Hands-on introduction of OpenMX
- Lecture -

Institute for Solid State Physics
Mitsuaki Kawamura

Schedule:
10:40～11:10 Lecture
11:10～12:00 Practice

2020/2/14
The 1st OpenMX hands-on workshop 2020

Outline

- Introduction : Basic OpenMX
  - What is OpenMX ?
  - What can OpenMX do ?
- Install OpenMX
- Structure of 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

Cf. all-electrons method

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

Cf. plane-waves (real-space grid), muffin-tin orbitals

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 (v3.9) 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
- Electronic polarization, Berry phase, Topological invariant
- Optical conductivity, dielectric function
- 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

Up

Download of OpenMX

Available packages in terms of GNU-GPL Version 3 (GPLv3)

- openmx3.9 (release date: 03/Dec./2019, 158 MB) + patch (11/Feb./2020)
- openmx3.8 (release date: 03/April/2016, 136 MB) + patch (12/June/2018)
- openmx3.7 (release date: 23/May/2013, 112 MB) + patch (21/Feb./2015)

Welcome to OpenMX

Open source package for Material eXplorer

- What's new
  - Patch3.9.2 to OpenMX Ver 3.9 (Feb. 11, 2020)
  - The 1st OpenMX hands-on workshop 2020 (Feb. 14, 2020)
  - Patch3.9.1 to OpenMX Ver 3.9 (Jan. 02, 2020)
- What is OpenMX?
- Download
- Manual of Ver. 3.9
- Manual of Ver. 3.8
- Technical Notes
- Video Lectures
- Publications
- OpenMX Forum
- OpenMX Viewer
- Workshop
- Database of Results
- Database of VPS and PAO
  - Ver. 2019
  - Ver. 2019 for core excitations
- ADPACK
- Miscellaneous informations
- Contributors
- Acknowledgment
- Opening positions

```
$ tar xzvf openmx3.9.tar.gz
$ cd openmx3.9/source
$ tar xzvf ../../patch3.9.2.tar.gz
```

- source/ : source code for OpenMX (C & fortran)
- work/ : sample inputs
- DFT_DATA19/ : 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 -O3 -xHOST -ip -no-prec-div -qopenmp ¥`
  `-I/opt/intel/mkl/include/fftw`
- FC : fortran compiler and compile option
  E.g./ `mpif90 -O3 -xHOST -ip -no-prec-div -qopenmp`
- LIB : linker option

E.g./
```
-L${MKLROOT}/lib/intel64 -lmkl_scalapack_lp64 -lmkl_intel_lp64 ¥
-lmkl_intel_thread -lmkl_core -lmkl_blacs_openmpi_lp64 ¥
-lmpi_usempif08 -lmpi_usempi_ignore_tkr -lmpi_mpifh -liomp5 ¥
-lpthread -lm -ldl
```

```
$ 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
- Berry phase, optical conductivity, topological invariant, etc.

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

The label of output files:

abc.out, abc.md, abc.Band, ・・・

```
System.CurrrentDirectory ./
System.Name abc
level.of.stdout 1
level.of.fileout 1
data.path /home/public/program/openmx3.9/DFT_DATA19/
```

Full path or relative path to DFT_DATA19 (pseudopotentials)

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)

```
Species.Number 2
<Definition.of.Atomic.Species
Fe Fe5.5H-s3p2d1 Fe_PBE19H
Pt Pt7.0-s3p2d2f1 Pt_PBE19
Definition.of.Atomic.Species>

Atoms.Number 2
Atoms.SpeciesAndCoordinates.Unit FRAC
<Atoms.SpeciesAndCoordinates
1 Fe 0.0000000 0.0000000 0.0000000 9.0 7.0
2 Pt 0.5000000 0.5000000 0.5000000 8.0 8.0
Atoms.SpeciesAndCoordinates>

Atoms.UnitVectors.Unit Ang
<Atoms.UnitVectors
2.7235000 0.0000000 0.0000000
0.0000000 2.7235000 0.0000000
0.0000000 0.0000000 3.7200000
Atoms.UnitVectors>
```

$\vec{a}_1$ $\vec{a}_2$ $\vec{a}_3$

Basis configuration
s:2 × 1
p:2 × 3
d:1 × 5

Atomic position

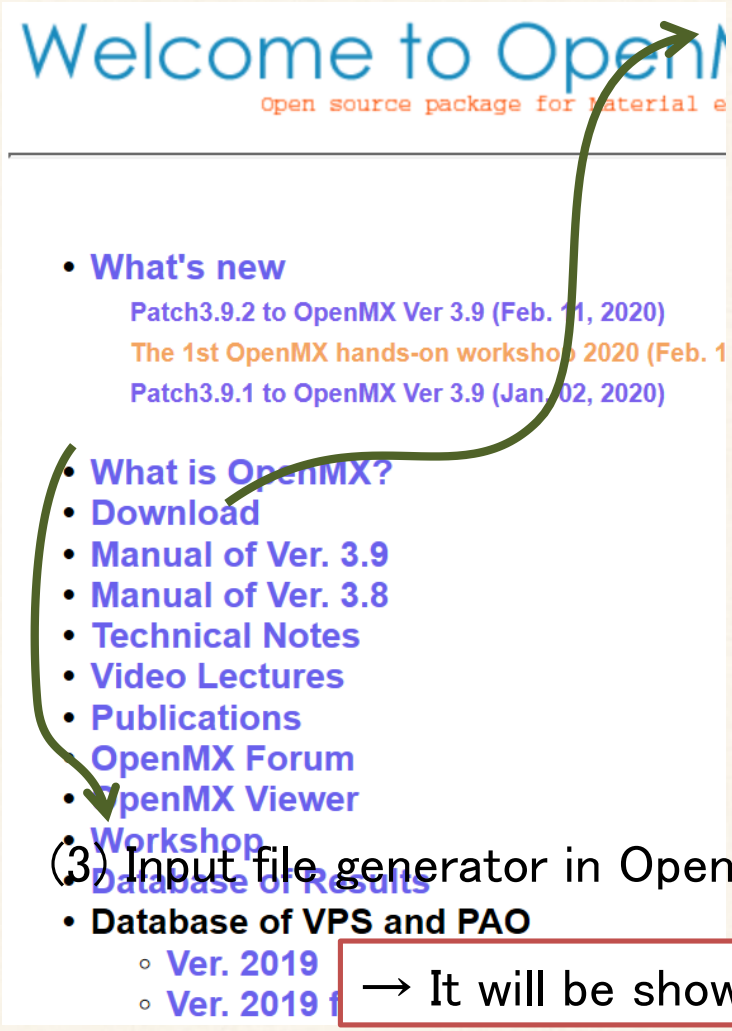
Occupation for initial guess

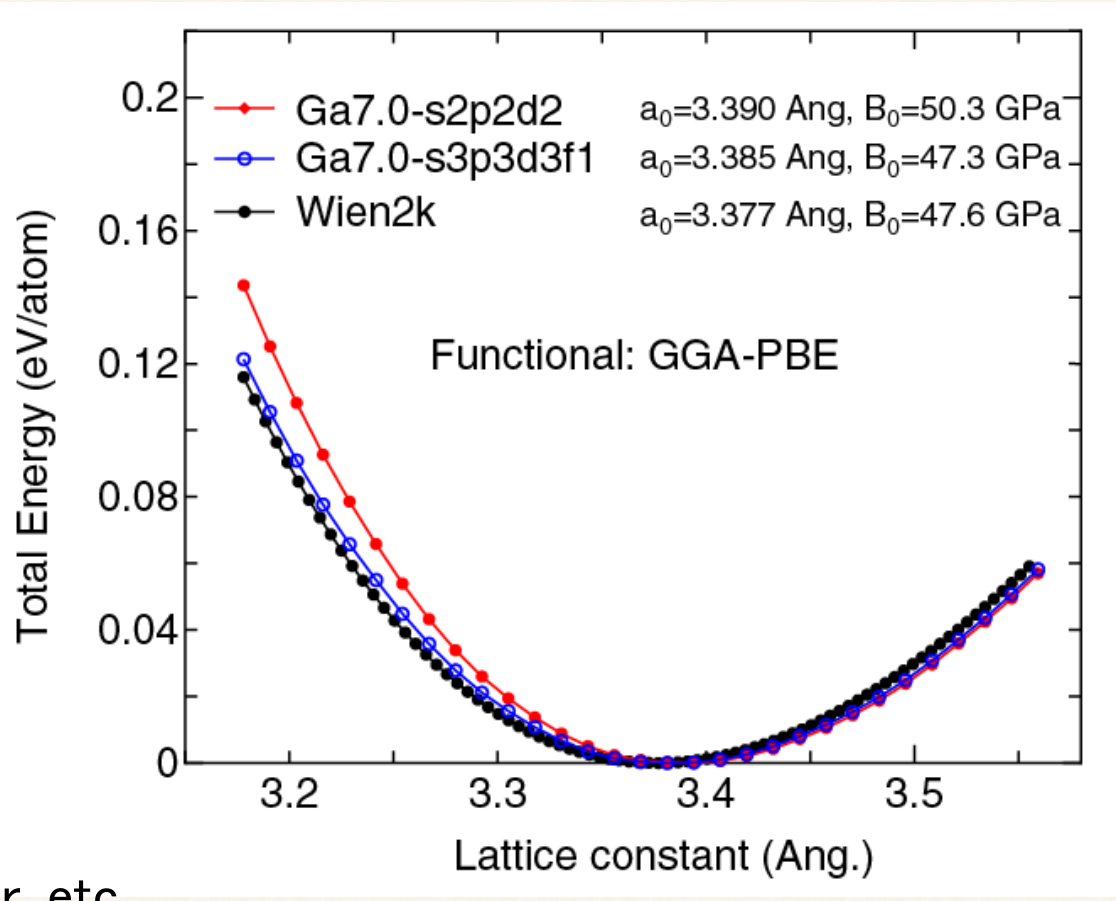
Input

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          on         # On|Off|NC
scf.SpinOrbit.Coupling        off         # On|Off, default=off
scf.energycutoff            220.0        # default=150 (Ry)
scf.EigenvalueSolver        band         # DC|GDC|Cluster|Band
scf.ElectronicTemperature   300.0        # default=300 (K)
scf.Kgrid                 12 12 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.Mixing.Type              rmm-diisk
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 weight
- Large mixing history
- Large start-pulay
- Large electronic temperature
- Large energy cutoff

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
```

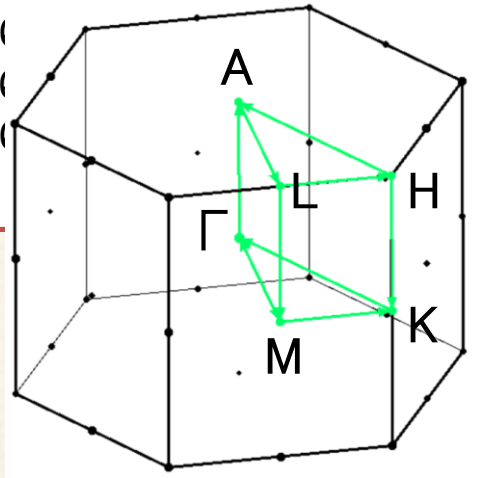
Input

Keyword for post process (1)

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

The post-process should be separated from the SCF calculation

```
Band.dispersion on # on|off, default=off
<Band.KPath.UnitCell
2.7235000000 0.0000000000 0.0000000000
0.0000000000 2.7235000000 0.0000000000
0.0000000000 0.0000000000 3.7200000000
Band.KPath.UnitCell>
Band.Nkpath 9
<Band.kpath
15 0.0000000000 0.0000000000 0.0000000000 0.0000000000 0.5000000000 0.0000000000 GAMMA X
15 0.0000000000 0.5000000000 0.0000000000 0.5000000000 0.5000000000 0.0000000000 X M
15 0.5000000000 0.5000000000 0.0000000000 0.0000000000 0.0000000000 0.0000000000 M GAMMA
15 0.0000000000 0.0000000000 0.0000000000 0.0000000000 0.0000000000 0.5000000000 GAMMA Z
15 0.0000000000 0.0000000000 0.5000000000 0.0000000000 0.5000000000 0.5000000000 Z R
15 0.0000000000 0.5000000000 0.5000000000 0.5000000000 0.5000000000 0.5000000000 R A
15 0.5000000000 0.5000000000 0.5000000000 0.0000000000 0.0000000000 (
15 0.0000000000 0.5000000000 0.0000000000 0.0000000000 0.5000000000 (
15 0.5000000000 0.5000000000 0.0000000000 0.5000000000 0.5000000000 (
Band.kpath>
```



Input

Keyword for post process (2)

DOS, PDOS

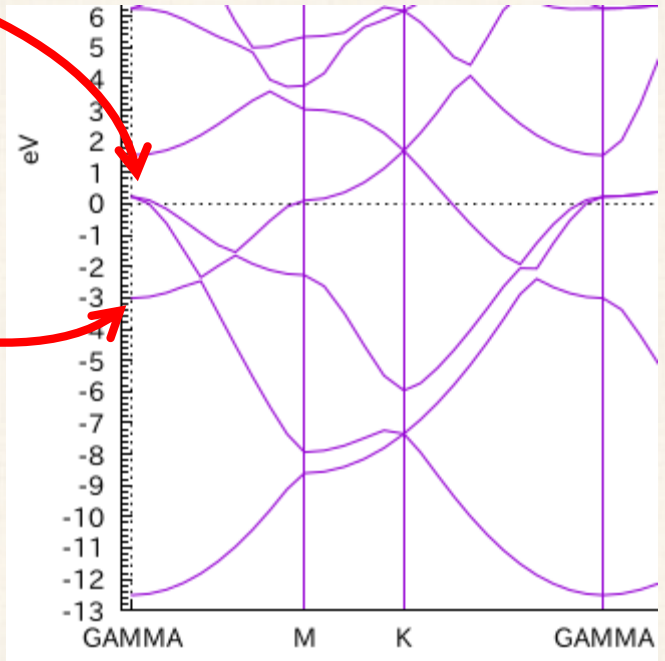
```
Dos.fileout       on
Dos.Erange        -3.0  3.0
Dos.Kgrid      28 28 20
```

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

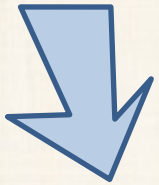
How can we generate input file ?

(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.

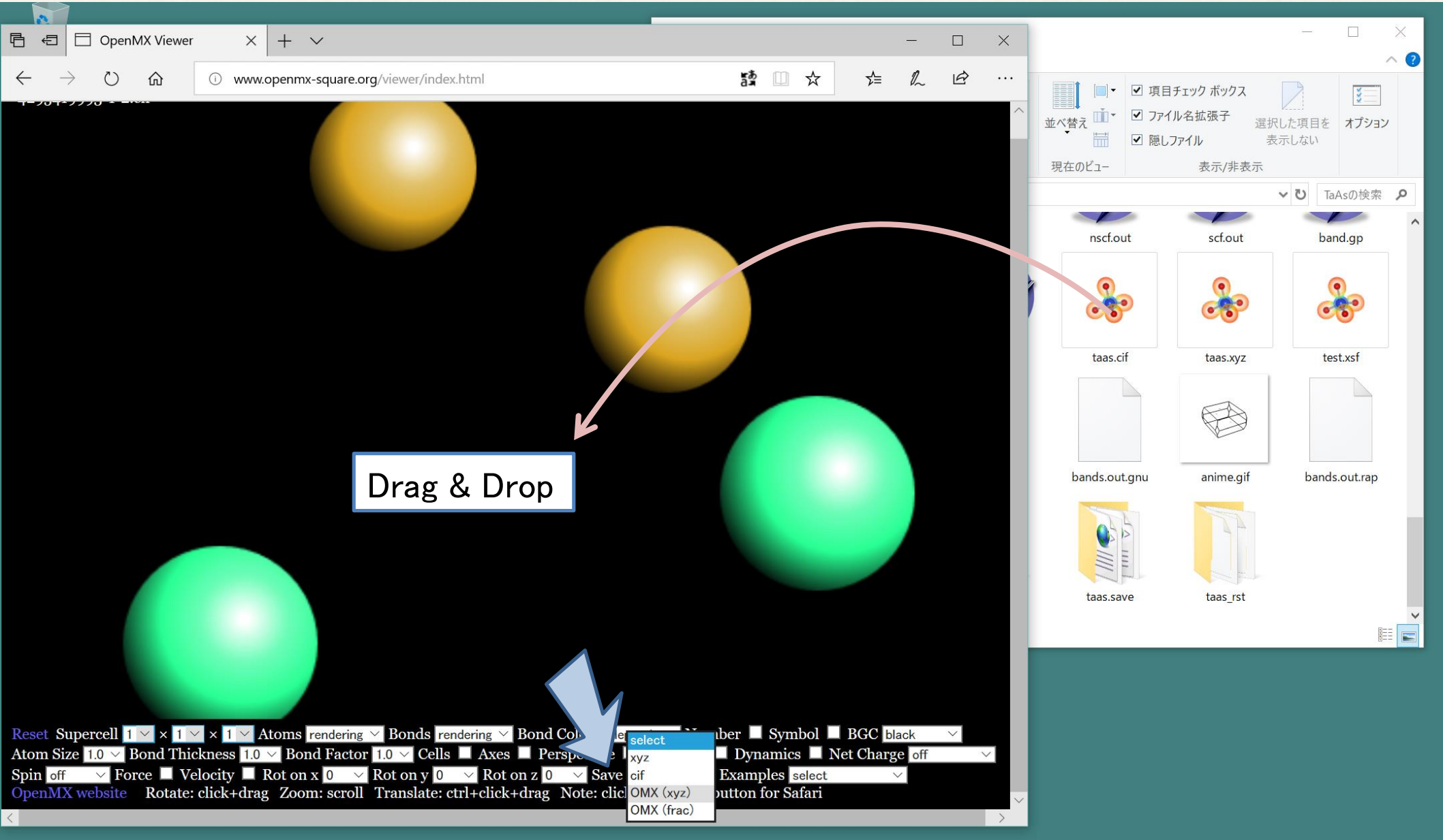
- ICSD (Commercial)
- Crystallography Open Database (http://www.crystallography.net/cod/)
- AtomWork (http://crystdb.nims.go.jp/) : requires sign-up
- Etc.



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

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`”.

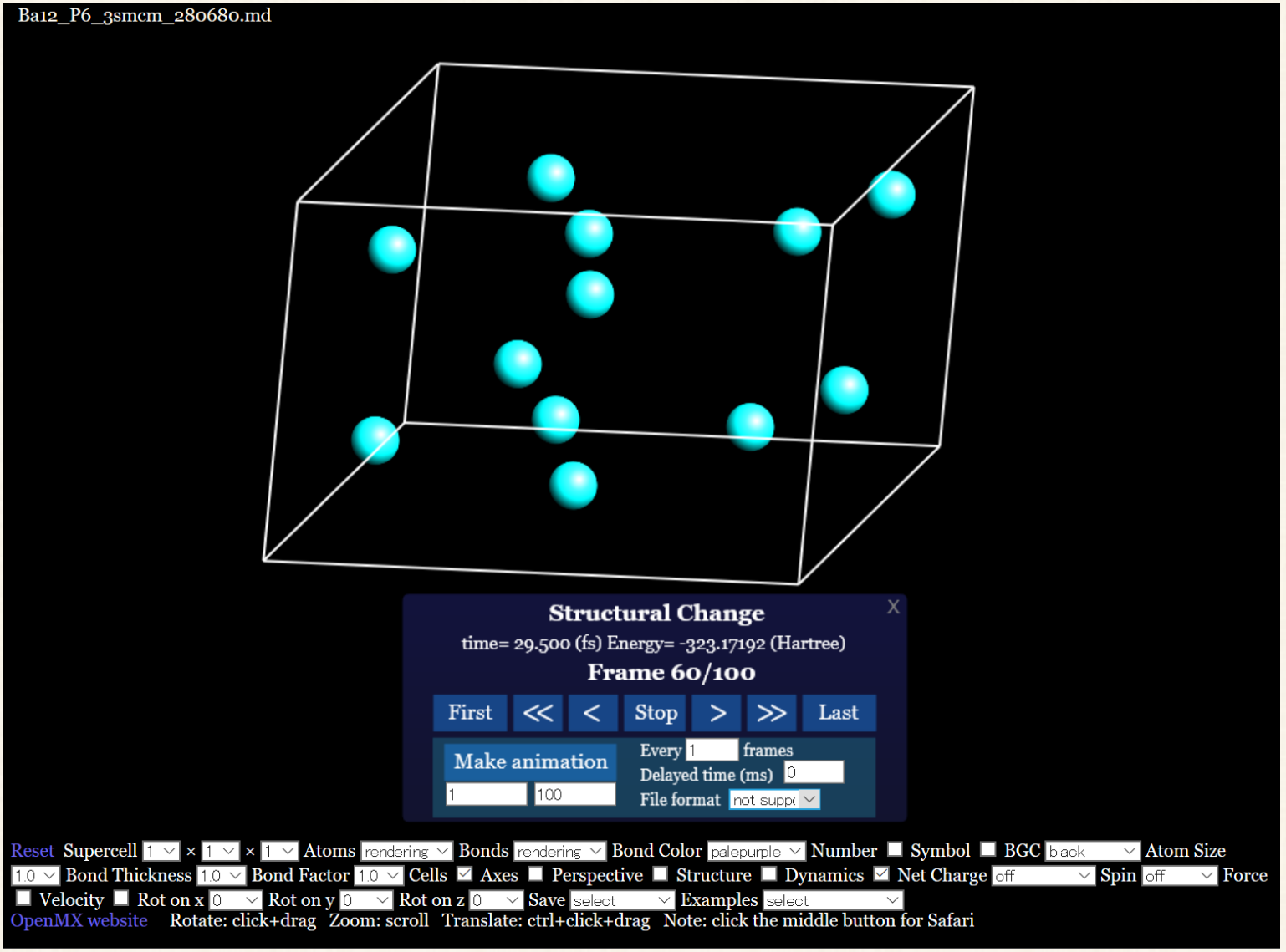
Output

Structural data for MD and optimization

XXX.md : Structure at each MD step

XXX.md2 : Final structure

OpenMX Viewer can display animation of MD.



Output

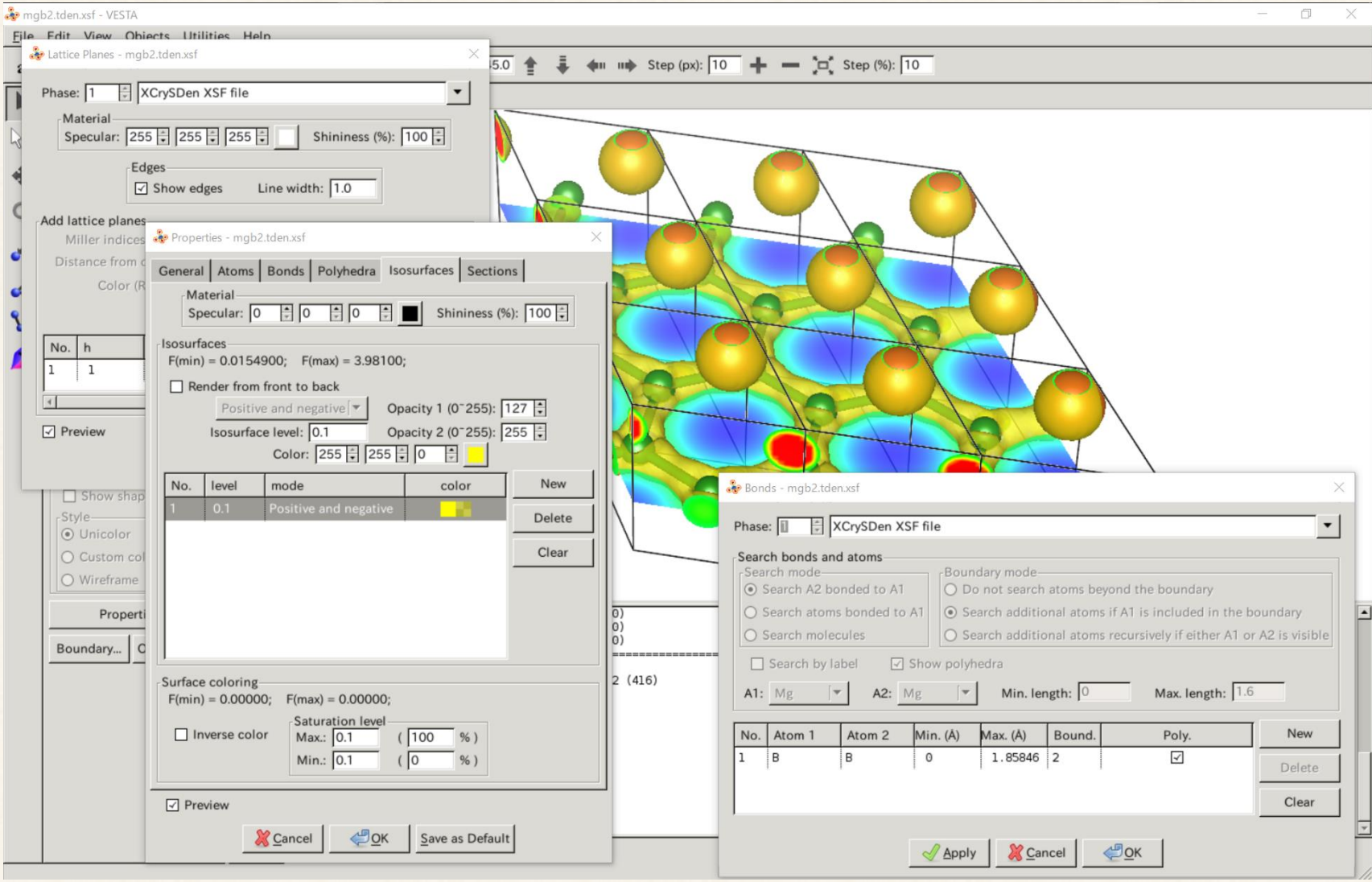
Charge density, potential

```
level.of.fileout  1
```

or

```
level.of.fileout  2
```

```
$ VESTA mgb2_tden.cube
```

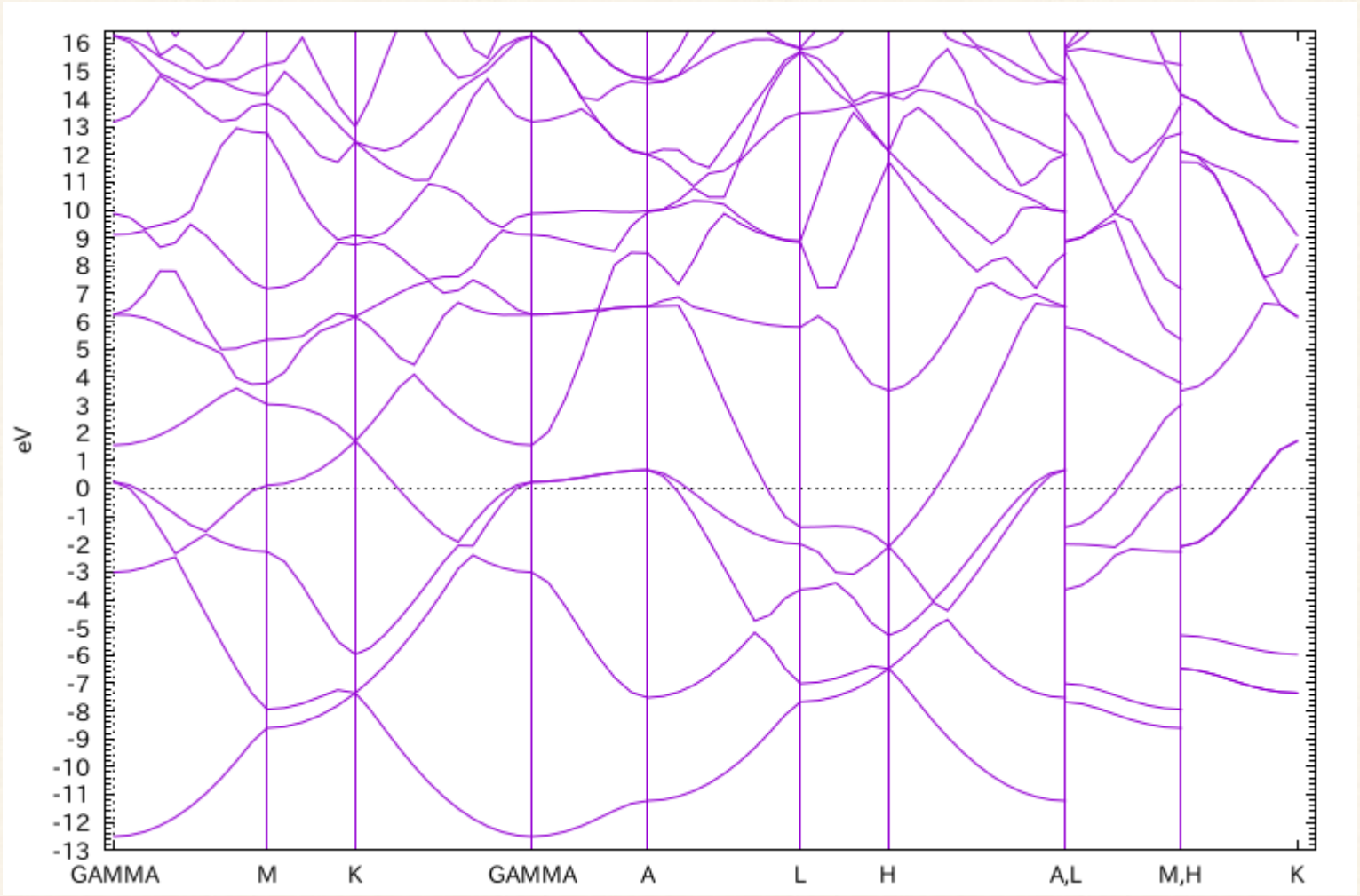


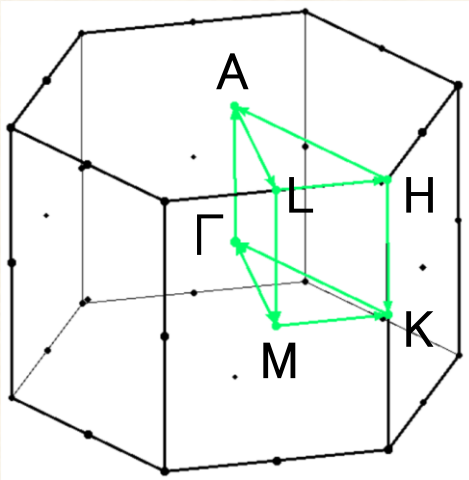
Output

Band structure

```
Band.dispersion                    on
```

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





Output

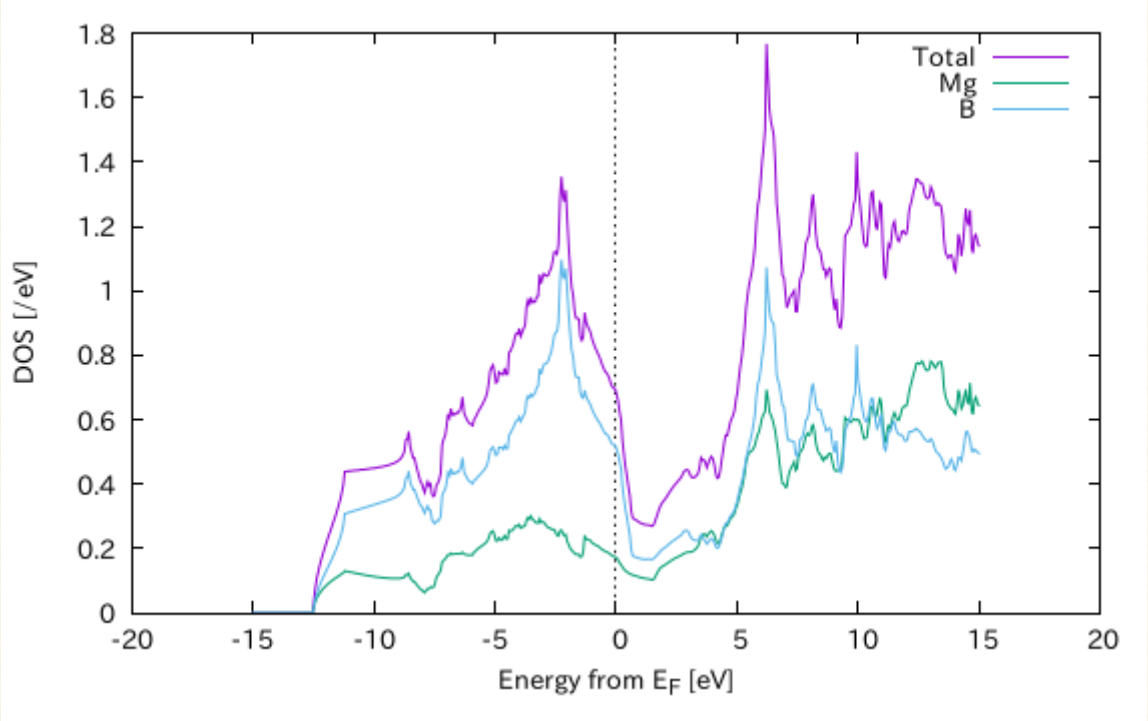
DOS and Fermi surface

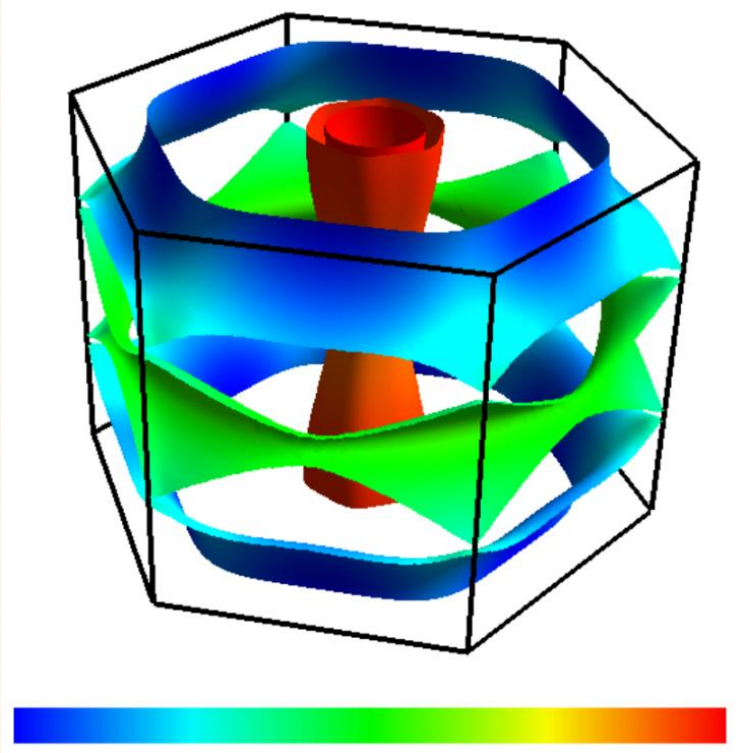
```
Dos.fileout       on
```

```
$ 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"
```



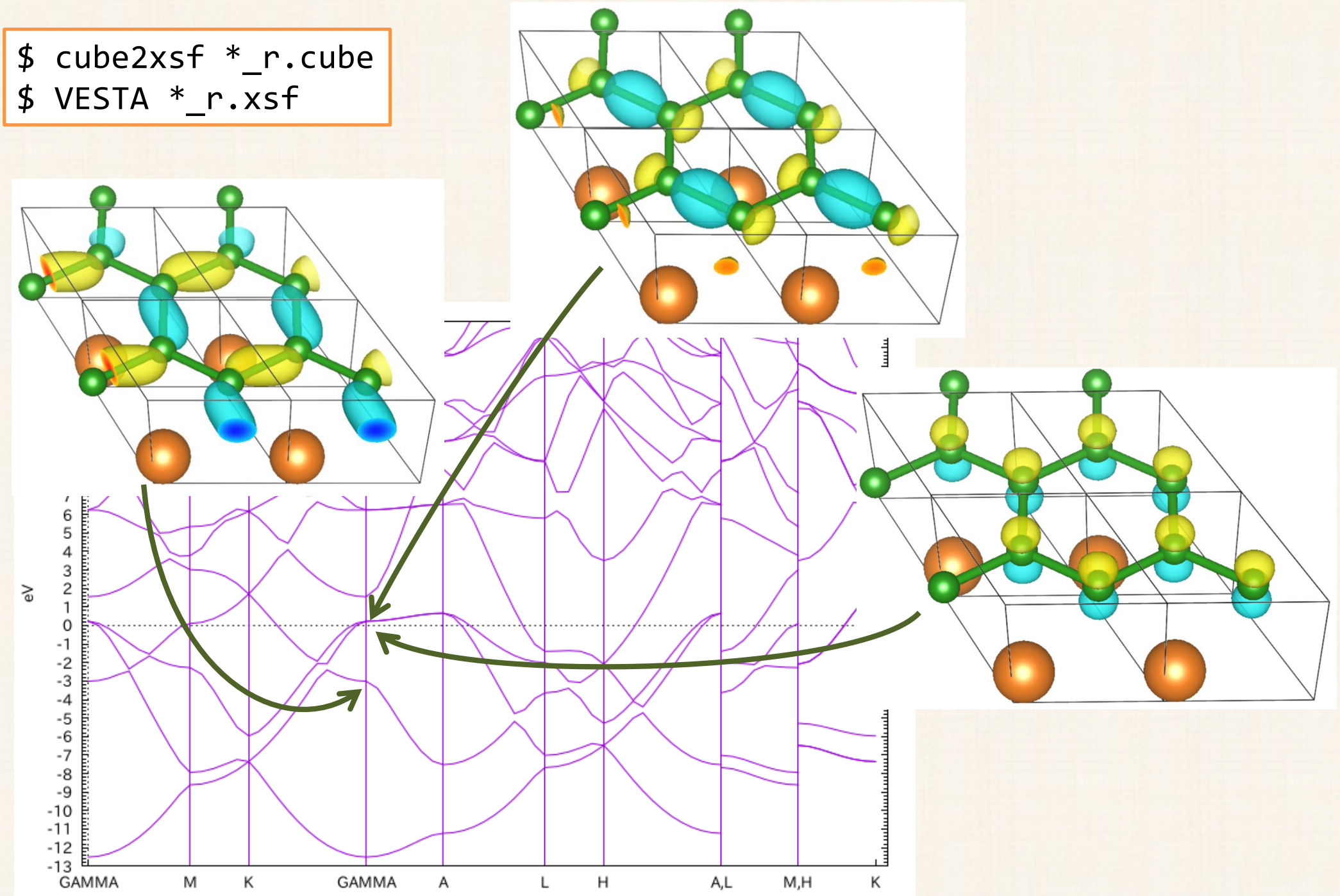


```
$ fermisurfer mgb2.FermiSurf_s0_a2.frmsf
```

Output

Kohn-Sham Bloch orbitals

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

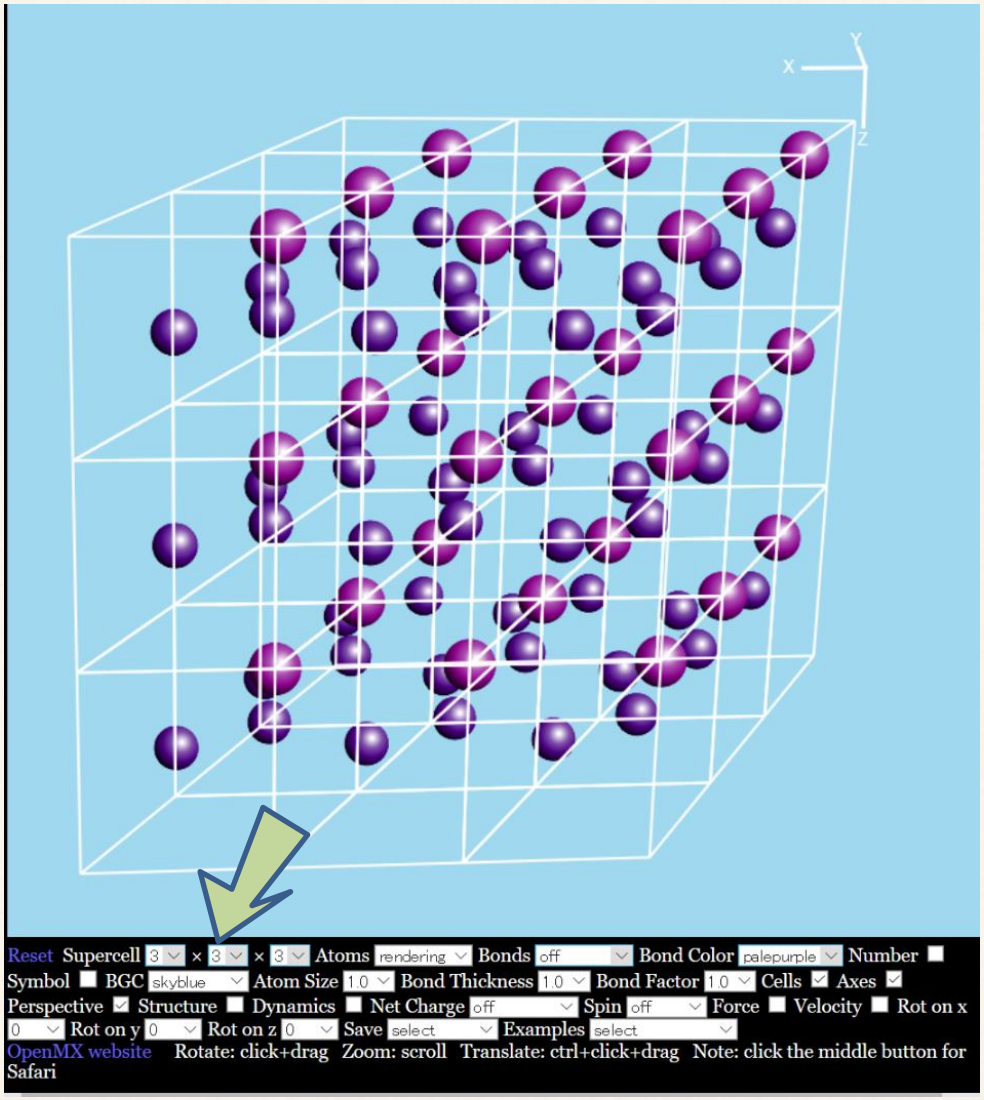


Remark

How can we construct supercell ?

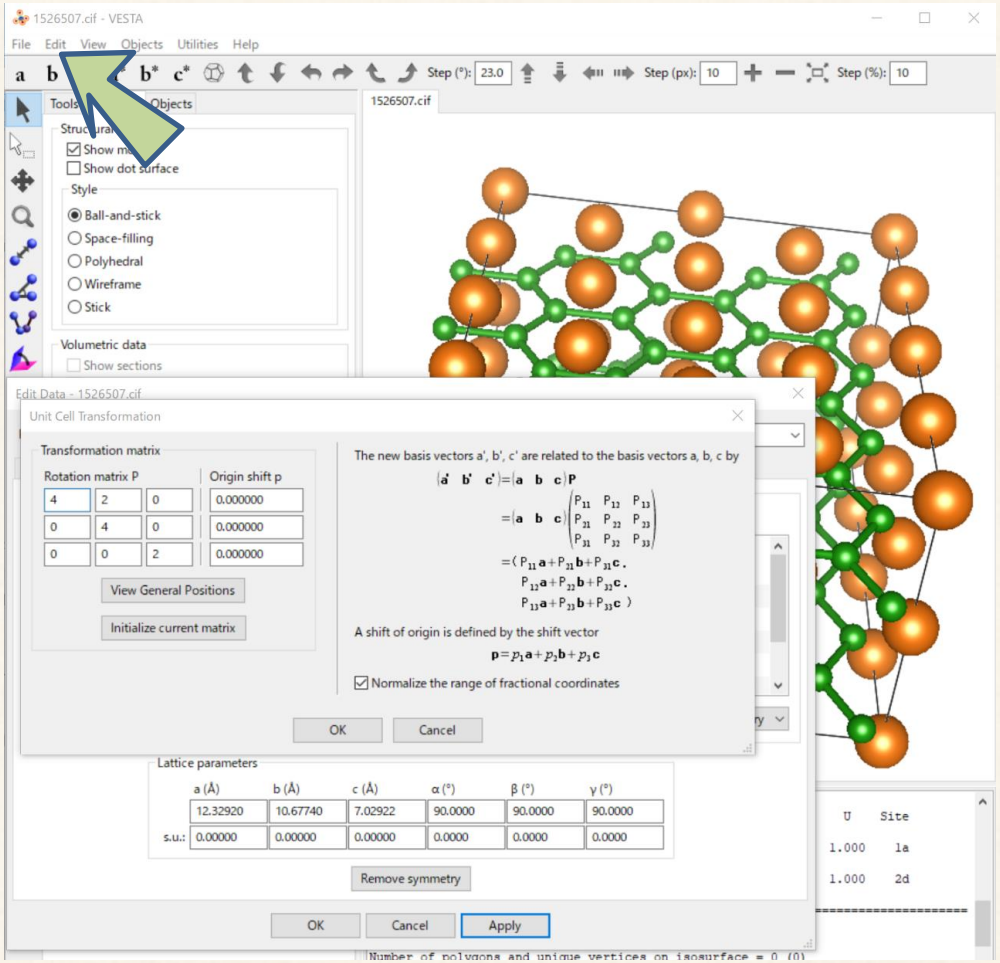
For the supercell written as $N_1 \times N_2 \times N_3$:

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

More information

Welcome to OpenMX

Open source package for Material eXplorer

Google Custom Search

- What's new
  - Patch3.9.2 to OpenMX Ver 3.9 (Feb. 11, 2020)
  - The 1st OpenMX hands-on workshop 2020 (Feb. 14, 2020)
  - Patch3.9.1 to OpenMX Ver 3.9 (Jan. 02, 2020)

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Remark

Contact, ask, discussion, bug report, ···

Known issue can be searched.

Get alert with e-mail

- What's new
  - Patch3.9.2 to OpenMX Ver 3.9 (Feb. 1
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OpenMX Forum

Google Custom Search

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

List of Threads

	Topics	Author	Replies	Views	Last Modified
⚠	From Administrator	Taisuke Ozaki	0	5769	2005/01/09 05:33 by Taisuke Ozaki
	Zeeman term in the OpenMx3.9 have problem	Umar farooq	4	51	2020/02/12 19:33 by Umar farooq
	Patch 3.9.2 to OpenMX Ver. 3.9	T. Ozaki	0	15	2020/02/11 22:44 by T. Ozaki
	installation error OpenMX ver 3.9	Maedeh	67	524	2020/02/11 19:38 by asad
	NEGF convergence making loop	Vikash	2	27	2020/02/07 01:02 by T. Ozaki
	Mailing list for the OpenMX Forum	T. Ozaki	0	42	2020/02/06 23:09 by T. Ozaki
	NEB simulation	Yuki Kamikawa	2	46	2020/01/30 21:00 by Yuki Kamikawa
	NEB memory and parallel problems	Reza	6	74	2020/01/29 00:41 by T. Ozaki
	DosMain issue in metal-graphene heterostructures	Samuel Dechamps	1	47	2020/01/25 13:51 by T. Ozaki

Summary

- We overview the typical usage of OpenMX. The following external utilities is useful to generate input file, visualize results.
  - OpenMX Viewer
  - 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.