

# Energy Band Calculation of Molecular Conductors

This is an instruction manual for computer program for energy band calculation particularly designed for molecular conductors. The molecular orbital calculation is performed by extended Hückel method.

## Contents

The programs are divided into the following independent programs:

extdh	extended Hückel molecular orbital calculation for a single molecule
scal	calculation of intermolecular orbital overlap integrals
tbmap	tight-binding energy band calculation

Instruction	Input File	Source	Indy	PC	Output File
extdh.doc	extdh.dat	extdh.f	extdh.out		hdat.d1
scal.doc	scal.dat	scal.f	scal.out		sdat.d1
tbmap.doc	tbmap.dat	tbmap.f	tbmap.out		tbmap.out tbmap.gra
planea.doc	planea.dat	planea.f	planea.out		pdat.d1
	atoms.dat	trmo.f	trmo.out		at.dat

The source is coded by FORTRAN, so the program is executable on any computer system which has FORTRAN compiler. Executable forms are supplied for Indy and PC.

## To run the test data

The supplied input files are for  $1-(\text{BETS})_2\text{FeCl}_4$ .

- (1) Download all input files and executable programs suitable for your computer.
- (2) Change the filename extdh.A.dat to extdh.dat. This is for the A BETS molecule.
- (3) Run extdh. This program generates hdat.d1 and fort.10. Open hdat.d1 and confirm that the calculation is normally ended.
- (4) Change the filename hdat.d1 to hdat.d2, extdh.dat back to extdh.A.dat, and extdh.B.dat to extdh.dat.
- (5) Run extdh. This program generates new hdat.d1 and fort.20. Open hdat.d1 to see the calculation is OK.
- (6) Run scal. This program reads data from fort.10 and fort.20 as well as scal.dat. This program generates sdat.d1. Open sdat.d1, and check the calculation is OK.
- (7) Run tbmap, which reads input data from tbmap.dat. This program generates tbmap.out and tbmap.gra. Tmap.gra is an input data for gnuplot to draw the energy band and the Fermi surface. To run gnuplot, consult tbmap.doc. This tbmap is an independent program, and you can use it without running other programs.
- (8) The program planea is for calculating the geometry of two molecules. This is an independent program.

## To calculate energy band of your own crystal,

- (1) In extdh.dat, change lattice constants, atomic coordinates, and electron number.

(2) For the user of teXsan, the format of atomic coordinates is transformed by trmo. Run trmo, which reads atomic coordinates from atoms.dat, and generates at.dat. Copy at.dat in extdh.dat and move the atomic coordinates to the appropriate place. Before doing this, calculate positions of hydrogen atoms. If there is a molecule located on an inversion center or other symmetry operations, make the complete molecule before changing the format.

(3) Run extdh. If there are more than one crystallographically independent molecules, repeat the calculation for each molecule, as shown in the above example.

(4) Copy extdh.dat on the top of scal.dat. Rearrange the atomic coordinates and the positions of lattice constants. Define the intermolecular vectors. Run the program.

(5) In tmap.dat, change lattice constants. Form sdat.d1, input the intermolecular overlap integrals calculated by scal. Define the molecular interactions.

(6) Run tmap and see tmap.out.

(7) Draw the energy band and Fermi surface by gnuplot.

## Hückel Parameters

When your crystal contains other atoms, see

<http://www.op.titech.ac.jp/lab/mori/EHTB/EHTB~1.html>

As for the theoretical background of this program, consult Refs. 1 and 2. When you publish any results calculated by the present programs, you are requested to cite Ref. 1.

- 1) T. Mori, A. Kobayashi, Y. Sasaki, H. Kobayashi, G. Saito, and H. Inokuchi, *Bull. Chem. Soc. Jpn.*, **57**, 627 (1984).
- 2) T. Mori, *Doctor Thesis*, Univ. Tokyo (1985), Chap. 4.