TEP

Temperature dependence of thermoelectric power from Tight-Binding Energy Band Calculation

Temperature dependence of thermoelectric power is calculated according to the relaxation time approximation and the energy band.

$$\mathbf{S}_{ij} = (1/eT)\sum (\mathbf{K}_0^{-1})_{ij}\, \mathbf{K}_{1,kj} \qquad (i,\ j,\ k = x,\ y,\ z)$$

$$\mathbf{K}_{0,\,ij} = (1/4\pi^3)(t/h) \int\int v_i v_j (-\partial f^0/\partial \varepsilon)(dS/v)d\varepsilon$$

$$\mathbf{K}_{1,\,ij} = (1/4\pi^3)(t/h) \int\int v_i v_j (-\partial f^0/\partial \varepsilon)\ (\varepsilon - E_F)\ (dS/v)d\varepsilon$$

Input data: tep.dat
Source: tep.f
Indy: tep
PC: tep.exe

This program generates the following output file:

Output: tep.out
Output: tep.grafor input of gnuplot

When you publish any results calculated by the present programs, you are requested to cite

T. Mori and H. Inokuchi, *J. Phys. Soc. Jpn.*, **57**, 3674 (1988).

Test Data

The supplied input files are for b -(BEDT-TTF)$_2$I$_3$.
(1) Download tep.dat and the tep executable program suitable for your computer.
(2) Run tep. This program generates tep.out and tep.gra. Open tep.out and check the calculation is OK.
(3) Run gnuplot to draw the energy band and the Fermi surface by opening tep.gra. The following is the example of the procedure.

```
set noborder
set noxtics
set noytics
set nokey
plot "tep.gra" with lines
set terminal postscript
set output "tep.ps"
replot
```

quit

Input Data

The following is an example of input data in tep.dat.
The input data are the same as tbmap.dat except the final four lines.

```
6.593      8.9757     15.093     93.79      94.97      110.54
    20.0   0.0
0.25  0.75 0.0   0.75 0.25  0.0
0.0062     0.0034     0.0039     0.0026     0.0039
10.0
0.0        0.0        0.0
 0  4  4  0
1.0        0.0        0.0
 5  0  1  5
0.0        1.0        0.0
 0  2  0  0
-1.0       1.0        0.0
 0  3  0  0
10.0
    2     1     3    20   -20     1                  1
 0.01        -0.2        0.3         0.75
1
 0  100.0   0.0   0.0
 0   51.0   -1.0  0.0
 1   51.0   -1.0  0.0   1.0   0.0   0.0        30.0
 0  101.0   0.0   0.0
 0  100.0   0.0   0.0
 0  100.0   1.0   0.0
 1  100.0   1.0   0.0   1.0   0.0   0.0        30.0
1
11

   13     2     0     0     0     1     0
  500   450   400   350   300   250   200   150   100    50    30    20    10
    0   300  -100   200   550
```

Line 13 `13  2  0  0  0  1` (7I5)

NTER = 13: The number of temperature points to be calculated.
NDC = 2: Upper 2 energy levels are used for the TEP calculation. These energy levels are those having the Fermi surfaces.
NDG1 = 0 : Zone boundary along the horizontal axis is non degenerated (= 0) or degenerated (= 1).
NDG2 = 0: Zone boundary along the vertical axis is non degenerated (= 0) or degenerated (= 1).
NWRIT = 0: To supress the output of V^2 map. =1 to output.

NDRAW = 1: To output S(T) graph to tep.gra. =0 to supress the output.

NTATE = 0: Normal output. Not zero to convert the tensor.

Line 14 500 450 400 350 300 250 200 150 100 50 30 20

(12I5)

Temperature points (K) to be calculated. NTER points from the previous line. If NTER < 0, the fist entry designates the highest temperature, and the second means the interval. If NTEP > 12, it needs the second line.

Line 15 0 300 -100 200 550 (5I5)

Specify the graph in tep.gra.

TMIN = 0: The temperature minimum.

TMAX = 300: The temperature maximum, by draw the S(T) curve up to TMAX2

SMIN = -100: The S(T) mimimum.

SMAX = 550: The S(T) maximum.

TMAX2: Maximum temperature for the S(T) curve.