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College on Computational Physics

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LMTO Programs

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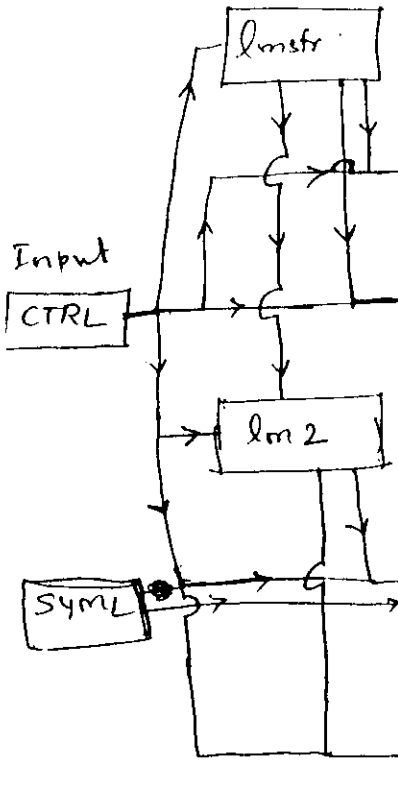
LMTO Programs

/home/lecturer/public/electron/lmto/source
" " " " " /plot



lmstr → Calculates the Structure Constants. Is a must before executing any other program.

lmhart → Calculates Hartree potential. Useful for looking into voids in the potential. (requires lmstr)

lmorl → To get the percentage overlap of the atomic spheres. (After lmstr).

lm2 → self-consistency (Requires the output of lmstr)

lmbnd → To get band structure after self-consistency at points specified by the file SYML

lmdos → Density of states calculation

- Whenever you want to redo the self-consistency from the scratch delete the files MIXM, MOMS and Atomic files (which have the name given as ATOM = CU)

- To plot bands: Execute 'gnubnd.x' after executing 'lmbnd'. It creates BNDS.GNU. Give 'gnuplot' command and give load 'BNDS.GNU' to get the plot. Use appropriate inputs in the interactive mode.

- To plot DOS: Execute 'gnudos.x' after 'lmdos'. Creates 'DOS.GNU'. Execute 'gnuplot' command. Give load 'DOS.GNU' to get the plot.
(important: When it asks for number of the DOS to be plotted give 1 2 3 / for s p d.)

(1)

Description of the 'CTRL' input file

HEADER — Any string for title.

VERS — Version of the program. It's 'LMASA-4'.

IO

SHOW = T

HELP = F — Give T if you need more information on the screen output.

VERBOS = 40 — Extent of the screen output. More the value more the detail you get.

WKP = F

OPTIONS

NSPIN = 1 for paramagnetic case, = 2 for spin-polarised case.

REL = T Relativistic, = F if non-relativistic

CCOR = T To include the combined correction term for structure constants; = F will not include.

ADNF = T for Automatic downfolding of s, p, or d character; = F is according to our input in IDXDN under CLASS (see below).

BEGIATOM = F For doing band structure calculations

= T for doing atomic calculation

NIATOM = no. of iterations needed in the atomic structure calculations (30 for atom; 5 for bands)

CHARGE = T if you want calculate charge density (A run of self consistency is essential before this)

= F do not calculate charge density.

Q = ATOM for atomic structure

= BAND for band structure (also default)

SYMGRP R4X MX R3D (for cubic symmetry)

Symmetry group of generator of the lattice.
R. stands for rotation followed by 4 indicates the 4-fold and X is generic for x, y and z axes.
M - mirror reflection about axes.
D - for ~~unit~~ Diagonal.

BZ NKABC. = 6 6 6
No. of k-points divisions along kx ky and kz directions.

METAL = T If the sample is metallic
: F .. .. non-metallic
(But always use METAL=T and introduce Empty Spheres ES if you want good Convergence and performance ; unless you are sure about the system).

TETRA = T use tetrahedral integration scheme for BZ.

TOL. : 1D-6 Tolerance or accuracy in the integration

STR RMAXS = 3.0 Indicates that the neighbours upto 3 times the lattice constant are considered.

NOCALC : F.

STRUC NBAS = 1 No. of basis atoms within the primitive cell (If more than one there would be as many positions specified and SITE).

NCLASS: 1 No. of different kinds of atoms involved. (CLASS will have as many (NCLASS) specifications)

NL = 3 No. of angular momentum symmetries used.
($NL = l_{max} + 1$)

ALAT : Lattice constant

PLAT : Primitive lattice vectors. (3)

CLASS

ATOM = Element (Symbol / name according to periodic Table.

Z = atomic number

R/W = ratio of the radii of the current specie with the average one.

LMX = maximum l-value

CONF = Valence electron configurations

e.g. for Cu 4S, 4P, 3d.

IDXDW = Level of downfolding or weightage given to the ang. mom. characters.

0 - automatic downfolding, if ADNF = T

1 high

2 low

3 not considered for calculation

(This line is repeated NCLASS times)

SITE

ATOM = Name same as above

(If more than type present each one is given separately)

POS = its position.

(This is repeated NBAS times)

START

NIT = No. of self consistency iterations

BROY = T For using Broyden mixing. This is very fast in bringing in convergence. If there is oscillation better use F option and use linear mixing.

WC = 3.0

NMIX = 2 For Broyden mixing utilise previous 2 iterations

1 for Anderson mixing with BROY = F

0 " linear " with BROY = F.

BETA = 0.4 mixing parameter (under relaxation).

CNVG = 1.D-6 convergence criterion for mag. moment

CNVGET = 1.D-6 " " for Total energy.

FREE = F for band structure

= T for atomic structure

(This should be used along with

BEGATOM = T, Q = ATOM, NIATOM = 80

to get atomic structure).

BEGMOM = T To begin with moments specified by us (with CONTROL=F or from previous iterations)

= F To begin with band structure

CONTROL = T use the parameters given by us.

= F ignore the parameters given by us but use the earlier results.

ATOM : Name.

P = $n + l_d$ n - principle quantum no. for the valence electrons. (Same as CONF above)

l_d - logarithmic derivative.

Curve l_d=0.5 if not sure.

$l_d < 0.5$ for diffused or free electron types

$l_d > 0.5$ for localised cases.

(For copper : 4.5^{s} 4.4^{p} 3.85^{d})

Q = Q_0 Q_1 Q_2

Q_0 = zeroth moment, charge

Q_1 = first moment

Q_2 = second moment of charge density.

HARTREE To run 'lmhart' program.

ORIGIN : 0 0 0 Origin for calculating Hartree potential in a plane.

R1, R2 : Span of the vectors defining the plane.

NDELR1; NDELR2 No of points along R1 and R2.

CHARGE : similar to above as in HARTREE. Used only when CHARGE=T