University Mohammed VI Polytechnic

Laboratory of Inorganic Materials for Sustainable Energy Technologies

DFT hands-on using quantum espresso

First edition of the African School on Computational Materials for Sustainable Energy Technologies (CMSET 2025)

November 26, 2025

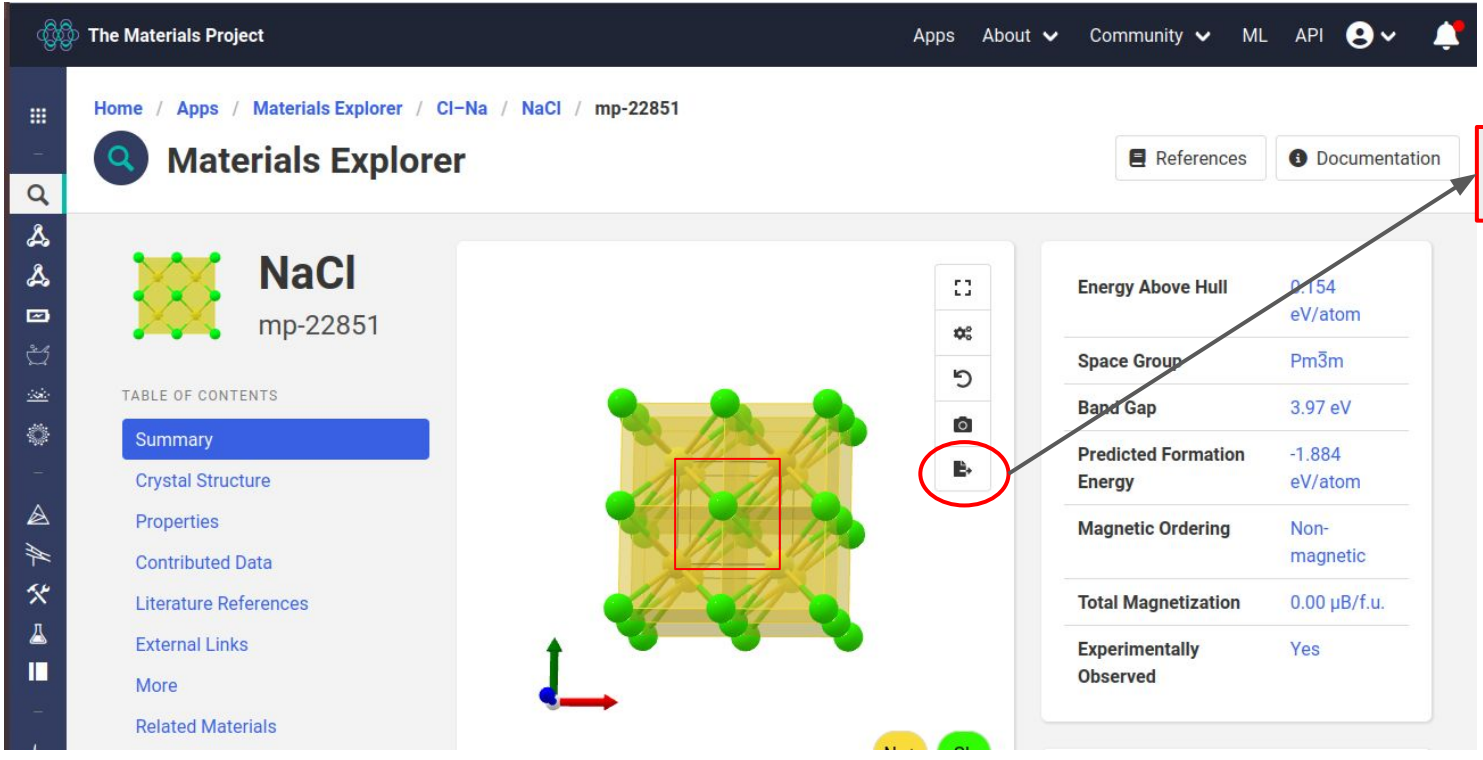
DFT Hands-on — Outline

- Download cif file using material project database
- Convert Cif file to input file for quantum espresso
- Read and visual input and output file
- Convergence test for Ecut, Ecutrho and kpoint mesh
- Cell relaxation
- Total and Partial Density of state (PDOS)
- Band structure

Download the NaCl Crystal Structure (CIF Format) from Public Databases

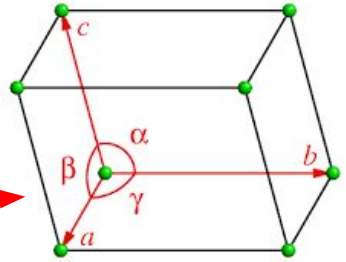
Material project | **Crystallography Open Database (COD)** | **Material cloud** | **AFLOW**

Material project → **Start exploring materials** → **Type your chemical formula: NaCl**

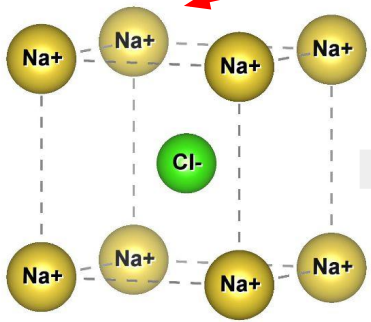


Understanding CIF Format: Key Structural Parameters

```
# generated using pymatgen
data_NaCl
_symmetry_space_group_name_H-M   Pm-3m
_cell_length_a   3.50219000
_cell_length_b   3.50219000
_cell_length_c   3.50219000
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   221
_chemical_formula_structural   NaCl
_chemical_formula_sum   'Na1 Cl1'
_cell_volume   42.95553287
_cell_formula_units_Z   1
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
  2  '-x, -y, -z'
  3  '-y, x, z'
  4  ……
```



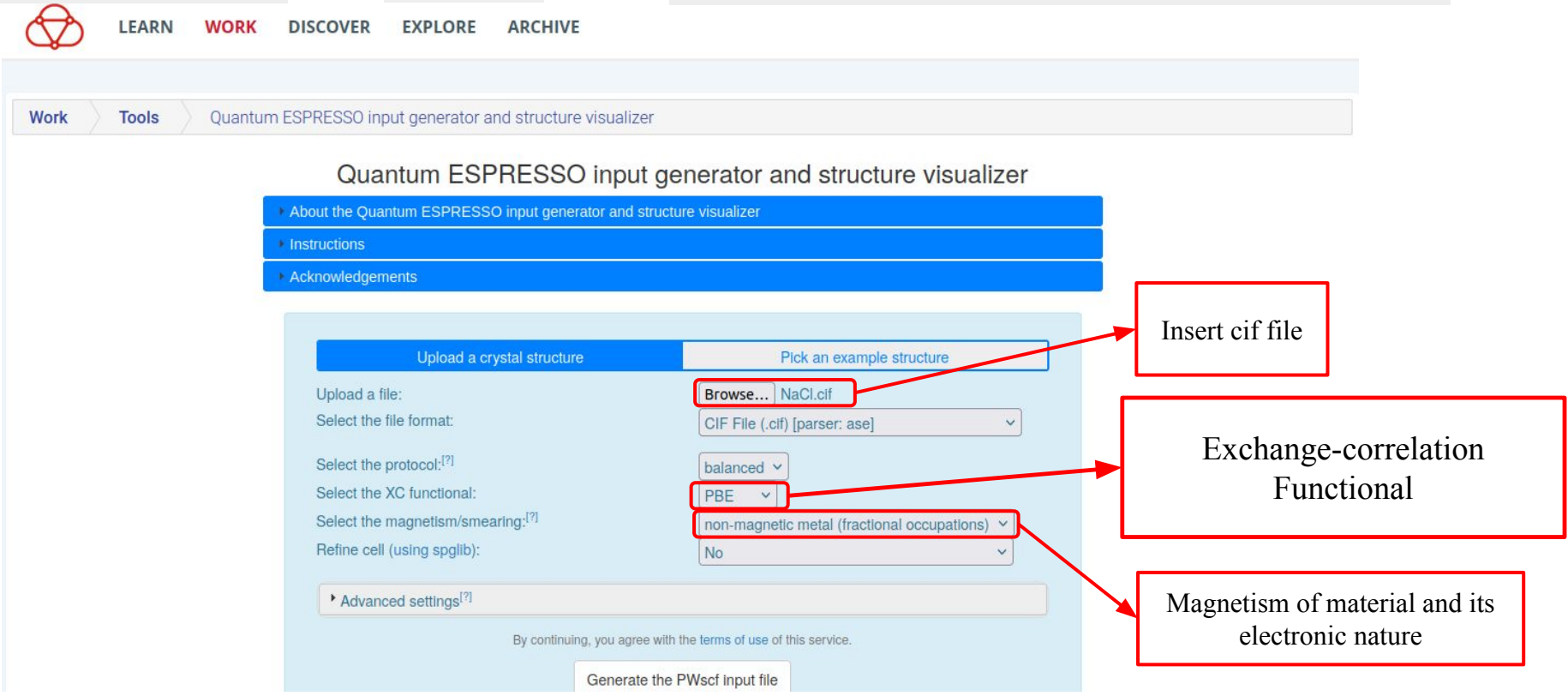

```
loop_
 _atom_type_symbol
 _atom_type_oxidation_number
  Na+  1.0
  Cl-  -1.0
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
  atom_site_occupancy
  Na+  Na0  1  0.00000000  0.00000000  0.00000000  1
  Cl-  Cl1  1  0.50000000  0.50000000  0.50000000  1
```



You can use vesta software for cif file visualisation

Converting CIF file to input file for quantum espresso (.in format)

cif2cell tool	**Open terminal and type**	**cif2cell file_name.cif -p quantum-espresso -o file_name.in**
Material cloud website	**Work**	**Quantum ESPRESSO input generator and structure visualizer**

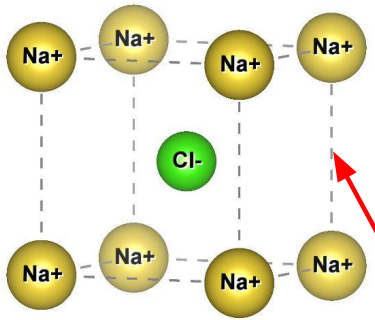


Input for for quantum espresso

```
&CONTROL
 calculation='scf',
 outdir='.',
 prefix='NaCl',
 pseudo_dir='/home/max/pseudo',
 verbosity='low',
 tprnfor=.true., tstress=.true.,
/
&SYSTEM
 ibrav = 0
 A =    3.4
 nat = 2
 ntyp = 2
 ecutwfc=40,
 ecutrho=200,
 input_dft='pbe',
 occupations='smearing',
 smearing='mv',
 degauss=0.005d0,
/
&ELECTRONS
 conv_thr=1d-08,
 mixing_beta=0.7d0,
/
```

Type of the calculation: scf, relax, vc-relax

Calculate forces and stress



Number and type of atoms in unit cell

Occupations “fixed” for semiconductor/insulator and “smearing” for metals

Convergence threshold for the energy

```
&IONS
 ion_dynamics='bfgs',
/
&CELL
 cell_dynamics='bfgs',
 press=0.d0,
 press_conv_thr=0.5d0,
/
ATOMIC_SPECIES
  Cl   35.45150  cl_pbe_v1.4.uspp.F.UPF
  Na   22.98900  na_pbe_v1.5.uspp.F.UPF
CELL_PARAMETERS {alat}
  1.000000000000000   0.000000000000000   0.000000000000000
  0.000000000000000   1.000000000000000   0.000000000000000
  0.000000000000000   0.000000000000000   1.000000000000000
ATOMIC_POSITIONS {crystal}
Cl   0.500000000000000   0.500000000000000   0.500000000000000
Na   0.000000000000000   0.000000000000000   0.000000000000000
K_POINTS {automatic}
 5 5 5 0 0 0
```

Ionic relaxation

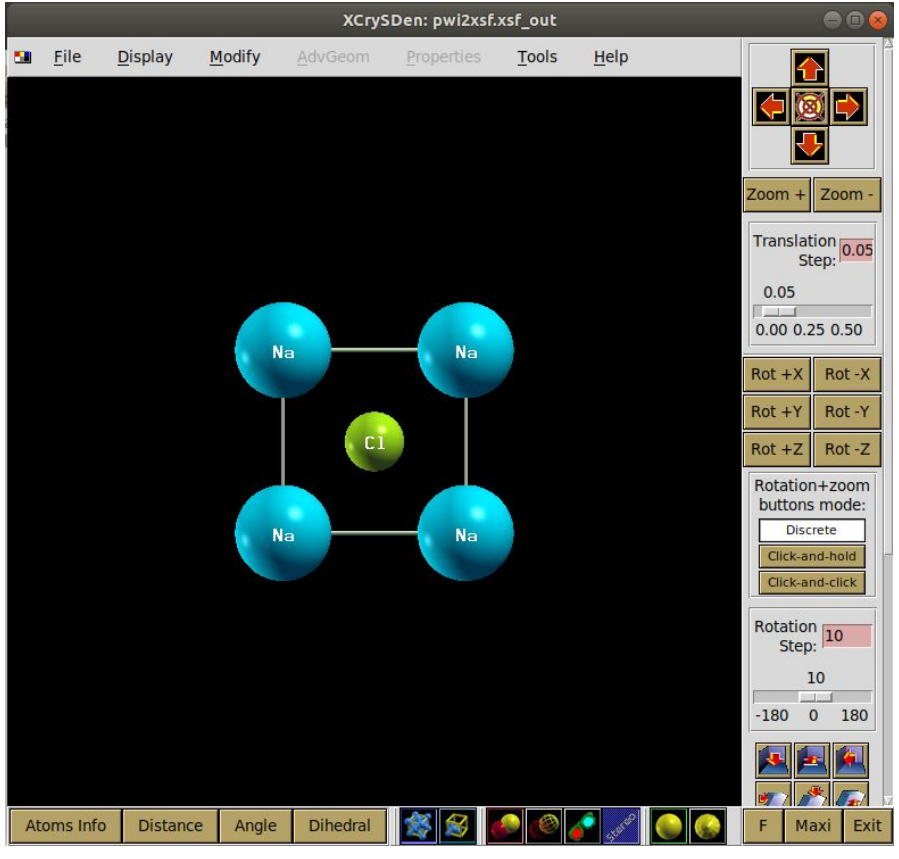
Cell relaxation

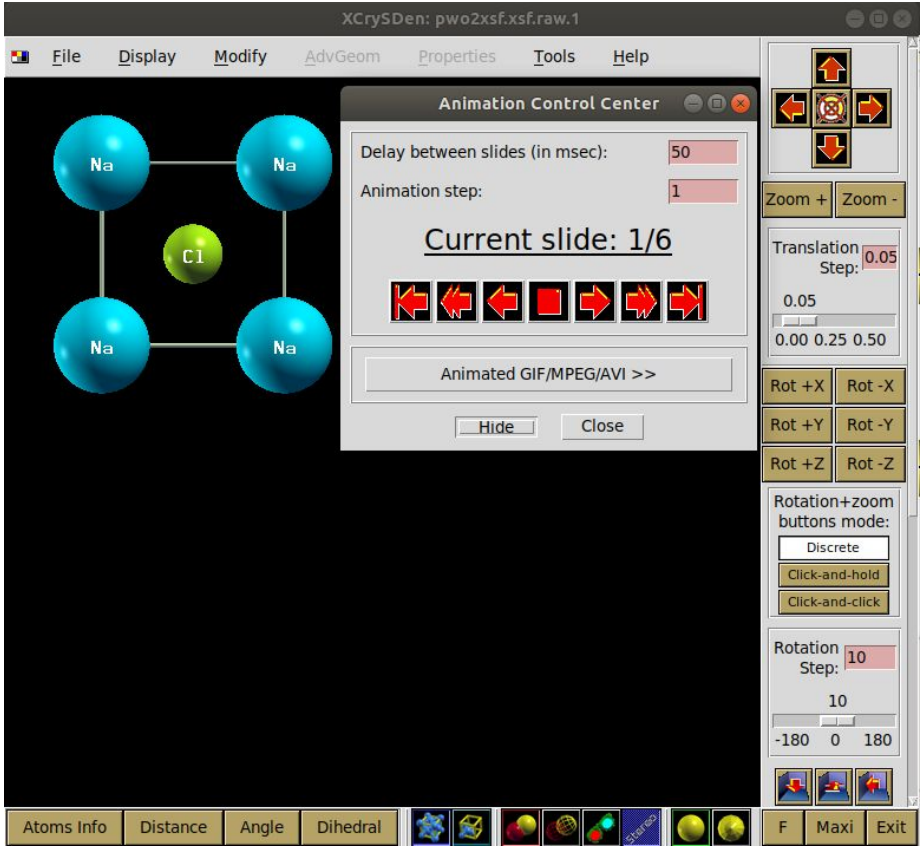
Complete description of input file in the website:
https://www.quantum-espresso.org/Doc/INPUT_PW.html

Using XCrySDen to Visualize Quantum ESPRESSO Input and Output Files

Open terminal and type: **conda activate visualise**

Open terminal and type **xcrysden** | **file** | **Open PWscf** | **Open PWscf Input file or Output file**

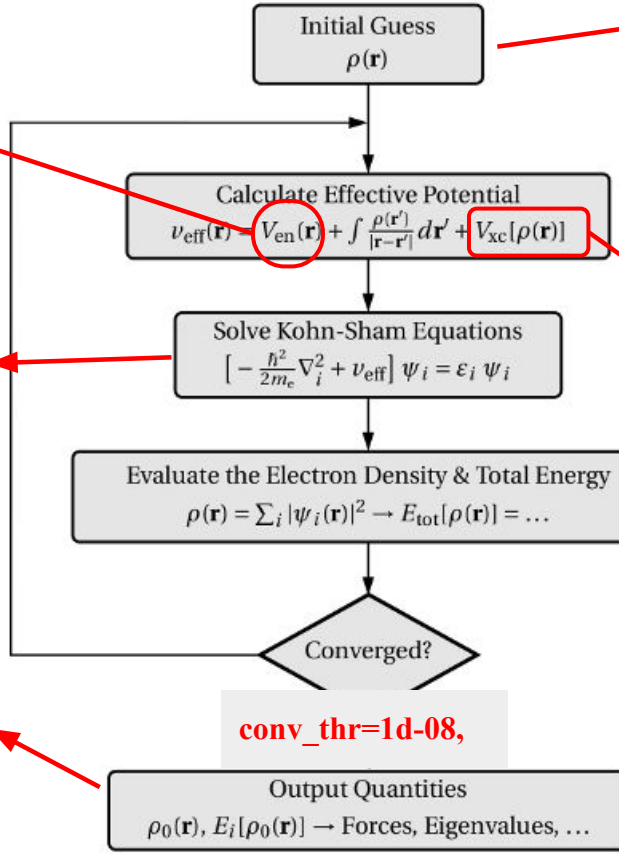




Input file and scf loop in quantum espresso

Calculated from ions positions

ATOMIC_POSITIONS {crystal}
Cl 0.50 0.50 0.50
Na 0.00 0.00 0.00



Will guessed from pseudo potential file or outdir file

startingwfc='atomic' —from pseudopotential
startingwfc='file' — from outdir file

exchange-correlation specified in input otherwise read from pseudopotential

input_dft='pbe',

Solved using iterative diagonalization

diagonalization='david'

mixing old and new density for better convergence stability

mixing_beta=0.7d0,

conv_thr=1d-08,

Calculate converged energy, forces and stress

tprnfor=.true.,
tstress=.true.,

Run input file and Read output file

Open input file directory | **activate quantum espresso: conda activate qespresso** | **run input using pw.x -input input.in > output.out**

```
bravais-lattice index     =            0
lattice parameter (alat)  =       6.4251  a.u.
unit-cell volume          =     265.2365 (a.u.)^3
number of atoms/cell      =            2
number of atomic types    =            2
number of electrons       =        16.00
number of Kohn-Sham states=           12
kinetic-energy cutoff     =      40.0000  Ry
charge density cutoff     =     200.0000  Ry
convergence threshold     =      1.0E-08
mixing beta               =       0.7000
number of iterations used =            8  plain     mixing
Exchange-correlation      = PBE ( 1  4  3  4 0 0)

celldm(1)=   6.425069  celldm(2)=   0.000000  celldm(3)=   0.000000
celldm(4)=   0.000000  celldm(5)=   0.000000  celldm(6)=   0.000000

crystal axes: (cart. coord. in units of alat)
          a(1) = (   1.000000   0.000000   0.000000 )
          a(2) = (   0.000000   1.000000   0.000000 )
          a(3) = (   0.000000   0.000000   1.000000 )

reciprocal axes: (cart. coord. in units 2 pi/alat)
          b(1) = (  1.000000  0.000000  0.000000 )
          b(2) = (  0.000000  1.000000  0.000000 )
          b(3) = (  0.000000  0.000000  1.000000 )
```

- **For an insulator is number of valence electrons /2**
- **For a metal, 20% more (minimum 4 more)**

celldm(1) = a

celldm(2)= b/a,

celldm(3)= c/a,

celldm(4)= cos(bc),

celldm(5)= cos(ac),

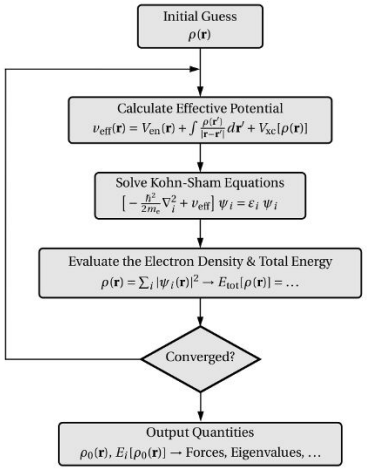
celldm(6)= cos(ab)

Reading output file

```
number of k points=    10  Marzari-Vanderbilt smearing, width (Ry)=  0.0050
                  cart. coord. in units 2pi/alat
   k(    1) = (   0.0000000   0.0000000   0.0000000), wk =   0.0160000
   k(    2) = (   0.0000000   0.0000000   0.2000000), wk =   0.0960000
   k(    3) = (   0.0000000   0.0000000   0.4000000), wk =   0.0960000
   k(    4) = (   0.0000000   0.2000000   0.2000000), wk =   0.1920000
   k(    5) = (   0.0000000   0.2000000   0.4000000), wk =   0.3840000
   k(    6) = (   0.0000000   0.4000000   0.4000000), wk =   0.1920000
   k(    7) = (   0.2000000   0.2000000   0.2000000), wk =   0.1280000
   k(    8) = (   0.2000000   0.2000000   0.4000000), wk =   0.3840000
   k(    9) = (   0.2000000   0.4000000   0.4000000), wk =   0.3840000
   k(   10) = (   0.4000000   0.4000000   0.4000000), wk =   0.1280000
```

As the k-point weight increase, the symmetry in this kpoint increase

```
iteration #  1     ecut=    40.00 Ry     beta=0.70
Davidson diagonalization with overlap
ethr =  1.00E-02,  avg # of iterations =  5.0

Threshold (ethr) on eigenvalues was too large:
Diagonalizing with lowered threshold

Davidson diagonalization with overlap
ethr =  3.31E-04,  avg # of iterations =  2.3

negative rho (up, down):  1.598E-02 0.000E+00

total cpu time spent up to now is        1.7 secs

total energy              =    -128.86376078 Ry
Harris-Foulkes estimate   =    -128.89603018 Ry
estimated scf accuracy    <       0.05107874 Ry
```



Kohn-Sham Hamiltonian matrix solved for each k-point

Scf loop has been solved for the first time

Reading output file

```
   The total energy is the sum of the following terms:

   one-electron contribution =     -74.18279152 Ry
   hartree contribution      =      42.36507042 Ry
   xc contribution           =     -23.92644874 Ry
   ewald contribution        =     -73.13425203 Ry
   smearing contrib. (-TS)   =       0.00000000 Ry
```

```
      k = 0.0000 0.0000 0.0000 (  1141 PWs)   bands (ev):

-47.0643 -18.9626 -18.9626 -18.9626 -10.6534   2.4857   2.4857   2.4857
  7.3475  11.4677  11.4677  19.6121
```

Eigenvalues of Kohn-Sham Hamiltonian for each kpoint

```
!    total energy              =    -128.87842187 Ry
     Harris-Foulkes estimate   =    -128.87842187 Ry
     estimated scf accuracy    <          7.6E-11 Ry
```

Converged total energy

```
atom    1 type  1   force =     0.00000000    0.00000000    0.00000000
atom    2 type  2   force =     0.00000000    0.00000000    0.00000000

Total force =     0.000000     Total SCF correction =     0.000000
```

Forces after converging scf loop

Reading output file

```
  negative rho (up, down):  1.517E-02 0.000E+00
      total   stress  (Ry/bohr**3)                   (kbar)     P=   31.25
0.00021242   0.00000000   0.00000000        31.25      0.00      0.00
0.00000000   0.00021242   0.00000000         0.00     31.25      0.00
0.00000000   0.00000000   0.00021242         0.00      0.00     31.25
```

Hydrostatic pressure on the cell

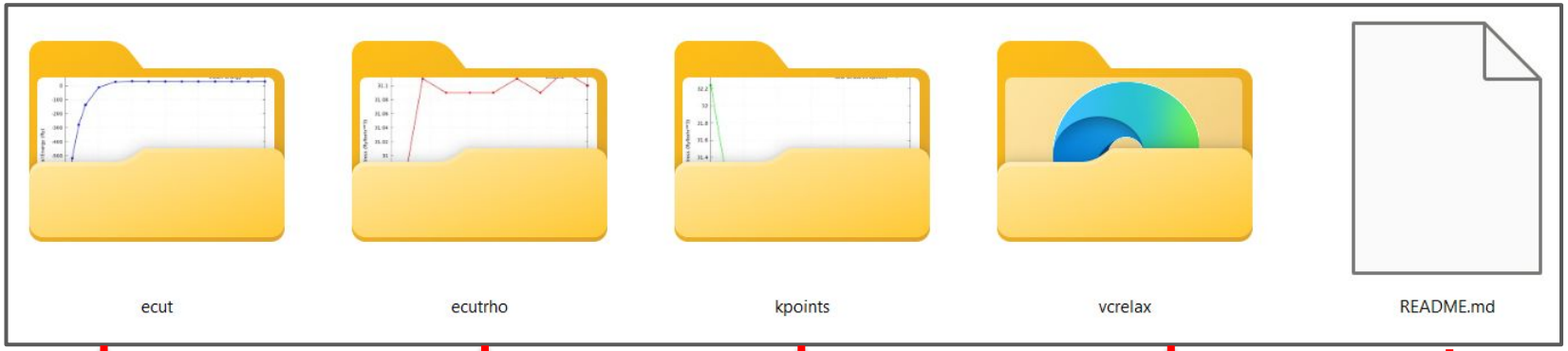
pw.x -input input.in > output.out

```
  Parallel routines
  fft_scatter  :      0.10s CPU      0.10s WALL (    6305 calls)

  PWSCF        :     4.76s CPU         5.08s WALL
```

mpirun --bind-to core --map-by core -np 2 (or 4 or 6) pw.x -input input.in > output.out

```
  Parallel routines
  fft_scatter  :      0.13s CPU      0.14s WALL (    6301 calls)

  PWSCF        :     3.00s CPU         3.12s WALL
```

Optimisation steps and folders



Ecut optimisation

Ecutrho optimisation

K-point meshes optimisation

Cell relaxation

Readme file

Cutoff-Energy (Ecut) Convergence Study

ecut.$ecut.in

```
&CONTROL
 calculation='scf',
 outdir='.',
 prefix='NaCl',
 pseudo_dir='../../../pseudo',
 verbosity='low',
 tprnfor=.true.,
 tstress=.true.,
/
&SYSTEM
 ibrav = 0
 A = 3.4
 nat = 2
 ntyp = 2
 ecutwfc = ${ecut},
 ecutrho = 200,
 input_dft='pbe',
 occupations='smearing',
 smearing='mv',
 degauss=0.005d0,
/
&ELECTRONS
 conv_thr=1d-8,
 mixing_beta=0.7d0,
/
&IONS
 ion_dynamics='bfgs',
/
&CELL
 cell_dynamics='bfgs',
 press=0.d0,
 press_conv_thr=0.5d0,
/
```

```
CELL_PARAMETERS {alat}
 1.0 0.0 0.0
 0.0 1.0 0.0
 0.0 0.0 1.0

ATOMIC_SPECIES
 Cl 35.45150 cl_pbe_v1.4.uspp.F.UPF
 Na 22.98900 na_pbe_v1.5.uspp.F.UPF

ATOMIC_POSITIONS {crystal}
 Cl 0.5 0.5 0.5
 Na 0.0 0.0 0.0

K_POINTS {automatic}
 5 5 5 0 0 0
```

Set cutoffs

for ecut in 20 22 24 26 30 35 40 45 50 55 60 65 70 75 80; do

Target parameter for accurate optimization

Hydrostatic pressure

```
          (kbar)     P= -924.42
-924.42     0.00      0.00
   0.00  -924.42      0.00
   0.00     0.00   -924.42
```

Total energy

```
!    total energy              =    -128.49580518 Ry
     Harris-Foulkes estimate   =    -128.49580519 Ry
     estimated scf accuracy    <          9.1E-09 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =     -73.12275949 Ry
     hartree contribution      =      41.52353047 Ry
     xc contribution           =     -23.76232413 Ry
     ewald contribution        =     -73.13425203 Ry
     smearing contrib. (-TS)   =      -0.00000000 Ry

     convergence has been achieved in   6 iterations
```

Cutoff-Energy (Ecut) Convergence Study

We will use Gnuplot to make the plot. Here is the script code for plotting:

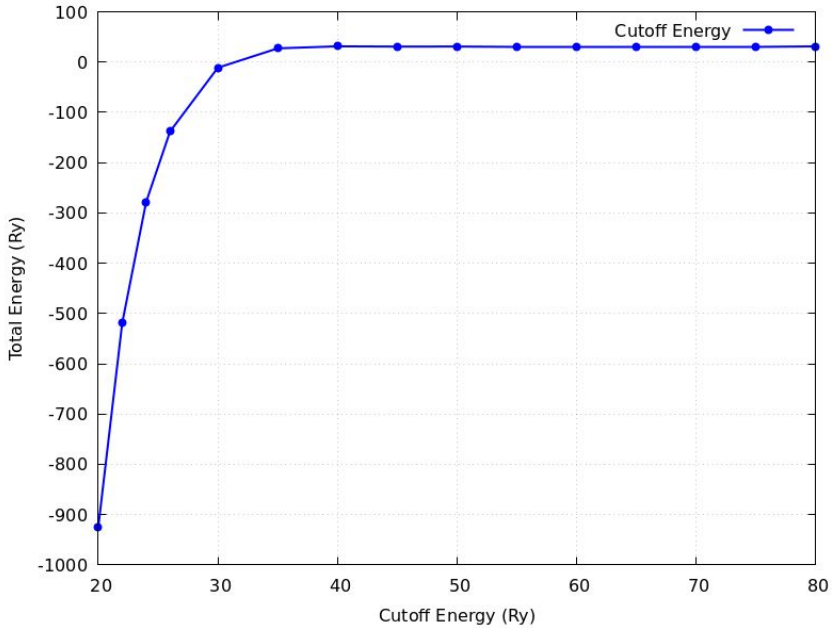
calc-pres.dat

```
20      -924.42
22      -518.80
24      -278.47
26      -138.08
30       -11.19
35        27.21
40        31.25
45        30.79
50        30.88
55        31.13
60        31.13
65        30.99
70        30.94
75        31.01
80        31.14
```

plot_ecut.gp

```
# plot_ecut.gp
# Gnuplot script to plot total energy vs. cutoff
energy
# Set output to PNG image file
set terminal pngcairo size 800,600
set output "ecut_convergence.png"
set xlabel "Cutoff Energy (Ry)"
set ylabel "Total Stress (Ry/Bohr**3)"
set style line 1 lc rgb "blue" lw 2 pt 7
# Plot the data
plot "ecutpres.dat" using 1:2 with linespoints
linestyle 1 title "Cutoff Energy«
# Close the output file
set output
```

Hydrostatic pressure as a function of Ecut energy



Based on Hydrostatic convergence test, an ecut value of 60 Ry is appropriate for a convergence within ~1-2 kbar.

Charge Density cutoff (Ecutrho) Convergence Study

ecut.$ecutrho.in

```
&CONTROL
 calculation='scf',
 outdir='.',
 prefix='NaCl',
 pseudo_dir='../../../pseudo',
 verbosity='low',
 tprnfor=.true.,
 tstress=.true.,
/
&SYSTEM
 ibrav = 0
 A = 3.4
 nat = 2
 ntyp = 2
 ecutwfc =60
 ecutrho = ${ecutrho},
 input_dft='pbe',
 occupations='smearing',
 smearing='mv',
 degauss=0.005d0,
/
&ELECTRONS
 conv_thr=1d-8,
 mixing_beta=0.7d0,
/
&IONS
 ion_dynamics='bfgs',
/
&CELL
 cell_dynamics='bfgs',
 press=0.d0,
 press_conv_thr=0.5d0,
/
```

```
CELL_PARAMETERS {alat}
 1.0 0.0 0.0
 0.0 1.0 0.0
 0.0 0.0 1.0

ATOMIC_SPECIES
 Cl 35.45150 cl_pbe_v1.4.uspp.F.UPF
 Na 22.98900 na_pbe_v1.5.uspp.F.UPF

ATOMIC_POSITIONS {crystal}
 Cl 0.5 0.5 0.5
 Na 0.0 0.0 0.0

K_POINTS {automatic}
 5 5 5 0 0 0
```

Set ecutrho

for ecutrho in 120 180 240 300 360 420 480 540 600; do

Charge Density cutoff (Ecutrho) Convergence Study

We will use Gnuplot to make the plot. Here is the script code for plotting:

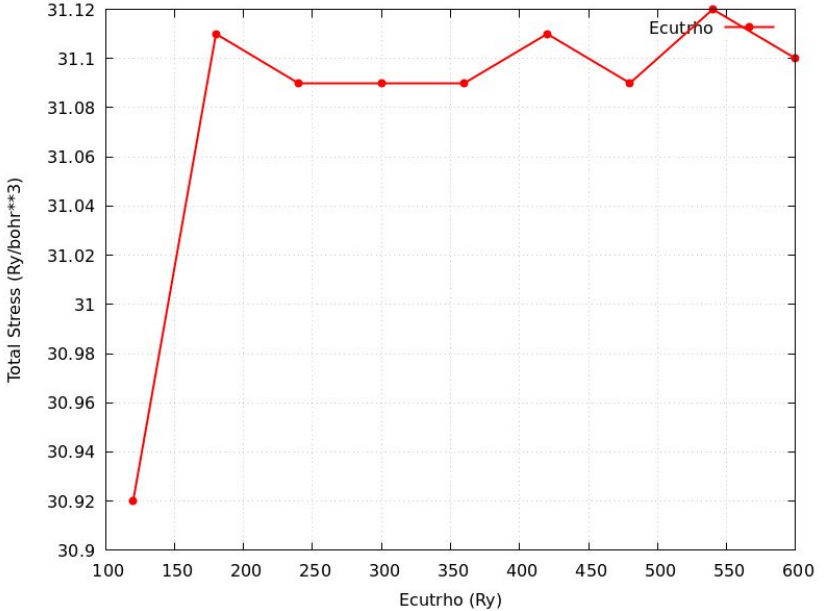
calc-ecutrho.dat

120	30.92
180	31.11
240	31.09
300	31.09
360	31.09
420	31.11
480	31.09
540	31.12
600	31.10

plot_ecutrho.gp

```
# plot_ecutrho.gp
# Gnuplot script to plot total Stress vs. ecutrho energy
# Set output to PNG image file
set terminal pngcairo size 800,600
set output « ecutrho-results.png"
set xlabel « Ecutrho (Ry) "
set ylabel "Total Stress (Ry/bohr**3)"
set style line 1 lc rgb  "red" lw 2 pt 7
# Plot the data
plot « file.dat" using 1:2 with linespoints linestyle 1 title " Ecutrho »
# Close the output file
set output
```

Hydrostatic pressure as a function of Ecutrho energy



Based on Hydrostatic convergence test, an ecutrho value of 300 Ry is appropriate for a convergence within ~1-2 kbar.

K-point meshes Convergence test

ecut.$ecutrho.in

```
&CONTROL
 calculation='scf',
 outdir='.',
 prefix='NaCl',
 pseudo_dir='../../../pseudo',
 verbosity='low',
 tprnfor=.true.,
 tstress=.true.,
/
&SYSTEM
 ibrav = 0
 A = 3.4
 nat = 2
 ntyp = 2
 ecutwfc =60,
 ecutrho = 300,
 input_dft='pbe',
 occupations='smearing',
 smearing='mv',
 degauss=0.005d0,
/
&ELECTRONS
 conv_thr=1d-8,
 mixing_beta=0.7d0,
/
&IONS
 ion_dynamics='bfgs',
/
&CELL
 cell_dynamics='bfgs',
 press=0.d0,
 press_conv_thr=0.5d0,
/
```

```
CELL_PARAMETERS {alat}
 1.0 0.0 0.0
 0.0 1.0 0.0
 0.0 0.0 1.0

ATOMIC_SPECIES
 Cl 35.45150 cl_pbe_v1.4.uspp.F.UPF
 Na 22.98900 na_pbe_v1.5.uspp.F.UPF

ATOMIC_POSITIONS {crystal}
 Cl 0.5 0.5 0.5
 Na 0.0 0.0 0.0

K_POINTS {automatic}
 ${mesh} ${mesh} ${mesh} 0 0 0
```

Set K-points

for mesh in 4 5 6 7 8 9 10 11 12 13 14 15 16 ; do

K-point mesh Convergence test

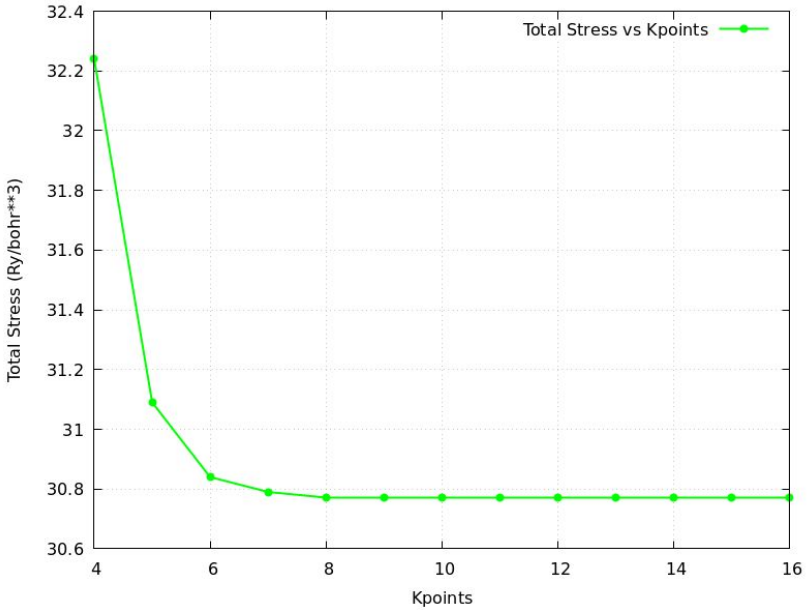
We will use Gnuplot to make the plot. Here is the script code for plotting:

calc-kpoints.dat	
4	32.24
5	31.09
6	30.84
7	30.79
8	30.77
9	30.77
10	30.77
11	30.77
12	30.77
13	30.77
14	30.77
15	30.77
16	30.77

plot_kpoints.gp

```
# plot_press.gp
# Gnuplot script to plot

# Set output to PNG image file
set terminal pngcairo size 800,600
set output "kpoints_convergence.png"  # Name of the output
  file

set xlabel "Kpoints"
set ylabel "Total Stress (Ry/bohr**3)"

set grid
set style line 1 lc rgb "green" lw 2 pt 7

# Plot the data
plot "calc-kpoints.dat" using 1:2 with linespoints
  linestyle 1 title "Total Stress vs Kpoints"

# Close the output file
set output
```

Hydrostatic pressure as a function of k-point mesh



Based on Hydrostatic convergence test, an kpoint mesh values of 9x9x9 is appropriate for a convergence within ~1-2 kbar.

Optimization using vc-relax

vc-relax.in

```
&CONTROL
 calculation   = 'vc-relax',
 outdir        = '.',
 prefix        = 'NaCl',
 pseudo_dir    = '../../../pseudo',
 verbosity     = 'low',
 tprnfor       = .true.,
 tstress       = .true.,
/
&SYSTEM
 ibrav         = 0
 A             = 3.4
 nat           = 2
 ntyp          = 2
 ecutwfc       = 60,
 ecutrho       = 300,
 input_dft     = 'pbe',
 occupations   = 'smearing',
 smearing      = 'mv',
 degauss       = 0.005d0,
/
&ELECTRONS
 conv_thr      = 1d-8,
 mixing_beta   = 0.7d0,
/
&IONS
 ion_dynamics  = 'bfgs',
/
&CELL
 cell_dynamics = 'bfgs',
 press         = 0.d0,
 press_conv_thr= 0.5d0,
/

CELL_PARAMETERS {alat}
 1.0 0.0 0.0
 0.0 1.0 0.0
 0.0 0.0 1.0

ATOMIC_SPECIES
 Cl 35.45150 cl_pbe_v1.4.uspp.F.UPF
 Na 22.98900 na_pbe_v1.5.uspp.F.UPF

ATOMIC_POSITIONS {crystal}
 Cl 0.5 0.5 0.5
 Na 0.0 0.0 0.0

K_POINTS {automatic}
 9 9 9 0 0 0
```

vc-relax.out

```
     negative rho (up, down):  1.454E-02 0.000E+00

     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  1   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  2   force =     0.00000000    0.00000000    0.00000000

     Total force =     0.000000     Total SCF correction =     0.000000


     Computing stress (Cartesian axis) and pressure

     negative rho (up, down):  1.454E-02 0.000E+00
          total   stress  (Ry/bohr**3)                   (kbar)     P=    0.04
  0.00000027   0.00000000   0.00000000          0.04      0.00      0.00
  0.00000000   0.00000027   0.00000000          0.00      0.04      0.00
  0.00000000   0.00000000   0.00000027          0.00      0.00      0.04

     bfgs converged in   6 scf cycles and   5 bfgs steps
     (criteria: energy <  1.0E-04 Ry, force <  1.0E-03Ry/Bohr, cell <  5.0E-01kbar)

     End of BFGS Geometry Optimization

     Final enthalpy =    -128.8814882949 Ry
Begin final coordinates
     new unit-cell volume =    291.83131 a.u.^3 (    43.24494 Ang^3 )
     density =      2.24403 g/cm^3

CELL_PARAMETERS (alat=  6.42506885)
   1.032363974   0.000000000   0.000000000
   0.000000000   1.032363974   0.000000000
   0.000000000   0.000000000   1.032363974

ATOMIC_POSITIONS (crystal)
Cl       0.500000000   0.500000000   0.500000000
Na       0.000000000   0.000000000   0.000000000
End final coordinates
```

Density of States (DOS)

To run a DOS calculation

1. Perform self-consistent (SCF) calculation using **pw.x**

2. Perform non-self-consistent (NSCF) calculation using **pw.x**

    - use denser k-point mesh than in the SCF step

    - set occupations = 'tetrahedra' in the &SYSTEM card

3. Run **projwfc.x** to obtain the total and projected density of states (PDOS)

Density of States (DOS)

scf.in

```
&CONTROL
 calculation='scf',
 outdir='.',
 prefix='NaCl',
 pseudo_dir='/home/max/work/pseudo',
 verbosity='low',
 tprnfor=.true.,
 tstress=.true.,
/

&SYSTEM
  ibrav = 0
  celldm(1) = 6.42506885
  nat = 2
  ntyp = 2
  ecutwfc=60,
  ecutrho=300,
  input_dft='pbe',
  occupations='smearing',
  smearing='mv',
  degauss=0.005d0,
/

&ELECTRONS
 conv_thr=1d-08,
 mixing_beta=0.7d0,
/

CELL_PARAMETERS (alat)
   1.032363974   0.000000000   0.000000000
   0.000000000   1.032363974   0.000000000
   0.000000000   0.000000000   1.032363974

ATOMIC_POSITIONS (crystal)
Cl       0.500000000   0.500000000   0.500000000
Na       0.000000000   0.000000000   0.000000000

K_POINTS {automatic}
 9 9 9 0 0 0
```

pw.x < scf.in > scf.out

nscf.in

```
&CONTROL
 calculation='nscf',
 outdir='.',
 prefix='NaCl',
 pseudo_dir='/home/max/work/pseudo',
 verbosity='low',
 tprnfor=.true.,
 tstress=.true.,
/

&SYSTEM
  ibrav = 0
  celldm(1) = 6.42506885
  nat = 2
  ntyp = 2
  ecutwfc=60,
  ecutrho=300,
  input_dft='pbe',
  occupations='tetrahedra',
/

&ELECTRONS
 conv_thr=1d-08,
 mixing_beta=0.7d0,
/

CELL_PARAMETERS (alat)
   1.032363974   0.000000000   0.000000000
   0.000000000   1.032363974   0.000000000
   0.000000000   0.000000000   1.032363974

ATOMIC_SPECIES
  Cl    35.45150  cl_pbe_v1.4.uspp.F.UPF
  Na    22.98900  na_pbe_v1.5.uspp.F.UPF

ATOMIC_POSITIONS (crystal)
Cl       0.500000000   0.500000000   0.500000000
Na       0.000000000   0.000000000   0.000000000

K_POINTS {automatic}
 18 18 18 0 0 0
```

pw.x < nscf.in > nscf.out

projwfc.in (PDOS)

```
&PROJWFC
 prefix='NaCl',
 outdir='.',
 Emin=-6,
 Emax=17,
 DeltaE=0.05,
 filpdos='NaCl',
 filproj='NaCl'
/
```

projwfc.x < projwfc.in > projwfc.out

Total and Partial Density of States (PDOS)

Total Density of States

Output Files: total_pdos

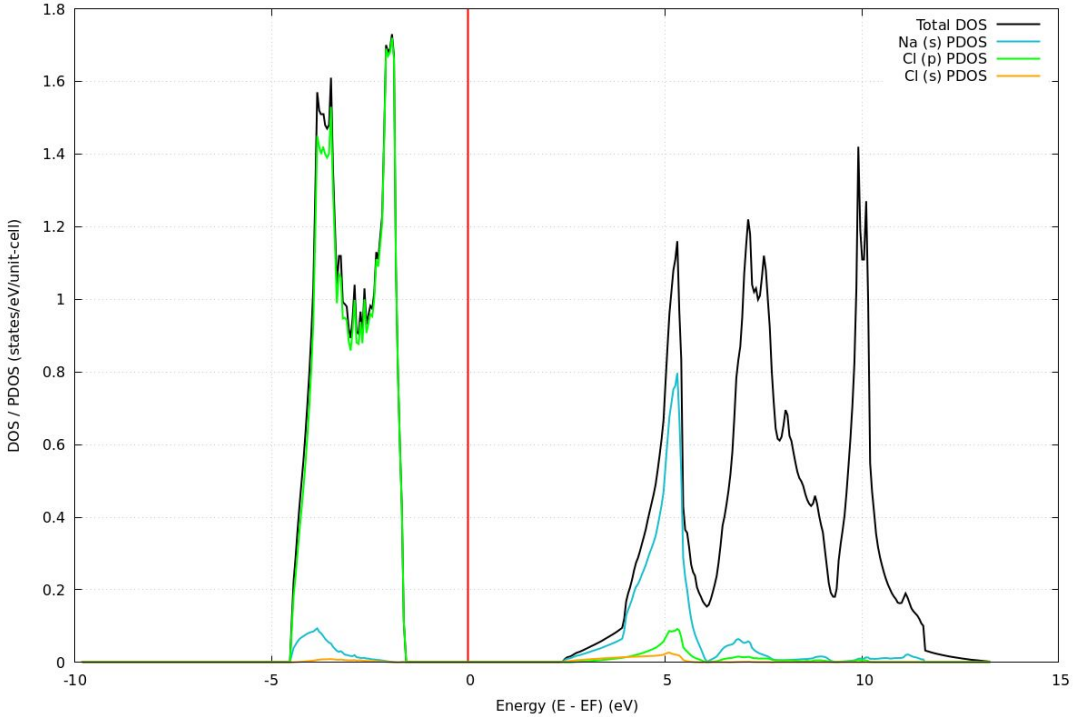
```
# E (eV)   dos(E)     pdos(E)
  -6.000   0.000E+00   0.000E+00
  -5.950   0.000E+00   0.000E+00
  -5.900   0.000E+00   0.000E+00
  -5.850   0.000E+00   0.000E+00
  -5.800   0.000E+00   0.000E+00
  -5.750   0.000E+00   0.000E+00
.....
```

Partial Density of States

Output Files: NaCl.pdos_atm#1(Na)_wfc#2(s)
NaCl.pdos_atm#2(Cl)_wfc#1(s)
NaCl.pdos_atm#2(Cl)_wfc#2(p)

```
# E (eV)   ldos(E)    pdos(E)    pdos(E)    pdos(E)
  -6.000   0.000E+00  0.000E+00  0.000E+00  0.000E+00
  -5.950   0.000E+00  0.000E+00  0.000E+00  0.000E+00
  -5.900   0.000E+00  0.000E+00  0.000E+00  0.000E+00
  -5.850   0.000E+00  0.000E+00  0.000E+00  0.000E+00
  -5.800   0.000E+00  0.000E+00  0.000E+00  0.000E+00
  -5.750   0.000E+00  0.000E+00  0.000E+00  0.000E+00
  -5.700   0.000E+00  0.000E+00  0.000E+00  0.000E+00
.....
```

conda activate visualise
Gnuplot plot_bands.gnu



Band Structure

To run the Band structure

1. Perform self-consistent (SCF) calculation using **pw.x**
2. Perform the non-self-consistent (NSCF) calculation using **pw.x**
    - use k-points along the high-symmetry path in the Brillouin zone
    - for insulators, occupations = 'tetrahedra' in the &SYSTEM card
3. Run **bands.x** to extract the band energies

Band Structure

scf.in

```
&CONTROL
 calculation='scf',
 outdir='.',
 prefix='NaCl',
 pseudo_dir='/home/max/work/pseudo',
 verbosity='low',
 tprnfor=.true.,
 tstress=.true.,
/

&SYSTEM
  ibrav = 0
  celldm(1) = 6.42506885
  nat = 2
  ntyp = 2
  ecutwfc=60,
  ecutrho=300,
  input_dft='pbe',
  occupations='smearing',
  smearing='mv',
  degauss=0.005d0,
/

&ELECTRONS
 conv_thr=1d-08,
 mixing_beta=0.7d0,
/

CELL_PARAMETERS (alat)
   1.032363974   0.000000000   0.000000000
   0.000000000   1.032363974   0.000000000
   0.000000000   0.000000000   1.032363974
ATOMIC_POSITIONS (crystal)
Cl       0.500000000   0.500000000   0.500000000
Na       0.000000000   0.000000000   0.000000000

K_POINTS {automatic}
 9 9 9 0 0 0
```

pw.x < scf.in > scf.out

bands.in

```
&CONTROL
 calculation='bands',
 outdir='.',
 prefix='NaCl',
 pseudo_dir='/home/max/work/pseudo',
 verbosity='low',
 tprnfor=.true.,
 tstress=.true.,
/

&SYSTEM
  ibrav = 0
  celldm(1) = 6.42506885
  nat = 2
  ntyp = 2
  ecutwfc=60,
  ecutrho=300,
  input_dft='pbe',
  occupations='smearing',
  smearing='mv',
  degauss=0.005d0,
  nbnd = 12,
/

&ELECTRONS
 conv_thr=1d-08,
 mixing_beta=0.7d0,
/

CELL_PARAMETERS (alat)
   1.032363974   0.000000000   0.000000000
   0.000000000   1.032363974   0.000000000
   0.000000000   0.000000000   1.032363974
```

pw.x < bands.in > bands.out

```
ATOMIC_SPECIES
  Cl   35.45150  cl_pbe_v1.4.uspp.F.UPF
  Na   22.98900  na_pbe_v1.5.uspp.F.UPF

ATOMIC_POSITIONS (crystal)
Cl       0.500000000   0.500000000   0.500000000
Na       0.000000000   0.000000000   0.000000000

K_POINTS {crystal_b}
8
 0.0000  0.0000  0.0000  30  ! G (Γ)
 0.0000  0.5000  0.0000  30  ! X
 0.5000  0.5000  0.0000  30  ! M
 0.0000  0.0000  0.0000  30  ! G (Γ)
 0.5000  0.5000  0.5000  30  ! R
 0.0000  0.5000  0.0000  30  ! X
 0.5000  0.5000  0.0000  30  ! M
 0.5000  0.5000  0.5000  30  ! R
```

pp.in

```
&BANDS
  outdir = '.'
  prefix = 'NaCl'
  filband = 'NaCl.dat'
/
```

bands.x < pp.in > pp.out

Special k-points – seek path

Upload your QE input file to https://www.materialscloud.org/work/tools/seekpath

SeeK-path: the k-path finder and visualizer

What SeeK-path does

SeeK-path definitions and advantages

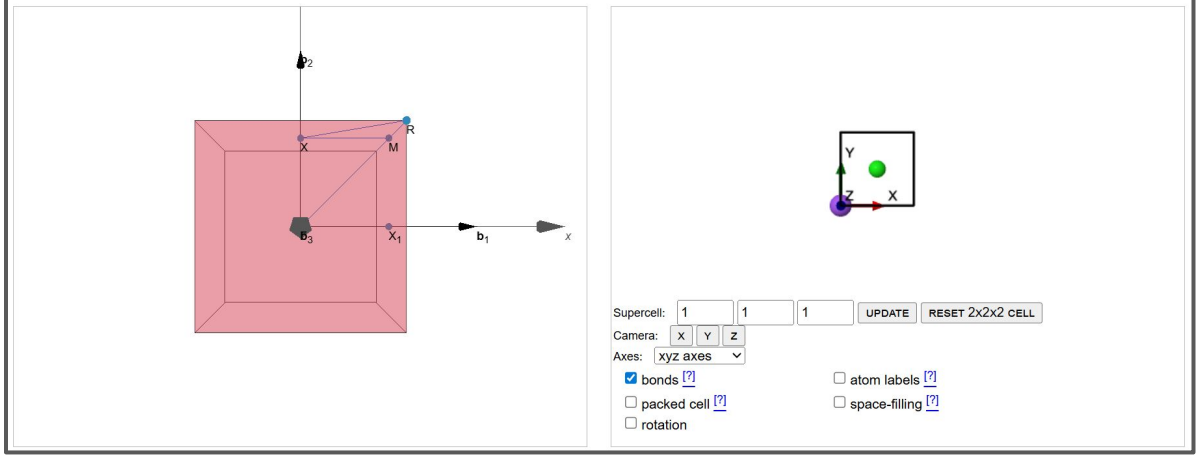
Upload your structure

Upload a crystal structure: Choisir un fichier scf.in

Select here the file format: Quantum ESPRESSO input [parser: qe-tools]

By continuing, you agree with the terms of use of this service.

Calculate my structure



Reciprocal space and Brillouin-zone information

Reciprocal cell vectors (1/Å)

b	x	y	z
b_1	1.8479956786	0.0000000000	0.0000000000
b_2	0.0000000000	1.8479956786	0.0000000000
b_3	0.0000000000	0.0000000000	1.8479956786

Suggested path

Γ—X—M—Γ—R—X|R—M

High-symmetry points (scaled units)

Label	k_1	k_2	k_3
Γ	0.0000000000	0.0000000000	0.0000000000
M	0.5000000000	0.5000000000	0.0000000000
R	0.5000000000	0.5000000000	0.5000000000
X	0.0000000000	0.5000000000	0.0000000000
X_1	0.5000000000	0.0000000000	0.0000000000

Band Structure

SCF file output:

```
the Fermi energy is     3.7918 ev
```

NSCF file output:

```
    0.0000  -48.0156
    0.0161  -48.0156
    0.0323  -48.0156
    0.0484  -48.0156
    0.0646  -48.0155
    0.0807  -48.0155
.....................
```

Postprocessing:

```
Reading collected, re-writing distributed wavefunctions
high-symmetry point:  0.0000 0.0000 0.0000   x coordinate   0.0000
high-symmetry point:  0.0000 0.4843 0.0000   x coordinate   0.4843
high-symmetry point:  0.4843 0.4843 0.0000   x coordinate   0.9687
high-symmetry point:  0.0000 0.0000 0.0000   x coordinate   1.6536
high-symmetry point:  0.4843 0.4843 0.4843   x coordinate   2.4925
high-symmetry point:  0.0000 0.4843 0.0000   x coordinate   3.1774
high-symmetry point:  0.4843 0.4843 0.0000   x coordinate   3.6617
high-symmetry point:  0.4843 0.4843 0.4843   x coordinate   4.1461
```

Gnuplot plot_bands.gnu