

TBMAP

Tight-Binding Energy Band Calculation

By using the overlap integrals calculated by SCAL, the energy band and the Fermi surface are calculated on the basis of the tight-binding approximation.

Input data: tbmap.dat
Source: tbmap.f
Indy: tbmap
PC: tbmap

This program generates the following output file:

Output: tbmap.out
Output: tbmap.gra for input of gnuplot

Test Data

The supplied input files are for λ -(BETS)₂FeCl₄.

- (1) Download tbmap.dat and the tbmap executable program suitable for your computer.
 - (2) Run tbmap. This program generates tbmap.out and tbmap.gra. Open tbmap.out and check the calculation is OK.
 - (3) Run gnuplot to draw the energy band and the Fermi surface by opening tbmap.gra.
- The following is the example of the procedure.

```
set yrange [0:10800]
set noborder
set noxtics
set noytics
set nokey
plot "tbmap.gra" with lines
pause -1 "Hit Return Key"
set terminal postscript
set output "tbmap.ps"
replot
quit
```

Input Data

The following is an example of input data in tbmap.dat.

```
6.593      8.975      15.093     93.79      94.97      110.54
  2
  0
-0.0245   -0.0084    -0.0127   -0.0068    -0.0050
      0.0      0.0      0.0
```

```

0 1 1 0
  0.0      1.0      0.0
0 3 0 0
  1.0      0.0      0.0
5 4 0 5
  1.0      1.0      0.0
0 2 0 0
10.0
  2      1      3      20      -25      1      0.0
0.02      -0.5      0.5      0.75
1
0 10 0.0 0.0 0.0
0 5 1.0 -1.0 0.0
1 5 1.0 -1.0 0.0 1.0 0.0 0.0 3 0.0
0 10 1.0 0.0 0.0
0 10 0.0 0.0 0.0
0 10 0.0 1.0 0.0
1 10 0.0 1.0 0.0 1.0 0.0 0.0 3 0.0
10
11

```

Line 1 6.593 8.975 15.093 93.79 94.97 110.54 (6F10.0)

Lattice constants. a, b, c, α , β , and γ . When the angles are 90° , the columns may remain blank.

Line 2 2 (15, 12F5.0)

A unit cell contains two molecules. If the energy levels of these molecules are different owing to charge separation, write the difference.

Line 3 0 (12F5.0)

Positions of molecules. All molecules may be put on (0.0, 0.0, 0.0).

Line 4 -0.0245 -0.0084 -0.0127 -0.0068 -0.0050 (6F10.0)

p1 p2 q1 q2 c

Overlap integrals calculated by SCAL. When zero appears at the n -th entry, the number of the overlap is assumed to be $n-1$. The maximum number of these lines is three, so that we can put maximum 18 overlaps. When the number of the overlaps are just six, input the second blank line. If n is less than six, the second line is not necessary.

Line 5 Blank (F10.0)

The value of E in $t = E \times S$. If this line is blank, $E = -10$ eV is assumed.

Line 6 0.0 0.0 0.0 (3F10.0)

Translation that specifies the neighboring cell.

Line 7 0 1 1 0 (30I2)

This means a matrix like:

```

0 1
1 0

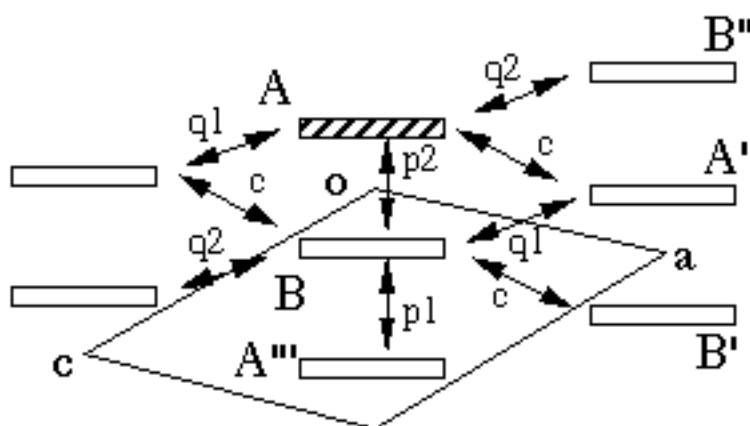
```

1 means the first overlap read in Line 4 is placed between the first molecule in the original cell and the second molecule in the translated cell. Now the translation is (0.0, 0.0, 0.0) so that this matrix represents the overlaps within the original cell.

The first translation should be always (0.0, 0.0, 0.0), in which the diagonal elements are zero and the non-diagonal elements are symmetrical.

Lines 6 and 7 are repeated until all interactions are covered. When $x \geq 10.0$ appears, proceed to the next input.

The above example is for β -(BEDT-TTF)₂I₃ shown in beta.gif.



Two molecules in the original unit cell are designated as A and B in Figure 1. Note these molecules are different from SCAL calculation. As for the original cell (0.0, 0.0, 0.0), the matrix is

$$\begin{matrix} 0 & 1 \\ 1 & 0 \end{matrix}$$

so that between A and B is the first overlap. The numbering of the overlap follows the order of Line 4, then the first overlap is p_1 . The second translation (0.0, 1.0, 0.0) is accompanied by the matrix

$$\begin{matrix} 0 & 3 \\ 0 & 0. \end{matrix}$$

From the first molecule (A) in the original cell to the second molecule (B') in the translated cell, there is the third overlap (q_1). The next translation is (1.0, 0.0, 0.0) with the matrix

$$\begin{matrix} 5 & 4 \\ 0 & 5. \end{matrix}$$

This translation generates A'' and B'', so that from A to A'' is the fifth overlap (c), from A to B'' is the fourth (q_2), from B to A'' is nothing (0), and from B to B'' is the fifth (c). The final translation (1.0, 1.0, 0.0) covers the A-B''' interaction designated as p_2 .

$$\begin{matrix} 0 & 2 \\ 0 & 0 \end{matrix}$$

Line 8 2 1 3 20 -25 1 0.0 (6I5, F10.0)

2: Horizontal axis of the map and the drawing of the Fermi surface is k_b -axis.

1: Vertical axis of the map and the drawing of the Fermi surface is k_a -axis.

3: Section of the map is k_c -axis.

20: The mesh of the horizontal axis is 20. Then the map is calculated from $k_b = 0.0$ to $k_b = \pi/b$ with the interval of $\pi/20b$.

-25: The mesh of the vertical axis is 25. Then the map is calculated from $k_a = -\pi/b$ to $k_a = \pi/b$ with the interval of $\pi/25a$.

1: The mesh of the k_c -axis is one, Then the map is calculated only at $k_c = 0.0$.

The map is written in meV unit. If you want to change this scale, the output energy is multiplied by this number. 1000 is the default.

Line 9 0.02 -0.5 0.5 0.75 (4F10.0)

Calculation of the density of states. The program counts the number of states starting from -0.5 eV to 0.5 eV with the interval of 0.02 eV. Fill 0.75 of this band. 1.0 corresponds to totally filled, 0.75 to quarter filled (2:1 composition), and 0.5 to half-filled. The Fermi surface is searched on the basis of this number.

Line 10 1 (11)

Draw the energy band diagram, when 1. Not draw when 0.

Line 11 0 10 0.0 0.0 0.0 (2I5, 3F10.0)
0 5 1.0 -1.0 0.0

Instruction for drawing the energy band diagram. The program calculates the energy band from the Γ point (0.0, 0.0, 0.0) to $(\pi/a, -\pi/b, 0.0)$ with 1/10 intervals. The above input generates the following sequence as shown in Figure 2. If the first number is not zero like,

1 5 1.0 -1.0 0.0 1.0 0.0 0.0 3 0.0

this means the crossing point of the lines going through $(\pi/a, -\pi/b, 0.0)$ and $(\pi/a, 0.0, 0.0)$, then the V point in Figure 2. The final "3 0.0" stands for $k_z = 0.0$ at this crossing point. When the first column is greater than 2, proceed to the next line.

Line 12 11 (2I1)

Draw the Fermi surface diagram, when 1. Not draw when 0.

For Your Own Crystal

Construct your input data according to the above instruction, and run tmap.