ecalj tutorial: Get started

Here we explain DFT/QSGW calculations with ecalj. Then we explain how to make band plots.
Further functionalities in ecalj listed at

To install ecalj, look into install. Then go to following steps.

This may give some help Qiita Japanese, but most of all are here.

Overview of QSGW calculation

- band calculations calculations (LDA level) are performed with the program `lmf`. The initial setting file is `ctrl.foobar` (`foobar` is user-defined). Before running `lmf`, it is necessary to run `lmfa`, which is a spherically symmetric atom calculation to determine the initial conditions for the electron density (`lmfa` finishes instantaneously).

- A file `sigm.foobar` is the key for QSGW calculations. The file `sigm.foobar` contains the non-local potential $V_{\rm xc}^{\rm QSGW}-V_{\rm xc}^{\rm LDA}$. By adding this potential term to the usual LDA calculation performed by `lmf`, we can perform QSGW calculations.

- Thus the problem is how to generate $V_{\rm xc}^{\rm QSGW}({\bf r},{\bf r}')$. This is calculated from the self-energy $\Sigma({\bf r},{\bf r}',\omega)$, which is calculated in the GW approximation. Roughly speaking, we obtain $V_{\rm xc}^{\rm QSGW}({\bf r},{\bf r}')$ with removing the omega-dependence in $\Sigma({\bf r},{\bf r}',\omega)$.

- Therefore, the calculation of $V_{\rm xc}^{\rm QSGW}$ is the major part of the QSGW cycle , and is calculated in a double-structure loop. That is, there is an inner loop of `lmf`, and an outer loop to calculates $V_{\rm xc}^{\rm QSGW}$ using the eigenfunctions given by `lmf`. This outer loop can be executed with a python script called gwsc (which runs fortran programs). The computational time for QSGW is much longer than that of LDA calculation. As a guideline, it takes about 10 hours for 20 atoms (depending on the number of electrons). See https://arxiv.org/abs/2506.03477

- We have GPU acceleration for QSGW, https://arxiv.org/abs/2506.03477. Thus we can handle large systems. With 4 GPU, we can compute systems with 40 atoms per cell with surfaces.

- We intend to perform calculations **without parameter settings by hands**.
  Thus I think ecalj is one of the easiest code to perform GW for users. See band database in QSGW at
  https://github.com/tkotani/DOSnpSupplement/blob/main/bandpng.md
  (this is supplement of https://arxiv.org/abs/2507.19189). This is away from complete one, but showing the abity of ecalj.

Install

install

Steps to perform QSGW in ecalj

For simplicity, we explain paramagetic cases, no 4f without SO at first.

0. POSCAR

We first need POSCAR (crystal structure in VASP format).
You can find samples of POSCAR in ecalj/ecalj_auto/INPUT/testSGA/POSCARALL as

```
cd ecalj
mkdir TEST
cd TEST
mkdir test1
mkdir test2
cat ecalj_auto/INPUT/testSGA/joblist.bk
cp ../ecalj_auto/INPUT/testSGA/POSCARALL/POSCAR.mp-2534 test1
cp ../ecalj_auto/INPUT/testSGA/POSCARALL/POSCAR.mp-8062 test2
```

For example, POSCAR of mp-2534 GaAs is given as:

```
Ga1 As1
1.0
   3.5212530000000002    0.0000000000000000    2.0329969999999999
   1.1737510000000000    3.3198690000000002    2.0329969999999999
   0.0000000000000000    0.0000000000000000    4.0659929999999997
Ga As
1 1
direct
   0.0000000000000000    0.0000000000000000    0.0000000000000000 Ga
   0.2500000000000000    0.2500000000000000    0.2500000000000000 As
```

This is another POSCAR for ba2pdo2cl2:

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```
POSCAR_ba2pdo2cl2
1.0
-2.06443 2.06443 8.40383
2.06443 -2.06443 8.40383
2.06443 2.06443 -8.40383
Ba Pd O Cl
2 1 2 2
Cartesian
0.0 0.0 6.5153213224
0.0 0.0 10.2923386776
0.0 0.0 0.0
0.0 2.06443 0.0
2.06443 0.0 0.0
0.0 0.0 3.1625293056
0.0 0.0 13.6451306944
```

If you have cif and like to convert it to `POSCAR`, do
`cif2cell foobar.cif -p vasp --vasp-cartesian --vasp-format=5`.

Step 1. convert POSCAR to ctrls file

Then we convert POSCAR to ctrls by vasp2ctrl.
ctrls is the structure file used in ecalj.

```
vasp2ctrl POSCAR.mp-2534
mv ctrls.POSCAR.mp-2534.vasp2ctrl ctrls.POSCAR.mp-2534
cat ctrls.mp-2534
```

ctrls.mp-2534 contains crystal structure equivalent to POSCAR:

```
cat ctrls.mp-2534
STRUC
     ALAT=1.8897268777743552
     PLAT=      3.52125300000       0.00000000000       2.03299700000
                1.17375100000       3.31986900000       2.03299700000
                0.00000000000       0.00000000000       4.06599300000
  NBAS=2
SITE
     ATOM=Ga POS=     0.00000000000       0.00000000000
0.00000000000
     ATOM=As POS=     1.17375100000       0.82996725000
2.03299675000
```

- MEMO:
    - ctrl2vasp ctrl.mp-2534 can convert back to VASP file. Check this by VESTA. We can use viewvesta (convert and invoke VESTA).
    - many unused files are generated (forget them).

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Step 2. Get ctrl from ctrls

ctrl is a basis input file for ecalj. We generate template of ctrl by ctrlgenM1.py.
Minimum explanations are embedded in the generated ctrl file.
Number of k points (nk1 nk2 nk3), APW cutoff (pwemax), nspin, so(spin orbit switch) are only what we need to tweak usually.

When we run lmf, we can add command line option such as -vnspin=2. Then const foobar=1 defined in the ctrl file is overridden (referred with {foobar}). save.* file show which -vfoobar you used.

It is possible to enforce symmetry, antiferro symmetry.

We only need ctrl file in the following calculations (while some tmp* kinds of files are generated).

```
ctrlgenM1.py mp-2534
cp ctrlgenM1.ctrl.mp-2534 ctrl.mp-2534
```

Edit `ctrl.foobar` if necessary. Explanations are embedded in ctrl.foobar (please let me know wrong descriptions). Possible points to rewrite in ctrl.foobar:

1. Number of k points (nk1,nk2,nk3).
2. nsp=2 if magnetic
3. SpinOrbitCoupling: so=0 (none), so=1 (LdotS), 2 (LzSz). nsp=2 is required for so=1,2. so=1 does not yet support QSGW. SOC axis can also be freely selected, but currently (0,0,1) default and (1,1,0) are supported (m_augmbl.f90). If you want to set SO=1 in QSGW, currently, run QSGW calculation with so=0 or so=2 to obtain ssig file, then set so=1
4. xcfun (choice of LDA exchange correlation term). Only =1:BH, =2:VWN, =103:PBE-GGA.
5. LDA+U settings (not explained yet).
6. ssig=1.0 (If you choose QSGW80, use ssig=0.8. Effective for QSGW calculations. $V^{\rm xc QSGW}-V^{\rm xc LDA}$ is stored in a file `sigm.foobar`. We add ssig $\times (V^{\rm xc QSGW}-V^{\rm xc LDA})$ to the potential in the lmf calculation as long as `sigm.foobar` file is available.

- `lmchk --pr60 foobar` allows you to check the recognized symmetries by `lmf`. Turning off --pr60 or reducing 60 will reduce the verbosity of output.

At this point, you can visually check the following check files.

- SiteInfo.chk
  MT radius Atomic positions
- PlatQlat.chk
  Primitive lattice vector (plat) Primitive reciprocal lattice vector (qlat)

Here we explain details of ctrl file.

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Hereafter, we only use `ctrl.foobar` (`ctrls.foobar` is used hereafter.). We can delete temporary files.

Step 3. LDA calculation

1. Run lmfa at first. It is for spherical atomic electron densities, contained in the crystals. lmfa ends instantaneously.

   ```
   lmfa ctrl.mp-2534
   ```

   gives spherical atom calculation for initialization.`lmfa` calculates spherically symmetric atoms and generates the files required for lmf below.
   Check `conf` section in the console output as

```
lmfa ctrl.mp-2534 |grep conf
```

. This shows atomic configuration (there are no side effects even if `lmfa` is repeated). The initial condition of electron density for lmf is given as the superposition of spherically symmetric atomic densities given by lmfa. In addition, lmfa calculations are performed with the logarithmic derivative of the radial wave function at the MT sphere edge fixed (READP True in default ctrlgenM1.py setting). The derivatives are contained in `atmpnu.*` files. So, `atmpnu.*` are needed for `lmf`.

2. After `lmfa`, we run LDA calculation as:

```
mpirun -np 8 lmf mp-2534 |tee llmf
```

   - mp-2534 (GaAs) gives 5.75 $\AA$ for GaAs, while the experimental value is 5.65$\AA$.
   - llmf contains information of iterations, check eigenvalue and fermi energies, band gap.
   - rst.mp-2534 is generated. Self-consistent charge included.
   - You can change lattice constant as ALAT=1.8897268777743552*5.65/5.75 in ctrl file. simple math operators such as `* + - / **` can be possible in ctrl.
   - Note: ctrlp is intermediate file generated by python from ctrl. Fortran calls a python code internally.(ctrl2ctrlp.py is responsible for the math)
   - check save.mp-2534. Show history of lmfa and lmf. one line per iteration. Show your console options. c,x,i,h
LDA energy shown two values need to be the same (but slight difference).
Repeat lmf stops with two iteration.
   - SiteInfo.lmchk : Site infor
   - PlatQlat.chk : Lattice info
   - estaticpot.dat : electrostatic potential of smooth part.

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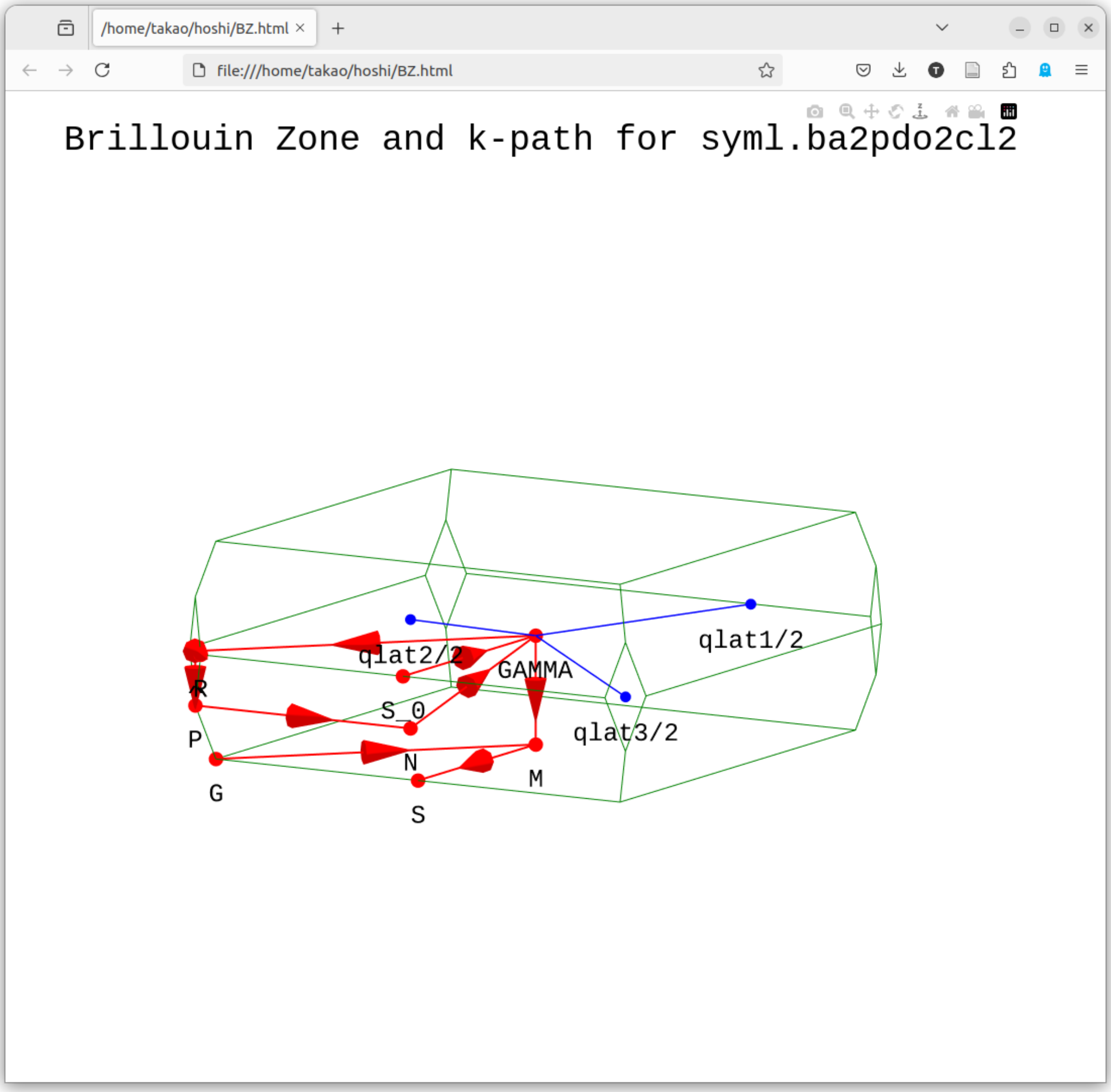
Step 4. Create k-path and BZ for band plot

After the calculation converges, it might be necessary to make a band plot with `job_band` command explain later on. The normality of the calculation of bands can be confirmed by the band plot (for magnetic systems, check the total magnetic moment and the magnetic moment for each site).

Before `job_band`, run `getsyml gaas`. Install any missing packages with pip. It is on spglib by Togo and seekpath. After finished, view BZ.html. It shows the k-path in the BZ ashow show below for ba2pdo2cl2. It is an interactive figure written with plotly, so you can read the coordinate values.

```
getsyml mp-2534
```

- Samples of BZ.html by getsyml are seen at https://ecalj.sakura.ne.jp/BZ/.



Brillouin Zone and k-path for syml.ba2pdo2cl2

Step 5. band plot

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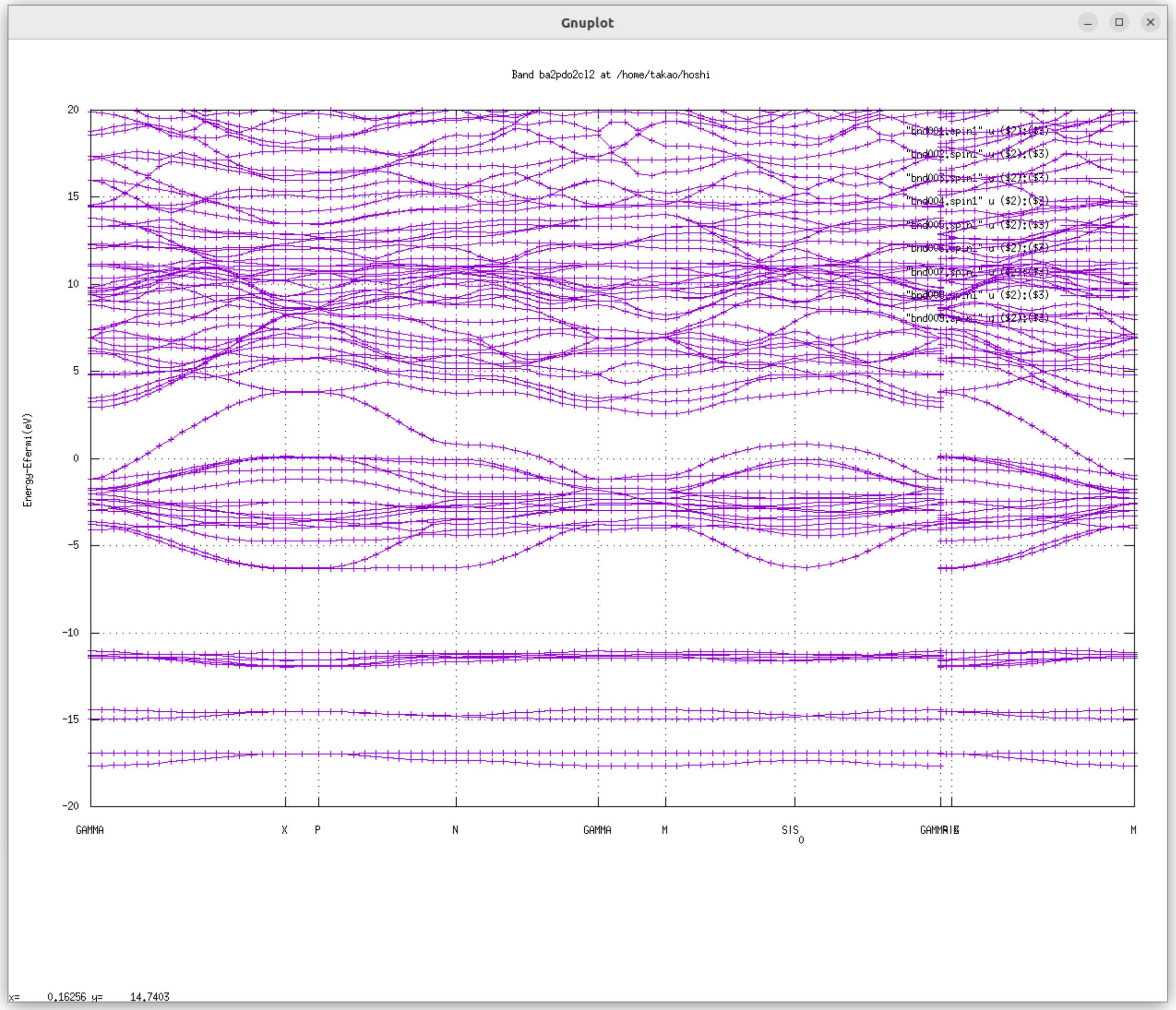
(this is a case for ba2pdo2cl2)

```
>job_band ctrl.ba2pdo2cl2 -np 8
```

A gnuplot script can be created. Edit it if necessary. If you edit syml.ba2pdo2cl2 before `job_band`, you can adjust the symmetry line and mesh size.

- The following picture is the LDA bands for the default calculation of ba2pdo2cl2 (the names of the symmetric points can be confirmed with BZ.html. In addition, look into `syml.foobar`). 0 eV is the Fermi energy. Since this is metallic, we see no band gap.



.

- The defaults are fine except for the k-mesh setting. For example, it is better to increase the k mesh for Fe. In general, for semiconductors, 4 4 4 for Si is a reasonable level, 6 6 6 is a level that can be used for a paper, and 8 8 8 is a level for checking accuracy. For metals such as Fe, 8 8 8 is a reasonable level.

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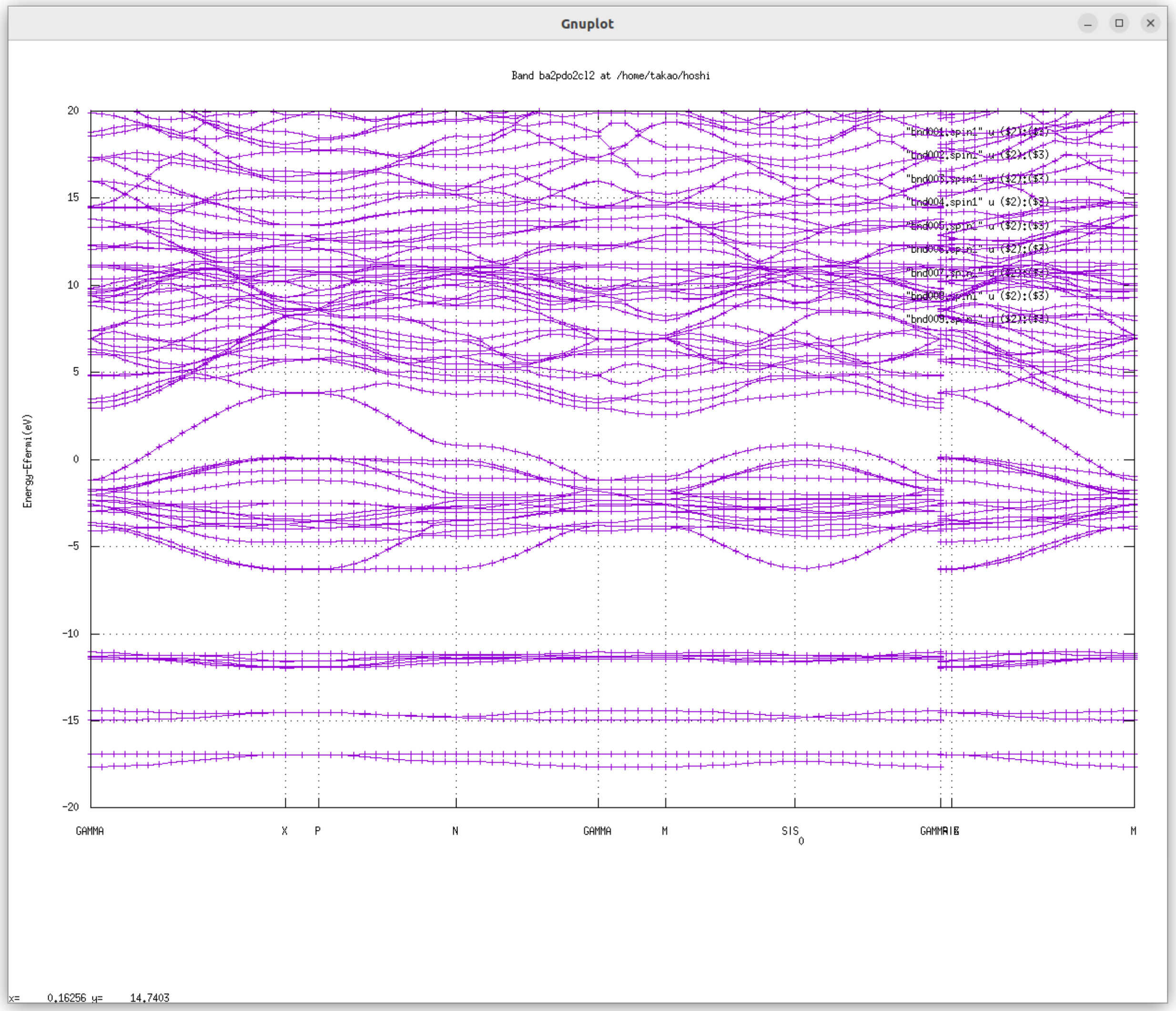
Here we are talking about band energies.

- In ecalj, the k mesh for `lmf` (ctrl) and the k mesh for GW (n1n2n3 specified in GWinput) can be different. The former has affected little on computational time, but the latter has a large effect (thus we want to reduce `n1n2n3` in `GWinput`).

- In ecalj's band plot mode, theoretically degenerated bands because of symmetry at the BZ edge are not degenerated. This is because there are limited numbers of APW basis functions, so run the band plot with pwemax=4, etc. (Temporary solution: We want to automate it).


Gnuplot
Band ba2pdo2cl2 at /home/takao/hoshi
"bnd001.spin1" u ($2):($3)
"bnd002.spin1" u ($2):($3)
"bnd003.spin1" u ($2):($3)
"bnd004.spin1" u ($2):($3)
"bnd005.spin1" u ($2):($3)
"bnd006.spin1" u ($2):($3)
"bnd007.spin1" u ($2):($3)
"bnd008.spin1" u ($2):($3)
"bnd009.spin1" u ($2):($3)
Energy-Efermi(eV)
20
15
10
5
0
-5
-10
-15
-20
GAMMA
X
P
N
GAMMA
M
SIS
0
GAMMRIB
M
x= 0.16256 y= 14.7403

job_tdos, job_fermisurface, job_pdos

`job_pdos` calculates PDOS, `job_tdos` calculates total DOS, and `job_fermisurface` draws the Fermi surface with Xcrysden.
`job_fermisurface` can be used to draw the shape of the CBM bottom as ellipsoid of Si.

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xxx

Step 6. QSGW calcualtion

We now run QSGW calculations. qSGW is compuationally very expensive. So we recommend you to run smaller systems at first.

For QSGW calculations, we need one additional input file `GWinput`, whose template is generated by mkGWinput GWinput as

```
mkGWinput ctrl.mp-2534
```

Then copy and edit GWimput.tmp to GWinput.

In GWinput, n1n2n3 should be smaller than nk1 nk2 nk3 in ctrl file
in order to reduce computational time (1/2 or 2/3 of ctrl, for example)
If 6x6x6 for Si, it is reasoble. Except k points, not need to modify so much (ask us).
GWinput is explained here. Input system is different from ctrl.

flow of QSGW calculation with the script gwsc

We run the QSGW calculations with gwsc. For semiconductors, several QSGW iterations are fine, close enough to final results.
QSGW is to obtain band structures (or one-body Hamiltonian), the total energy is not yet.

QPU file contains diagonal components of GW calculations.
Note that our Mixed Produce basis is a key technology for the GW calculation.

```
gwsc -np NP [--phispinsym] [--gpu] [--mp] nloop extension
```

(--phispinsym is for magnetic materials to keep the same basis for up and down)

Then console outputs of gwsc is somthing like

```
### START gwsc: ITERADD= 1, MPI size=  4, 4 TARGET= si
===== Ititial band structure ======
---> No sigm. LDA caculation for eigenfunctions
0:00:00.226245   mpirun -np 1 /home/takao/bin/lmfa si     >llmfa
0:00:00.807062   mpirun -np 4 /home/takao/bin/lmf  si     >llmf_lda
===== QSGW iteration start iter 1 ===
0:00:03.071054   mpirun -np 1 /home/takao/bin/lmf si     --jobgw=0
>llmfgw00
0:00:03.904403   mpirun -np 1 /home/takao/bin/qg4gw    --job=1 > lqg4gw
0:00:04.431022   mpirun -np 4 /home/takao/bin/lmf si     --jobgw=1
>llmfgw01
0:00:05.918216   mpirun -np 1 /home/takao/bin/heftet --job=1    > leftet
0:00:06.444439   mpirun -np 1 /home/takao/bin/hbasfp0 --job=3    >lbasC
0:00:07.064558   mpirun -np 4 /home/takao/bin/hvccfp0 --job=3    > lvccC
0:00:07.812283   mpirun -np 4 /home/takao/bin/hsfp0_sc --job=3    >lsxC
0:00:08.545956   mpirun -np 1 /home/takao/bin/hbasfp0 --job=0    > lbas
0:00:09.156775   mpirun -np 4 /home/takao/bin/hvccfp0 --job=0    > lvcc
0:00:09.884064   mpirun -np 4 /home/takao/bin/hsfp0_sc --job=1    >lsx
0:00:10.644292   mpirun -np 4 /home/takao/bin/hrcxq   > lrcxq
0:00:11.482931   mpirun -np 4 /home/takao/bin/hsfp0_sc --job=2    > lsc
0:00:12.460776   mpirun -np 1 /home/takao/bin/hqpe_sc    > lqpe
0:00:13.019735   mpirun -np 4 /home/takao/bin/lmf si     >llmf
===== QSGW iteration end   iter 1 ===
OK! ==== All calclation finished for  gwsc ====
```

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...

The log files of console outputs are `l*`. C at the end of the lof file means Core-related parts. `lsxC` is the exchange self-energy due to cores.
`lsx` is for exchange. `lsc` is correlation. `lvc`c is for Coulomb matrix。
In this calculation we run `gwsc -np 8 1 si`, where 1 is the number of QSGW iteration.

If you repeat gwsc, we have additional QSGW iterations on top the previous calculations.

Here is a case of ba2pdo2cl2.

Run

```
mkGWinput ba2pdo2cl2
```

to generate GWinput.tmp, which is a setting file for QSGW.
After copying this to GWinput, you may need to edit GWinput.
Minimum thing to edit is the number of k points for the self energy (n1n2n3).
Compared with k points in ctrl (nk1,nk2,nk3), we use small numbers.
(We often use 1/2 or 2/3 of k points given in ctrl as nk1,nk2,nk3).

There are another setting in GWinput. However, we usually do not need to touch things except n1n2n3 if you treat non-magnetic semiconductors.

Then you can run QSGW calculation with

```
gwsc -np 32 1 ba2pdo2cl2
```

. Here 1 means the number of QSGW iterations. QSGW iteration is quite time-consuming. `gwsc` gives minimum help (we need to explain options elsewhere).

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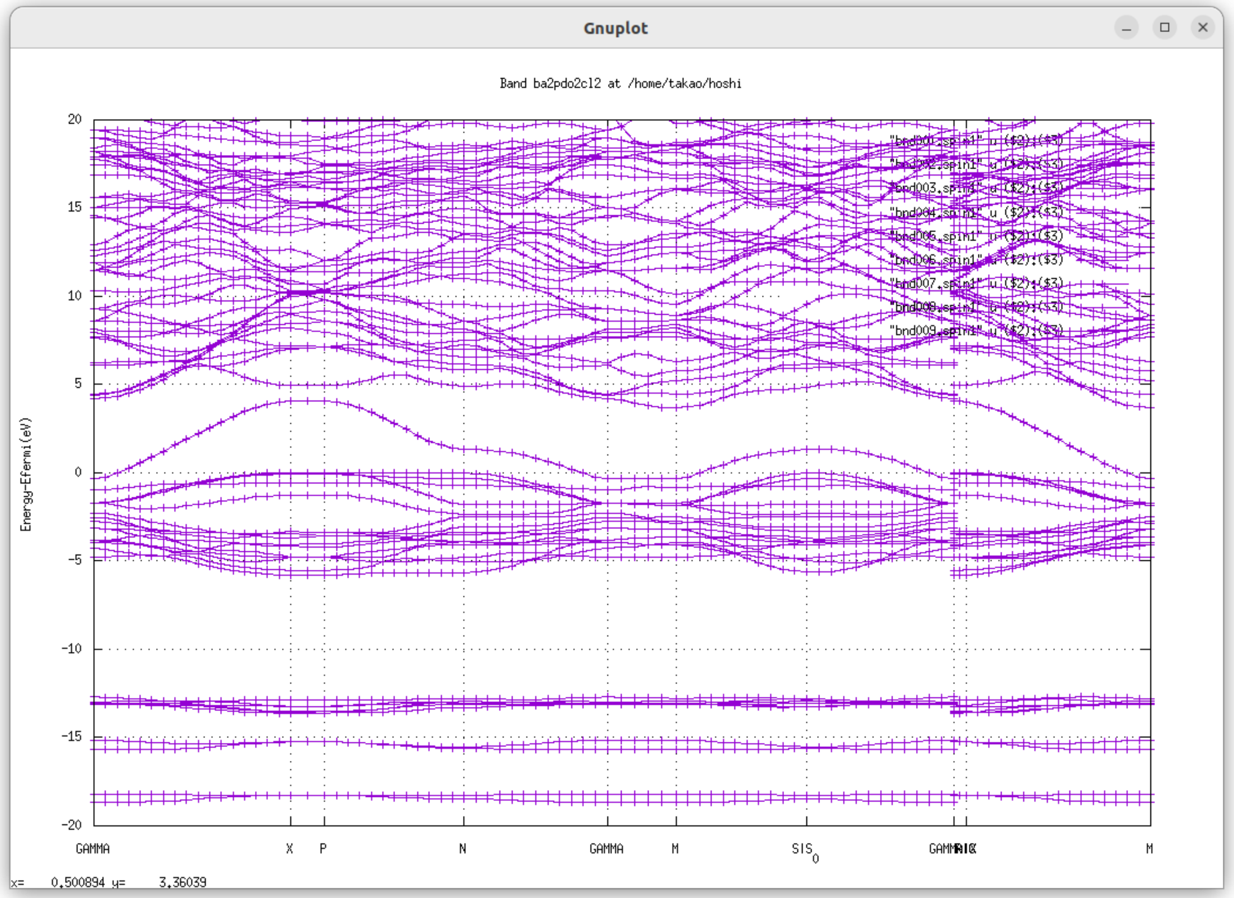
The iteration is kept in `rst.foobar`:electron density, `sigm.*`:vxcqsgw.
(Remove these files in addition to *run files/directories if you like to start from the beginning).

- It requires 53 minutes to run one iteration of QSGW.
- job_band ba2pdo2cl2 -np 32 gives the following picture. QSGW one-shot changes band structure around Ef from that in LDA.But still metallic, no band gaps.


Gnuplot
Band ba2pdo2cl2 at /home/takao/hoshi
Energy-Efermi(eV)
20
15
10
5
0
-5
-10
-15
-20
GAMMA
X
P
N
GAMMA
M
SIS
0
GAMMRIX
M
"bnd001.spin1" u ($2):($3)
"bnd002.spin1" u ($2):($3)
"bnd003.spin1" u ($2):($3)
"bnd004.spin1" u ($2):($3)
"bnd005.spin1" u ($2):($3)
"bnd006.spin1" u ($2):($3)
"bnd007.spin1" u ($2):($3)
"bnd008.spin1" u ($2):($3)
"bnd009.spin1" u ($2):($3)
x= 0.500894 y= 3.36039

- To continue QSGW iteration, run

```
gwsc -np 32 nx ba2pdo2cl2
```

Since you did 1 already. You will have the results of 1+nx QSGQ iteration.

- when we run 8 iterations as for ba2pdo2cl2, we had band gap 2.1 eV. We saw band gap after 4th iteration.

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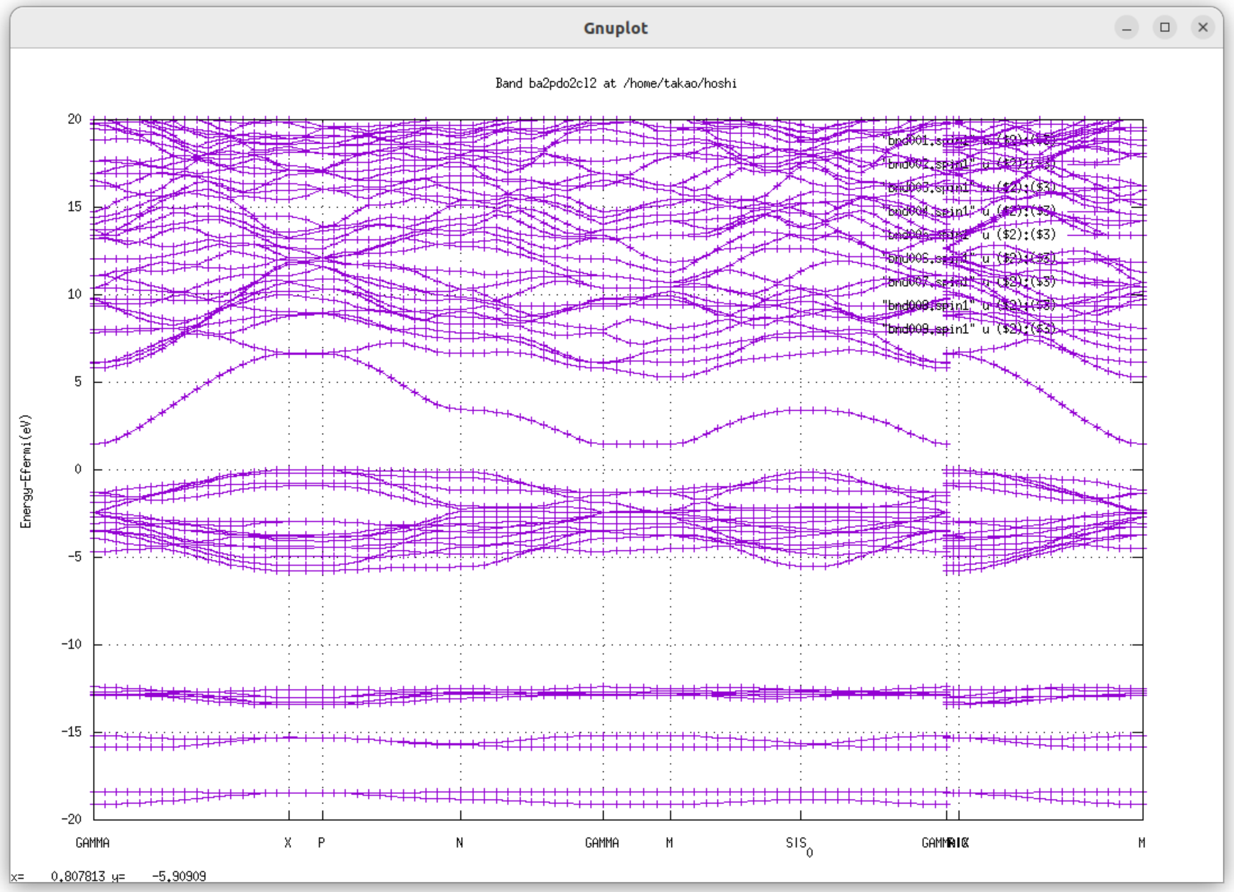

- For comparison with experiments, we recommend to use ssig=0.8
  (set in ctrl.foobar file), which is called as QSGW80.

- Spin-orbit coupling. After you obtain `sigm.foobar`, you set SO=1 (LdotS scheme) and run lmf. Then you can include effect of SOC. Sinc SO=1
  is not implemented in the whole gwsc cycle, we have to include SOC just at the end step (We include SOC after we fix VxcQSGW).

- If you run

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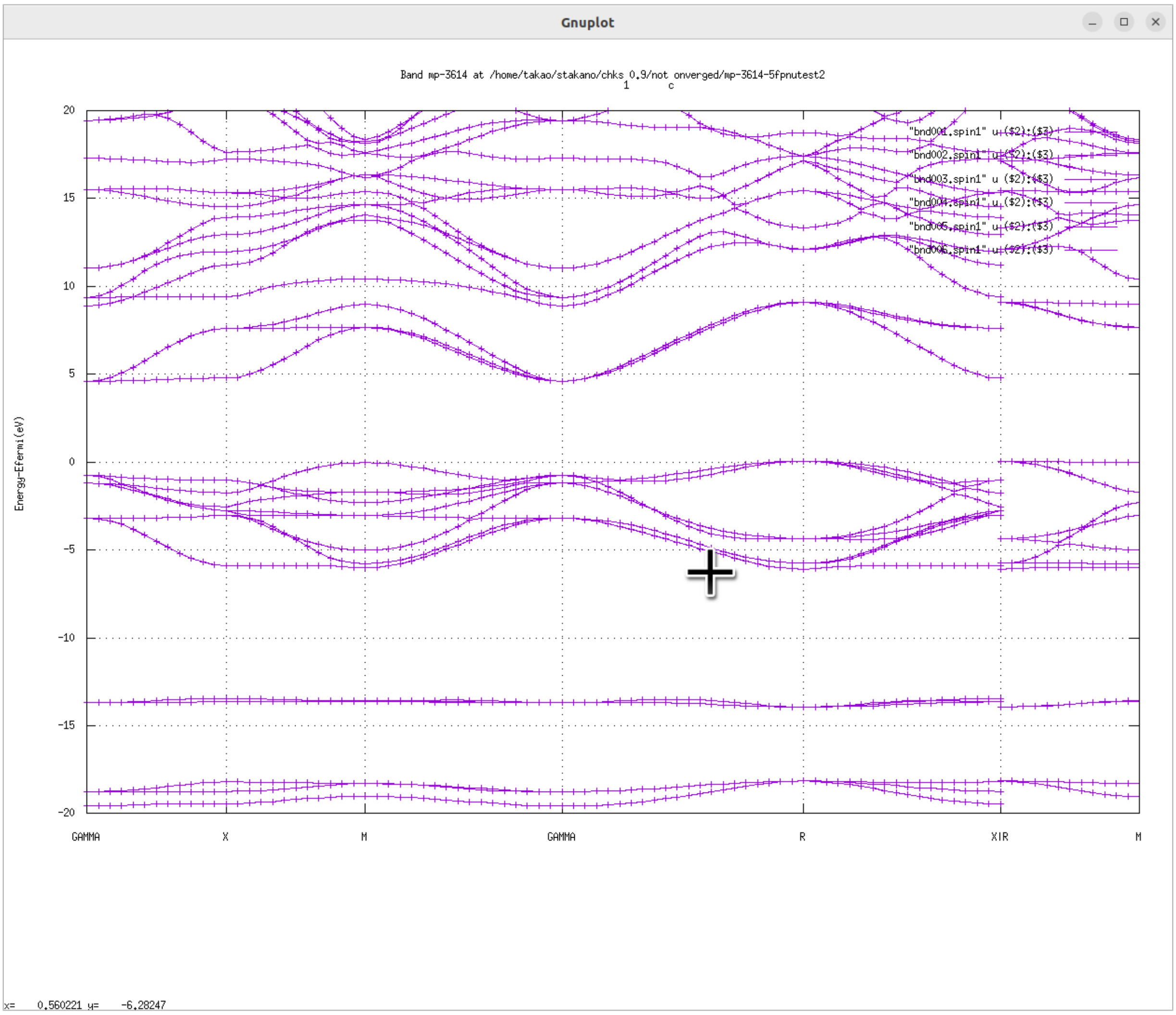
```
gwsc -np 32 5 ba2pdo2cl2 -vssig=0.8
```

, this overide ssig, which is defined in ctrl.ba2pdo2cl2, in lmf calculations. (Check it in save.ba2pdo2cl2)

- Example of QSGW for KTaO3 (perovskite,mp-3614)


Gnuplot
Band mp-3614 at /home/takao/stakano/chks_0.9/not_onverged/mp-3614-5fpnutest2
1 c
"bnd001.spin1" u ($2):($3)
"bnd002.spin1" u ($2):($3)
"bnd003.spin1" u ($2):($3)
"bnd004.spin1" u ($2):($3)
"bnd005.spin1" u ($2):($3)
"bnd006.spin1" u ($2):($3)
Energy-Efermi(eV)
20
15
10
5
0
-5
-10
-15
-20
GAMMA
X
M
GAMMA
R
X|R
M
x= 0.560221 y= -6.28247

How to start over calcualtions

Remove mix* rst* (mix* is mixing files)
If MT changes, start over from lmfa (remove atm* files)

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- As long as converged, no problem.
- If you have 3d spagetti bands at Ef, need caution.

A mini database for tests.

ecalj contains a mini database and auto calculation for test purpose (at LDA level).

At ecalj/MATERIALS/, you can run ./jobmaterials.py.
Then you can perform LDA calculations for simple materials whose crystal structures are already contained in a mini database.

```
./job_materials.py
```

gives a help, showing a list of materials. Then

```
./job_materials.py Si
```

performs LDA calculation of Si at ecalj/MATERIALS/Si/.

- Key input files are
  `ctrls.si,ctrl.si`
  . See sections below. `rst.si` contains self-consistent electron density. Check iterations with the output file `save.si`. The console output of lmf is in llmf. Not need to know all the console outputs.
- Before QSGW, it is better to confirm the LDA level calculations are fine. In order to do the confirmation, band plot is convenient.
  For band plot we need the symmetry line as `syml.si` which can
  be generated by

  ```
  getsyml si
  ```

  Then run

  ```
  job_band si -np 8
  ```

  results band plots in the gnuplot.

lmchk

```
lmchk mp-2534
```

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is to check the crystal symmetry. In addition determine MT radius. and Check the ovarlap of MTs. Defaults setting is with -3% overlap.(no overlap).

- symmetry
- MT overlap
  If you have less symmetry rather than than the symmetry of lattice for magnetic systems,
  you have to set crystal symmetry by hand.
  This can be done by adding space group symmetry generator to SYMGRP (instead of find).
  We need to pay attention for this point in the case of SOC.

Summary of other manuals

Spin poralized case

Here we explain magnetic systems.
We have to set MMOM (ititial spin magnatic moments) in addition to set nspin=2.
For example, we set ctrl.nio as

```
SITE    ATOM=Niup POS=  .0   .0   .0
        ATOM=Nidn POS= 1.0  1.0  1.0
        ATOM=O POS=  .5   .5   .5
        ATOM=O POS= 1.5  1.5  1.5
SPEC
    ATOM=Niup Z=28 R=2.12
      MMOM=0 0  1.2 0
      EH=-1 -1 -1 -1  RSMH=1.06 1.06 1.06 1.06
      EH2=-2 -2 -2  RSMH2=1.06 1.06 1.06
      KMXA={kmxa}  LMX=3 LMXA=4 NMCORE=1
    ATOM=Nidn Z=28 R=2.12
      MMOM=0 0 -1.2 0
      EH=-1 -1 -1 -1  RSMH=1.06 1.06 1.06 1.06
      EH2=-2 -2 -2  RSMH2=1.06 1.06 1.06
      KMXA={kmxa}  LMX=3 LMXA=4 NMCORE=1
```

Here we have two sites named Niup and Nidn. They both have MMOM. 1.2 means spin moment for d channel.
That is `MMOM {s} {p} {d} {f}`, where `{s} {p} {d} {f}` are number of spin moments for each $l$ at atomic sites.
In addition, we set `nspin=2` defined at the `% const` line in ctrl file.
We can read magnetic moments within MT at 'true mm' column in the console output in the `mmom.nio.chk` as

```
# Qtrue    MagMom(up-dn) Rmt   MT
1 8.527587  1.200085  2.120000 Niup
2 8.527604 -1.200081  2.120000 Nidn
3 5.380352 -0.000002  1.700000 O
4 5.380352 -0.000002  1.700000 O
```

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Note it is overwritten at every iteration. These are shown in concole output as `true mm' as well.
Atomic site index are given in 'Siteinfo.chk'. Total Magnetic Moments are shown as

```
 Magnetic moment=     2.241805 !this is a case of bulk Fe
```

Antiferro symmetry

We can set Antiferro symmetry (not yet for SOC=1).
We have README_AF.md and samples at ~/ecalj/Samples/AFsymmetry/

Spin-orbit coupling

We have a switch `HAM_SO` in the ctrl file

If we assume antiferro symmetry, look into

Dielectric function, ESM, spin fluctuation, life time of QP, Wannier method,...
Ask us.

band plot with spin orbit coupling.

method 1: only band plot

```
job_band mp-2534 -np 8 -vso=1 -vnspin=2: band plot only
```

Caution: when you set nspin=2, rst is twiced. No way to move it back to rst for nspin=1.

method 2. single iteration and SO=1

```
mpirun -np 8 lmf -vso=1 -vnspin=2 -vnit=1
```

job_band mp-2534 -np 8 : band plot only

method 3. full iteration SO=1

```
mpirun -np 8 lmf -vso=1 -vnspin=2 -vnit=1
```

job_band mp-2534 -np 8 : band plot only

PROF

Caution: when you set nspin=2, rst is twiced. No way to move it back to rst for nspin=1.

ecalj/Samples/MgO_PROCAR

This is a sample of fat band. Run job_procarを実行する。You will have eps file.

Pointer to ecalj manuals