

Hands-on introduction of OpenMX – Practice –

Ozaki group
Mitsuaki Kawamura

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

Outline

- Introduction
- Computer in this tutorial
 - Configuration
 - Login
- Input file generation
- Job submit
- Check results
- Post processing and visualization
 - Band structure
 - Kohn–Sham orbitals
 - DOS, PDOS, Fermi surfaces
- Free excise

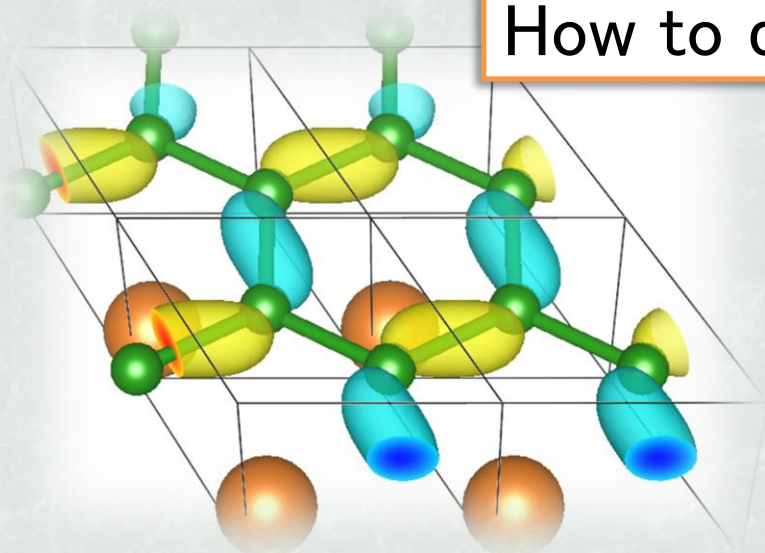
3/14 Intro Introduction : Purpose

We will overview

How to generate and modify the input file

and

How to display the result



Search results

Result: there are 2 entries in the selection

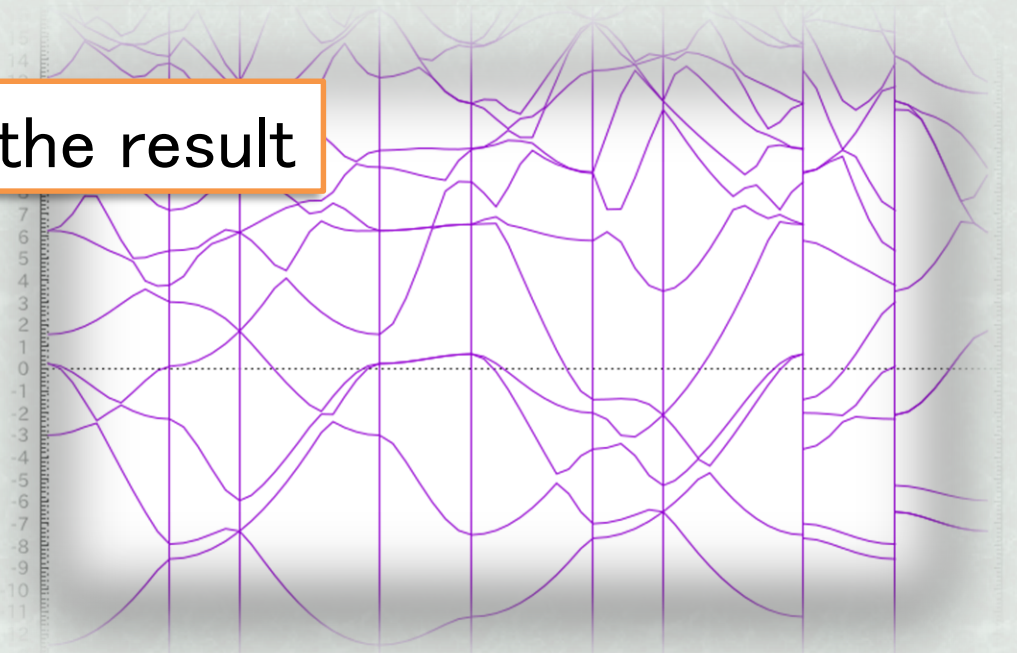
[Return to the old layout of the page](#)

Download all results as: [list of COD numbers](#) | [list of CIF URLs](#) | [data in CSV format](#) | [archive of CIF files \(ZIP\)](#)

Searching formula like 'B2 Mg'

100 200 300 500 1000 entries per page

Cell volume ▲	
90; 90; 120	J. Appl. Chem. USSR
3.0823; 3.0823; 3.51461	Jorgensen, J.D.; Hinchey, J.L. Lattice properties of MgB ₂ . <i>Physical Review B</i> 1998, 58, 10052-10055.
90; 90; 120	Physical Review B



Flow of this practice

Intro

Log-in workstation

Input file

Get CIF file from database



Convert cif to input file



View structure

SCF

Submit job for SCF



Check the result

Band structure

Modify input for band



Submit job



Plot band structure

Kohn-Sham orbital

Modify input for displaying orbital



Submit job



Plot Kohn-Sham orbital

DOS and Fermi surface

Modify input for DOS



Submit job



Interactive queue for DOS



Plot DOS and Fermi surface

Free exercise time

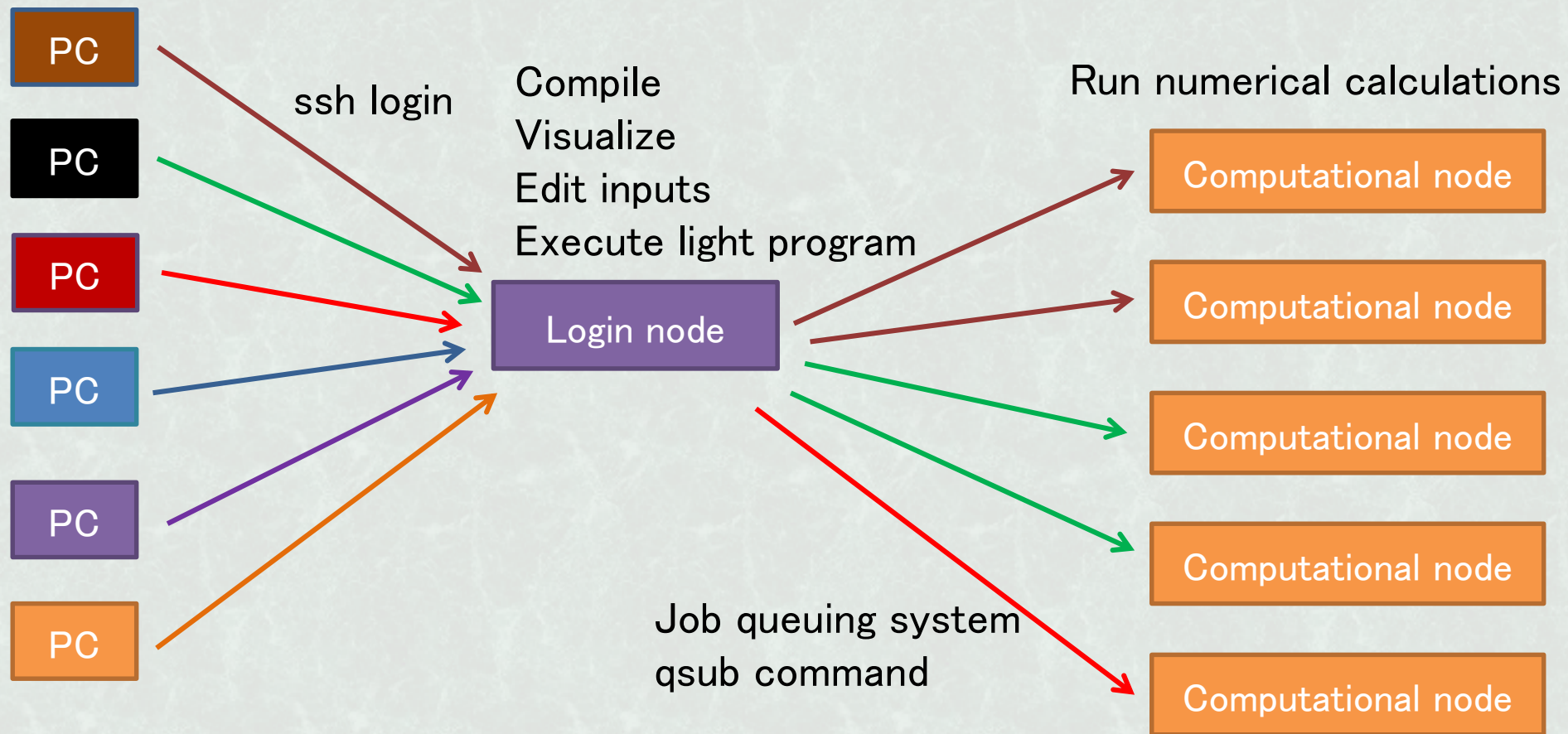
Computer for this summer school

CPU : Intel Xeon Broadwell 14cores × 2 (28 cores/node)

RAM : 64 GB / node

Compiler : Intel compiler & MKL library

Utilities : /home/public/bin/ (already added to PATH)



Login to workstation

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”

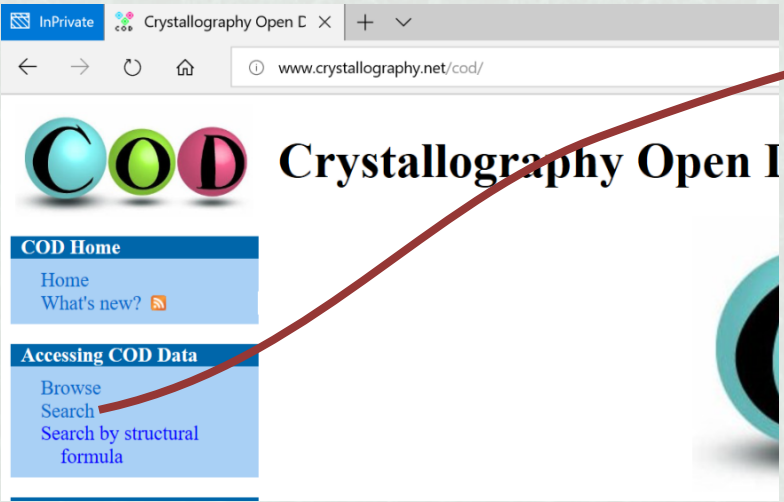
The screenshot shows a Google search for "xming putty". The search bar contains "xming putty" and a magnifying glass icon. Below the search bar are navigation tabs: "すべて", "動画", "画像", "ショッピング", "ニュース", "もっと見る", "設定", "ツール". The search results show approximately 84,800 items in 0.28 seconds. Several search 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/): Includes instructions for downloading Xming and PuTTY.
- PuTTY + Xming でX を使おう** (www.ep.sci.hokudai.ac.jp/~epnetfan/tebiki/server-login/xming.html): A guide on using Xming and PuTTY for server login.
- 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): A guide for using PuTTY and Xming to access Sun and Moodle from outside a university.
- 【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): A blog post about creating a development environment on Windows using Xming and PuTTY.
- Installing/Configuring PuTTY and Xming** (www.geo.mtu.edu/geoschem/docs/putty_install.html): A guide for installing and configuring PuTTY and Xming.

WinSCP is also required in this case.

7/14 Get CIF file from COD

Google "Crystallography Open Database"



Search

(For more information on search see the [hints and tips](#))

Search by COD ID:

[OpenBabel FastSearch:](#) Enter **SMILES:**

Note: substructure search by SMILES is currently available in a subset of COD containing 162172 structures.

text (1 or 2 words)	<input type="text"/>
journal	<input type="text"/>
year	<input type="text"/>
volume	<input type="text"/>
issue	<input type="text"/>
DOI	<input type="text"/>
Z (min, max)	<input type="text"/>
Z' (min, max)	<input type="text"/>
chemical formula (in Hill notation)	<input type="text" value="B2 Mg"/>
1 to 8 elements	<input type="text"/>
NOT these elements	<input type="text"/>
volume min and max	<input type="text"/>
number of distinct elements min and max	<input type="text"/>
filters	<input type="checkbox"/> has Fobs <input type="checkbox"/> include duplicates <input type="checkbox"/> include structures with errors <input type="checkbox"/> include theoretical structures
<input type="button" value="Reset"/>	<input type="button" value="Send"/>

Search results

Result: there are 2 entries in the selection

[Switch to the old layout of the page](#)

Download all results as: [list of COD numbers](#) | [list of CIF URLs](#) | [data in CSV format](#) | [archive of CIF files \(ZIP\)](#)

Searching formula like 'B2 Mg'

◀ First | ◀ Previous 5 | Page 1

COD ID	Links	Formula	Space Group	Cell Parameters	Volume	Reference
1000026	CIF	B2 Mg	P 6/m m m	3.085; 3.085; 3.523 90; 90; 120	29.04	J. Appl. Chem. USSR, eng
1526507	CIF	B2 Mg	P 6/m m m	3.0823; 3.0823; 3.51461 90; 90; 120	28.917	Jorgensen, J.D.; Hinks, D. Lattice properties of Mg B Physical Review, Serie 3 2245225

"Copy URL", "Copy Link", etc.

In the workstation:

```
$ wget paste-url-here
$ fixcod.sh 1000026.cif
$ cif2input.py 1000026.cif mgb2
```

→ Input file "openmx.in" is generated.

"B2 Mg" into "chemical formula"
Alphabetic order

```
$ VESTA 1000026.cif
```

Queuing system

```
$ cp /home/public/iss2018/openmx.sh .
$ qsub openmx.sh
```

MPI processes per node

```
#!/bin/sh
#PBS -l nodes=1:ppn=7
#
source ~/.bashrc
#
export OMP_NUM_THREADS=4
#
cd $PBS_O_WORKDIR
#
mpiexec -hostfile $PBS_NODEFILE /home/public/openmx openmx.in -nt $OMP_NUM_THREADS ¥
> openmx.out
```

Number of OpenMP threads

Job status

$\text{ppn} \times \text{OMP_NUM_THREADS} \leq \text{number of cores par node (28)}$

```
$ qstat -a
```

```
gauss:
```

Job ID	Username	Queue	Jobname	SessID	NDS	TSK	Req'd Memory	Req'd Time	S	Elap Time
168.gauss	kawamura	default	openmx.sh	23466	1	7	--	--	R	00:00:00

Nodes

R: Running

Q: Waiting to start

```
$ qdel job-ID
```

Stop job

Check results

```
$ less mgb2.out  
$ less openmx.out
```

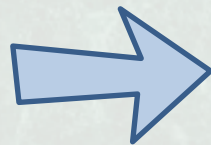
```
*****  
*****  
SCF history at MD= 1  
*****  
*****  
  
SCF=   1  NormRD=  1.000000000000  Uele= -14.025399913227  
SCF=   2  NormRD=  0.589538957582  Uele= -14.093889873889  
SCF=   3  NormRD=  0.249943571587  Uele= -14.122239227622  
      :  
SCF=  16  NormRD=  0.000350260351  Uele= -14.150623623150  
SCF=  17  NormRD=  0.000216964658  Uele= -14.150651456947  
SCF=  18  NormRD=  0.000134457940  Uele= -14.150668805936  
SCF=  19  NormRD=  0.000083360095  Uele= -14.150679594319  
SCF=  20  NormRD=  0.000051699263  Uele= -14.150686290499  
SCF=  21  NormRD=  0.000032833716  Uele= -14.150689700063  
SCF=  22  NormRD=  0.000020911680  Uele= -14.150692116404  
SCF=  23  NormRD=  0.000000083022  Uele= -14.150697139160  
SCF=  24  NormRD=  0.000000081048  Uele= -14.150697139607
```

10/14 Band structure

Edit "openmx.in" with emacs, vim, etc.

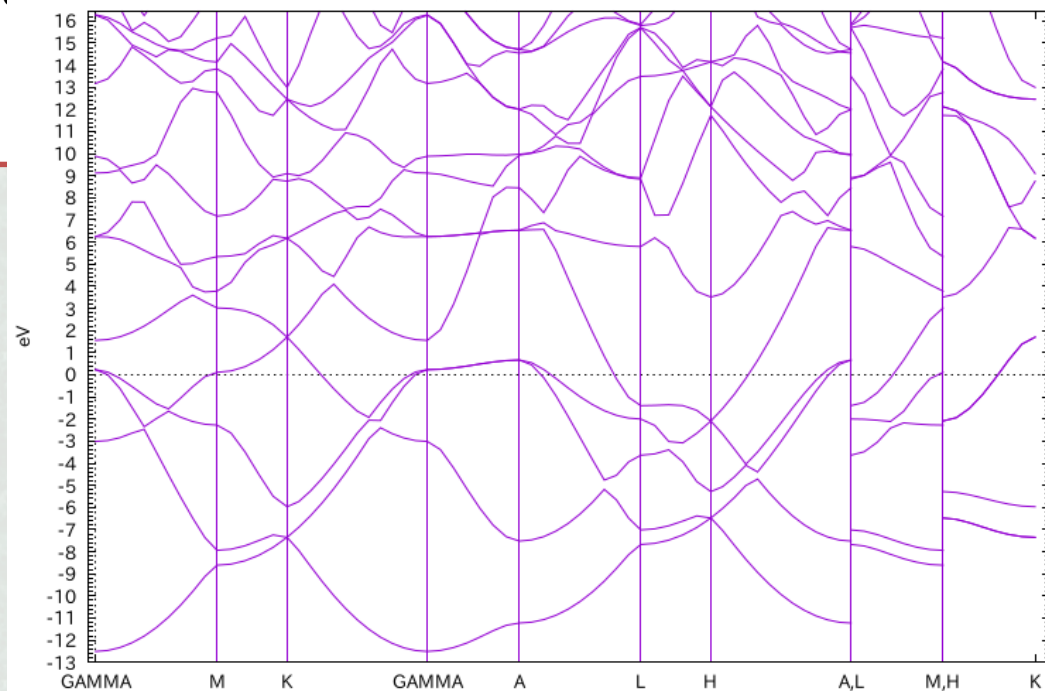
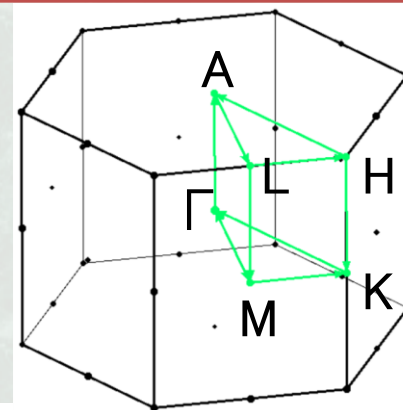
```
scf.restart      off
orbitalOpt.Force.Skip  off
Band.dispersion  off
```

Line 10
Line 100
Line 137



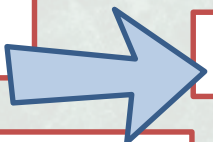
```
scf.restart      on
orbitalOpt.Force.Skip  on
Band.dispersion  on
```

```
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
8  0.333333 0.333333 0.500000 0.333333 0.333333
Band.kpath>
```

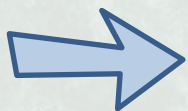


```
$ qsub openmx.sh
```

```
mgb2.Band
```



```
$ bandgnu13 mgb2.Band
```



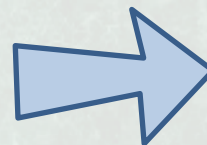
```
mgb2.GNUBAND
```

```
$ gnuplot mgb2.GNUBAND
```

Kohn-Sham orbitals

Modify openmx.in

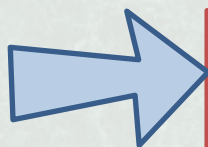
```
Band.dispersion    on   Line 137
MO.fileout        off  Line 311
num.LUMOs         1    Line 313
```



```
Band.dispersion    off
MO.fileout         on
num.LUMOs         2
```

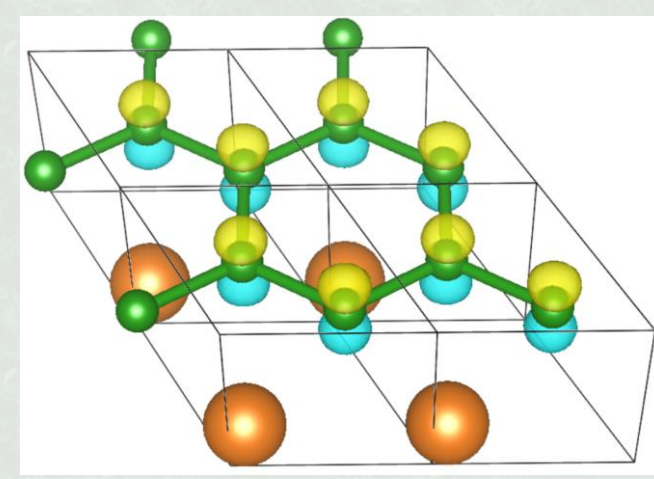
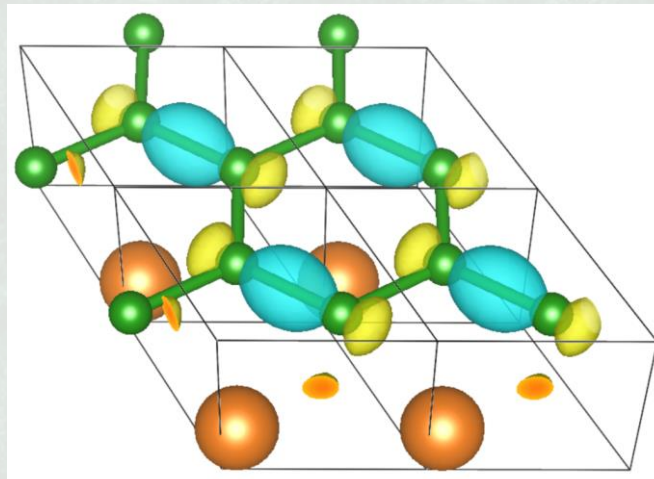
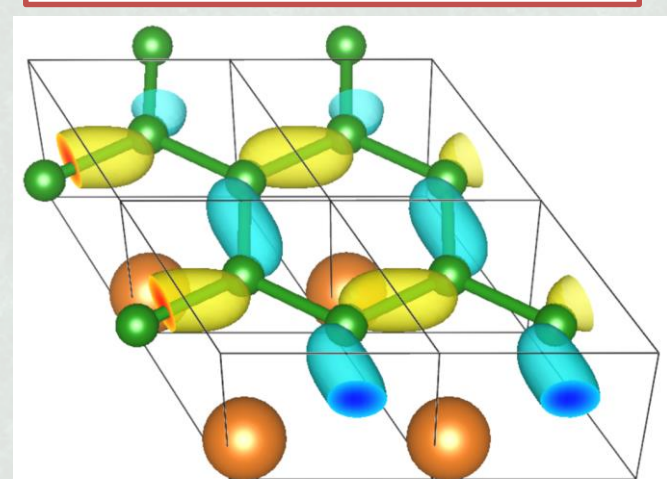
```
$ qsub openmx.sh
```

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



```
mgb2.homo0_0_0_i.cube  mgb2.lumo0_0_0_i.cube  mgb2.lumo0_0_1_i.cube
mgb2.homo0_0_0_r.cube  mgb2.lumo0_0_0_r.cube  mgb2.lumo0_0_1_r.cube
```

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



12/14 Fermi surface, DOS, PDOS (1)

```
MO.fileout      on  
DOS.fileout     off
```

```
Line 311  
Line 207
```

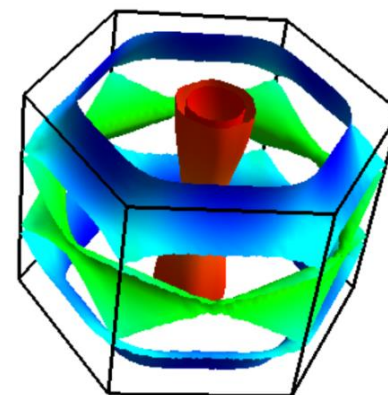
```
MO.fileout      off  
DOS.fileout     on
```

```
Dos.Erange      -20.0 20.0  
Dos.Kgrid       28 28 20
```

```
$ qsub openmx.sh
```

```
mgb2.Dos.val, mgb2.Dos.vec,  
mgb2.FermiSurf_s0_a1.frmsf,  
mgb2.FermiSurf_s0_a2.frmsf,  
mgb2.FermiSurf_s0_a3.frmsf
```

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



13/14 Fermi surface, DOS, PDOS (2)

```
[XXX@gauss] $ qsub -I
[XXX@gaussXX] $ DosMain mgb2.Dos.val mgb2.Dos.vec
:
Which method do you use?, Tetrahedron(1), Gaussian Broadening(2)
1 ↵
Do you want Dos(1) or PDos(2)?
2 ↵
Which atoms for PDOS : (1,...,3), ex 1 2
1 2 3 ↵
[XXX@gaussXX] $ exit
```

Interactive queue

```
$ gnuplot
```

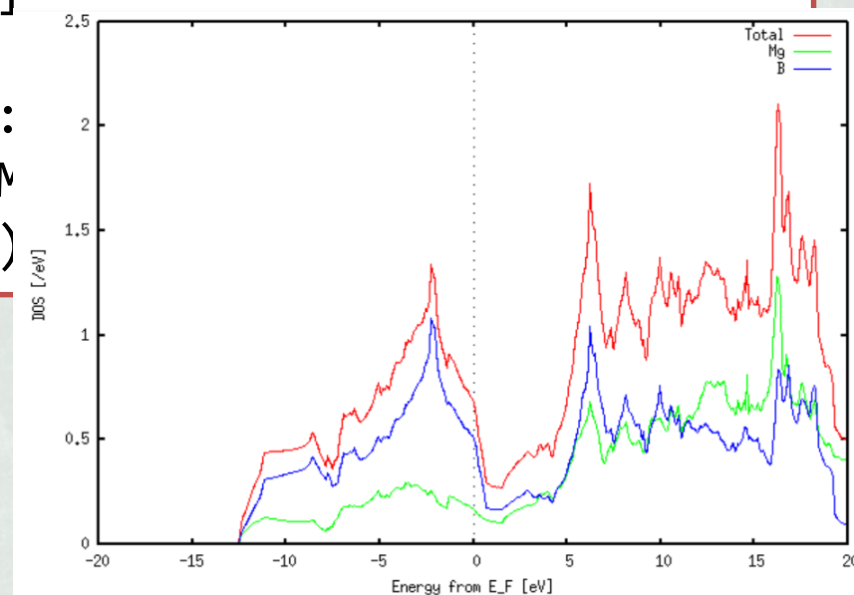
```
gnuplot> set yzeroaxis
```

```
gnuplot> set xlabel "Energy from E_F [eV]"
```

```
gnuplot> set ylabel "DOS [/eV]"
```

```
gnuplot> plot "mgb2.DOS.Tetrahedron" u 1:
"mgb2.PDOS.Tetrahedron.atom1" w l tit "M"
"mgb2.PDOS.Tetrahedron.atom2" u 1:($2*2)
```

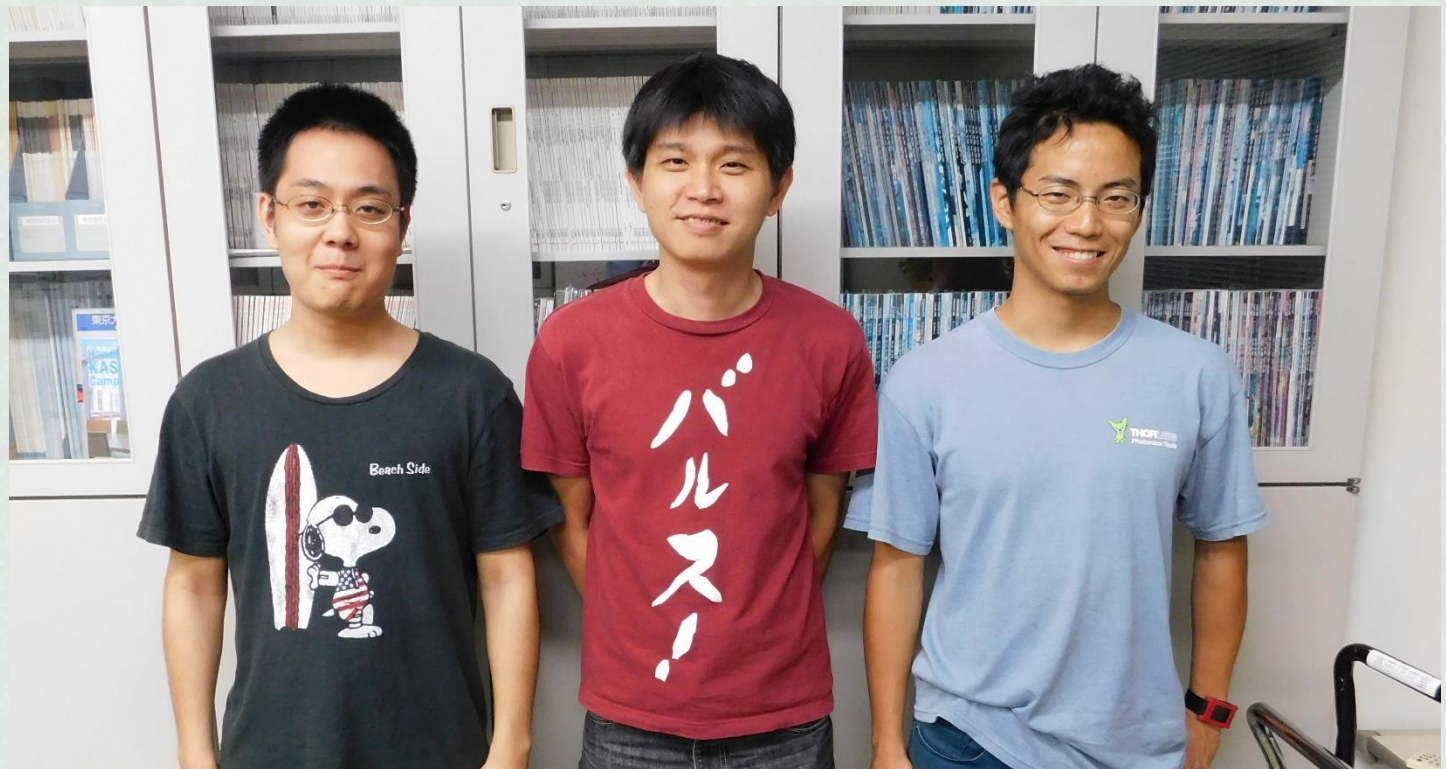
As well as DOS



Free exercise time

- Compute other materials from COD database. Explain the result of band structure, PDOS, Fermisurface.
- Install the following visualization tools into your own PC.
 - VESTA
 - XCrysDen
 - FermiSurfer
- Try other functions of OpenMX (Wannier function, etc.).
- Etc.

Tutors



Masahiro Fukuda

Yung-Ting Lee

Mitsuaki Kawamura