

Hands-on introduction of OpenMX – Lecture –

Institute for Solid State Physics
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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

What is OpenMX

First-principles program package based on density functional theory with

pseudopotentials

and

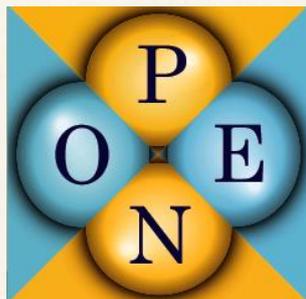
numerical local orbitals basis set

Cf. all-electrons method

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

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/>

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 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

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\${MKLRROOT}/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 file : General rule of Keywords

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

Key.Word Value

```
#
#
# Definition of Atomic Species
#
```

comment

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

Uppercase and Lowercase are not distinguished.

Keyword for path, title, IO

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

The label of output files:

abc.out, abc.md, abc.Band, ...

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.).

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 Fe5.51-s3p2d1 Fe_PBE19H
Pt Pt7.0-s3p2d2f1 Pt_PBE19H
Definition.of.Atomic.Species>
```

Basis configuration

s:2 × 1
p:2 × 3
d:1 × 5

```
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>
```

Atomic position

```
Atoms.UnitVectors.Unit Ang
<Atoms.UnitVectors
2.7235000 0.0000000 0.0000000  $\vec{a}_1$ 
0.0000000 2.7235000 0.0000000  $\vec{a}_2$ 
0.0000000 0.0000000 3.7200000  $\vec{a}_3$ 
Atoms.UnitVectors>
```

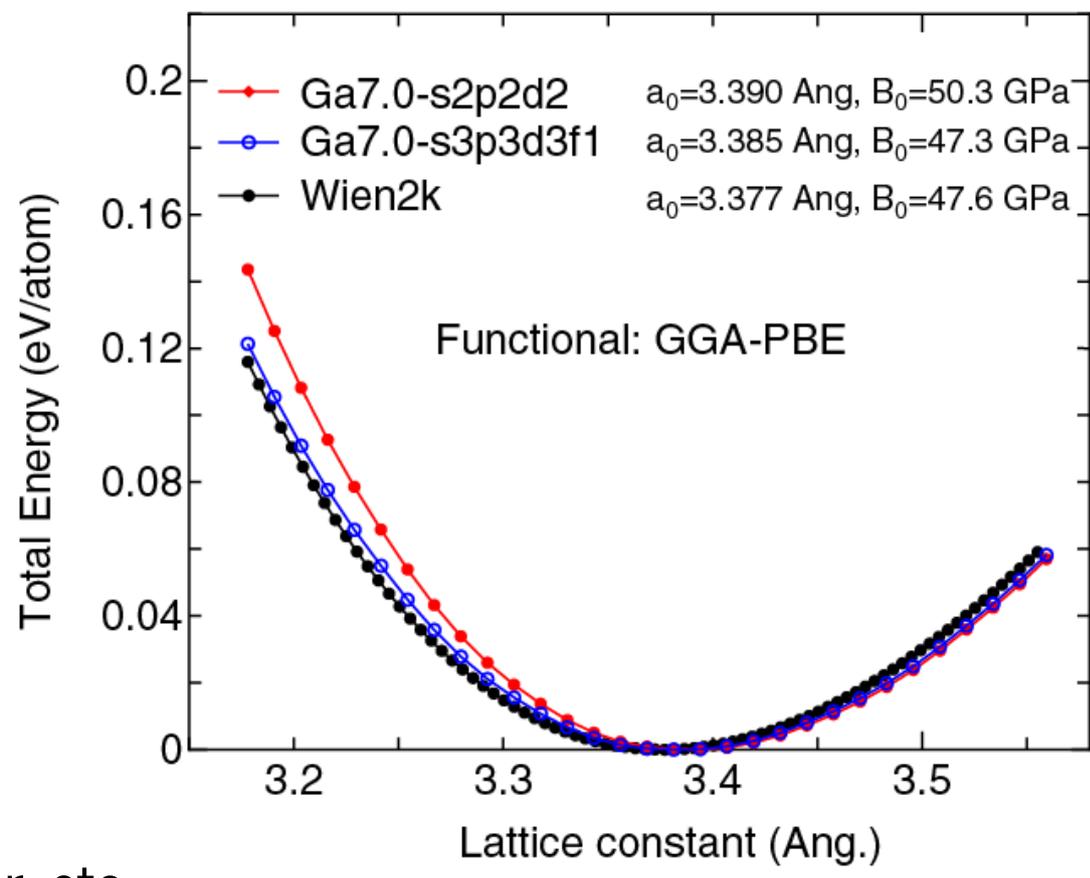
Occupation for
initial guess

How we choose basis configuration ?

- (1) Follow the configuration in literature if we reproduce it.
- (2) Suggestion in the OpenMX Web page

Welcome to OpenMX
open source package for material e

- **What's new**
 - Patch3.9.2 to OpenMX Ver 3.9 (Feb. 11, 2020)
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- **Database of VPS and PAO**
 - Ver. 2019
 - Ver. 2019 f



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

→ It will be shown in this lecture and practice.

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.

12/29 **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
```

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
```

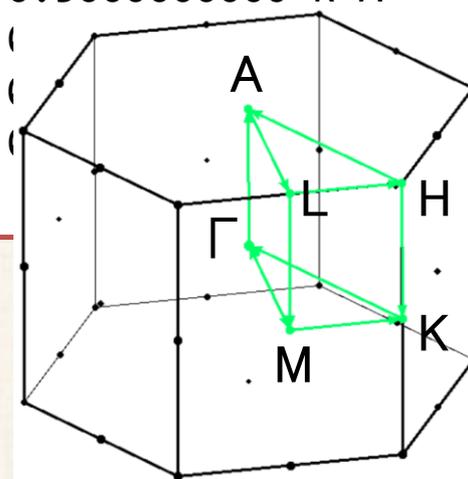
```
15 0.0000000000 0.5000000000 0.5000000000 0.5000000000 0.5000000000 0.5000000000 R A
```

```
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>
```



Keyword for post process (2)

DOS, PDOS

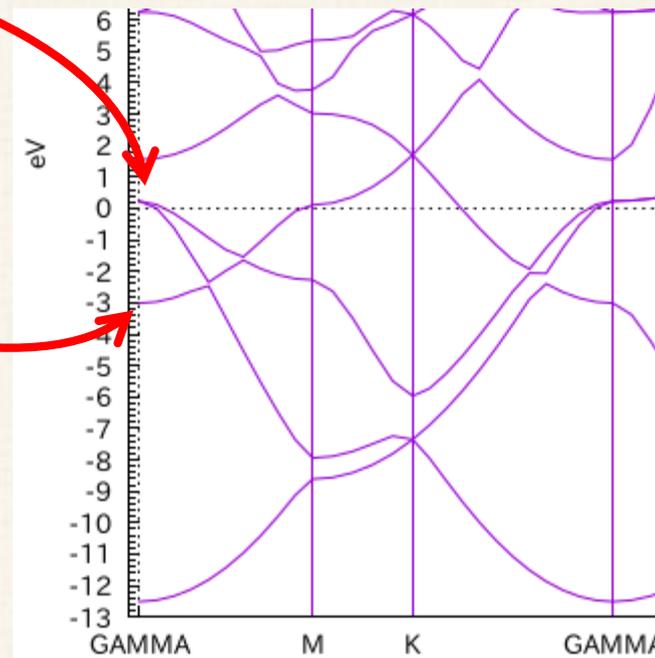
```
Dos.fileout      on
Dos.Erange      -3.0  3.0
Dos.Kgrid       28 28 20
```

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>
```



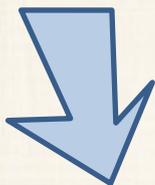
How can we generate input file ?

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

(2) Generate input file from CIF (Crystallographic 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 generator in OpenMX Viewer

The image shows a screenshot of the OpenMX Viewer web application. The browser window displays the URL `www.openmx-square.org/viewer/index.html`. The main area shows a 3D molecular model with several atoms represented as spheres (yellow and green) and bonds. A pink arrow points from a file explorer window to the model, and a blue arrow points from the model to the control panel.

A text box labeled "Drag & Drop" is positioned over the model. The file explorer window on the right shows a directory containing files such as `nscf.out`, `scf.out`, `band.gp`, `taas.cif`, `taas.xyz`, `test.xsf`, `bands.out.gnu`, `anime.gif`, `bands.out.rap`, `taas.save`, and `taas_rst`.

The control panel at the bottom includes various settings for the visualization, such as `Reset`, `Supercell`, `Atoms rendering`, `Bonds rendering`, `Bond Color`, `Atom Size`, `Bond Thickness`, `Bond Factor`, `Cells`, `Axes`, `Perspective`, `Spin`, `Force`, `Velocity`, `Rot on x`, `Rot on y`, `Rot on z`, `Save`, `OpenMX website`, `Rotate: click+drag`, `Zoom: scroll`, `Translate: ctrl+click+drag`, `Note: click`, `select`, `xyz`, `cif`, `OMX (xyz)`, `OMX (frac)`, `Number`, `Symbol`, `BGC black`, `Dynamics`, `Net Charge off`, `Examples select`, and `button for Safari`.

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

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

```

XXX.out file

Output

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

```

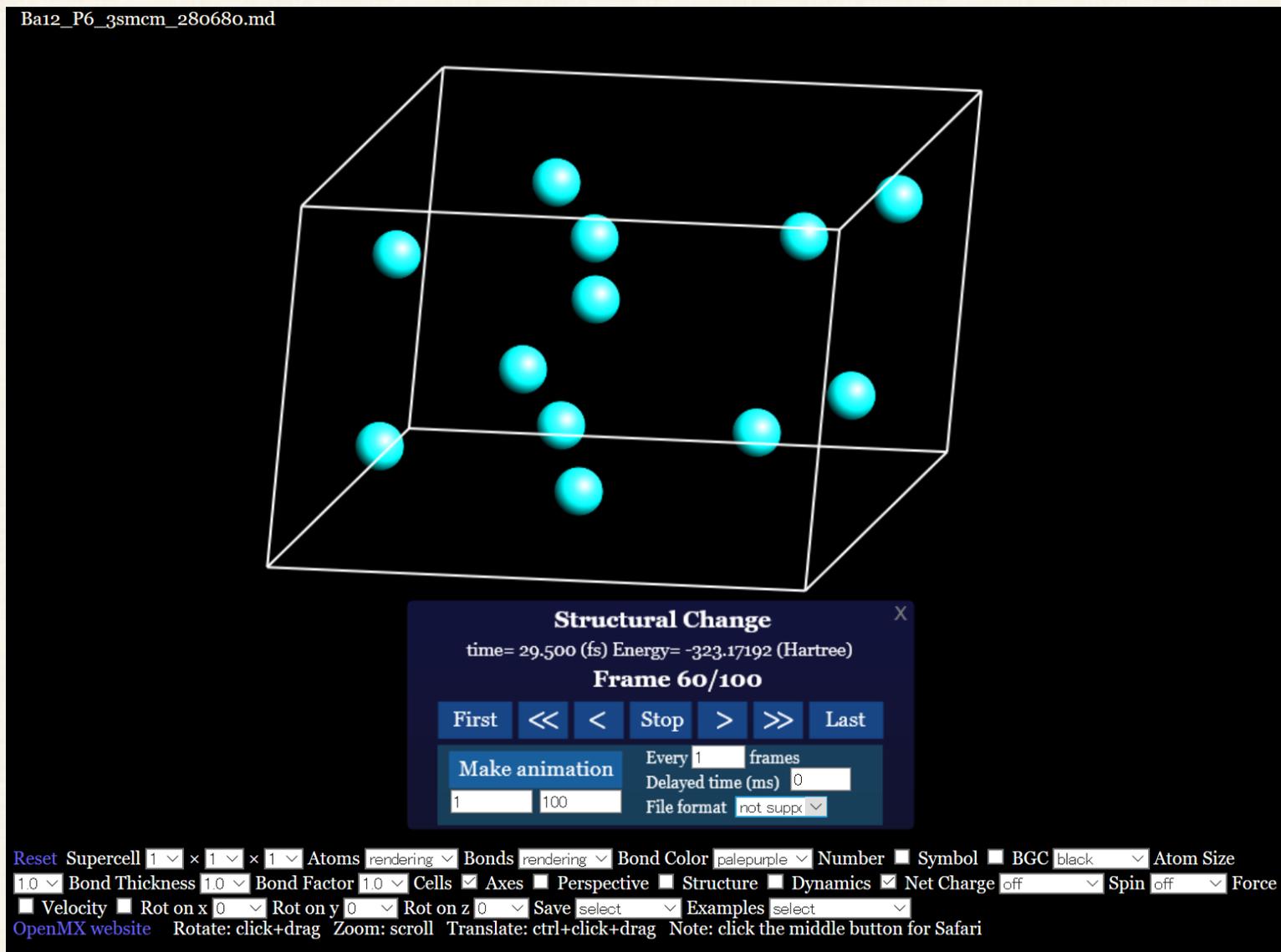
The amount of information depends on “level.of.fileout”.

Structural data for MD and optimization

XXX.md : Structure at each MD step

XXX.md2 : Final structure

OpenMX Viewer can display animation of MD.



Charge density, potential

level.of.fileout 1

or

level.of.fileout 2

\$ VESTA mgb2_tden.cube

The screenshot shows the VESTA software interface with the file 'mgb2_tden.xsf' open. The main window displays a 3D model of the crystal structure with yellow and red spheres representing atoms and a blue-to-yellow color map representing the charge density. Several dialog boxes are open, including 'Lattice Planes', 'Properties', and 'Bonds'.

Lattice Planes - mgb2_tden.xsf

Phase: 1 | XCrySDen XSF file

Material
Specular: 255 | 255 | 255 | Shininess (%): 100

Edges
 Show edges | Line width: 1.0

Properties - mgb2_tden.xsf

General | Atoms | Bonds | Polyhedra | Isosurfaces | Sections

Material
Specular: 0 | 0 | 0 | Shininess (%): 100

Isosurfaces
F(min) = 0.0154900; F(max) = 3.98100;
 Render from front to back
Positive and negative | Opacity 1 (0~255): 127
Isosurface level: 0.1 | Opacity 2 (0~255): 255
Color: 255 | 255 | 0

No.	level	mode	color
1	0.1	Positive and negative	

Surface coloring
F(min) = 0.00000; F(max) = 0.00000;
 Inverse color
Saturation level
Max.: 0.1 (100 %)
Min.: 0.1 (0 %)

Bonds - mgb2_tden.xsf

Phase: 1 | XCrySDen XSF file

Search bonds and atoms
Search mode:
 Search A2 bonded to A1
 Search atoms bonded to A1
 Search molecules
Boundary mode:
 Do not search atoms beyond the boundary
 Search additional atoms if A1 is included in the boundary
 Search additional atoms recursively if either A1 or A2 is visible

Search by label | Show polyhedra

A1: Mg | A2: Mg | Min. length: 0 | Max. length: 1.6

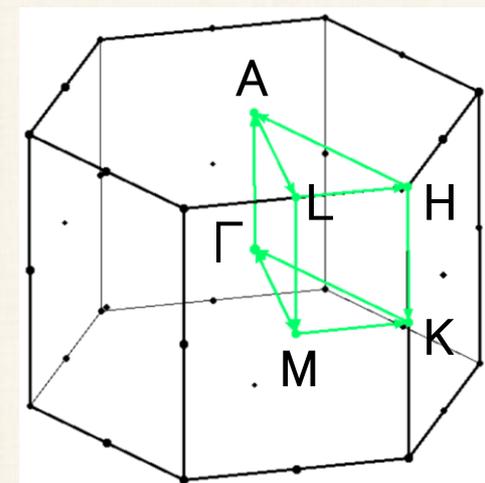
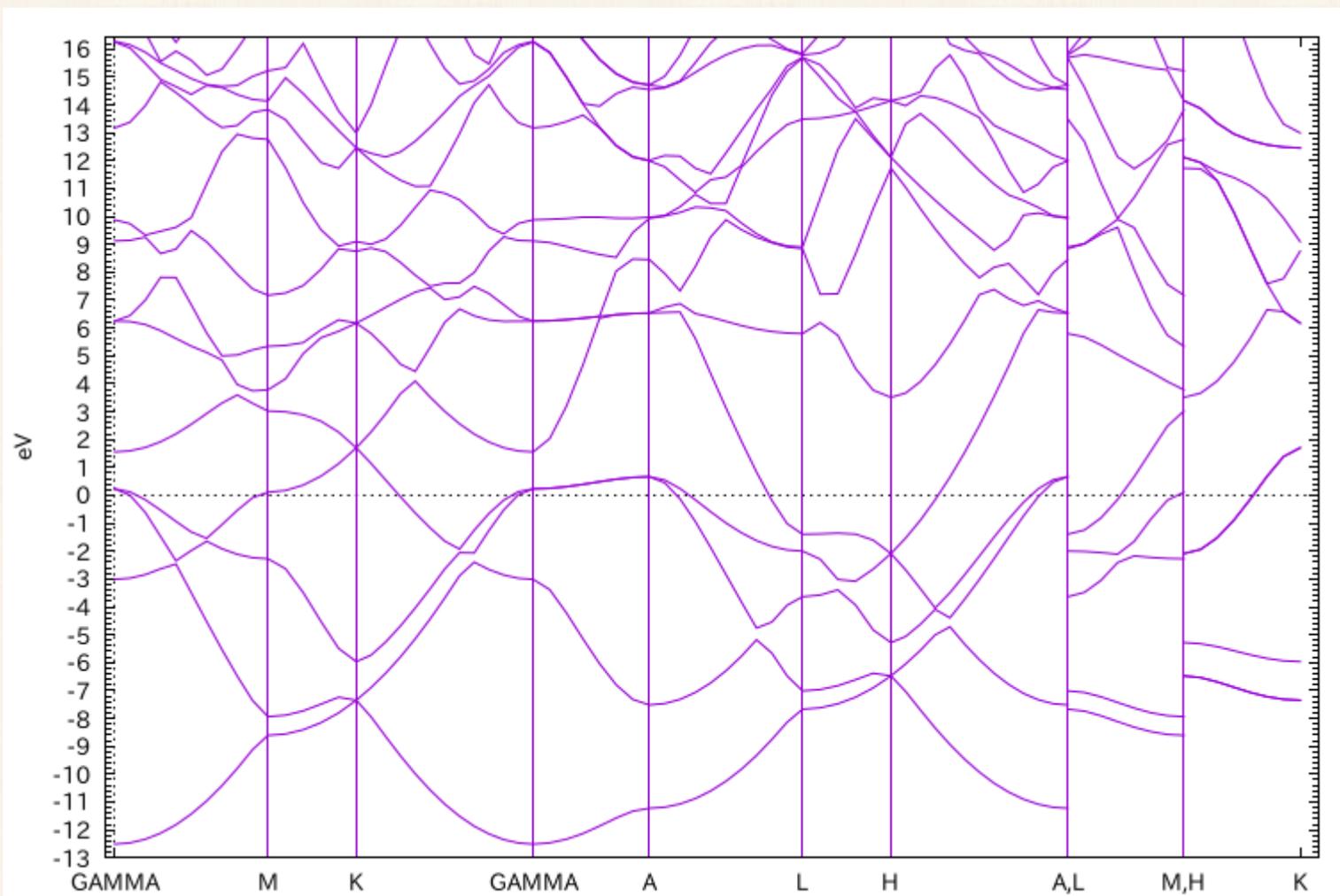
No.	Atom 1	Atom 2	Min. (Å)	Max. (Å)	Bound.	Poly.
1	B	B	0	1.85846	2	<input checked="" type="checkbox"/>

Band structure

Output

```
Band.dispersion      on
```

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



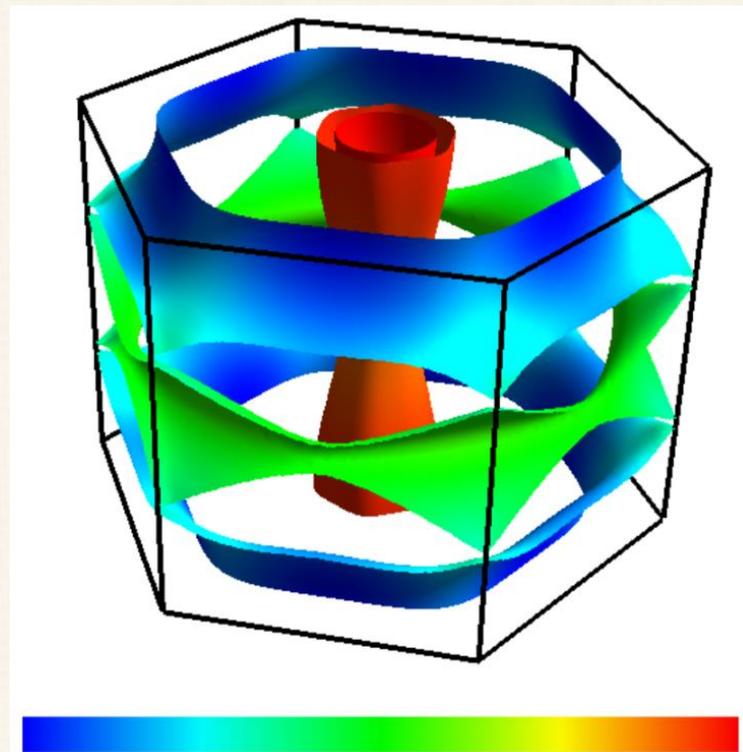
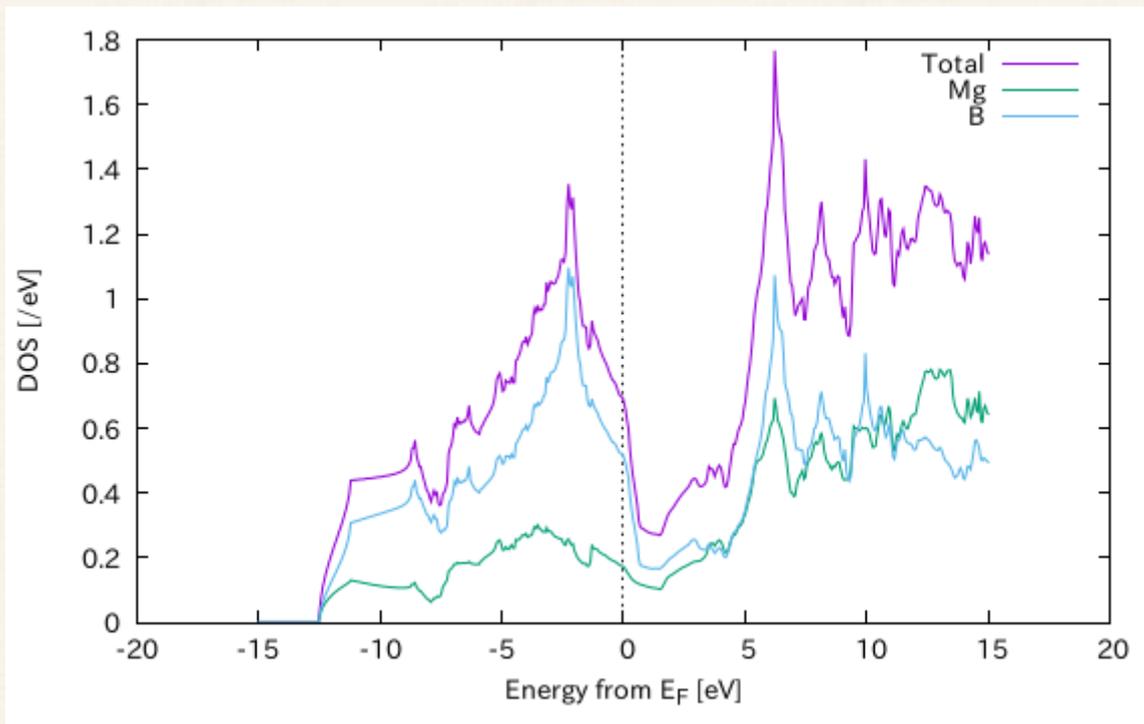
DOS and Fermi surface

```
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"
```

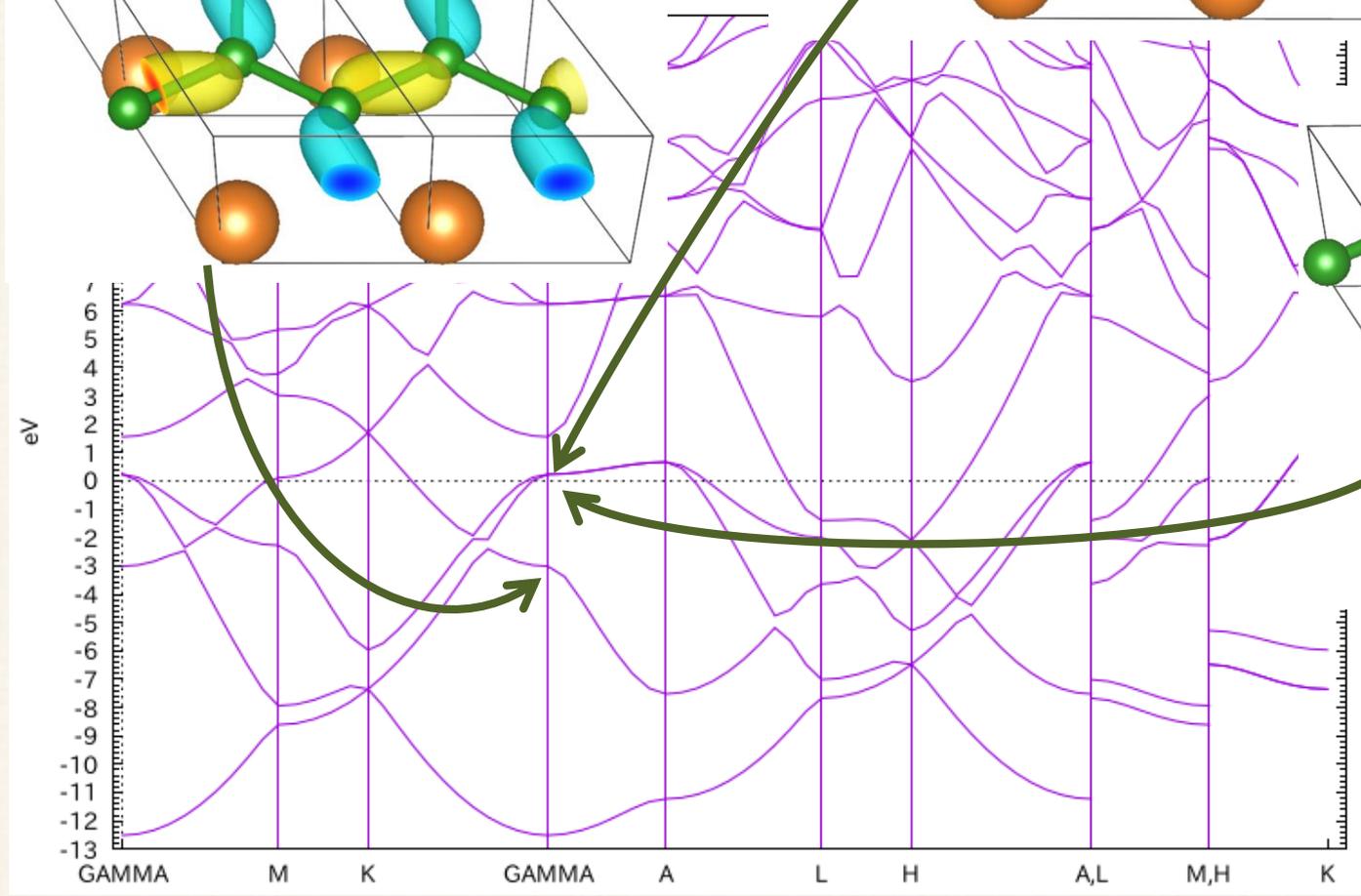
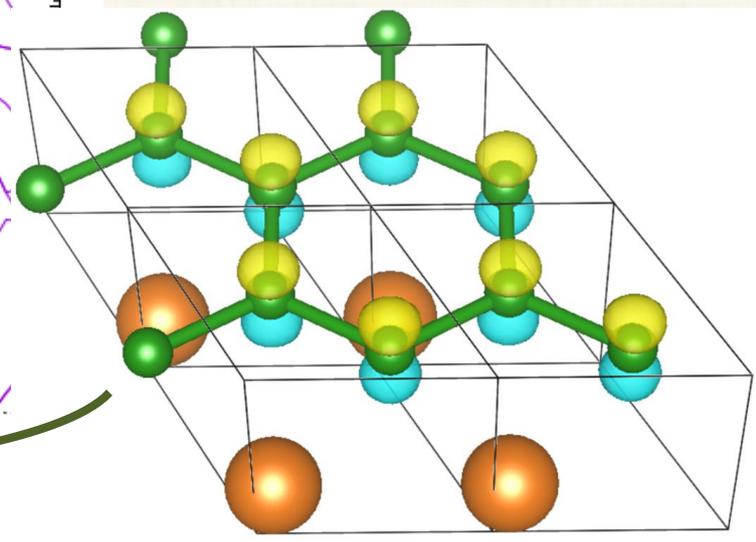
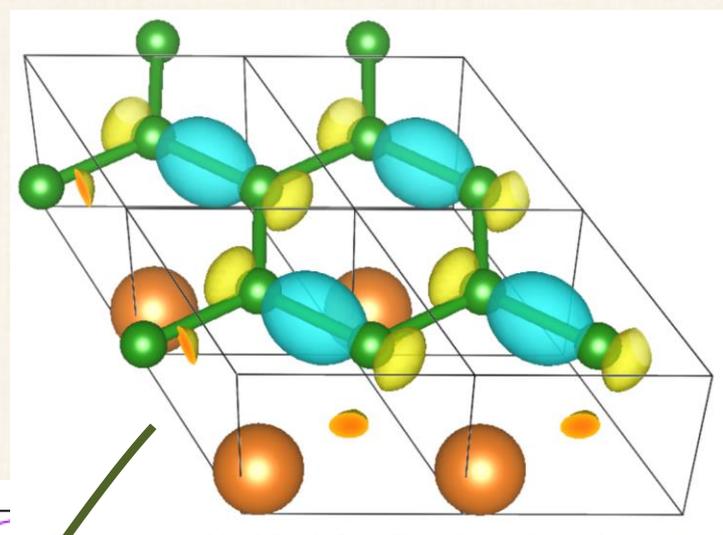
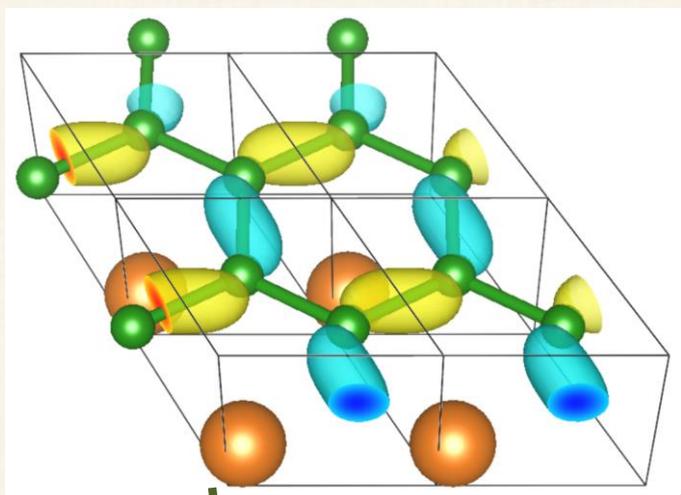


```
$ fermisurfer mgb2.FermiSurf_s0_a2.frmsf
```

Output

Kohn-Sham Bloch orbitals

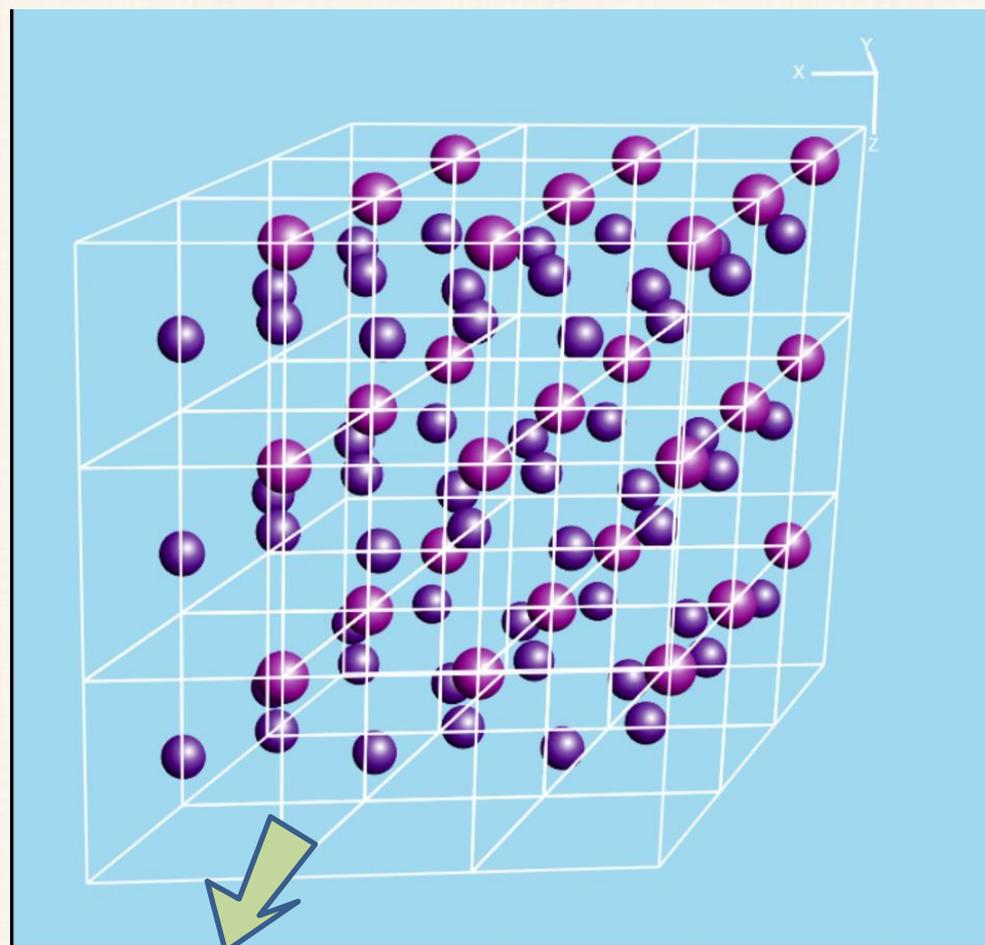
```
$ cube2xsf *_r.cube  
$ VESTA *_r.xsf
```



How can we construct supercell ?

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

OpenMX Viewer



Reset Supercell 3 x 3 x 3 Atoms rendering Bonds off Bond Color palepurple Number
 Symbol BGC skyblue Atom Size 1.0 Bond Thickness 1.0 Bond Factor 1.0 Cells Axes
 Perspective Structure Dynamics Net Charge off Spin off Force Velocity Rot on x
 0 Rot on y 0 Rot on z 0 Save select Examples select
 OpenMX website Rotate: click+drag Zoom: scroll Translate: ctrl+click+drag Note: click the middle button for Safari

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

VESTA → "Edit" → "Edit Data"

Unit Cell Transformation

Rotation matrix P

4	2	0
0	-4	0
0	0	2

Origin shift p

0.000000
0.000000
0.000000

The new basis vectors a', b', c' are related to the basis vectors a, b, c by

$$(\vec{a}' \ \vec{b}' \ \vec{c}') = (\vec{a} \ \vec{b} \ \vec{c}) P$$

$$= (\vec{a} \ \vec{b} \ \vec{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$

$$= (P_{11}\vec{a} + P_{21}\vec{b} + P_{31}\vec{c}, P_{12}\vec{a} + P_{22}\vec{b} + P_{32}\vec{c}, P_{13}\vec{a} + P_{23}\vec{b} + P_{33}\vec{c})$$

A shift of origin is defined by the shift vector

$$\vec{p} = p_1\vec{a} + p_2\vec{b} + p_3\vec{c}$$

Normalize the range of fractional coordinates

Lattice parameters

a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
12.32920	10.67740	7.02922	90.0000	90.0000	90.0000
s.u.: 0.00000	0.00000	0.00000	0.0000	0.0000	0.0000

Remove symmetry

OK Cancel Apply

Then, export CIF and read from OpenMX Viewer

More information

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. 3.9.1**

- **Technical Notes**

- **Video Lecture**

- **Publications**

- **OpenMX Forum**

- **OpenMX Viewer**

- **Workshop**

- **Database of Results**

- **Database of VPS and PAO**

- [Ver. 2019](#)

- [Ver. 2019 for core excitations](#)

- **ADPACK**

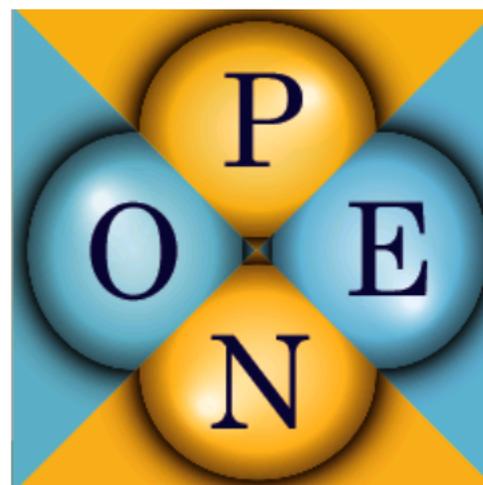
- **Miscellaneous informations**

- **Contributors**

- **Acknowledgment**

- **Opening positions**

- **Links**



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](#)

[The 1st OpenMX hands-on workshop](#)

[Patch3.9.1 to OpenMX Ver 3.9 \(Jan. 0](#)

• What is OpenMX?

• Download

• Manual of Ver. 3.9

• Manual of Ver. 3.8

• Technical Notes

• Video Lectures

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OpenMX Forum

Google Custom Search

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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”

The screenshot shows a Google search for "xming putty". The search bar contains "xming putty" and a magnifying glass icon. Below the search bar are navigation tabs: "すべて", "動画", "画像", "ショッピング", "ニュース", "もっと見る", "設定", "ツール". The search results show approximately 84,800 items found in 0.28 seconds. Several search results are highlighted with blue arrows:

- xming+puttyでのXの使い方マニュアル** (zodiac30.cse.kyutech.ac.jp/~fujiwara/setup/xming-putty/) - Arrow pointing to the title.
- PuTTY + Xming でX を使おう** (www.ep.sci.hokudai.ac.jp/~epnetfan/tebiki/server-login/xming.html) - Arrow pointing to the title.
- WindowsでPuTTYとXmingを利用して、大学外からSun, Moodleに...** (www.rc.mce.uec.ac.jp/sun_moodle/windows/putty_xming2.htm) - Arrow pointing to the title.
- 【今更感】XmingとPuttyでWindowsに最高の開発環境を作る - 波打際の...** (alfa.hatenablog.jp/entry/2016/05/19/101456) - Arrow pointing to the title.
- Installing/Configuring PuTTY and Xming** (www.geo.mtu.edu/geoschem/docs/putty_install.html) - Arrow pointing to the title.

WinSCP is also required in this case.