OpenMX tutorials

Computational Materials Physics Bootcamp

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Tutorial of OpenMX

OpenMX: basics

- File name
  - **System.CurrrentDir**
  - **System.Name**
  - **DATA.PATH**
  - **level.of.stdout**
  - **level.of.fileout**

```
# File Name
System.CurrrentDirectory        ./                                        # 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                          # Ang|AU|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                           # Ang|AU
<Atoms.UnitVectors
    3.540460000000000  0.000000000000000  0.000000000000000
    0.000000000000000  4.755470000000000  0.000000000000000
    0.000000000000000  0.000000000000000  30.00000000000000
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                  # On|Off, default=Off
scf.DFTU.Type                2                   # 1:Simplified(Dudarev)|2:General, default=1
scf.Hubbard.Occupation       Dual                # Onsite|Full|Dual, default=Dual
scf.dc.Type                  sFLL                # sFLL|sAMF|cFLL|cAMF, default=sFLL
#scf.Slater.Ratio             0.957136           # default=0.625
scf.Yukawa                   On                  # default=Off
scf.XcType                   GGA-PBE             # LDA|LSDA-CA|LSDA-PW|GGA-PBE
scf.SpinPolarization         NC                  # On|Off|NC
#scf.Constraint.NC.Spin       On                  # On|On2|Off, default=off
#scf.Constraint.NC.Spin.v     0.5                 # default=0.0(eV)
scf.SpinOrbit.Coupling       On                  # On|Off, default=off
HS.fileout                   Off                 # on|off, default=off
scf.ElectronicTemperature    300.0               # default=300 (K)
scf.energycutoff             150.0               # default=150 (Ry)
scf.maxIter                  200                 # default=40
scf.EigenvalueSolver         band                # Recursion|Cluster|Band
scf.Kgrid                    8 6 1               # means nk1xnk2xnk3
scf.Mixing.Type              rmm-diisk           # Simple|Rmm-Diis|Gr-Pulay
scf.Init.Mixing.Weight       0.300               # default=0.30
scf.Min.Mixing.Weight        0.001               # default=0.001
scf.Max.Mixing.Weight        0.400               # default=0.40
scf.Mixing.History           5                   # default=5
scf.Mixing.StartPulay        6                   # default=6
scf.criterion                1.0e-7              # 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   G X
    100    0.5000    0.0000    0.0000     0.5000    0.5000    0.0000   X S
    100    0.5000    0.5000    0.0000     0.0000    0.5000    0.0000   S Y
    100    0.0000    0.5000    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        # NOMD|OptC1|OptC2|OptC3|OptC4|OptC5|OptC6|OptC7|RFC5|RFC6|RFC7
MD.maxIter                      1           # default=1
MD.Opt.criterion                3.0e-4      # default=0.0003 (Hartree/Bohr)
```

OpenMX: basics

- DOS and PDOS

- **Dos.fileout**
- **Dos.Erange**
- **Dos.Kgrid**

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

- 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.in

```
# File Name
System.CurrrentDirectory          ./                                    # default=./
System.Name                       Si
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)

# Definition of Atomic Species
Species.Number                    1
<Definition.of.Atomic.Species
   Si    Si7.0-s2p2d1    Si_PBE19
Definition.of.Atomic.Species>

# Atoms
Atoms.Number                      2
Atoms.SpeciesAndCoordinates.Unit  AU                                    # Ang|AU
<Atoms.SpeciesAndCoordinates
 1   Si   0.0000     0.0000     0.0000   2.0   2.0
 2   Si   0.2500     0.2500     0.2500   2.0   2.0
Atoms.SpeciesAndCoordinates>

Atoms.UnitVectors.Unit            Ang                                   # Ang|AU
<Atoms.UnitVectors
   0.00000   2.71530   2.71530
   2.71530   0.00000   2.71530
   2.71530   2.71530   0.00000
Atoms.UnitVectors>
```

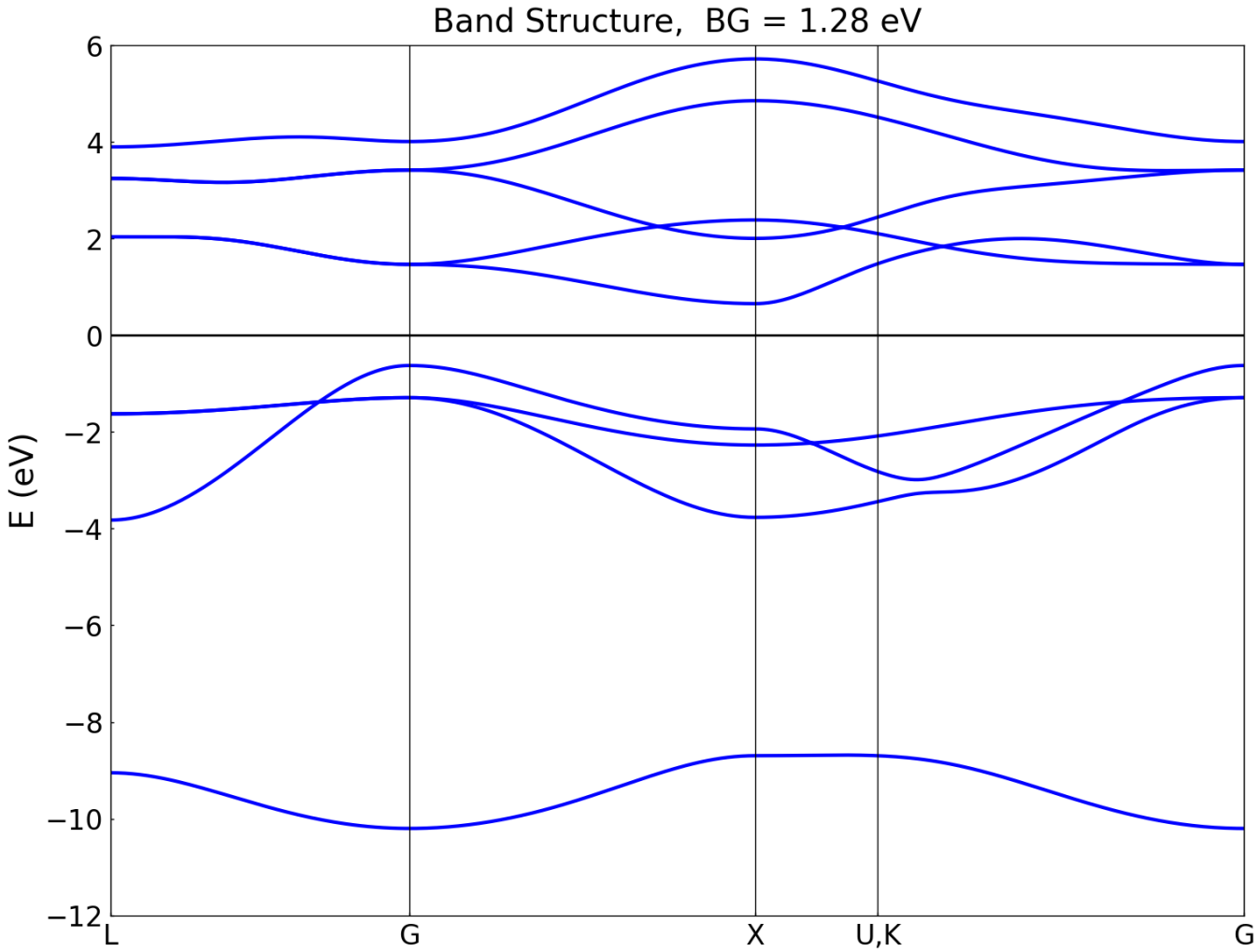
Si using OpenMX: Ground-State, Band Structure, DOS

```
# SCF or Electronic System
scf.XcType                      GGA-PBE                     # LDA|LSDA-CA|LSDA-PW|GGA-PBE
scf.SpinPolarization            Off                         # On|Off|NC
scf.SpinOrbit.Coupling          Off                         # On|Off, default=off
HS.fileout                      Off                         # on|off, default=off
scf.ElectronicTemperature       300.0                       # default=300 (K)
scf.energycutoff                200.0                       # default=150 (Ry)
scf.maxIter                     100                         # default=40
scf.EigenvalueSolver            band                        # Recursion|Cluster|Band
scf.Kgrid                       9 9 9                       # means nk1xnk2xnk3
scf.Mixing.Type                 rmm-diisk                   # Simple|Rmm-Diis|Gr-Pulay
scf.Init.Mixing.Weight          0.300                       # default=0.30
scf.Min.Mixing.Weight           0.001                       # default=0.001
scf.Max.Mixing.Weight           0.400                       # default=0.40
scf.Mixing.History              5                           # default=5
scf.Mixing.StartPulay           6                           # default=6
scf.criterion                   1.0e-7                      # default=1.0e-6 (Hartree)
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 discritization

Band.dispersion                 on                          # on|off, default=off
Band.Nkpath                     4
<Band.kpath
    80   0.5000  0.5000  0.5000    0.0000  0.0000  0.0000   L G
    100  0.0000  0.0000  0.0000    0.5000  0.0000  0.5000   G X
    30   0.5000  0.0000  0.5000    0.6250  0.2500  0.6250   X U
    100  0.3750  0.3750  0.7500    0.0000  0.0000  0.0000   K G
Band.kpath>

# MD or Geometry Optimization
MD.Type                         NOMD                        # NOMD|OptC1|OptC2|OptC3|OptC4|OptC5|OptC6|OptC7|RFC5|RFC6|RFC7
MD.maxIter                      1                           # default=1
MD.Opt.criterion                3.0e-4                      # default=0.0003 (Hartree/Bohr)
```

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 discritization
```

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