

OpenMX tutorials

Computational Materials Physics Bootcamp

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19-22 August, 2024

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Tutorial of OpenMX



OpenMX: basics

- File name

- System.CurrentDir

- System.Name

- DATA.PATH

- level.of.stdout

- level.of.fileout

```
# File Name
System.CurrentDirectory      ./                      # default=./
System.Name                  CrSBr
DATA.PATH                    /home/opt/pkg/openmx/3.9.9-intel-2020.3/DFT_DATA19
level.of.stdout              1                        # default=1 (1-3)
level.of.fileout             0                        # default=1 (0-2)
```

- Atomic Species

- Species.Number

- Denition.of.Atomic.Species

```
# Definition of Atomic Species
Species.Number              3
<Definition.of.Atomic.Species
  Cr  Cr6.0-s3p2d2f1      Cr_PBE19
  S   S7.0-s3p2d2f1      S_PBE19
  Br  Br7.0-s3p2d2f1      Br_PBE19
Definition.of.Atomic.Species>
```

OpenMX: basics

- Atoms

- Atoms.Number

- Atoms.SpeciesAndCoordinates.Unit

- Atoms.SpeciesAndCoordinates

- Atoms.UnitVectors.Unit

- Atoms.UnitVectors

```
# Atoms
Atoms.Number 12
Atoms.SpeciesAndCoordinates.Unit FRAC
<Atoms.SpeciesAndCoordinates
1 Cr 0.749999182310 0.250000097256 0.326171526313 8.0 6.0 90.0 90.0 0.0 0.0 0 Off
2 Cr 0.749999182310 0.250000097256 0.605972937979 6.0 8.0 90.0 -90.0 0.0 0.0 0 Off
3 Cr 0.249999727437 0.750000291769 0.673828473687 6.0 8.0 90.0 -90.0 0.0 0.0 0 Off
4 Cr 0.249999727437 0.750000291769 0.394027062021 8.0 6.0 90.0 90.0 0.0 0.0 0 Off
5 S 0.749999182310 0.750000291769 0.340373694760 3.0 3.0 0.0 0.0 0.0 0.0 0 Off
6 S 0.749999182310 0.750000291769 0.620175106427 3.0 3.0 0.0 0.0 0.0 0.0 0 Off
7 S 0.249999727437 0.250000097256 0.659626305240 3.0 3.0 0.0 0.0 0.0 0.0 0 Off
8 S 0.249999727437 0.250000097256 0.379824893573 3.0 3.0 0.0 0.0 0.0 0.0 0 Off
9 Br 0.249999727437 0.250000097256 0.266633831839 3.5 3.5 0.0 0.0 0.0 0.0 0 Off
10 Br 0.249999727437 0.250000097256 0.546435243505 3.5 3.5 0.0 0.0 0.0 0.0 0 Off
11 Br 0.749999182310 0.750000291769 0.733366168161 3.5 3.5 0.0 0.0 0.0 0.0 0 Off
12 Br 0.749999182310 0.750000291769 0.453564756495 3.5 3.5 0.0 0.0 0.0 0.0 0 Off
Atoms.SpeciesAndCoordinates>

Atoms.UnitVectors.Unit Ang
<Atoms.UnitVectors
3.5404600000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 4.7554700000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000
Atoms.UnitVectors>
```

OpenMX: basics

- SCF or Electronic System

scf.XcType

scf.SpinPolarization

scf.partialCoreCorrection

scf.Hubbard.U

scf.Hubbard.Occupation

Hubbard.U.values

scf.Constraint.NC.Spin

scf.Constraint.NC.Spin.v

scf.ElectronicTemperature

scf.energycutoff

scf.Ngrid

scf.maxIter

scf.EigenvalueSolver

scf.Kgrid

scf.ProExpn.VNA

scf.Mixing.Type

scf.Init.Mixing.Weight

scf.Min.Mixing.Weight

scf.Max.Mixing.Weight

scf.Kerker.factor

scf.Mixing.History

scf.Mixing.StartPulay

scf.Mixing.EveryPulay

scf.criterion

scf.Electric.Field

scf.system.charge

scf.SpinOrbit.Coupling

OpenMX: basics

```
# SCF or Electronic System
scf.Hubbard.U          On
scf.DFTU.Type          2
scf.Hubbard.Occupation Dual
scf.dc.Type            sFLL
#scf.Slater.Ratio      0.957136
scf.Yukawa             On
scf.XcType             GGA-PBE
scf.SpinPolarization   NC
#scf.Constraint.NC.Spin On
#scf.Constraint.NC.Spin.v 0.5
scf.SpinOrbit.Coupling On
HS.fileout             Off
scf.ElectronicTemperature 300.0
scf.energycutoff        150.0
scf.maxIter            200
scf.EigenvalueSolver   band
scf.Kgrid              8 6 1
scf.Mixing.Type         rmm-diisk
scf.Init.Mixing.Weight  0.300
scf.Min.Mixing.Weight   0.001
scf.Max.Mixing.Weight   0.400
scf.Mixing.History      5
scf.Mixing.StartPulay   6
scf.criterion           1.0e-7

# On|Off, default=Off
# 1:Simplified(Dudarev)|2:General, default=1
# Onsite|Full|Dual, default=Dual
# sFLL|sAMF|cFLL|cAMF, default=sFLL
# default=0.625
# default=Off
# LDA|LSDA-CA|LSDA-PW|GGA-PBE
# On|Off|NC
# On|On2|Off, default=off
# default=0.0 (eV)
# On|Off, default=off
# on|off, default=off
# default=300 (K)
# default=150 (Ry)
# default=40
# Recursion|Cluster|Band
# means nk1xnk2xnk3
# Simple|Rmm-Diis|Gr-Pulay
# default=0.30
# default=0.001
# default=0.40
# default=5
# default=6
# default=1.0e-6 (Hartree)
```

OpenMX: basics

- Hubbard U settings

- Hubbard.U.values

- Hund.J.values

```
<Hubbard.U.values                                     # eV
Cr  1s 0.0 2s 0.0 3s 0.0 1p 0.0 2p 0.0 1d 2.8
S   1s 0.0 2s 0.0 1p 0.0 2p 0.0 1d 0.0 1f 0.0
Br  1s 0.0 2s 0.0 3s 0.0 1p 0.0 2p 0.0 1d 0.0 2d 0.0
Hubbard.U.values>
```

```
<Hund.J.values                                       # eV
Cr  1s 0.0 2s 0.0 3s 0.0 1p 0.0 2p 0.0 1d 0.0
S   1s 0.0 2s 0.0 1p 0.0 2p 0.0 1d 0.0 1f 0.0
Br  1s 0.0 2s 0.0 3s 0.0 1p 0.0 2p 0.0 1d 0.0 2d 0.0
Hund.J.values>
```

- Band structure setting

- Band.dispersion

- Band.KPath.UnitCell

- Band.Nkpath

- Band.kpath

```
Band.dispersion                                     On          # on|off, default=off
Band.Nkpath                                         4
<Band.kpath>
100  0.0000  0.0000  0.0000  0.5000  0.0000  0.0000  0.0000  G X
100  0.5000  0.0000  0.0000  0.5000  0.5000  0.0000  0.0000  X S
100  0.5000  0.5000  0.0000  0.0000  0.5000  0.0000  0.0000  S Y
100  0.0000  0.5000  0.0000  0.0000  0.0000  0.0000  0.0000  Y G
Band.kpath>
```

OpenMX: basics

- MD or Geometry Optimization

- MD.Type
- MD.Fixed.XYZ
- MD.maxIter
- MD.TimeStep
- MD.Opt.criterion

- MD.Opt.DIIS.History
- MD.Opt.StartDIIS
- MD.TempControl
- NH.Mass.HeatBath
- MD.Init.Velocity

```
# MD or Geometry Optimization
```

```
MD.Type          NOMD
```

```
MD.maxIter       1
```

```
MD.Opt.criterion 3.0e-4
```

```
# NOMD|OptC1|OptC2|OptC3|OptC4|OptC5|OptC6|OptC7|RFC5|RFC6|RFC7
```

```
# default=1
```

```
# default=0.0003 (Hartree/Bohr)
```

OpenMX: basics

- DOS and PDOS

➤ Dos.fileout	# DOS or PDOS		
	Dos.fileout	on	# DOS calculation
➤ Dos.Erange	Dos.Erange	-25.0 25.0	# DOS energy range (0=chemical potential)
➤ Dos.Kgrid	Dos.Kgrid	18 18 22	# DOS k-point discretization

- Output Files :

- The output files are determined by 'level.of.fileout' parameter.
- The general format is 'System.Name.xxx'.

- If you want to repeat the calculation without restarting from the previous calculation you should delete all the output files first. Use the following command:

```
rm -r !(*.py|*.png|*.in|slurm.qs)
```

Silicon using OpenMX: Ground-State, Band Structure, DOS



Si using OpenMX: Ground-State, Band Structure, DOS

1. Create a subdirectory inside your main directory using 'mkdir' command:

```
mkdir OMX-Si
```

2. Copy all data from the following directory to your own subdirectory using cp command:

```
cp /home/cmpb/OpenMX/Si/* ./ OMX-Si
```

3. Go to your subdirectory using 'cd' command:

```
cd ./OMX-Si
```

4. Open the Si.in file and try to understand the keywords.

5. Now, if you feel ready for the run, it's time to submit the job. We need first to activate the module using:

```
module unload openmpi/4.1.4-intel-2023.0.0
```

```
module unload intel/2023.0.0
```

```
module load intel/2020.3
```

```
module load openmx
```

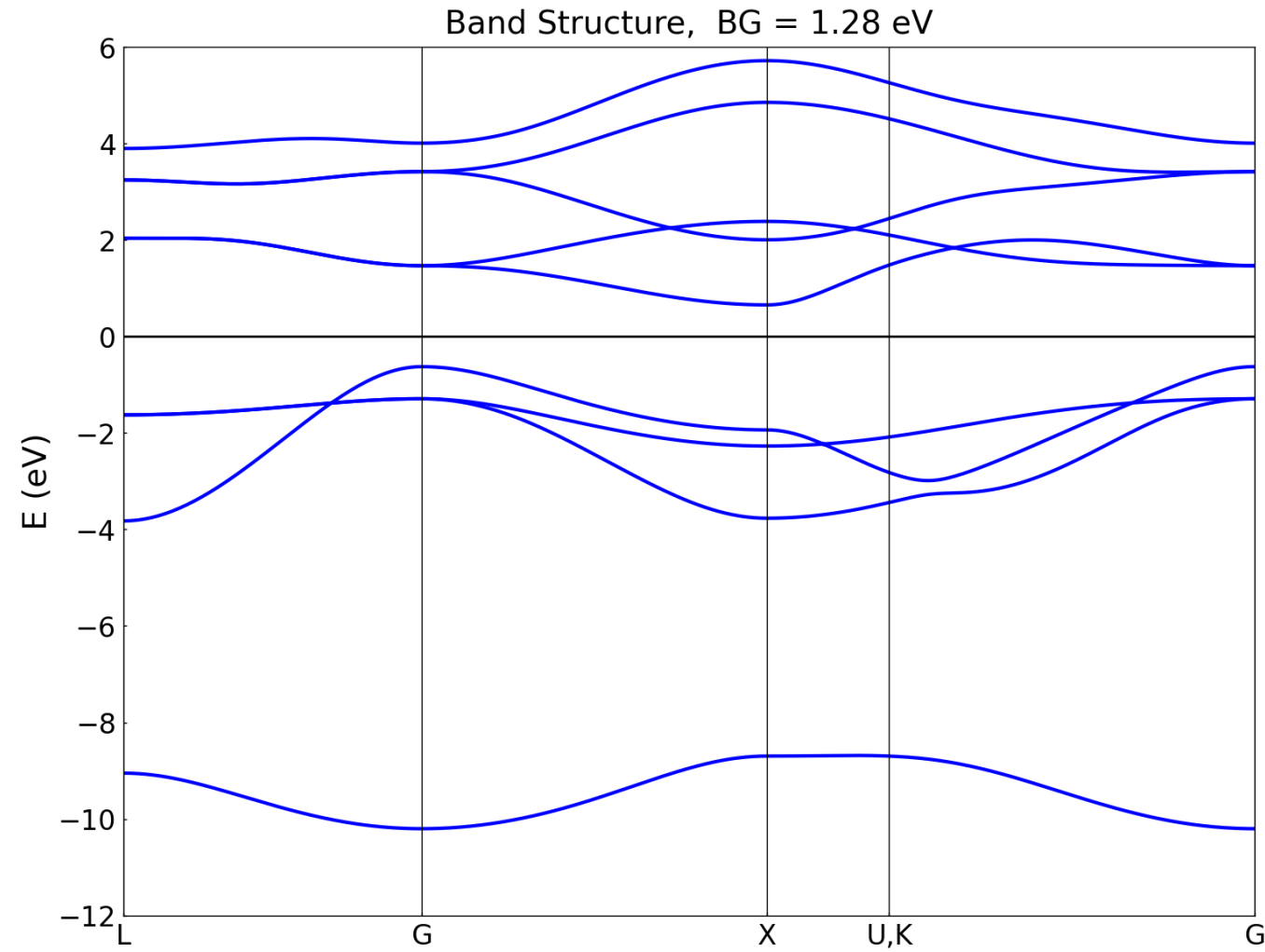
Si using OpenMX: Ground-State, Band Structure, DOS

6. Now, you can submit the job using the following command,

```
nohup mpirun -np 5 openmx Si.in > Si.out -f openmp &
```

7. The Si.out is the job log and you can see the progress of the scf loops by opening it.
8. When the job is finished open the Si.out and answer these questions. What is the ground state energy? How many scf loops are performed?
9. Use the following command to prepare the band structure data for plotting,
- ```
bandgnu13 Si.Band
```
10. Next use the python script in your directory to plot the band structure using the command,
- ```
Python3 Plot_band.py
```

Si using OpenMX: Ground-State, Band Structure, DOS



Si using OpenMX: Ground-State, Band Structure, DOS

11. Now, we are ready to calculate the DOS. The keyword setting in the code are:

```
Dos.fileout      on          # DOS calculation
Dos.Erange      -25.0 25.0   # DOS energy range (0=chemical potential)
Dos.Kgrid       27 27 27    # DOS k-point discretization
```

Since the keyword is already set in the input files, you just need to do the post processing. Use the following command to calculate the total DOS (PDOS)

```
DosMain Si.Dos.val Si.Dos.vec
```

Then, you are interactively asked from the program as follow:

```
DosMain Si.Dos.val Si.Dos.vec
Max of Spe_Total_CNO = 13
1 1 101 102 103 101 102 103 201 202 203 204 205
<Si.Dos.val>
<Si>
Which method do you use?, Tetrahedron(1), Gaussian Broadening(2)
1
Do you want Dos(1) or PDos(2)?
2

Number of atoms=2
Which atoms for PDOS : (1,...,2), ex 1 2
```

By answering these questions, you can calculate DOS or PDOS for a specific atom and orbitals.

Si using OpenMX: Ground-State, Band Structure, DOS

Now, use the following command to plot the DOS: `python3 Plot-DOS.py`

