Hands-on introduction of OpenMX
- Lecture -

Ozaki group
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Schedule:
14:30～15:30 Lecture
15:50～17:20 Practice

2018/7/2
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Outline

- Introduction : Basic OpenMX
  - What is OpenMX ?
  - What can OpenMX do ?
- Install OpenMX
- Input file
  - Keywords
  - OpenMX viewer
- Run, Parallelization
- Output
  - Standard output and *.out file
  - Visualization
  - Post process
- Remarks and Tips for OpenMX
- Post query into OpenMX forum

Intro

What is OpenMX

First-principles program package based on density functional theory with

pseudopotentials and numerical local orbitals basis set

Reduce numerical cost by using carefully constructed potential for the valence electrons

Describe efficiently Kohn-Sham orbitals in atomic, molecular, solid systems.

Open source package for Material eXplorer

Main developer : T. Ozaki

More than 20 contributors

http://www.openmx-square.org/

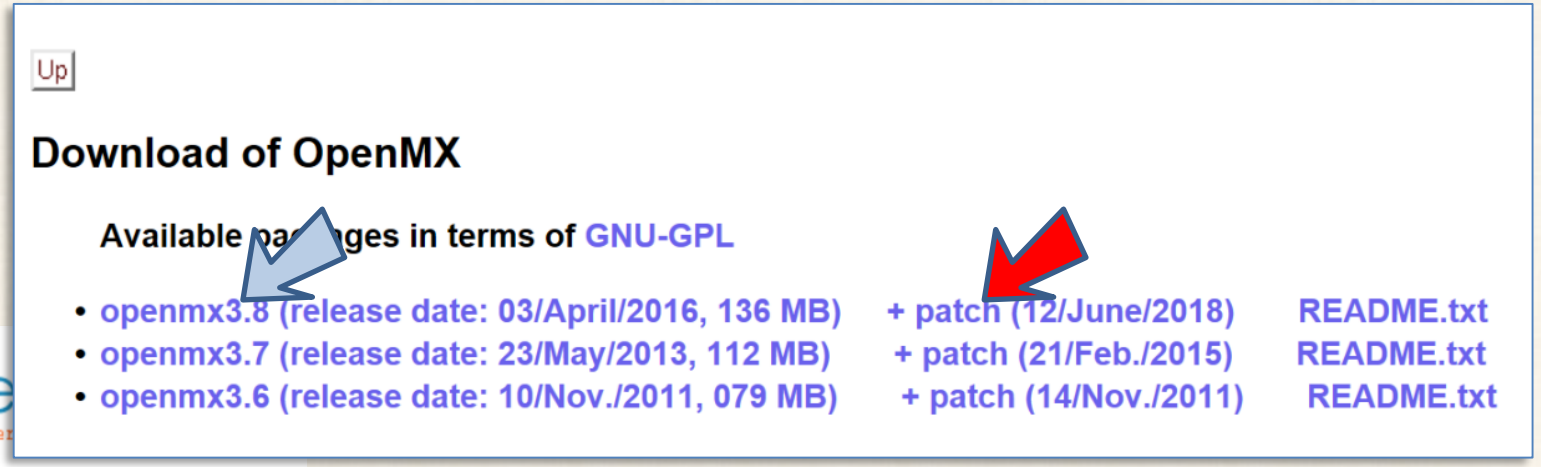
Intro

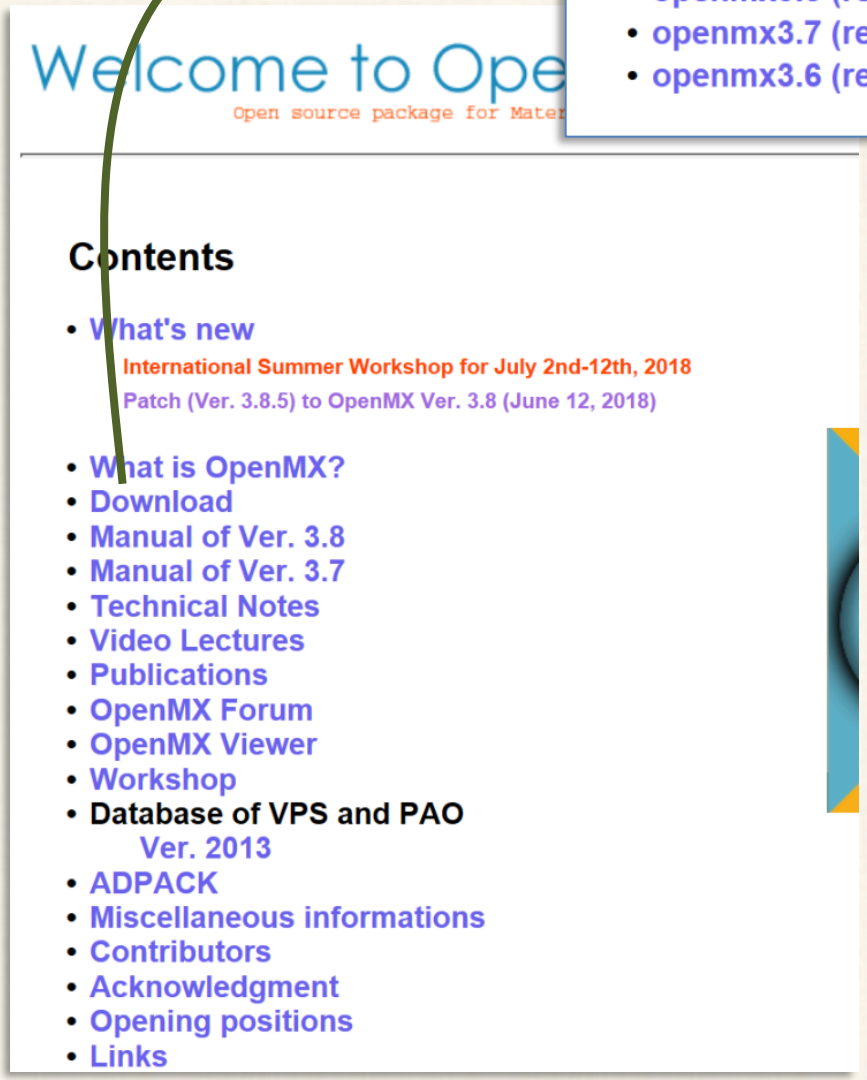
What can OpenMX do ?

- Total energy, charge/spin density, force, stress
- Band, DOS, PDOS, Fermi surface, Wannier function
- Variable-cell MD, structural optimization, reaction path (NEB)
- LDA, GGA, vdW functional, DFT+U
- Non-collinear magnetism, spin-orbit coupling
- Order-N
- Electronic transport with NEGF method
- Spin-Spin coupling constant
- Unfolding of band structure of surface, interface, etc.
- OpenMP + MPI hybrid parallelism
- Visualization and GUI input generation
- Etc.

Install

Install OpenMX : Download






```
$ tar xzvf openmx3.8.tar.gz
$ cd openmx3.8/source
$ tar xzvf ../../patch3.8.5.tar.gz
```

- source/ : source code for OpenMX (C & fortran)
- work/ : sample inputs
- DFT_DATA13/ : pseudo potential & basis set

Install

Build OpenMX

Edit makefile in source/directory to apply your system

Macro for make command

- CC : C compiler and compile option.
  E.g./ mpicc -fopenmp -O3 -I /usr/local/include/ -Dscalapack
- FC : fortran compiler and compile option
  E.g./ mpif90 -fopenmp -O3 -I /usr/local
- LIB : linker option
  E.g./ -mkl=parallel -lmpi_f90 -lmpi_f77

```
$ make all
```

- openmx : Main program
- bandgnu13 : Utility for plotting band structure
- DosMain : Utility for DOS and PDOS
- jx : Utility for exchange (spin-spin) coupling
- bin2txt, cube2xsf, md2axsf : File-format converter

Input

Input file : General rule of Keywords

```
#
# File Name
#

System.CurrrentDirectory    ./     # default=./
System.Name                 GaAs
level.of.stdout         1     # default=1 (1-3)
level.of.fileout        1     # default=1 (0-2)

#
#
# Definition of Atomic Species
#

Species.Number          3
<Definition.of.Atomic.Species
 Ga    Ga7.0-s2p2d1    Ga_CA13
 As    As7.0-s2p2d1    As_CA13
proj   As7.0-s1p1d1    As_CA13
Definition.of.Atomic.Species>
```

Key.Word Value

comment

<Key.Word.List
Value1a Value1b Value1c
Value2a Value2b Value2c
Value3a Value3b Value3c
Key.word.List>

Uppercase and Lowercase are not distinguished.

Input

Keyword for path, title, IO

Full path or relative path to DFT_DATA13 (pseudopotentials)

The label of output files:

GaAs.out, GaAs.md, GaAs.Band, …

```
DATA.PATH  /home/public/program/openmx3.8/DFT_DATA13/
System.CurrrentDirectory          ./    # default=./
System.Name                      mgb2
level.of.stdout                   1     # default=1 (1-3)
level.of.fileout                  1     # default=1 (0-2)
```

Amount of output data:

It should be ≧1 if we want to produce some volumetric files (charge-density, potential, etc.).

Input

Keyword for atomic species and structure

Basis file DFT_DATA13/PAO/B7.0.pao
(omitting .pao)

"7.0" is the radius of basis

Pseudopotential file
DFT_DATA13/VPS/B_PBE13.vps
(omitting ".vps")

Functional (GGA-PBE)

Basis configuration

```
Species.Number  4
<Definition.of.Atomic.Species
 B  B7.0-s2p2d1  B_PBE13
 Mg  Mg7.0-s3p3d2  Mg_PBE13
Definition.of.Atomic.Species>
Atoms.Number  3
Atoms.SpeciesAndCoordinates.Unit   Ang
<Atoms.SpeciesAndCoordinates
1 Mg 0.000000 0.000000 0.000000 4.000000 4.000000
2 B 1.542500 0.890563 1.761500 1.500000 1.500000
3 B 0.000000 1.781126 1.761500 1.500000 1.500000
Atoms.SpeciesAndCoordinates>
Atoms.UnitVectors.Unit  Ang
<Atoms.UnitVectors
 3.085000 0.000000 0.000000
 -1.542500 2.671688 0.000000
 0.000000 0.000000 3.523000
Atoms.UnitVectors>
```

Atomic position

Occupation for initial guess

$\vec{a}_1$

$\vec{a}_2$

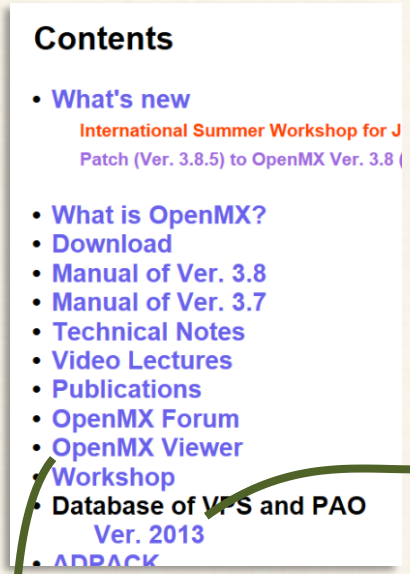
$\vec{a}_3$

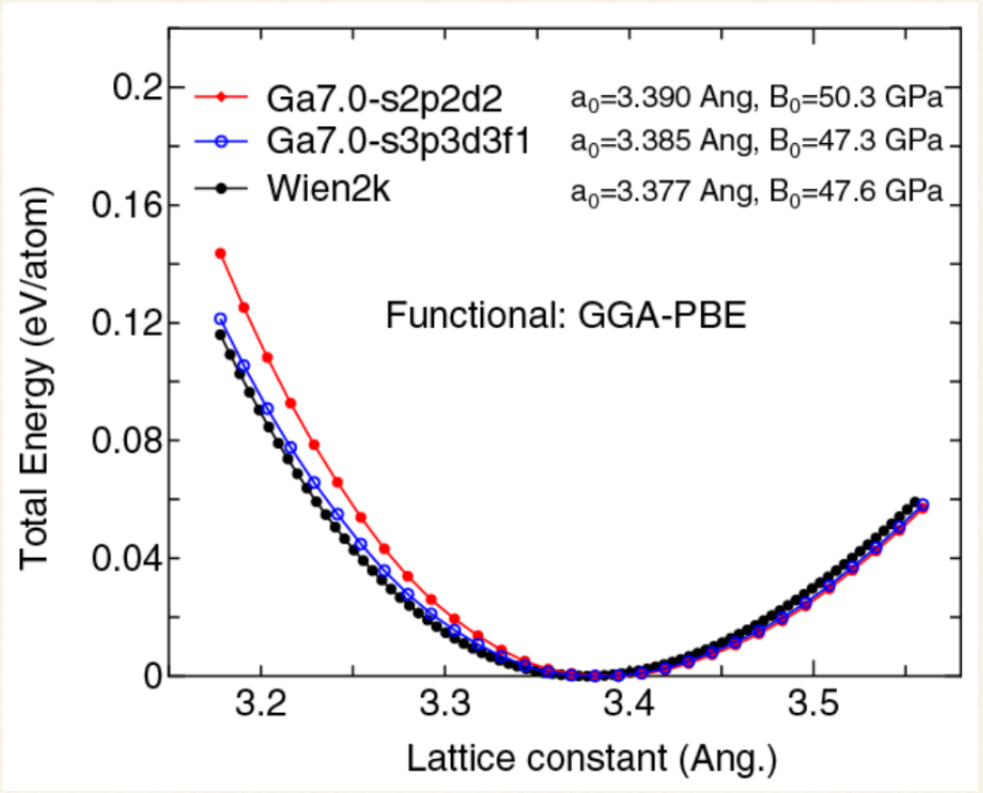
Input

How we choose basis configuration ?

(1) Follow the configuration in literature if we reproduce it.

(2) Suggestion in the OpenMX Web page





(3) Input file generator in OpenMX Viewer, etc.

→ It will be shown in this lecture and practice.

Input

Condition of DFT calculation

Cutoff energy for FFT grid.
Small "scf.energycutoff" causes bad SCF convergence (See manual).

```
scf.XcType                  GGA-PBE     # LDA|LSDA-CA|LSDA-PW|GGA-PBE
scf.SpinPolarization          off       # On|Off|NC
scf.SpinOrbit.Coupling        off       # On|Off, default=off
scf.energycutoff            300.0       # default=150 (Ry)
scf.EigenvalueSolver        band        # DC|GDC|Cluster|Band
scf.ElectronicTemperature   5000.0       # default=300 (K)
scf.Kgrid                 14 14 10       # means n1 x n2 x n3
```

Denser *k*-grid is required for metallic system.

For the Brillouin-zone integration.
It is not the same as the real temperature.

Input

Keyword for convergence

SCF convergence

```
scf.maxIter                50          # default=40
scf.criterion            1.0e-7        # default=1.0e-6 (Hartree)
scf.Init.Mixing.Weight    0.20         # default=0.30
scf.Min.Mixing.Weight     0.001        # default=0.001
scf.Max.Mixing.Weight     0.500        # default=0.40
scf.Mixing.History         7           # default=5
scf.Mixing.StartPulay      7           # default=6
scf.Mixing.EveryPulay      1           # default=6
```

For good convergence:

- Small mixing
- Large mixing history
- Large startpulay
- Large electronic temperature
- Large enegycutoff

See section "SCF convergence" In OpenMX manual

Structural optimization

```
MD.Type     OPT
MD.Opt.DIIS.History     3
MD.Opt.StartDIIS       30
MD.Opt.EveryDIIS       200
MD.maxIter             100
MD.Opt.criterion      0.0005
MD.Opt.Init.Hessian        Schlegel  # Schlegel|iden
```

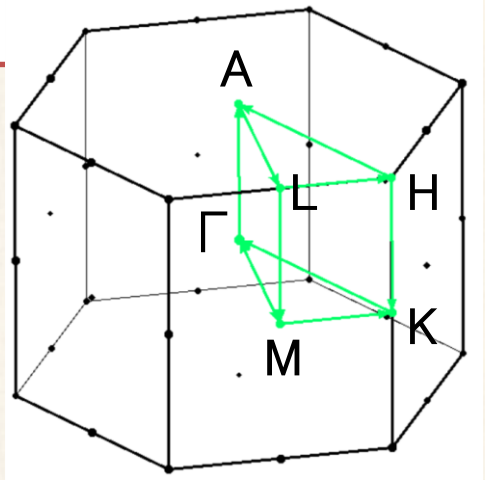
Input

Keyword for post process (1)

```
scf.restart      on
orbitalOpt.Force.Skip        on
```

The post-process should be separated from the SCF calculation

```
Band.dispersion                off
Band.Nkpath  9
<Band.kpath
11  0.000000 0.000000 0.000000 0.500000 0.000000 0.000000 GAMMA M
6  0.500000 0.000000 0.000000 0.333333 0.333333 0.000000 M K
13  0.333333 0.333333 0.000000 0.000000 0.000000 0.000000 K GAMMA
8  0.000000 0.000000 0.000000 0.000000 0.000000 0.500000 GAMMA A
11  0.000000 0.000000 0.500000 0.500000 0.000000 0.500000 A L
6  0.500000 0.000000 0.500000 0.333333 0.333333 0.500000 L H
13  0.333333 0.333333 0.500000 0.000000 0.000000 0.500000 H A
8  0.500000 0.000000 0.500000 0.500000 0.000000 0.000000 L M
8  0.333333 0.333333 0.500000 0.333333 0.333333 0.000000 H K
Band.kpath>
```



Input

Keyword for post process (2)

DOS, PDOS

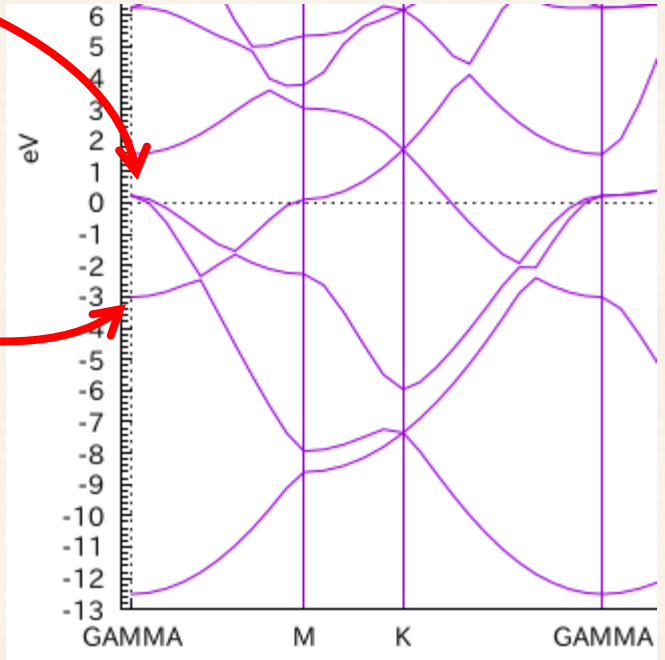
```
Dos.fileout       on
Dos.Erange        -3.0  3.0
Dos.Kgrid      28 28 20
```

Energy range is measured from E_F

k-grid for DOS should be denser than that for SCF (e.g. twice as large as)

Display Kohn-Sham orbitals

```
MO.fileout on
num.LUMOs   2
num.HOMOs   1
MO.Nkpoint   1
<MO.kpoint
0.0   0.0   0.0
MO.kpoint>
```



Input

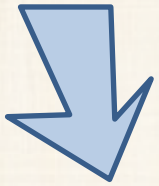
How can we generate input file ?

(1) Write input-file by our own hand.

(2) Generate input file from CIF (Crystalographic information format) file

(a) Get CIF file from any database.

- ICSD (Commercial)
- Crystallography Open Database (http://www.crystallography.net/cod/)
- AtomWork (http://crystdb.nims.go.jp/) : requires sign-up
- Etc.

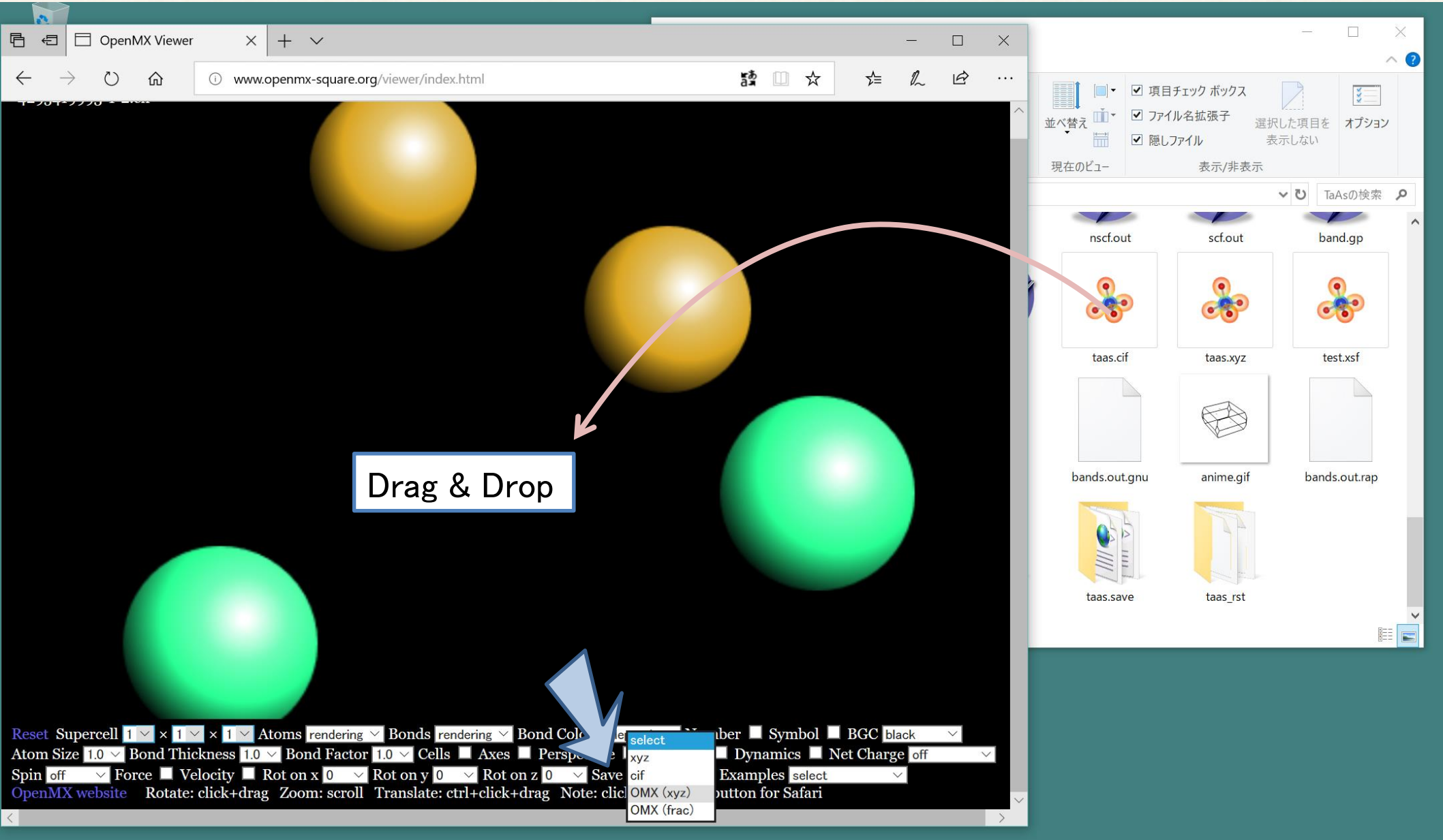


- OpenMX Viewer (http://www.openmx-square.org/)
- C-Tools (https://sourceforge.net/projects/c-tools/)
- Python script by kawamura

C↔TOOLS

Input

Input generator in OpenMX Viewer



Run

```
$ mpirun -np 7 openmx input-file -nt 4
```

Parallelization:

- MPI parallelization for atoms
- MPI for k-parallelization
- Eigenvalue solver (ELPA)
- Real-space grid (FFT etc.)
- Frequency in NEGF
- More parallelization in O(N)
- Etc.

Outputs

- Standard output, *.out file
- Structural data
  - *.md, *.md2
- Volumetric data
  - Charge/Spin density, potential, Orbital
- Post-processing
  - Band
  - Dos, Partial DOS

Output

Standard output

Check the progress of the SCF calculation from the standard output.

```
****************** MD= 1  SCF= 4 ******************
<Poisson>  Poisson's equation using FFT...
<Set_Hamiltonian>  Hamiltonian matrix for VNA+dVH+Vxc...
<Band>  Solving the eigenvalue problem...
 KGrids1:  -0.46428  -0.39286  -0.32143  -0.25000  -0.17857  -0.10714 ...
 KGrids2:  -0.46429  -0.39286  -0.32143  -0.25000  -0.17857  -0.10714 ...
 KGrids3:  -0.45000  -0.35000  -0.25000  -0.15000  -0.05000   0.05000 ...
<Band_DFT>  Eigen, time=2.525886
<Band_DFT>  DM, time=7.088623
    1   Mg  MulP   4.0500  4.0500 sum   8.1000
    2    B  MulP   1.4750  1.4750 sum   2.9500
    3    B  MulP   1.4750  1.4750 sum   2.9500
 Sum of MulP: up   =     7.00000 down          =     7.00000
              total=    14.00000 ideal(neutral)=    14.00000
<DFT>  Total Spin Moment (muB) =  0.000000000000
<DFT>  Mixing_weight= 0.400000000000
<DFT>  Uele    =  -14.134678018779  dUele     =   0.012438791157
<DFT>  NormRD =    0.127025852654  Criterion =   0.000001000000
```

Output

XXX.out file

This file is generated at the end of the calculation.

- SCF history
- Structure optimization/MD history
- Each contribution of the total energy
- All eigenvalues, eigenvectors (optional)
- Mulliken populations
- Computational time at each procedure

When we browse with “less” command,
We can jump each section as :

```
/¥* ⏎
```

```
**********************************************************
**********************************************************
              SCF history at MD= 1
**********************************************************
**********************************************************

  SCF=   1  NormRD=  1.000000000000  Uele= -14.025400095131
  SCF=   2  NormRD=  0.589538767138  Uele= -14.093890088826
  SCF=   3  NormRD=  0.249943520955  Uele= -14.122239457714
  SCF=   4  NormRD=  0.127025831723  Uele= -14.134678255608
  SCF=   5  NormRD=  0.073388775646  Uele= -14.140692161282
  SCF=   6  NormRD=  0.044342510992  Uele= -14.144151844345
  SCF=   7  NormRD=  0.027111841578  Uele= -14.146375438069
  SCF=   8  NormRD=  0.016634903597  Uele= -14.147860482646
  SCF=   9  NormRD=  0.010224951888  Uele= -14.148853983324
```

The amount of information depends on “`level.of.fileout`”.

Output

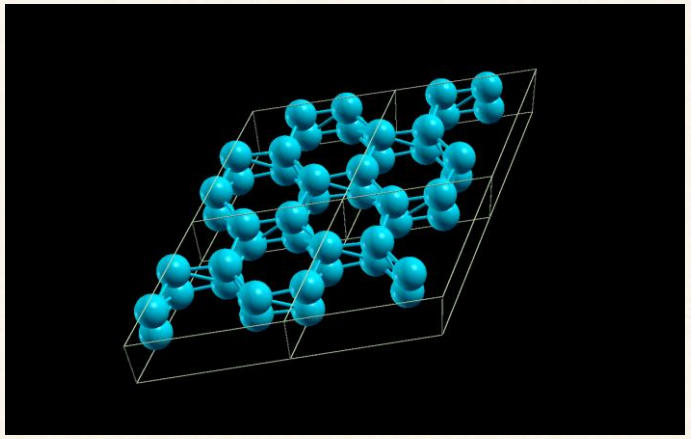
Structural data for MD and optimization

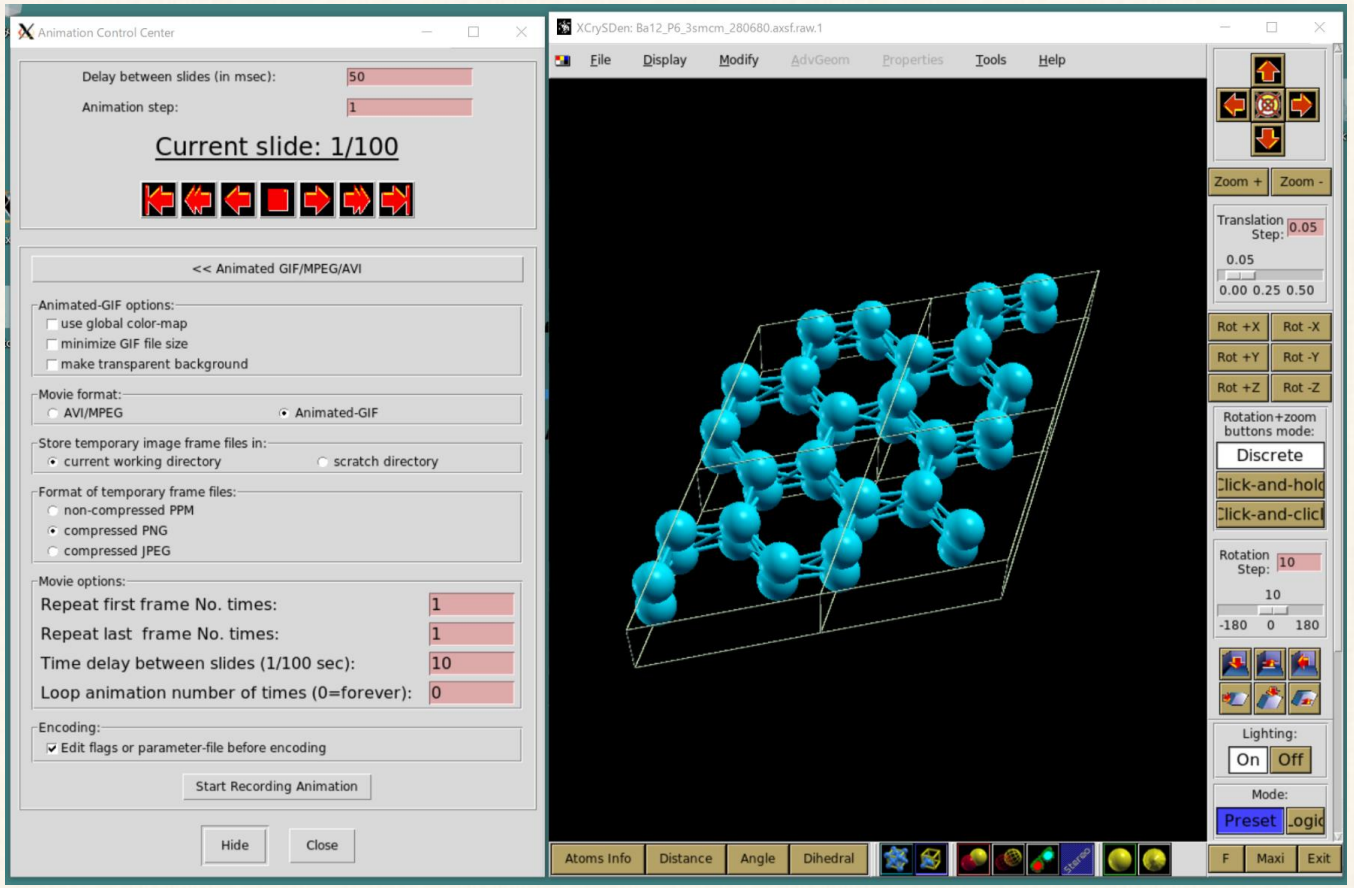
XXX.md : Structure at each MD step

XXX.md2 : Final structure

XCrysDen can read “.axsf” file.

```
$ md2axsf XXX.md XXX.axsf
$ xcrysden --axsf XXX.axsf
```





OpenMX Viewer also can display animation of MD.

It can read *.md file.

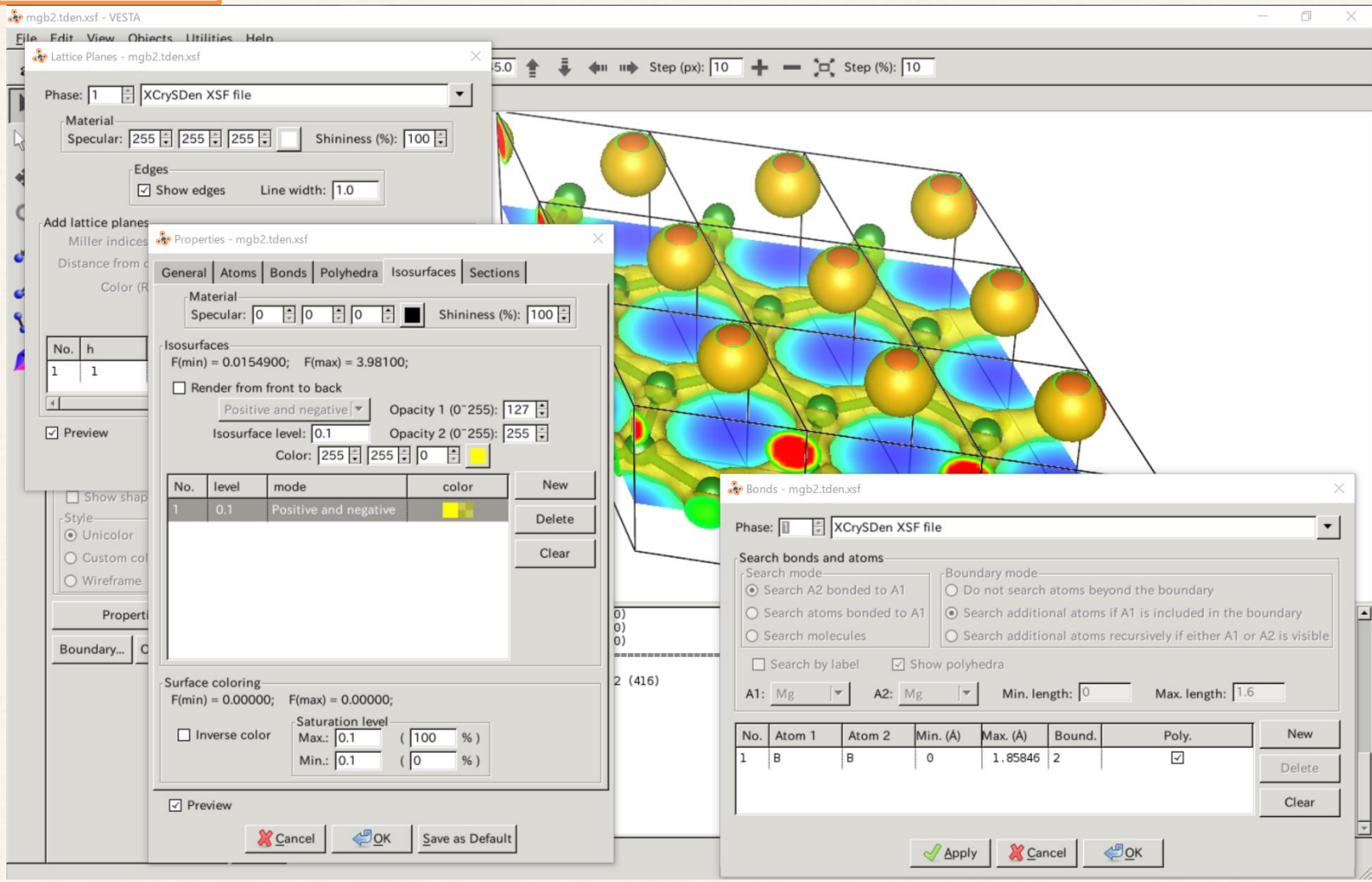
Output

Charge density, potential

`level.of.fileout 1` or `level.of.fileout 2`

```
$ cube2xsf *.cube
$ VESTA mgb2_tden.xsf
```

Gaussian Cube format is not suitable for the periodic system.

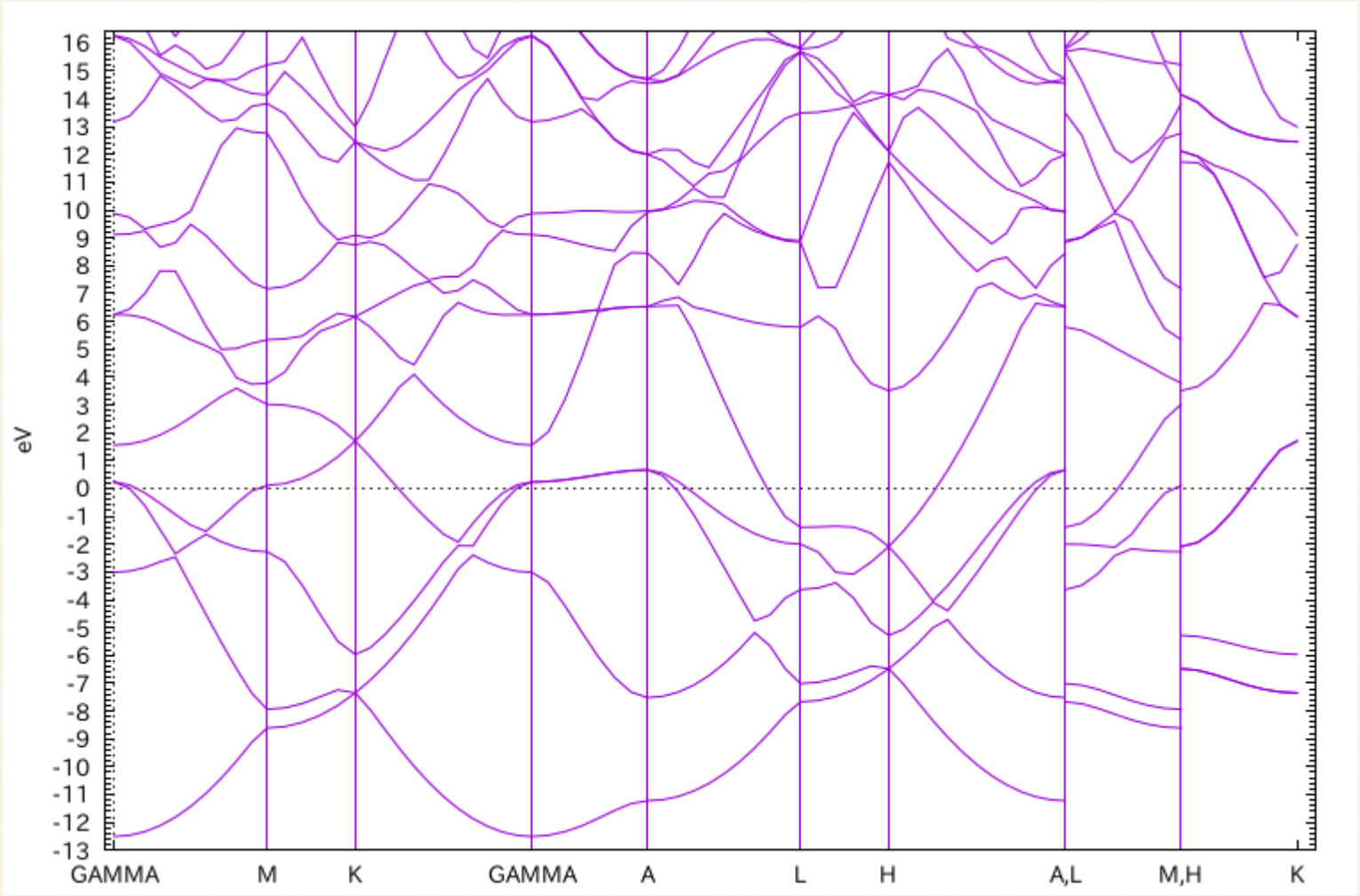


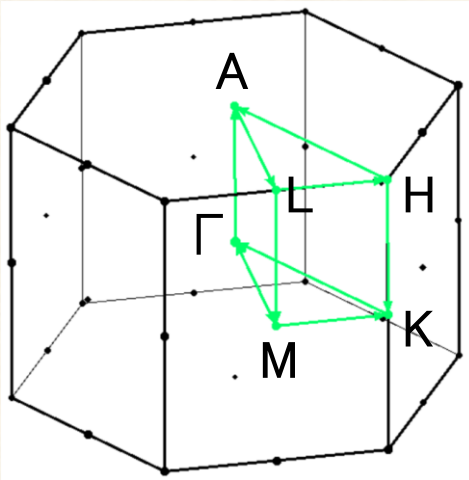
Output

Band structure

```
Band.dispersion                    on
```

```
$ bandgnu13 mgb2.Band
$ gnuplot mgb2.GNUBAND
```





Output

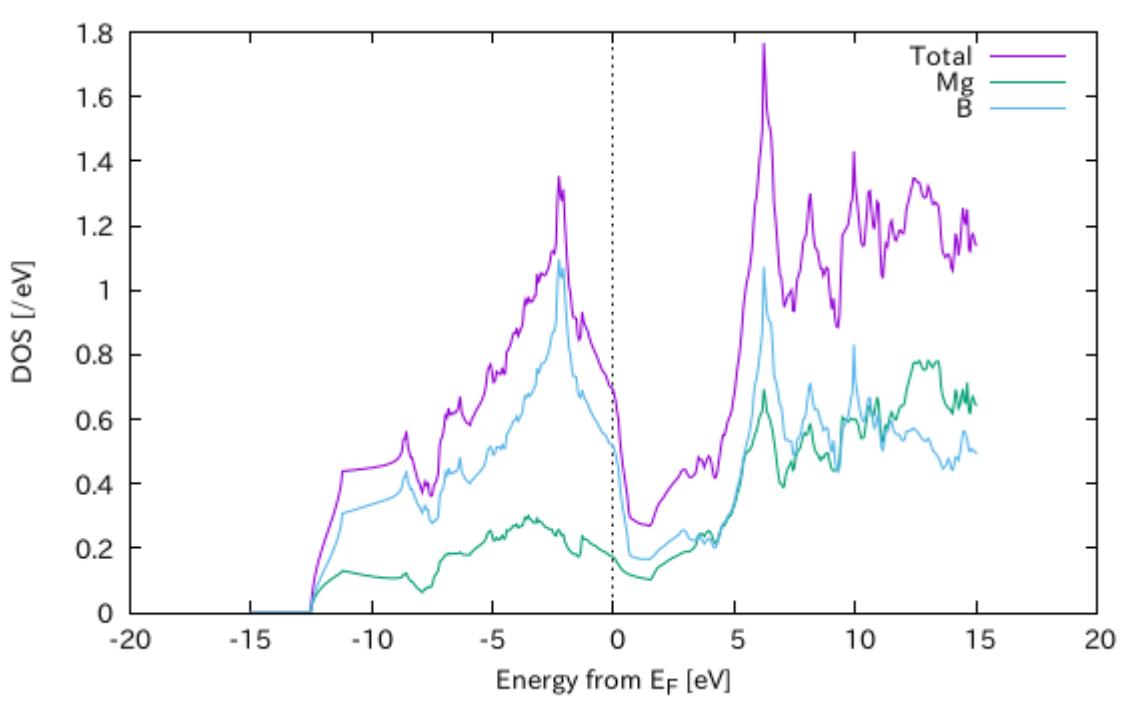
DOS and Fermi surface

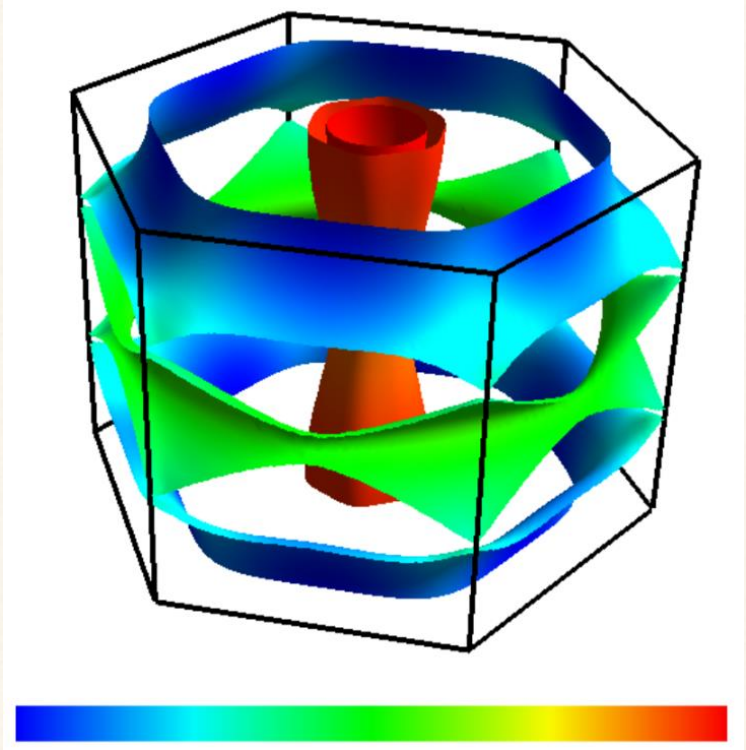
```
Dos.fileout       on
```

```
$ DosMain mgb2.Dos.val mgb2.Dos.vec
```

The tetrahedron method is highly recommended.

```
gnuplot> plot “mgb2.DOS.Tetrahedron” u 1:2 w l tit “Total”, ¥
 "mgb2.PDOS.Tetrahedron.atom1" w l tit "Mg", ¥
 "mgb2.PDOS.Tetrahedron.atom2" u 1:($2*2) w l tit "B"
```



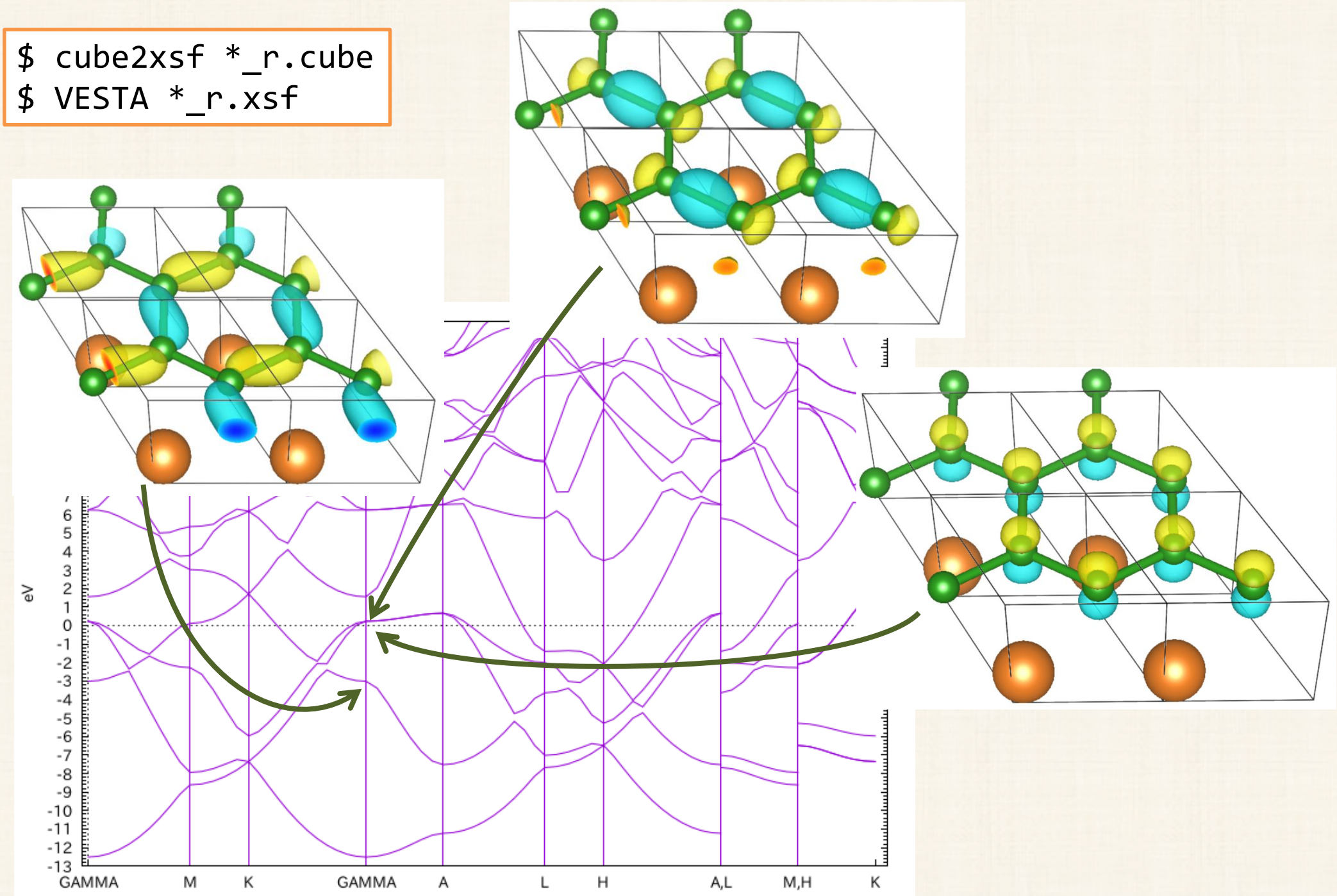


```
$ fermisurfer mgb2.FermiSurf_s0_a2.frmsf
```

Output

Kohn-Sham Bloch orbitals

```
$ cube2xsf *_r.cube
$ VESTA *_r.xsf
```

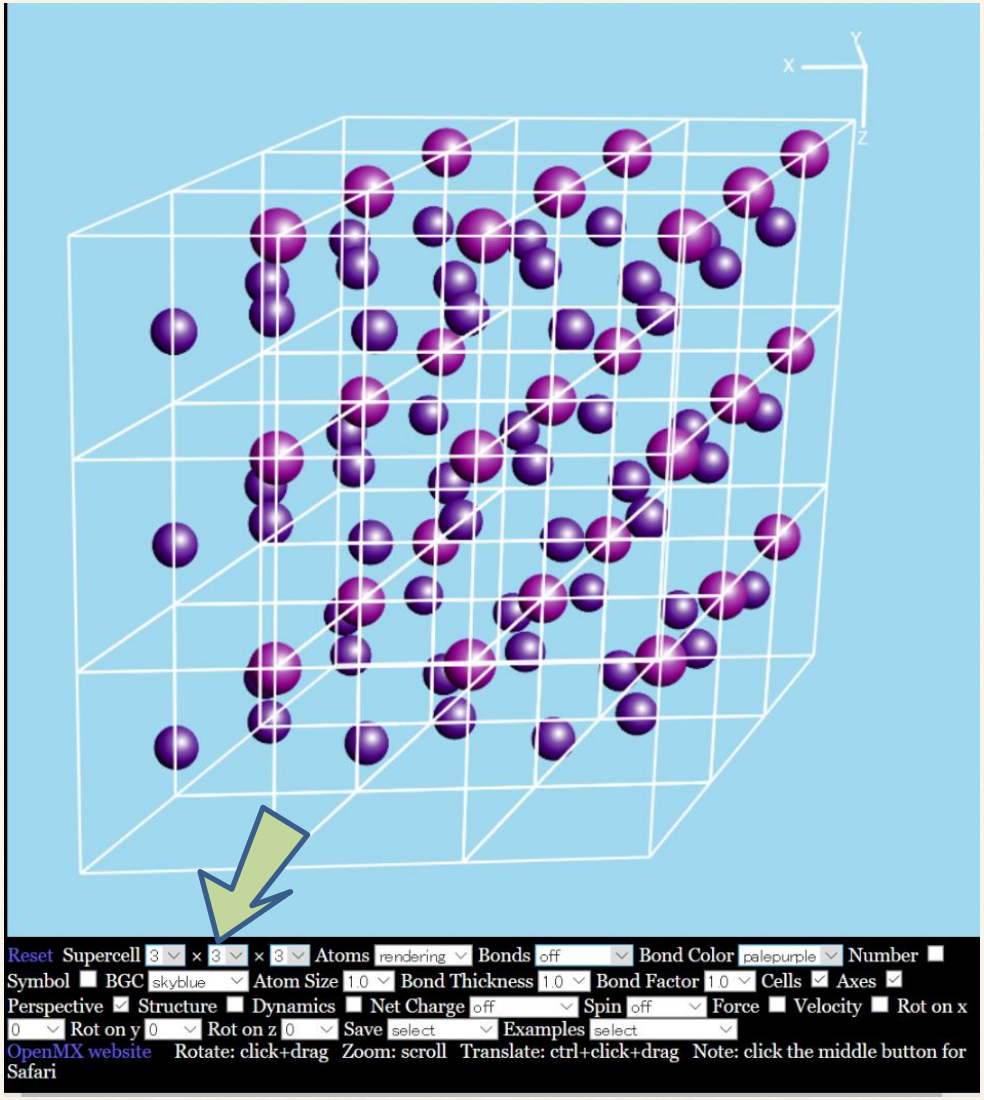


Remark

How can we construct supercell ?

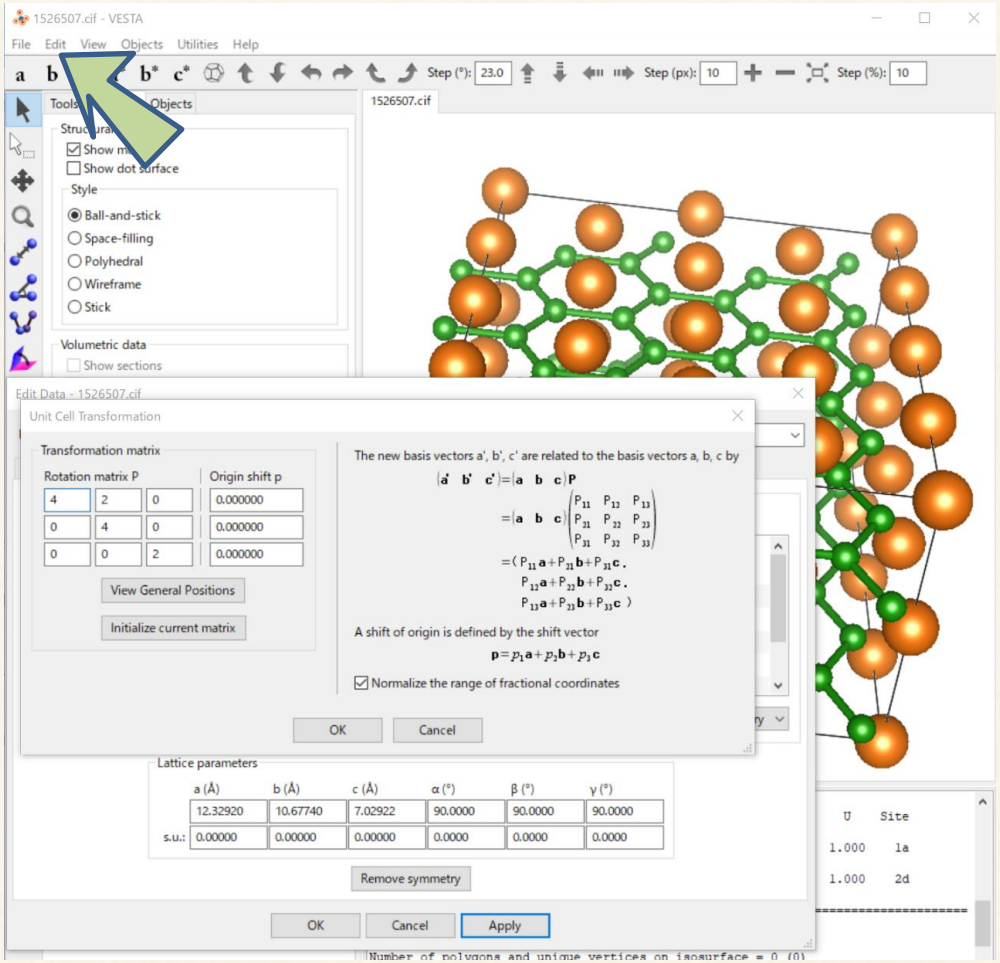
For the supercell written as $N_1 \times N_2 \times N_3$:

OpenMX Viewer



$$(\vec{a}'_1, \vec{a}'_2, \vec{a}'_3) = (\vec{a}_1, \vec{a}_2, \vec{a}_3) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$

VESTA→"Edit"→"Edit Data"

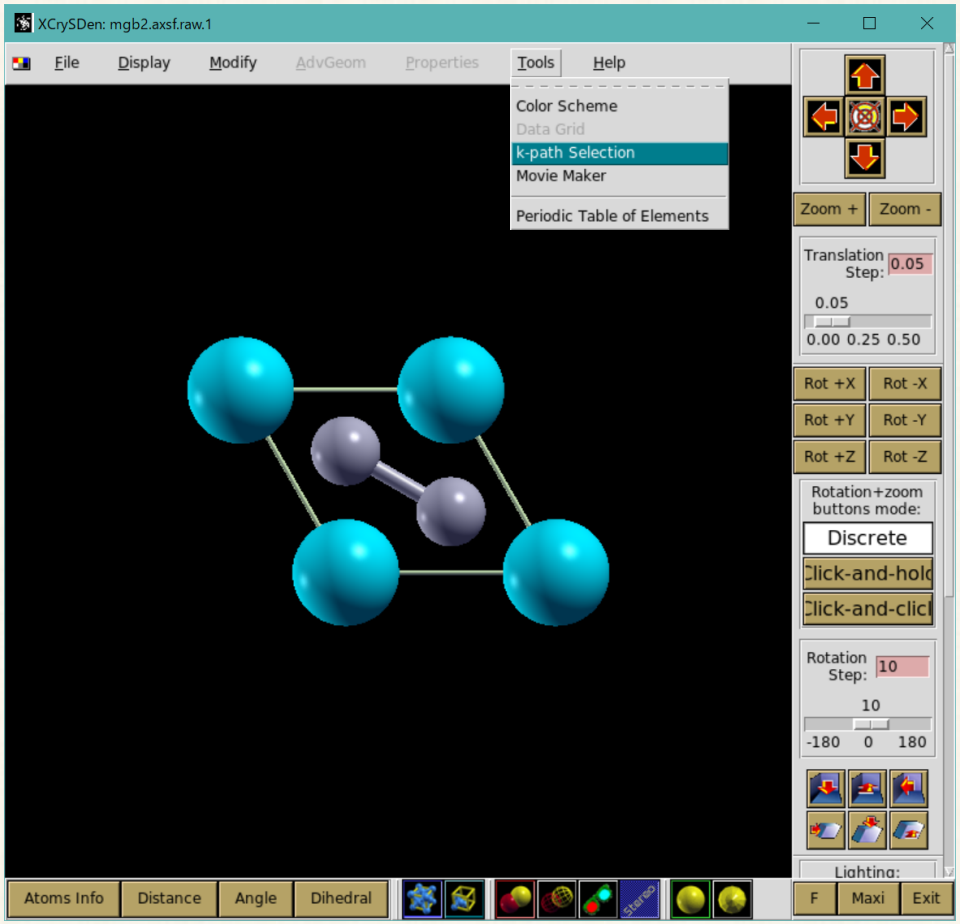


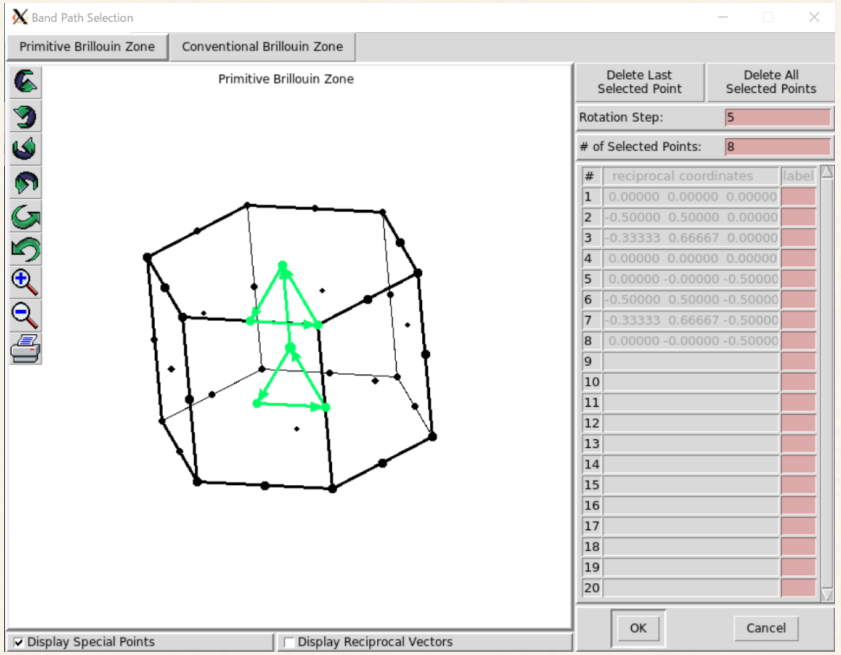
Then, export CIF and read from OpenMX Viewer

Remark

Specifying your own *k*-path

```
$ md2axsf XXX.md XXX.axsf
$ xcrysden --axsf XXX.axsf
```





Save k-points in arbitrary format.

The label of each special k-point is shown in “Wikipedia brillouin-zone” (English).

Remark

More information

Welcome to OpenMX

Open source package for Material eXplorer

Google Custom Search

Contents

- What's new
  - International Summer Workshop for July 2nd-12th, 2018
  - Patch (Ver. 3.8.5) to OpenMX Ver. 3.8 (June 12, 2018)
- What is OpenMX?
- Download
- Manual of Ver. 3.8
- Manual of Ver. 3.7
- Technical Notes
- Video Lecture
- Publications
- OpenMX Forum
- OpenMX Viewer
- Workshop
- Database of VPS and PAO
  - Ver. 2013
- ADPACK
- Miscellaneous informations
- Contributors

Remark

Contact, ask, discussion, bug report, …

Contents

- What's new
  - International Summer Workshop for Ju
  - Patch (Ver. 3.8.5) to OpenMX Ver. 3.8 (
- What is OpenMX?
- Download
- Manual of Ver. 3.8
- Manual of Ver. 3.7
- Technical Notes
- Video Lectures
- Publications
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- Workshop
- Database of VPS and PAO Ver. 2013
- ADPACK
- Miscellaneous informations
- Contributors
- Acknowledgment
- Opening positions
- Links

Known issue can be searched.

OpenMX Forum

Google Custom Search

New Thread | Return Home | Points of Concern | Search | Past Log | Administration

List of Threads

Topics	Author	Replies	Views	Last Modified
From Administrator	Taisuke Ozaki	0	5222	2005/01/09 05:33 by Taisuke Ozaki
convergence for ESM calculation with on2+EF	jiang	0	9	2018/06/21 10:20 by jiang
error in make all	sara.shafaei	1	15	2018/06/20 01:26 by Naoya Yamaguchi
calculations of Z2 and Chern number	Wenliang Liu	1	46	2018/06/16 12:03 by T. Ozaki
Geometry optimization of metal slab yields nan forces	Dechamps Samuel	9	69	2018/06/12 23:39 by Dechamps Samuel
How to solve this problem:APPLICATION TERMINATED WITH THE EXIT STRING: Killed (signal 9)	xmzhang	1	42	2018/06/12 10:12 by T. Ozaki
Patch 3.8.5 to OpenMX Ver. 3.8	T. Ozaki	0	51	2018/06/12 10:05 by T. Ozaki
transport direction for thin film	Prashant	2	69	2018/06/11 22:50 by T. Ozaki
a bad relaxed structure from the RFC5 geometry optimizaiton	Jack	2	36	2018/06/05 09:18 by Jack
Work Function of graphene	Renato	2	56	2018/05/26 00:02 by Renato
How to plot Vhart in a given direction.	Carlos	2	44	2018/05/23 03:16 by Carlos
Step3 of Transport Calculation is not successful	Mobin	5	87	2018/05/22 02:04

Summary

- We overview the typical usage of OpenMX. The following external utilities is useful to generate input file, visualize results.
  - OpenMX Viewer
  - XCrysDen
  - VESTA
  - FermiSurfer
- In the next practice, we will gain the experience of OpenMX with these programs.

Prepare for practice : ssh client

Case 1: Use ssh command (Linux, UNIX, macOS, WSL)

```
$ ssh -Y user-name@server-name
```

Your PC may ask you to add this workstation to “known-hosts”.

Enter your password.

Case 2: GUI ssh-client in Windows

Google “xming putty”

WinSCP is also required in this case.