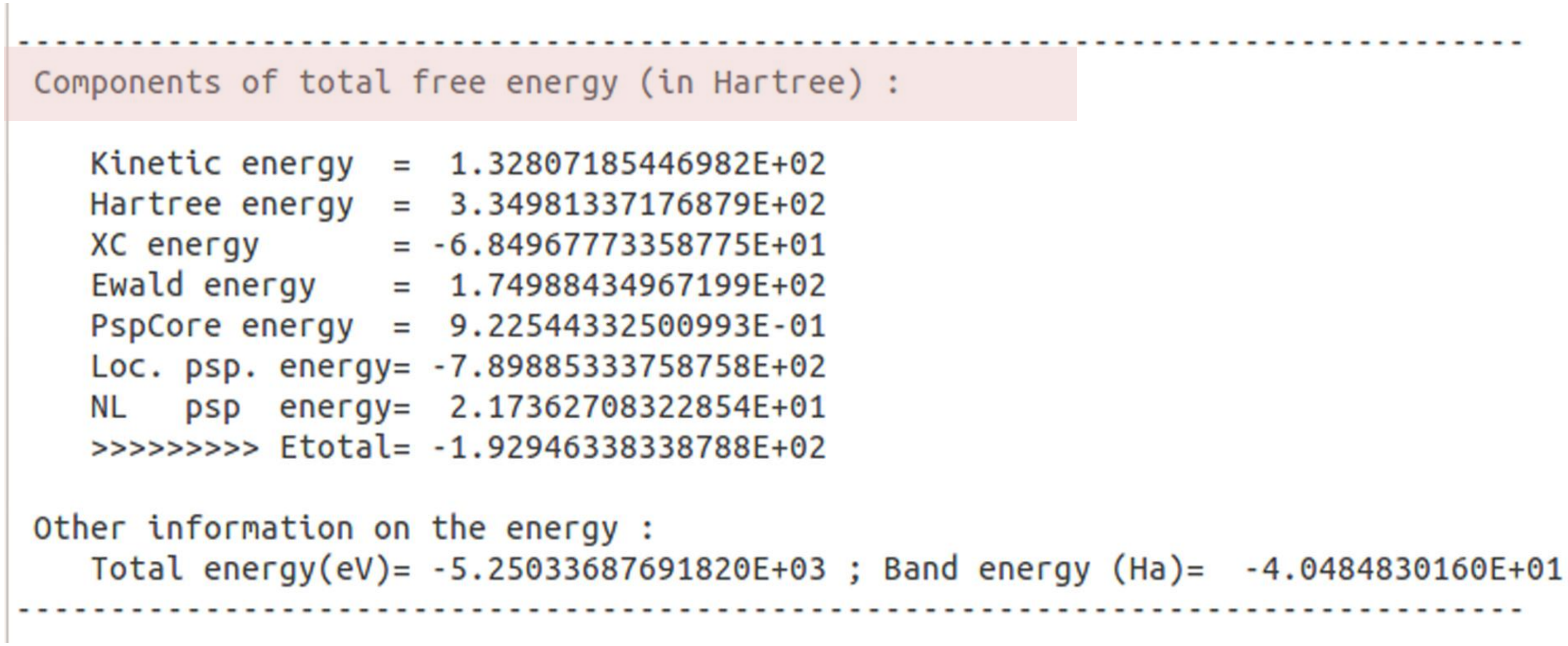


```
=====================================================================================

     iter   Etot(hartree)       deltaE(h)  residm     vres2    diffor    maxfor
 ETOT  1  -192.51535842173    -1.925E+02 2.935E-02 2.012E+03 1.005E-02 1.005E-02
 ETOT  2  -192.94185314536    -4.265E-01 4.779E-03 1.888E+02 9.015E-03 1.133E-02
 ETOT  3  -192.94411972884    -2.267E-03 3.191E-03 1.039E+02 1.076E-03 1.036E-02
 ETOT  4  -192.94533386782    -1.214E-03 1.304E-03 5.619E+01 1.026E-03 9.975E-03
 ETOT  5  -192.94596140680    -6.275E-04 6.241E-04 2.009E+01 1.154E-03 1.097E-02
 ETOT  6  -192.94611366814    -1.523E-04 3.498E-04 1.177E+01 3.102E-04 1.076E-02
 ETOT  7  -192.94618446602    -7.080E-05 1.981E-04 4.938E+00 4.406E-04 1.056E-02
 ETOT  8  -192.94629701340    -1.125E-04 2.587E-04 2.174E+00 3.768E-04 1.050E-02
 ETOT  9  -192.94631777877    -2.077E-05 1.731E-04 1.685E+00 1.563E-04 1.061E-02
 ETOT 10  -192.94632029460    -2.516E-06 2.174E-04 1.275E+00 8.082E-05 1.058E-02
 ETOT 11  -192.94632779717    -7.503E-06 1.131E-04 8.336E-01 5.599E-05 1.059E-02
 ETOT 12  -192.94632892236    -1.125E-06 1.292E-04 6.001E-01 2.124E-05 1.060E-02
 ETOT 13  -192.94633377238    -4.850E-06 5.727E-05 3.020E-01 5.375E-05 1.059E-02
 ETOT 14  -192.94633560568    -1.833E-06 6.280E-05 6.457E-02 5.789E-05 1.060E-02
 ETOT 15  -192.94633777224    -2.167E-06 3.446E-05 5.161E-02 2.788E-05 1.060E-02
 ETOT 16  -192.94633807816    -3.059E-07 2.932E-05 2.235E-02 2.920E-05 1.059E-02
 ETOT 17  -192.94633833879    -2.606E-07 2.354E-05 1.389E-02 2.792E-05 1.060E-02

 At SCF step   17, etot is converged :
  for the second time, diff in etot=  2.606E-07 < toldfe=  1.000E-06
```

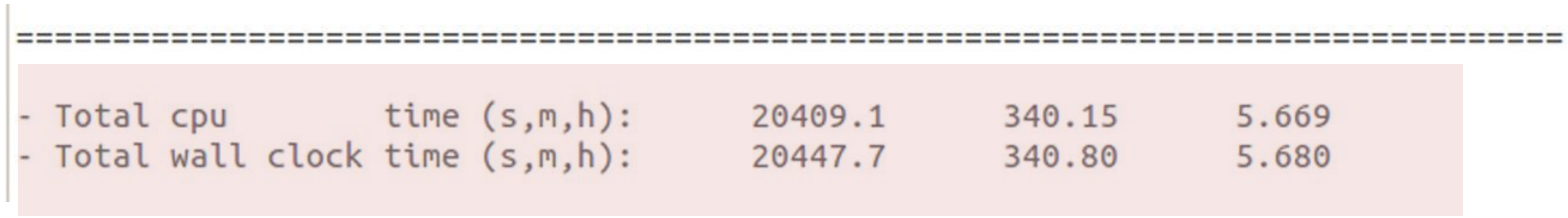
The main output files



```
 --------------------------------------------------------------------------------
 Components of total free energy (in Hartree) :

    Kinetic energy  =  1.32807185446982E+02
    Hartree energy  =  3.34981337176879E+02
    XC energy       = -6.84967773358775E+01
    Ewald energy    =  1.74988434967199E+02
    PspCore energy  =  9.22544332500993E-01
    Loc. psp. energy= -7.89885333758758E+02
    NL   psp  energy=  2.17362708322854E+01
    >>>>>>>>> Etotal= -1.92946338338788E+02

 Other information on the energy :
    Total energy(eV)= -5.25033687691820E+03 ; Band energy (Ha)=  -4.0484830160E+01
 --------------------------------------------------------------------------------
```



```
==============================================================================

- Total cpu        time (s,m,h):       20409.1       340.15       5.669
- Total wall clock time (s,m,h):       20447.7       340.80       5.680
```

How I can plot band Structures from Abinit output files?

STEP 1 : produce a .dbs file

The first thing to do is to extract datas from an Abinit output file and produce a **.dbs file** (dbs stands for Data for Band Structure). To do so, you must execute the program and specify the name of the .out file you wish to use.

- Copy your output file in the following path:

  abinit-7.10.2/scripts/post_processing

- Then in the commond line type:

```
> python AbinitBandStructureMaker.py file.out
```

the program will extract all the necessary datas and produce a .dbs file.
If everything goes well, you'll get the following message in the commond line:

```
> "file.out.dbs " file created successfully
```

STEP 2: produce a .agr file

Now that you have a customized .dbs file, you must extract datas from this file to produce a **.agr file** (a formatted file readable by xmgrace).
To produce a .agr file, execute the program and specify the name of the .dbs file you wish to use:

```
> python AbinitBandStructureMaker.py file.out.dbs
```

If everything goes well, you'll get the following message :

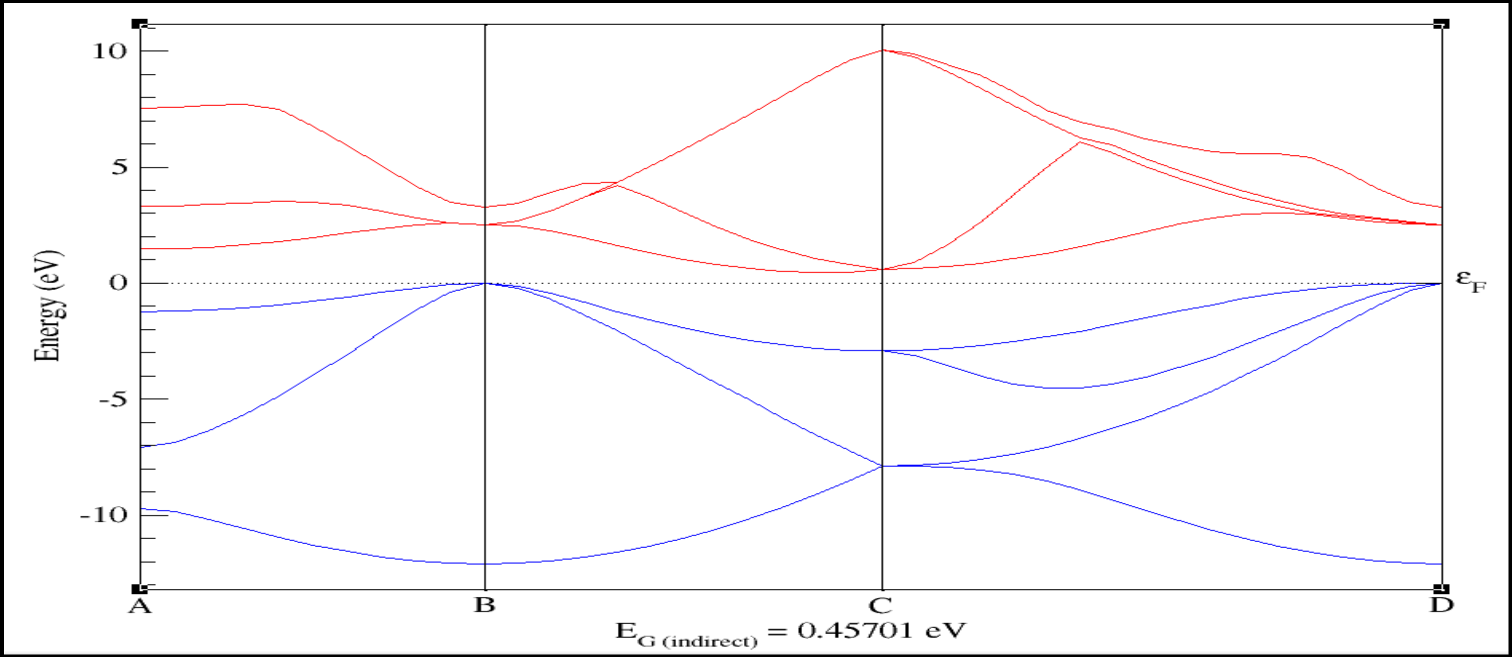
```
> "file.out.agr " file created successfully
```

STEP 3 : plot the band structure

Now that you possess a .agr file, you just need to execute xmgrace and use the .agr file to plot the band structure.

```
> xmgrace file.out.agr
```

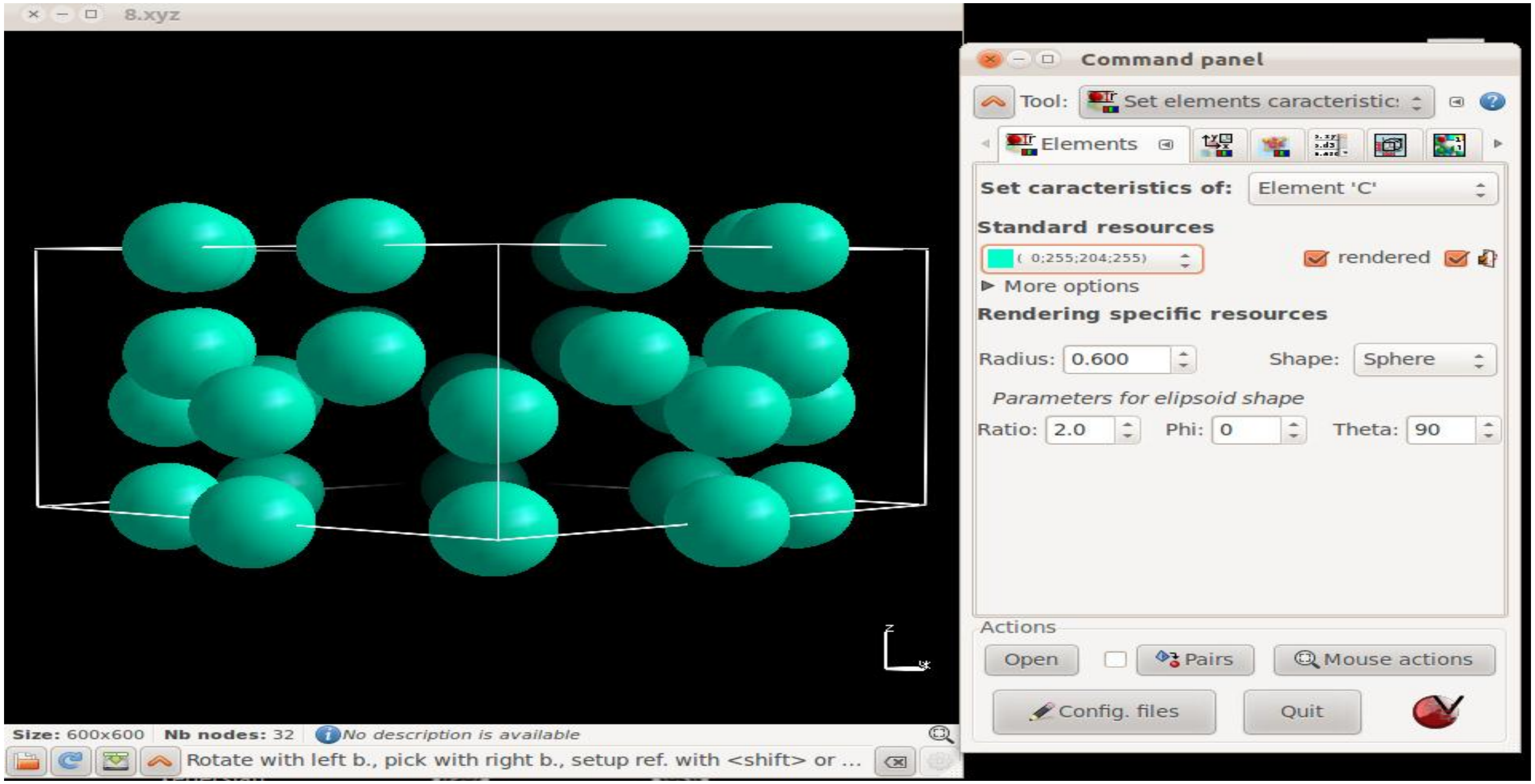
Your plot is ready:



V_Sim visualizes atomic structures □□□□□□□□□□□■

Nasim Moradi

http://inac.cea.fr/L_Sim/V_Sim/



8.xyz

Command panel

Tool: Set elements caracteristic:

Elements

Set caracteristics of: Element 'C'

Standard resources

(0;255;204;255) rendered

▶ More options

Rendering specific resources

Radius: 0.600 Shape: Sphere

Parameters for elipsoid shape

Ratio: 2.0 Phi: 0 Theta: 90

Actions

Open Pairs Mouse actions

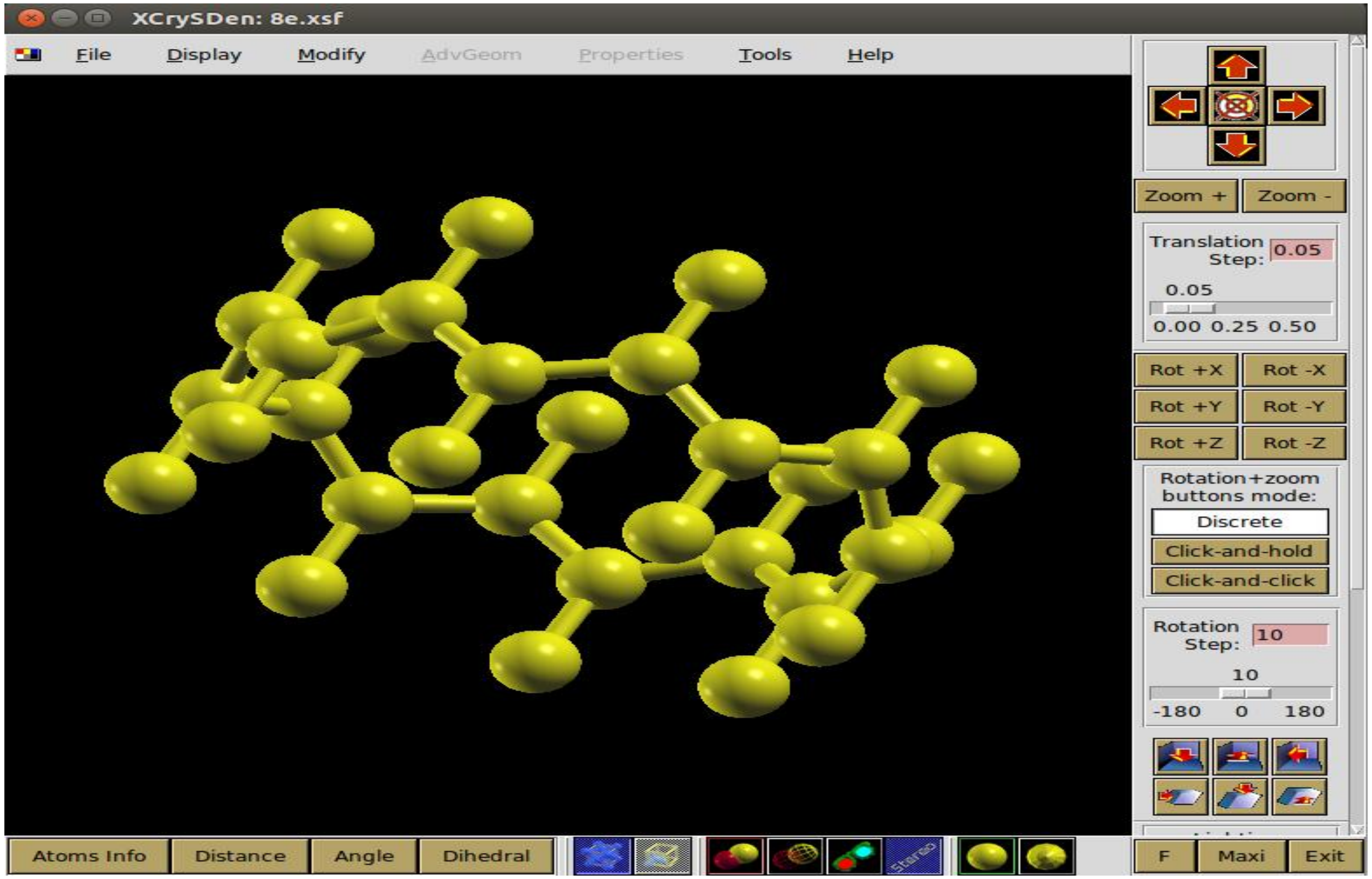
Config. files Quit

Size: 600x600 **Nb nodes:** 32 *No description is available*

Rotate with left b., pick with right b., setup ref. with <shift> or ...

XcrysDen visualizes atomic structures □□□□□□□□□□□■

http://www.xcrysden.org



DESCRIPTION

ABINIT

Input files

ABINIT Run

Output files

SUBJECTS

Let's play with:

abinit

Thank you…