User Guide

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This is a guide for TB package users.

1. TBIN

TBIN is a file containing most of the material parameters, excluding hopping terms and k points.

Here are the rules.

Name xxx # Name of the material, default value is “Material”.

Dim 2 or 3 # Dimension, default value is 3

Spin 0 or 1 # Consider spin or not, default value is 0

SGN NO.SG # Number of space group (1~230), default value is 1

Nbr N or N1 N2 (N3) # Farthest of unit cells

LatVecSG # Lattice vectors of space group operators

A1 # 1st Lattice vector (space group)

A2 # 2nd Lattice vector (space group)

A3 # 3rd Lattice vector (space group)

LatVec # Lattice vectors

a1 # 1st Lattice vector

a2 # 2nd Lattice vector

a3 # 3rd Lattice vector

AtTpNum n # Number of atom types

Bases # Atoms and orbitals

AtomName1 AtomNumber1 OrbitalName1

AtomName2 AtomNumber2 OrbitalName2

…

AtomSite # Atoms sites

Site1

Site2

…

The order is not important.

Orbital name can be 1S, 2S, 2P, 3S, 3P, 3D, 4S, 4P, 4D, 4F, 5S, 5P, 5D, 5F, 6S, 6P, 6D, 6F, 7S, 7P, 7D, 7F and 1s, 2s, 2px, 2py, 2pz, 3s, 3px, 3py, 3pz, 3dxy, 3dyz, 3dzx, 3dx2-y2, 3dz2, 4s, 4px, 4py, 4pz, 4dxy, 4dyz, 4dzx, 4dx2-y2, 4dz2, 4fz3, 4fxz2, 4fyz2, 4fxyz, 4fz(x2-y2), 4fx(x2-3y2), 4fy(3x2-y2), 5s, 5px, 5py, 5pz, 5dxy, 5dyz, 5dzx, 5dx2-y2, 5dz2, 5fz3, 5fxz2, 5fyz2, 5fxyz, 5fz(x2-y2), 5fx(x2-3y2), 5fy(3x2-y2), 6s, 6px, 6py, 6pz, 6dxy, 6dyz, 6dzx, 6dx2-y2, 6dz2, 6fz3, 6fxz2, 6fyz2, 6fxyz, 6fz(x2-y2), 6fx(x2-3y2), 6fy(3x2-y2), 7s, 7px, 7py, 7pz, 7dxy, 7dyz, 7dzx, 7dx2-y2, 7dz2, 7fz3, 7fxz2, 7fyz2, 7fxyz, 7fz(x2-y2), 7fx(x2-3y2), 7fy(3x2-y2).

Missed principal quantum number is also allowed: S, P, D, F and s, px, py, pz, dxy, dyz, dzx, dx2-y2, dz2, fz3, fxz2, fyz2, fxyz, fz(x2-y2), fx(x2-3y2), fy(3x2-y2).

In Nbr, N means N N for 2D and N N N for 3D. N1 N2 is for 2D, and N1 N2 N3 is for 3D. All the atoms in the unit cells [n1, n2 (, n3)] with will be considered. But those are symmetrically related to atoms outside the region will be neglected.

Lattice vectors should be chosen as the bases of space group symmetry operations in Bilbao (<https://www.cryst.ehu.es/cryst/get_gen.html>).

Example of graphene

Name Graphene

Dim 2

Spin 0

SGN 191

Nbr 1

LatVecSG

0.50000000 -0.86602540 0.00000000

0.50000000 0.86602540 0.00000000

0.00000000 0.00000000 1.00000000

LatVec

0.50000000 -0.86602540 0.00000000

0.50000000 0.86602540 0.00000000

0.00000000 0.00000000 1.00000000

AtTpNum 1

Bases

C 2 pz

AtomSite

0.33333333 0.66666666 0.00000000

0.66666666 0.33333333 0.00000000

1. HopValIN

HopValIN is a file containing values of hopping terms according to HopFree in data/Name/.

In HopFree, each line is the index of a free hopping term. The first 5 integers are n1, n2, n3, iAt, jAt, and the last two strings are iOrb and jOrb. It means hopping from iOrb of iAt in cell [0,0,0] to jOrb of jAt in cell [n1, n2, n3]. The redundant terms will be neglected, and the missing ones will be completed with zeros.

The form of HopValIN should be like the follows.

HopVal1

HopVal2

…

HopValN

Each HopValn should be a float number.

Example (h-BN):

1.0

1.1

1.2

0.01

0.02

0.03

0.04

0.0

0.0

1. KptIN

HopValIN is a file containing information of k points.

First line is Method, including “Volume”, “Line”, “Point”.

For Method “Volume”, it calculates uniformly distributed k points in the whole Brillouin zone. The second line is nk1 nk2 (nk3), all of whom are integers. For 2D, it is nk1 nk2 or nk1 nk2 1 and nk = [nk1, nk2, 1]. For 3D, it is nk1 nk2 nk3 and nk = [nk1, nk2, nk3].

Form:

Volume

nk1 nk2 (nk3)

Example:

Volume

10 10 1

For Method “Line”, it calculates almost uniformly distributed k points on a fold line. The second line is nk, an integer, which is the total number of k points. The following three lines are lattice vectors. The following lines are k points in form of m1 m2 m3 (“KptName”). [m1, m2, m3] are endpoints (in unit of reciprocal lattice vectors) of the fold line. And “KptName” is the name of k points.

Form:

Line

nk

a1

a2

a3

m11 m12 m13 (“KptName1”)

m21 m22 m23 (“KptName2”)

…

mN1 mN2 mN3 (“KptNameN”)

Example (Graphene):

Line

100

0.50000000 -0.86602540 0.00000000

0.50000000 0.86602540 0.00000000

0.00000000 0.00000000 1.00000000

0.0000 0.0000 0.0000 ${\Gamma}$

0.0000 0.5000 0.0000 M

-0.3333 0.6667 0.0000 K

0.0000 0.0000 0.0000 ${\Gamma}$

For Method “Point”, it calculates any inputted k points.

Form:

Point

m11 m12 m13

m21 m22 m23

…

mN1 mN2 mN3

Example:

Point

0.0000 0.0000 0.0000

0.0000 0.5000 0.0000

-0.3333 0.6667 0.0000

0.0000 0.0000 0.0000

1. BerIN

BerIN is a file containing information of Intrinsic AHC & ANC calculations.

First line is nk0. The number of k points is nk0^Dim, where Dim is the dimension.

Second line is temperature.

Third line is Fermi energy.

Form:

nk0

Tem1 Tem2 … TemN

EF1 EF2 … EFN

Example:

10

0.0 0.0 0.0 0.0 0.0

-0.2 -0.1 0.0 0.1 0.2

1. DosIN

DosIN is a file containing information of density of states (DOS).

First line is Method including “Diag”-“Diagonalization of Hamiltonian”, “Inv”-“Inverse to calculate Green’s function”, “KPM”-“Kernel Polynomial Method”. It will be further explained in DOS.docx.

If Method is “Diag” or “Inv”:

Second line is Emin, Emax, nE, eta. The input energy is np.linspace(Emin,Emax,nE). eta is the in definition of Green’s function .

Third line is nk0. The number of k points is nk0^Dim, where Dim is the dimension.

If Method is “KPM”:

Second line is Emin, Emax, nE.

Third line is nk0.

Forth line is nsr. The number of series in Chebyshev polynomials expansion.

Form:

Method

Emin Emax nE (eta)

nk0

(nsr)

Example1:

Diag

-5 5 1001 0.01

100

Example2:

KPM

-5 5 1001

100

100

1. QcIN

QcIN is a file containing information of quantum conductance in 2D material.

First line is Method including “Eigsolution” and “Iteration”

Second line is Emin, Emax, nE, eta. The input energy is np.linspace(Emin,Emax,nE). eta is add to the imaginary part of energy: .

Third line is c1, c2, Dir. c1 and c2 are parameters to extend the cell that Lattice vector become . Dir is the 1 or 2, which labels the extension direction of strip.

Fourth line is Wid, Len. Wid is the width (number of cells) of strip including center meterial and lead. Len is the length (number of cells) of center meterial

Form:

Method

Emin Emax nE eta

c1 c2 Dir

Wid Len

Example:

Eigsolution

-5 5 201 0.000001

1 1 1

4 10