DFT calculations by OpenMX #2

- Getting started with a cif file

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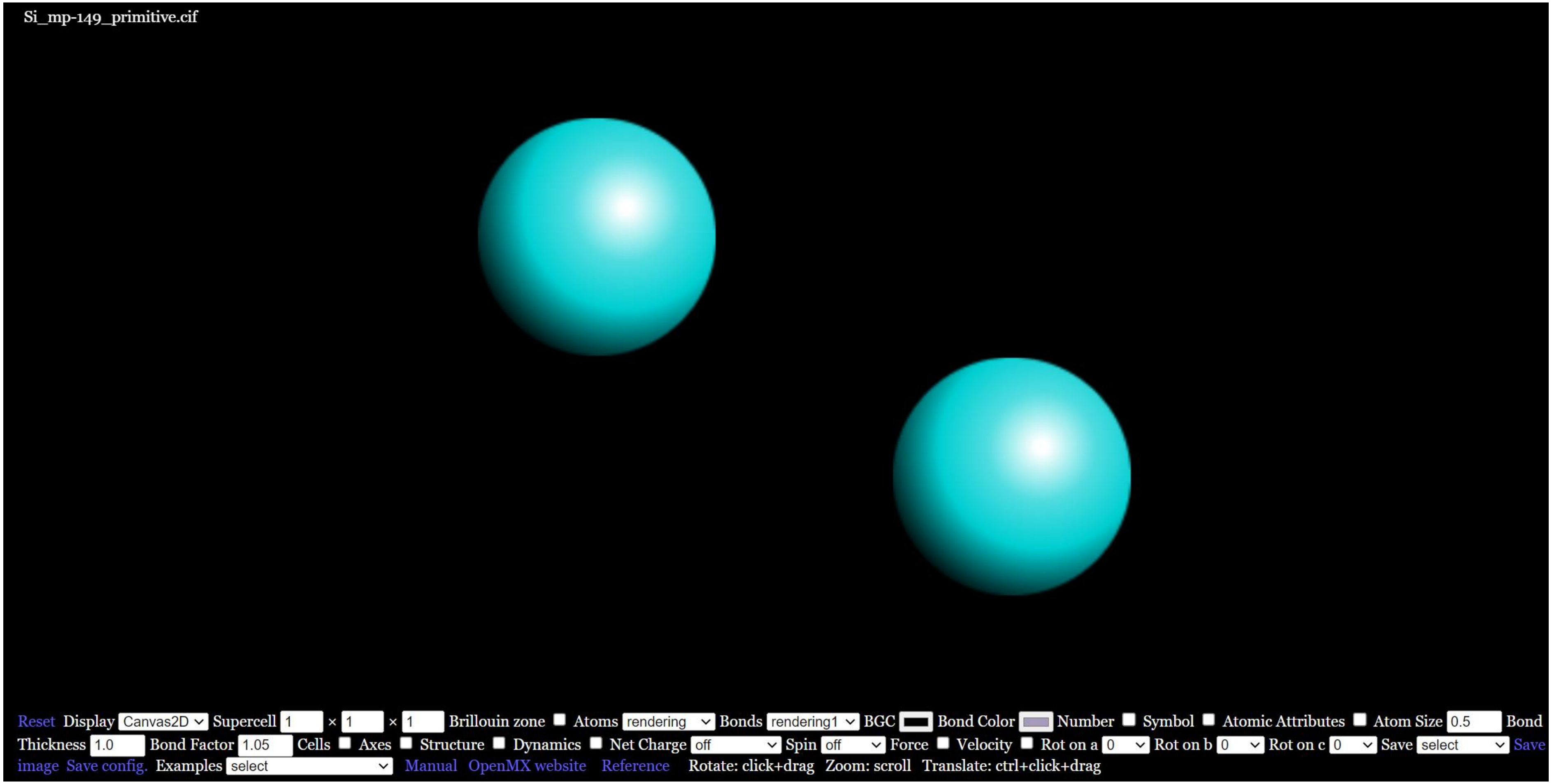
Getting started with a cif file #1

Drag and drop the following cif file on OpenMX Viewer

Si_mp-149_primitive.cif https://www.openmx-square.org/examples/Si_mp-149_primitive.cif

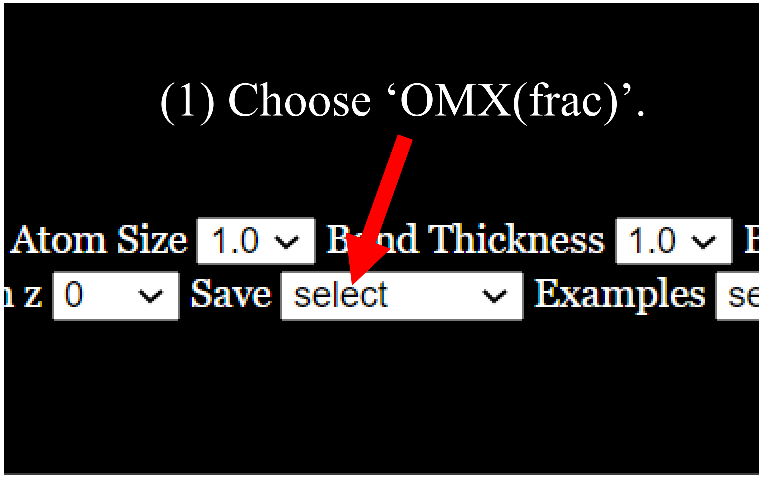
OpenMX Viewer: http://www.openmx-square.org/viewer/



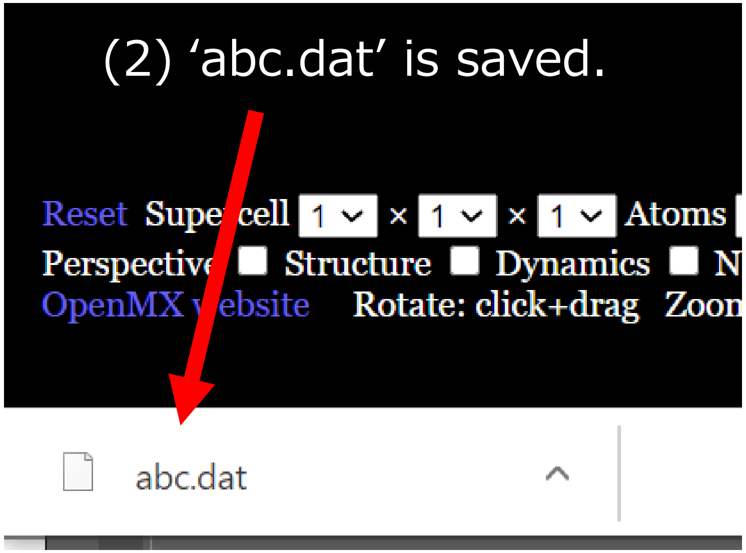
Si_mp-149_primitive.cif

Reset Display Canvas2D Supercell 1 × 1 × 1 Brillouin zone ☐ Atoms rendering Bonds rendering1 BGC ■ Bond Color ▨ Number ☐ Symbol ☐ Atomic Attributes ☐ Atom Size 0.5 Bond Thickness 1.0 Bond Factor 1.05 Cells ☐ Axes ☐ Structure ☐ Dynamics ☐ Net Charge off Spin off Force ☐ Velocity ☐ Rot on a 0 Rot on b 0 Rot on c 0 Save select Save image Save config. Examples select Manual OpenMX website Reference Rotate: click+drag Zoom: scroll Translate: ctrl+click+drag

Getting started with a cif file #2

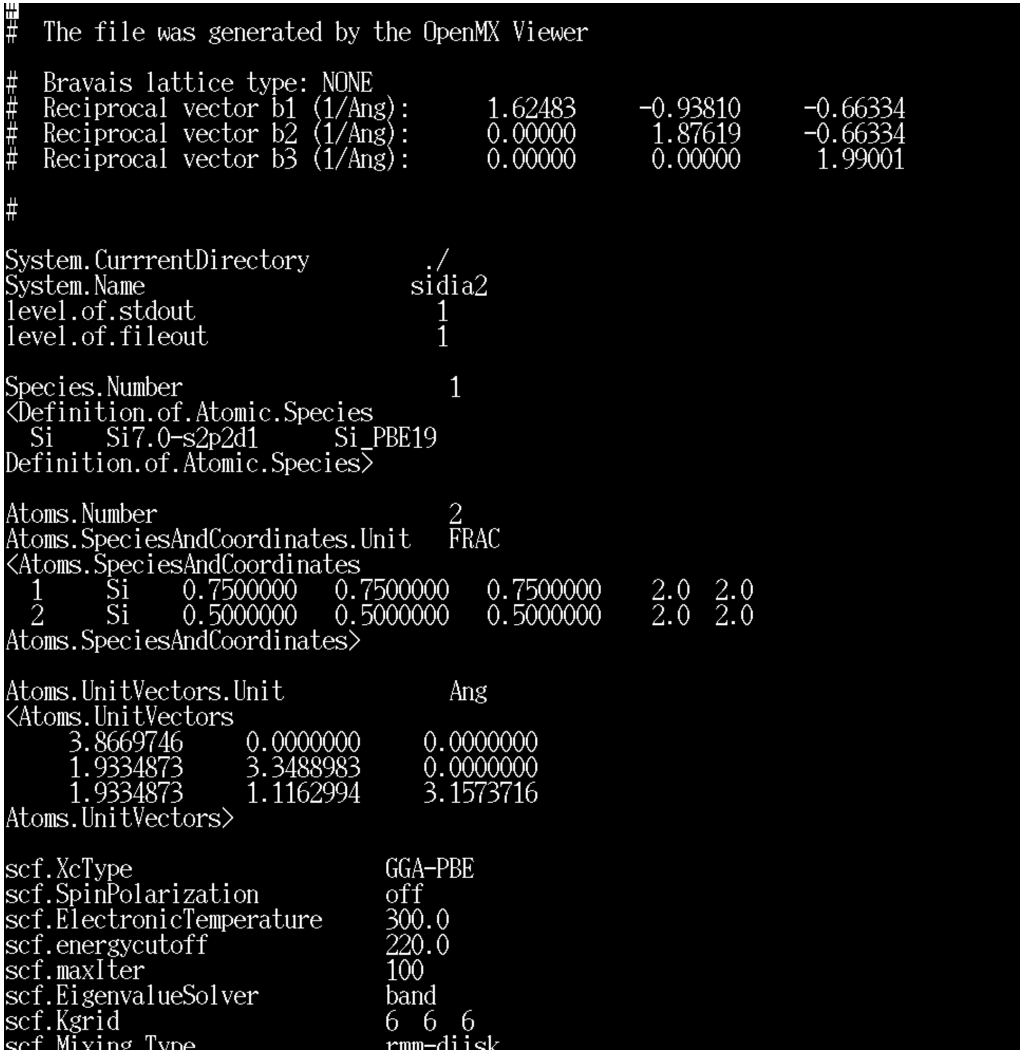


(1) Choose ‘OMX(frac)’.



(2) ‘abc.dat’ is saved.

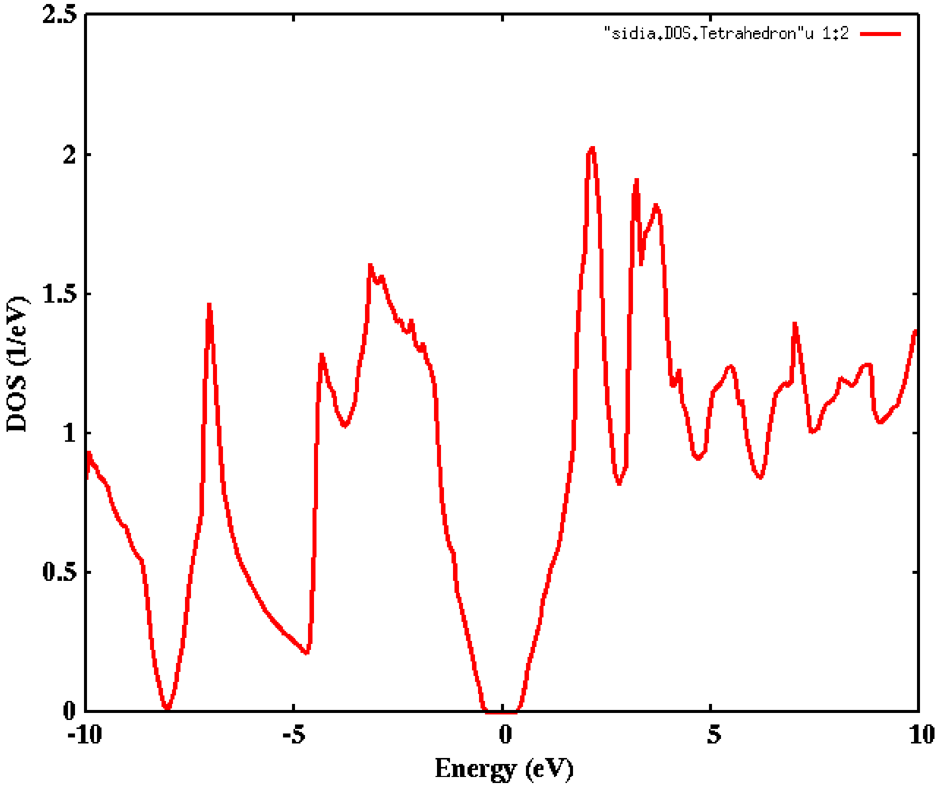
‘abc.dat’ is an input file for OpenMX.



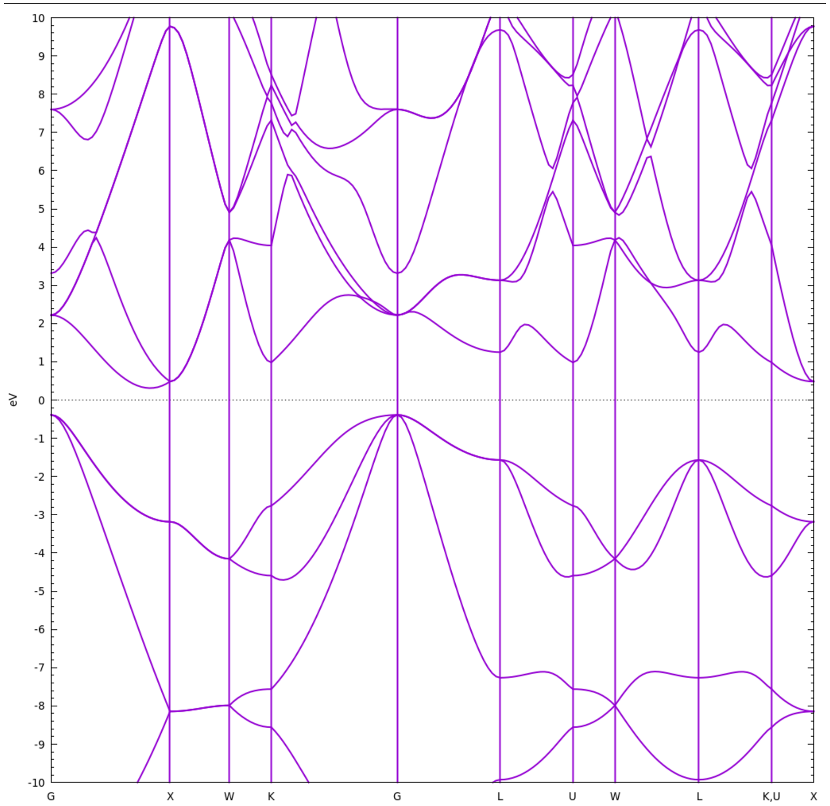
```
#
#  The file was generated by the OpenMX Viewer

#  Bravais lattice type: NONE
#  Reciprocal vector b1 (1/Ang):     1.62483     -0.93810     -0.66334
#  Reciprocal vector b2 (1/Ang):     0.00000      1.87619     -0.66334
#  Reciprocal vector b3 (1/Ang):     0.00000      0.00000      1.99001

#

System.CurrrentDirectory         ./
System.Name                     sidia2
level.of.stdout                   1
level.of.fileout                  1

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

Atoms.Number                       2
Atoms.SpeciesAndCoordinates.Unit   FRAC
<Atoms.SpeciesAndCoordinates
  1      Si     0.7500000   0.7500000   0.7500000    2.0  2.0
  2      Si     0.5000000   0.5000000   0.5000000    2.0  2.0
Atoms.SpeciesAndCoordinates>

Atoms.UnitVectors.Unit             Ang
<Atoms.UnitVectors
     3.8669746     0.0000000     0.0000000
     1.9334873     3.3488983     0.0000000
     1.9334873     1.1162994     3.1573716
Atoms.UnitVectors>

scf.XcType                    GGA-PBE
scf.SpinPolarization          off
scf.ElectronicTemperature     300.0
scf.energycutoff              220.0
scf.maxIter                   100
scf.EigenvalueSolver          band
scf.Kgrid                     6  6  6
scf.Mixing.Type               rmm-diisk
```

Getting started with a cif file #3

Please rename ‘abc.dat’ to ‘Sidia.dat’, and change the keywords as “Dos.fileout on” and “Band.dispersion on” to calculate DOS and band dispersion. By performing the calculation, one can get the following figures.



How to calculate the DOS can be found at
http://www.openmx-square.org/openmx_man3.9jp/node70.html



How to calculate the band dispersion can be found at
http://www.openmx-square.org/openmx_man3.9jp/node68.html

Input file for the band calculation of Si #1

Keyword is not case sensitive.
The order of the Keyword is arbitrary.

```
System.CurrrentDirectory          ./
```

The output directory of output files is specified by this keyword.
The default is './'.

```
System.Name                 sidia
```

The file name of output files is specified by this keyword.

```
level.of.stdout            1
```

The amount of the standard output during the calculation is controlled by the keyword 'level.of.stdout'. In case of 'level.of.stdout=0', minimum information. In case of 'level.of.stdout=1', standard information. In case of 'level.of.stdout=2', additional information together with the minimum output information. 'level.of.stdout=3' is for developers. The default is 1.

```
level.of.fileout           1
```

The amount of information output to the files is controlled by the keyword 'level.of.fileout'. In case of 'level.of.fileout=0', minimum information (no Gaussian cube and grid files). In case of 'level.of.fileout=1', standard output. In case of 'level.of.fileout=2', additional information together with the standard output. The default is 1.

```
data.path                 ../
```

The path to the VPS and PAO directories can be specified in your input file by the keyword. Both the absolute and relative specifications are available. The default is '../DFT_DATA19'.

Input file for the band calculation of Si #2

```
Species.Number                 1
```

The number of atomic species in the system is specified by the keyword.

```
<Definition.of.Atomic.Species
  Si    Si7.0-s2p2d1     Si_PBE19
Definition.of.Atomic.Species>
```

Specify the prototype species by specifying the filenames of both pseudoatomic basis functions and pseudopotentials. These files are located in the directories "DFT_DATA19/PAO" and "DFT_DATA19/VPS", respectively.

- ‘Si7.0’ corresponds to ‘Si7.0.pao’.
- '-s2p2d1' means to select two s-orbitals, two p-orbitals, and one d-orbital as the radial function. In this case, $2 \times 1 + 2 \times 3 + 1 \times 5 = 13$ bases will be assigned to silicon Si.

The destination of Si7.0.pao and Si_PBE19.vps is specified by the following keyword.

```
DATA.PATH    ../DFT_DATA19     # default=../DFT_DATA19
```

Default setting is ‘../DFT_DATA19’

Input file for the band calculation of Si #3

```
Atoms.Number                    2
```

The total number of atoms in the system is specified by the keyword.

```
Atoms.SpeciesAndCoordinates.Unit   FRAC
```

The unit of the atomic coordinates is specified by the keyword

Angstrom → Ang
Atomic unit → AU
fractional coordinate → FRAC

In the fractional coordinates, the coordinates can range from 0.0 to 1.0, and the coordinates beyond its range will be automatically adjusted after the input file is read.

Input file for the band calculation of Si #4

The atomic coordinates and the number of spin charge are given by the keyword.

```
<Atoms.SpeciesAndCoordinates
  1    Si   0.7500000  0.7500000  0.7500000   2.0  2.0
  2    Si   0.5000000  0.5000000  0.5000000   2.0  2.0
Atoms.SpeciesAndCoordinates>
```

1st column: a sequential serial number for identifying atoms
2nd column: Specify the species defined in the first column of ‘Definition.of.Atomic.Species’
3-5 columns: Specify x, y, and z coordinates, respectively
When 'FRAC' is chosen for the keyword 'Atoms.SpeciesAndCoordinates.Unit', the third, fourth, and fifth columns are fractional coordinates spanned by **a**, **b**, and **c**-axes, where the coordinates can range from 0.0 to 1.0, and the coordinates beyond its range will be automatically adjusted after the input file is read.
6-7 columns:
The sixth and seventh columns give the number of initial charges for up and down spin states of each atom, respectively. The number of valence electron for each atom can be found at
http://www.openmx-square.org/openmx_man3.9jp/node27.html

When you calculate spin-polarized systems using 'LSDA-CA' or 'LSDA-PW', you can give the initial spin charges for each atom, which might be those of the ground state, to accelerate the SCF convergence.

Input file for the band calculation of Si #5

```
Atoms.UnitVectors.Unit          Ang
```

The unit of the vectors for the unit cell is specified by the keyword 'Atoms.UnitVectors.Unit'. Please specify 'Ang' when you use the unit of Angstrom, and 'AU' when the unit of atomic unit.

```
<Atoms.UnitVectors
  3.8669746   0.0000000   0.0000000
  1.9334873   3.3488983   0.0000000
  1.9334873   1.1162994   3.1573716
Atoms.UnitVectors>
```

Keywords specifying the vectors **a**, **b**, and **c** of the unit cell. The first, second and third rows correspond to vectors **a**, **b**, and **c** of the unit cell, respectively.

Input file for the band calculation of Si #6

```
scf.XcType                  GGA-PBE
```

The keyword ‘scf.XcType’ specifies the exchange-correlation potential.

Ceperley-Alder LDA ⇒ LDA、
Ceperley-AlderLSDA ⇒ LSDA-CA
Perdew-Wang LSDA ⇒ LSDA-PW
GGA by PBE ⇒ GGA-PBE

```
scf.SpinPolarization        off
```

The keyword 'scf.SpinPolarization' specifies the non-spin polarization or the spin polarization for the electronic structure. If the calculation for the spin polarization is performed, then specify 'ON'. If the calculation for the non-spin polarization is performed, then specify 'OFF'. When you use 'LDA' for the keyword 'scf.XcType', the keyword 'scf.SpinPolarization' must be 'OFF'. In addition to these options, 'NC' is supported for the non-collinear DFT calculation. For this calculation, see also the Section 'Non-collinear DFT'.

```
scf.ElectronicTemperature   300.0
```

The electronic temperature (K) is given by the keyword. The default is 300 (K).

```
scf.energycutoff            220.0
```

The keyword 'scf.energycutoff' specifies the cutoff energy which is used in the calculation of matrix elements associated with difference charge Coulomb potential and exchange-correlation potential and the solution of Poisson's equation using fast Fourier transform (FFT). The default is 150 (Ryd).

Input file for the band calculation of Si #7

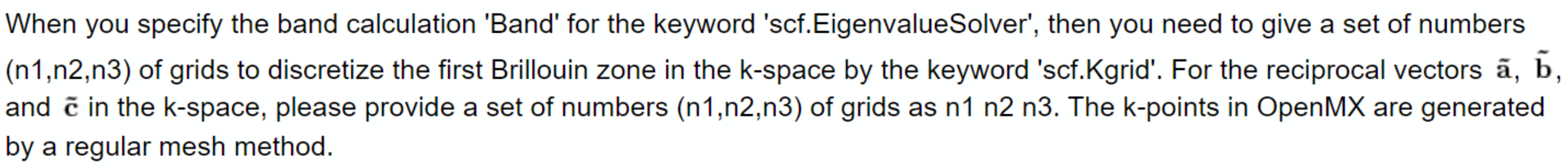
scf.maxIter 100

The maximum number of SCF iterations is specified by the keyword 'scf.maxIter'. The SCF loop is terminated at the number specified by 'scf.maxIter' even if a convergence criterion is not satisfied. The default is 40.

scf.EigenvalueSolver band

The solution method for the eigenvalue problem is specified by the keyword 'scf.EigenvalueSolver'. An O(N) divide-conquer method 'DC', an O(N) divide-conquer method with localized natural orbitals 'DC-LNO', an O(N) Krylov subspace method 'Krylov', a numerically exact low-order scaling method 'ON2', the cluster calculation 'Cluster', and the band calculation 'Band' are available.

scf.Kgrid 6 6 6



When you specify the band calculation 'Band' for the keyword 'scf.EigenvalueSolver', then you need to give a set of numbers (n1,n2,n3) of grids to discretize the first Brillouin zone in the k-space by the keyword 'scf.Kgrid'. For the reciprocal vectors $\tilde{\mathbf{a}}$, $\tilde{\mathbf{b}}$, and $\tilde{\mathbf{c}}$ in the k-space, please provide a set of numbers (n1,n2,n3) of grids as n1 n2 n3. The k-points in OpenMX are generated by a regular mesh method.

Input file for the band calculation of Si #8

scf.Mixing.Type rmm-diisk

This keyword specifies the electron density mixing method for generating the electron density (or density matrix) that will be input to the next iteration step of the SCF calculation. Select one of the following methods: Simple Mixing (Simple), Guaranteed-Reduction Pulay (GR-Pulay), RMM-DIIS, Kerker, RMM-DIISK, RMM-DIISV, or RMM-DIISH.

scf.Init.Mixing.Weight 0.05

A keyword specifying the initial mixing ratio. Valid range is 0<scf.Init.Mixing.Weight<1. Default value is 0.3.

scf.Min.Mixing.Weight 0.01

The keyword 'scf.Min.Mixing.Weight' gives the lower limit of a mixing weight in the simple and Kerker mixing methods. The default is 0.001.

scf.Max.Mixing.Weight 0.30

The keyword 'scf.Max.Mixing.Weight' gives the upper limit of a mixing weight in the simple and Kerker mixing methods. The default is 0.4.

scf.Mixing.History 25

In the GR-Pulay method, the RMM-DIIS method, the Kerker method, the RMM-DIISK method, the RMM-DIISV method, and the RMM-DIISH method, the input electron density (Hamiltonian) at the next SCF step is estimated based on the output electron densities (Hamiltonian) in the several previous SCF steps. The keyword 'scf.Mixing.History' specifies the number of previous SCF steps which are used in the estimation. For example, if 'scf.Mixing.History' is specified to be 3, and when the SCF step is 6th, the electron densities at 5, 4, and 3 SCF steps are taken into account. Around 30 is a better choice.

scf.Mixing.StartPulay 15

The SCF step which starts the GR-Pulay, the RMM-DIIS, the Kerker, the RMM-DIISK, the RMM-DIISV method, or the RMM-DIISH methods is specified by the keyword 'scf.Mixing.StartPulay'. The SCF steps before starting these Pulay-type methods are then performed by the simple or Kerker mixing methods. The default is 6.

scf.criterion 1.0e-7

Convergence criterion for the SCF calculation (in Hartree units)

Input file for the band calculation of Si #9

Keywords for the DOS calculation:

```
Dos.fileout             on
Dos.Erange           -15.0  10.0
Dos.Kgrid             12 12 12
```

How to calculate the DOS can be found at
http://www.openmx-square.org/openmx_man3.9jp/node70.html

Keywords for the calculation of band dispersion:

```
Band.dispersion          on
Band.Nkpath             10
<Band.kpath
  30  0.000000 0.000000 0.000000   0.500000 0.000000 0.500000   G X
  15  0.500000 0.000000 0.500000   0.500000 0.250000 0.750000   X W
  11  0.500000 0.250000 0.750000   0.375000 0.375000 0.750000   W K
  32  0.375000 0.375000 0.750000   0.000000 0.000000 0.000000   K G
  26  0.000000 0.000000 0.000000   0.500000 0.500000 0.500000   G L
  19  0.500000 0.500000 0.500000   0.625000 0.250000 0.625000   L U
  11  0.625000 0.250000 0.625000   0.500000 0.250000 0.750000   U W
  22  0.500000 0.250000 0.750000   0.500000 0.500000 0.500000   W L
  19  0.500000 0.500000 0.500000   0.375000 0.375000 0.750000   L K
  11  0.625000 0.250000 0.625000   0.500000 0.000000 0.500000   U X
Band.kpath>
```

How to calculate the band dispersion can be found at
http://www.openmx-square.org/openmx_man3.9jp/node68.html