

HiLAPW

— BASIC EDITION —

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1 Introduction

In these days, band calculation is often called first-principles or *ab initio* calculation. This means that a theoretical study on the basis of band calculation becomes calculating not only band structure but also several physical quantities directly from first principles. There have been three important issues in progress of the first-principles calculation. The first is the establishment of the basic theory, typically density-functional and related theory. The density-functional theory provides a practical approach of one-electron theory through local-density approximation (LDA) and more recently generalized gradient approximation (GGA). The second is the highly-developed band-structure calculation methods which make possible a realistic calculation for a very complicated material system with reasonable computer resource. In the calculation, it is almost inevitable to assume numerical approximations and modeling in addition to the basic ones such as the Born-Oppenheimer approximation and LDA. Both kinds of the approximation are often used without making any distinction and mixed up in the everyday calculations. In order to discuss physics and validity of the basic approximations, it is indispensable to minimize the numerical ones and at least to evaluate their limitation and errors. Further development of the numerical techniques and algorithms is highly desired for large-scale systems and complex phenomena to be investigated in recent materials science. The third is rapid progress in high performance computing. A desktop computer in every researcher's office has computing power comparable to a computer called "supercomputer" ten years ago. (Concerning the first and second issues, beginner-course students are recommended to study first fundamentals of the electronic structure theory [1].)

Under these circumstances, a computer code for the first-principles calculation becomes a gigantic package including a lot of state-of-the-art techniques and related know-how. Usefulness and wide applicability of the first-principles calculation in materials science research have been acknowledged. However, there has never been a general application code available until quite recently as in quantum chemistry field. In this decade, a number of research groups have developed first-principles calculation codes and, in many cases, made them open to public.

HiLAPW introduced in this article is a first-principles calculation package originally developed by a theory group in Hiroshima University. The current developments of the package are being made in collaboration between Osaka University and Hiroshima University. In section 2, the basic specifications of HiLAPW are explained. The package contains several executables, which perform part of the first-principles calculation. The executables are

linked via data files, as described in section 3. In section 4, the way to install the package is given. Finally, some application examples are shown in the following sections.

2 Basic Specifications

The HiLAPW program package is designed to perform first-principles calculations based on the density functional theory. Main features include the followings.

2.1 Linearized Augmented Plane Wave Basis Functions

The linearized augmented plane wave (LAPW) functions have high variational degrees of freedom and practically good efficiency without using pseudopotentials. Original non-linearized APW was proposed by Slater [2] with muffin-tin potential approximation.

This program utilizes LAPW basis functions by Soler and Williams [5, 6], which are slightly different in a practical sense from the original ones by Andersen [3] and Koelling and Arbman [4].

2.2 Scalar Relativistic Treatment

When the atomic number increases the relativistic effects cannot be neglected. A proper treatment of the relativity can be made with use of Dirac equation instead of Schrödinger one. In this package, the scalar relativistic treatment is used including all the relativistic effects except the spin-orbit coupling (SOC) [7]. Additional inclusion of SOC in a second-variation process provides an approximated but accurate description equivalent to solving Dirac equation.

2.3 Self-Consistent Field Method

The Kohn-Sham equations should be determined in a self-consistent-field (SCF) manner and usually solved by an iterative scheme. The essential part of the iterative scheme is how to guess input electron density for next iteration from the input and output electron density distribution functions in the previous iterations. Simple mixing method and extended Anderson method [8] can be employed depending on the SCF convergence behavior in different material systems.

2.4 Full Potential Method

The muffin-tin potential approximation assumed in the original APW and LAPW methods often leads to a less accurate or unphysical solution in cases of sparsely packing or low-symmetry systems. The full-potential method [9] assumes no shape approximation for the electron density and potential functions and may be applicable to any crystal symmetry even surface and interface systems. Note that the muffin-tin sphere is still assumed in the full-potential method but only divides the regions where a plane-wave or spherical-wave representation is adopted to express the electron density and potential functions. The final results such as the total energy are unchanged by a different choice of the muffin-tin sphere radius with well converged parameters for the representations.

2.5 Atomic Forces

In pseudopotential methods with the plane wave basis, atomic forces, which are defined as a minus gradient of the total energy with respect to the atomic coordinates, are simply given by the Hellmann-Feynman theorem, leading to great success in the Car-Parrinello molecular dynamics simulations. In the LAPW method, where the augmentation functions have explicit dependence of the atomic coordinates, the so-called Pulay term must be evaluated additionally to obtain the atomic forces accurately. In the package, Soler and Williams' formulation [5, 6] is used for the atomic forces. With the forces, structural optimization and phonon mode calculation can be easily carried out.

2.6 Tetrahedron Integration Scheme with the Second-Order Corrections

Integration within the Brillouin zone is frequently performed to compute any of the physical quantities such as the electron density and the density of states. Blöchl's tetrahedron scheme [10] is utilized in the code. The other integration schemes with the occupation given by the error function or the Fermi distribution function can be also used optionally.

2.7 Irreducible Representation of the Eigenstates

The group theory tells that each one-electron eigestate belongs to an irreducible representation of the k group. With the irreducible representation, one can understand how the eigenstate is transformed by the symmetry operation (rotation or mirror). For example, the matrix element of the electric dipole with respect to the initial and final states gives the selection rule for photo-excitation spectra.

3 Executables

The HiLAPW program package is composed of kernel executables such as `xsets` and `xlapw`, and some other optional ones. All the executables can be made with use of `makefile` attached with the package and `FORTRAN90` compiler on user's computer. List of the executables and related data files are summarized in Table 1.

4 Installation

The first thing to install the package is to download the package `hilapw.tar.gz` to the home directory on your computer and to extract it as

```
# cd ~
# gunzip hilapw.tar
# tar xvf hilapw.tar
```

Hereinafter, the symbol `#` at the first column denotes the prompt in the UNIX system and is not needed to be typed. The following directory structure under the home directory is expanded with this.

Table 1: Executables and related data files in HiLAPW.

executable	role	input files	output files
xsets	generation of the initial data	atomdata atomdens spgrdata sets.in	wavout sets.out
xlapw	SCF FLAPW calculation	wavin lapw.in	wavout ekn dis foa tau ten lapw.out
xdoss	DOS calculation	wavin doss.in	pdos pdos.index doss.out
xnewa	k-point update	wavin	wavout newa.out
xwbox	electron density calculation on 3D mesh	wavin wbox.in	wbox.list wbox.out
xpbox	potential calculation on 3D mesh	wavin pbox.in	pbox.list pbox.out
xspin	addition of spin degree	wavin	wavout spin.out
xwcon	format conversion of wav file	wavin wavin.frm wcon.in	wavout wavout.frm wcon.out
xsymm	symmetry calculation	wavin	ekl cml symm.out
xrept	reorder of the eigenstates	ekl cml	eig1 eig2 rept.out

```
hilapw/  
  bin/  
  bz/  
  data/  
  lib/  
  ps/  
  sources/
```

Some of the tool commands and all of the executables after the proper installation are located in the directory `bin/`. The directory `bz/` contains the data for the typical Brillouin zone used for the band-structure plotting. In `data/`, the default databases, `atomdata`, `atomdens` and `spgrdata`, and some example archived data, `Cu.tar`, `Si.tar` and `Fe.tar`, are placed.

Before compilation, check the FORTRAN90 compiler name and its appropriate options available on your computer and modify `makefile` in three directories `/hilapw/sources`, `/hilapw/lib` and `/hilapw/ps` if necessary. In addition to the FORTRAN90 compiler, the libraries of linear algebra routines BLAS and LAPACK are required for installation of HiLAPW.

After the proper specifications in `makefile`, one can compile by typing `make` to install.

```
# cd hilapw/sources  
# make clean  
# make all  
# make install
```

The same process is needed in the directories `/hilapw/sources` and `/hilapw/lib`.

```
# cd ~/hilapw/ps  
# make clean  
# make all  
# make install  
# cd ~/hilapw/lib  
# make clean  
# make all  
# make install
```

In order to make all the executables activated, the directory `/hilapw/bin` should be added in your path. For example, when the `csh` or `tcsh` environment is used, the following line after the last `set path` line in `.cshrc` can be inserted.

```
set path = ( . $home/hilapw/bin $path)
```

To activate it, just type.

```
# source ~/.cshrc
```

For example calculations, let us create a new directory `hilapw1` under your home directory.

```
# cd ~  
# mkdir hilapw1
```

5 Cu with fcc Structure

5.1 SCF Calculation

Under the directory `hilapw1` just made above, another new directory `Cu` is created for calculations of fcc Cu. By typing `getdata`, three database files `atomdata`, `atomdens` and `spgrdata` are imported from the default database directory `~/hilapw/data`.

```
# cd hilapw1
# mkdir Cu
# cd Cu
# getdata
```

To perform example calculations for fcc Cu, extract eleven files from the directory `~/hilapw/data`.

```
# tar xvf ~/hilapw/data/Cu.tar
```

For starting the SCF calculation, just type the shell-script as

```
# ./JOB-SCF
```

The students are recommended to look inside the script `JOB-SCF` and to understand how all the processes are executed.

After the execution `xlapw`, the tool command `LAcopy` is used for attaching a particular modifier (`A1` or `A2`) to the output files.

5.2 Density of States

For the total density of states (DOS), type

```
# xdoss
# mv pdos pdosA2
# getfermi outA2 > fermiA2
# PSP < psp_tdos > tdos.ps
```

to get a PostScript (PS) file `tdos.ps` as shown in Fig. 1. Here, the tool command `getfermi` is for extracting the Fermi energy from a file. `PSP` is a general-purpose PS plotting tool with the specifications of a standard input file, `psp_tdos` in this case.

For plotting partial DOS, since the required data are already generated and stored in the file `pdosA2`, type

```
# PSP < psp_pdos > pdos.ps
```

to get projected DOS on cubic harmonics s , p , $d(e_g)$ and $d(t_{2g})$ as shown in Fig. 2.

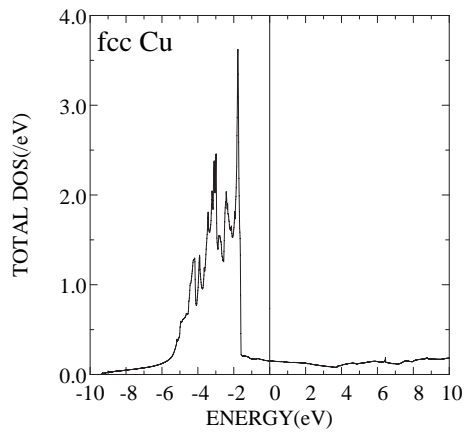


Figure 1: Total density of states in fcc Cu. The origin of energy is taken at the Fermi energy.

5.3 Band Structure

Next, let us try to plot the band structure of fcc Cu.

```
# JOB-EK
# JOB-SYM
```

The shell-script `JOB-EK` demands energy-eigenvalue calculations for k points along the high-symmetry lines of the fcc Brillouin zone in Fig. 3. The script `JOB-SYM` requests to extract the irreducible representation for each eigenstate. To obtain the band structure (Fig. 4), just type

```
# PSP < psp_ek > ek.ps
```

6 Si with Diamond Structure

6.1 SCF Calculation

Following the previous example for fcc Cu, get started with some preparations.

```
# cd ~/hilapw1
# mkdir Si
# cd Si
# getdata
# tar xvf ~/hilapw/data/Si.tar
```

With the present data set, an example for calculating the total energy by changing the lattice constant for Si with diamond structure is provided.

```
# JOB-TEN
```

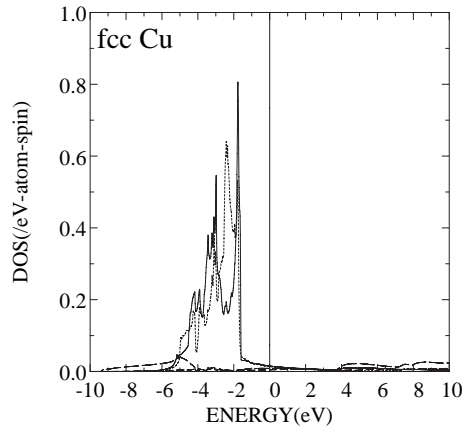


Figure 2: Partial density of states in fcc Cu. The origin of energy is taken at the Fermi energy. Long broken, short broken, dotted and solid lines denote components of the partial DOS of s , p , $d(e_g)$ and $d(t_{2g})$, respectively.

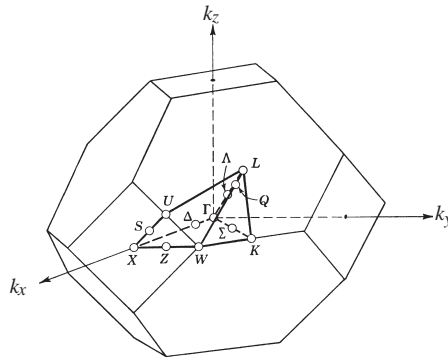


Figure 3: Brillouin zone of the fcc structure.

SCF calculations at eleven lattice constants between $a = 5.20\text{\AA}$ and $a = 5.60\text{\AA}$ are performed. Using calculated results, total energies as a function of the unitcell volume are fitted to Murnaghan's equation of state[11].

```
# GET-TEN > TEN
# xefitm < TEN > fit_TEN
```

The executable `xefitm` is a tool program to fit the data to Murnaghan's equation of state by the least-square method. Inside the output file `fit_TEN`, you can find the results as

```
Coefficients for Murnaghan fitting
c1   =   0.3072618807D+07
c2   =   0.1652098587D-02
E'   =  -1156.7411297535
V0   =    266.2218508318
E0   =  -1156.1556676775
```

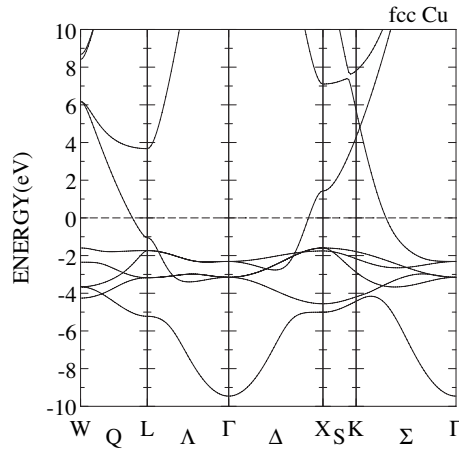



Figure 4: Band structure of fcc Cu. The origin of energy is taken at the Fermi energy.

B' = 4.0200000000
 B0 = 0.0066414363 97.6955282824 GPa

where V_0 is the equilibrium unitcell volume in atomic units, B_0 is the bulk modulus and B' is its volume derivative defined as

$$B_0 = B(V_0) = \left(V \frac{d^2 E_{\text{total}}}{dV^2} \right)_0$$

$$B' = -\frac{1}{B_0} \left(V \frac{dB(V)}{dV} \right)_0$$

Figure 5 shows the volume dependence of the total energy obtained by typing

```
# tail -103 fit_TEN > TEN2
# PSP < psp_TEN > TEN.ps
```

where dots represent calculated data points and solid line is the fitted equation of state.

7 Ferromagnetic Fe with bcc Structure

7.1 SCF Calculation

Again, let's create a new directory and take all the data files for the present example.

```
# cd ~/hilapw1
# mkdir Fe
# cd Fe
# getdata
# tar xvf ~/hilapw/data/Fe.tar
```

In this section, an SCF calculation is carried out and DOS and band structure are plotted in a similar manner to the calculations for fcc Cu. To start the SCF calculation, type the shell-script

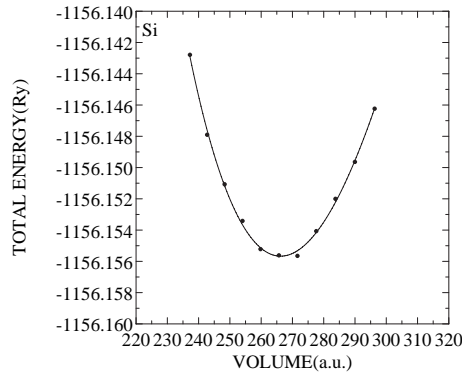


Figure 5: Volume dependence of calculated total energy in diamond Si. Dots represent calculated data points and solid line is the fitted equation of state.

```
# JOB-SCF
```

Detailed scripts in JOB-SCF should be checked carefully.

7.2 Density of States

全状態密度を計算するには In order to perform a DOS calculation and to get the total DOS plot, type

```
# xdoss
# mv pdos pdosA2
# getfermi outA2 > fermiA2
# PSP < psp_tdos > tdos.ps
```

The output PS file `tdos.ps` is shown in Fig. 6.

Partial DOS can be obtained by

```
# PSP < psp_pdos > pdos.ps
```

Figure 2 shows projected partial DOS on cubic harmonics, s , p , $d(e_g)$, $d(t_{2g})$.

7.3 Spin Magnetic Moment

Results of `xlapw` are output in a file `lapw.out`. (With use of the prepared shell-scripts, the file is rename as `outA1` or `outA2`.)

One can find the following output data in the file as

```
===== ELECPR
NUMBER OF ELECTRONS WITHIN MUFFIN-TIN
TYPE SPIN      TOTAL          S          P          D          F
   1   UP    4.02803    0.09164    0.07447    3.86191
   1  DOWN    1.84418    0.09370    0.08735    1.66313
      U+D    5.87221    0.18534    0.16182    5.52504
      U-D    2.18385   -0.00206   -0.01287    2.19878
```

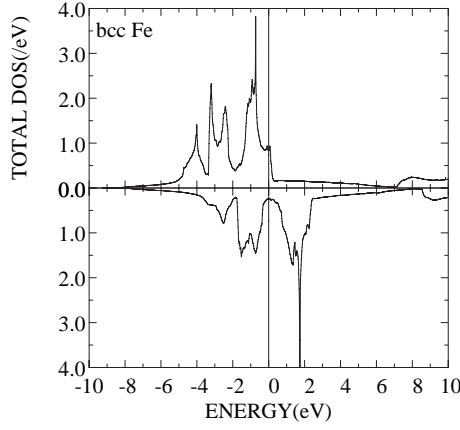


Figure 6: Total density of states in ferromagnetic bcc Fe. Upper and lower panels show density of states for up and down spin bands, respectively. The origin of energy is taken at the Fermi energy.

Here, the numerical data are the number of electrons, which is defined as an integrated density of states at the Fermi energy for each partial (spin and orbital-angular-momentum projected) state within the muffin-tin sphere. The spin magnetic moment inside the muffin-tin sphere (1\AA) is $2.18\mu_B$, most of which comes from the d states. The s and p states are weakly and negatively spin-polarized.

Note that the magnitude of the spin magnetic moment here is an integrated value of the spin density, depending on the muffin-tin sphere radius assumed. In the case of a ferromagnetic system, total spin magnetic moment per unitcell including contributions outside the spheres can be evaluated by summing up the occupation for each spin band and by subtracting them as

----- BAND OCCUPATION

BAND	UP-SPIN			DOWN-SPIN		
	E-MIN	E-MAX	WEIGHT	E-MIN	E-MAX	WEIGHT
1	0.06570	0.44910	1.00000	0.09416	0.55769	1.00000
2	0.34063	0.52660	1.00000	0.46359	0.66445	1.00000
3	0.44597	0.68832	0.99998	0.55620	0.84957	0.88590
4	0.51715	0.68832	0.99983	0.65867	0.84957	0.00781
5	0.56364	0.70814	0.89049	0.71533	0.86892	0.00000
6	0.60697	1.38338	0.21600	0.78281	1.41846	0.00000
7	1.17953	2.48901	0.00000	1.26695	2.49821	0.00000
8	1.30182	2.48901	0.00000	1.38167	2.49821	0.00000
9	1.43833	2.50566	0.00000	1.49335	2.51826	0.00000
10	1.83505	3.37425	0.00000	1.92887	3.20781	0.00000

SUM			5.10629			2.89371
U-D			2.21257			

to get the total spin moment of $2.21\mu_B$. Therefore, the spin magnetic moment in bcc Fe is mostly localized within the muffin-tin sphere.

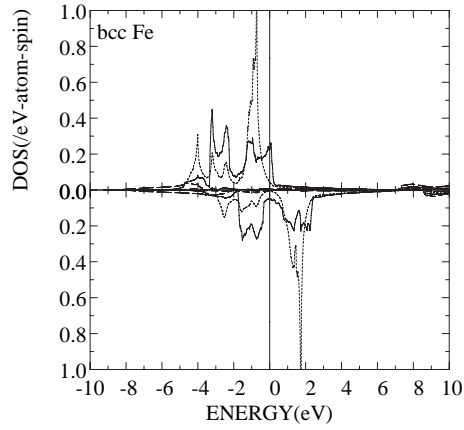


Figure 7: Partial density of states in ferromagnetic bcc Fe. Long broken, short broken, dotted and solid lines denote components of the density of states projected on cubic harmonics s , p , $d(e_g)$, $d(t_{2g})$. Upper and lower panels show density of states for up and down spin bands, respectively. The origin of energy is taken at the Fermi energy.

7.4 Band Structure

Band structure of ferromagnetic bcc Fe is calculated and plotted along the high-symmetry lines of the bcc Brillouin zone (Fig. 8).

```
# JOB-EK
# JOB-SYM
```

The PS file containing the band structure can be generated by

```
# PSP < psp_ek > ek.ps
```

and shown in Fig. 9.

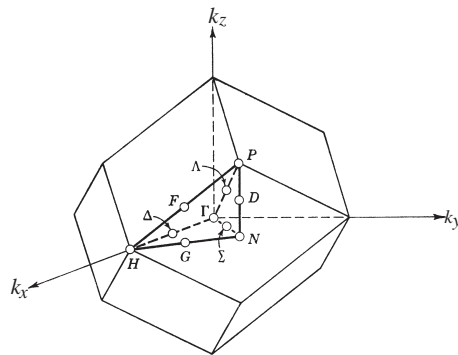


Figure 8: Brillouin zone of bcc lattice.

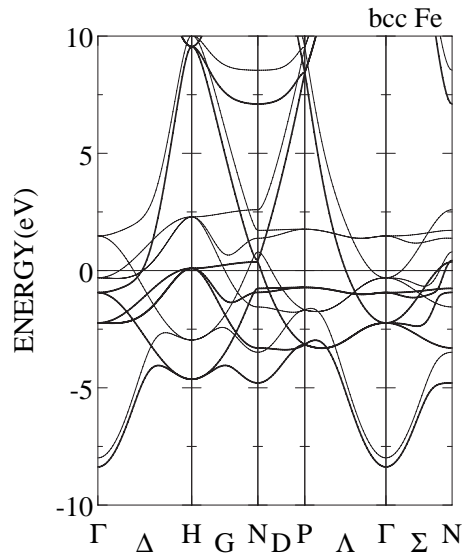


Figure 9: Band structure of ferromagnetic bcc Fe. The majority-spin and minority-spin bands are plotted with thick and thin lines, respectively. The origin of energy is taken at the Fermi energy.

8 Input Data

In this section, three input data `sets.in`, `lapw.in` and `doss.in` are briefly explained for the fcc Cu example.

8.1 Input Data for `xsets: sets.in`

The input file `sets.in` includes data about the target material system such as crystal structure, atomic information and k-point grid. (In the following data, 01: and so represent the line number of the file for sake of explanation and is not included in the actual data.)

```

01: fcc Cu
02: -----nspin
03: 1
04: -----space group
05: Fm-3m
06: 3.61 3.61 3.61
07: 90.0 90.0 90.0
08: -----atoms
09: 1
10: Cu 1
11: 0.0 0.0 0.0
12: -----k points
13: 0
14: 8 8 8

```

The line 01 is a comment within 80 characters. This comment is also used as a header line in some output files. The line 02 is a comment used for a data separator. The line 03 contains an integer number used as a flag `NSPIN` of spin-polarization treatment. `NSPIN=1` for non-spin-polarized and `NSPIN=2` for spin-polarized calculation. In non-spin-polarized case, up and down spin states are treated equally and all the occupations are multiplied by the spin degeneracy of two when summing up the states. The line 04 is a comment used for a data separator. In line 05, name of the space group of the system is declared. Only the space group names included in the file `spgrdata` are allowed to use. In line 06 the lattice constants a, b, c are given in Å units and α, β, γ are in degrees. If the lattice constants are incompatible with the space group given above, the lattice system of the space group has the priority. For example, if a different b value from a is given, b is replaced with the a value. In Table 2, relations of the lattice constants to the lattice system and type are listed. The line 08 is a comment used for a data separator. An integer number in line 09

Table 2: Lattice constants $a, b, c, \alpha, \beta, \gamma$, lattice system, lattice type. The c axis in monoclinic lattice is taken as the unique axis.

lattice system	a	b	c	α	β	γ	lattice types
cubic	a	a	a	90	90	90	P, I, F
tetragonal	a	a	c	90	90	90	P, I
orthorhombic	a	b	c	90	90	90	P, I, F, C
hexagonal	a	a	c	90	90	120	P
trigonal	a	a	a	α	α	α	P(R)
monoclinic	a	b	c	90	90	γ	P, B
triclinic	a	b	c	α	β	γ	P

indicates crystallographically independent atomic kinds `NTTP`. Two atoms which have the same atomic number should be counted two when no symmetry operation exists between both atomic sites. Line 10 contains name of the element and number of atomic sites of one kind. In the following lines starting 11, atomic position vectors of all the atomic sites of the kind are given in the conventional lattice units. The line 12 is a comment used for a data separator. An integer number in line 13 denotes how to set up the k-point grid. A Uniform grid including (excluding) Γ point is constructed for 0 (-1). If it's a positive integer, it represents the number of k-points to be calculated, and coordinates of k-point in $(2\pi/a, 2\pi/b, 2\pi/c)$ units with the sampling weight should be given in the following lines.

8.2 Input Data for `xlapw`: `lapw.in`

A file `lapw.in` is the input data for `xlapw` and contains parameters controlling the calculations.

```
01:HiLAPW 1.0
02:      20.0          emax
03:      80.0          egmax
04:      -1           lbroad
05:      0.005        deltae
```

```

06:          10                      ne
07: c 0.0 c 0.0 c 0.0              ezr
08:          -1                      atomic_loop_mode
09:      loop dta  scf cmix smix field
10:          10 0.00      5 0.20 0.00 0.00 0.00

```

The line 01 is a comment within 80 characters. Real numbers in lines 02 and 03 are the cutoff energy in Ry used in the wavefunction and the electron density, respectively. An integer number in line 04 specifies the method of k-point integration. The number is -1 for the tetrahedron method with corrections, 0 for the standard linear tetrahedron method, 1 for the broadening method with the error function and 2 for the broadening method with the Fermi function. In the case of the broadening method, a broadening width in Ry should be given in line 05. In line 06, number of the valence states should be given, which must be equal to or greater than half of the number of the valence electrons in insulating systems and must be sufficiently larger than that in metallic cases. An appropriate number of the valence states is proposed in the output file `sets.out` after the execution of `xsets` as

```

NUMBER OF VALENCE STATES
MINIMUM      =      6
APPROPRIATE=      9

```

In line 07, the way to choose the energy parameter for each orbital-angular-momentum wave of the atom kind is specified. Usually the example data set `c 0.0 c 0.0 c 0.0` are expected to work and all the energy parameters for s , p and d waves are taken at the center of the occupied partial DOS. Sometimes, a higher energy parameter such as 1Ry above the Fermi energy given as `f 1.0` is needed for a particular partial wave in the case of a shallow core state existing with the same orbital angular momentum. An integer number in line 08 controls atomic force calculation. If it's -1 , no atomic force is calculated. Atomic forces are calculated for 0 and greater. When it's a positive integer, atomic positions are relaxed according to a different algorithm with some extra data specified (not described here because of advanced calculation). Line 09 is a comment. Input data in line 10 give control parameters for SCF calculation. The example data denote 10 SCF iteration with the electron density mixing of 0.2 by the 5th order extended Anderson scheme. In the case of spin-polarized calculation, the spin-density mixing ratio is also specified.

8.3 Input Data for `xdoss: doss.in`

The file `doss.in` contains the control parameters when calculation the density of states.

```

01:doss.in
02:-0.2 1.8 2000
03:1
04:0 0 0

```

The line 01 is a comment within 80 characters. In line 02, the energy range in Ry and energy mesh number are given for DOS calculation. You may get some information about the position of the bands from the output file of `xlapw`. The range of each band can be given in `BAND OCCUPATION` part of the output file. An integer in line 03 specifies kind of

the harmonics on which the partial DOS is projected. Spherical harmonics for 0, cubic harmonics for 1 and hexagonal harmonics for 2. The principal axes of the harmonics can be changed by specifying the Euler angles (α, β, γ) in degrees in line 04. After the execution of `xdoss`, all the DOS data are output in the file `pdos`. An extra file `pdos.index` tells each column of the data corresponds to which partial DOS.

References

- [1] For example, see: R.M. Martin, "Electronic Structure" (Cambridge University Press, 2004).
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HiLAPW

— version 1.12 —

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The original edition of HiLAPW document describe practical procedures and examples based on HiLAPW2002 (version 1.0) and additional issues introduced in version 1.12 are given in this article.

1 Additional Specifications and Tools in version 1.1

In HiLAPW version 1.1, several functionalities are included in addition to some patches to fix the bugs found in version 1.0.

1.1 Choice of Functional Form in the Local-Density or Generalized-Gradient Approximation

In version 1.0, it is not possible to choose the adopted functional form explicitly in the local-density approximation (LDA). On the occasion that the generalized-gradient approximation (GGA) is installed, the functional form used can be specified when `xlapw` is running. Available functional form is written in the file `excodata`, in which the form in the first line is adopted. The default file `excodata` can be obtained by typing `getdata` in addition to the previous database files.

1.1.1 Choice of Exchange-Correlation Functional: `excodata`

Before the execution of `xsets`, typing `getdata` gives three of the database files `atomdata`, `atomdens` and `spgrdata` as described previously. In version 1.1, a new default file `excodata` is also copied on your working directory. Exchange-correlation functional form used in `xlapw` can be chosen by specifying the name of functional on the first line of the file `excodata`. The default `excodata` file is following:

```
LDA MJW
GGA PBE
LDA BH
LDA GL
LDA VWN
LDA PZ
```

In the present version 1.1, LDA functionals by Moruzzi-Janak-Williams (MJW) [1], Barth-Hedin (BH) [2], Gunnarsson-Lundqvist (GL) [3], Vosko-Wilk-Nusair (VWN) [4] and Perdew-Zunger [5] and GGA one by Perdew-Burke-Ernzerhof (PBE) [6] can be used.

The choice of the functional form is NOT a kind of adjustable parameters. Instead, it should be used for checking the validity and reliability of the calculated results. Nevertheless, it is also of reality that either LDA or GGA works well for some particular systems and physical phenomena and vice versa.

1.2 Modifications in Core Functions and Atomic-Force Calculation

Since GGA includes the second derivatives of the electron density, one has to pay more attention to the representation of the electron density. Especially, as different representations are assumed for the electron density inside and outside the muffin-tin spheres in the full-potential method, a consistent numerical treatment must be paid to achieve the continuous representation of the electron density on the sphere boundary. Previously, the valence electron density has been expressed in such a consistent manner but no such an accurate treatment has been made on the core density, resulting to some serious problems in the case of GGA.

Certain amplitude of a shallow core state may penetrate into the outer region of the muffin-tin sphere. The amplitude outside the sphere was treated in the plane-wave representation and a constant density was assumed inside the sphere when the Fourier transformation is performed, leading to some spurious noise due to its discontinuity. A gaussian type function is now used inside the sphere so as to fulfill the continuity on the sphere boundary. However, the previous treatment on the core density gives only very minor error in the atomic forces but the corrected representation requires an explicit consideration of the core density in the plane-wave part of the atomic forces. With the present corrections, the core density can be treated in GGA and atomic-force calculations in a consistent and accurate way.

2 Additional Specifications and Tools in version 1.11

In HiLAPW version 1.11, new functionality for input method of atomic positions is included in addition to some patches to fix the bugs found in version 1.1.

2.1 Input Method of Atomic Positions

When the atomic positions are given in the previous version, the position vectors of all atoms in unitcell should be input and their consistency to the space group is checked. It is highly desired to simplify the input method in cases of many-atom systems and/or displacing the atoms for a given space group. Therefore, it is now possible in this version to input only one position vector for one kind of atom.

For example, the input data `sets.in` for Y_2C_3 in the previous version are following.

```
Y2C3 #220 I-43d a=8.18976 x(Y)=0.05017 x(C)=0.29481
-----nspin
1
```

```

-----space group
I-43d
 8.18976 8.18976 8.18976
 90.0 90.0 90.0
-----atoms
  2
Y   8
 0.05017  0.05017  0.05017  x,x,x
 0.30017  0.30017  0.30017  1/4+x,1/4+x,1/4+x
 0.55017  0.44983 -0.05017  1/2+x,1/2-x,-x
 0.80017  0.19983  0.69983  3/4+x,1/4-x,3/4-x
-0.05017  0.55017  0.44983  -x,1/2+x,1/2-x
 0.69983  0.80017  0.19983  3/4-x,3/4+x,1/4-x
 0.44983 -0.05017  0.55017  1/2-x,-x,1/2+x
 0.19983  0.69983  0.80017  1/4-x,3/4-x,3/4+x
C  12
 0.29481  0.00000  0.25000  x,0,1/4
-0.29481  0.50000  0.25000  -x,1/2,1/4
 0.54481  0.50000  0.25000  1/4+x,1/2,1/4
 0.45519  0.00000  0.25000  3/4-x,0,1/4
 0.25000  0.29481  0.00000  1/4,x,0
 0.25000 -0.29481  0.50000  1/4,-x,1/2
 0.25000  0.54481  0.50000  1/4,1/4+x,1/2
 0.25000  0.45519  0.00000  1/4,3/4-x,0
 0.00000  0.25000  0.29481  0,1/4,x
 0.50000  0.25000 -0.29481  1/2,1/4,-x
 0.50000  0.25000  0.54481  1/2,1/4,1/4+x
 0.00000  0.25000  0.45519  0,1/4,3/4-x
-----k-points
  0
  4   4   4

```

The present version 1.11 may accept the previous data and also the following simplified data format as

```

Y2C3 #220 I-43d a=8.18976 x(Y)=0.05017 x(C)=0.29481
-----nspin
  1
-----space group
I-43d
 8.18976 8.18976 8.18976
 90.0 90.0 90.0
-----atoms
  2
Y   0
 0.05017  0.05017  0.05017  x,x,x
C   0
 0.29481  0.00000  0.25000  x,0,1/4

```

```

-----k-points
      0
      4      4      4

```

where the value 0 following the element name denotes only one position vector for one kind of atom.

Note that since all the atomic position vectors are generated according to the input atomic position and the space group, the generated position vectors should be checked.

3 Additional Specifications and Tools in version 1.12

In HiLAPW version 1.12, a modification in linearization for preventing the ghost band is made in addition to some patches to fix the bugs found in version 1.11.

3.1 Modification in Linear Method

In linear method [7, 8], the energy dependence of the radial function $R_l(r, E)$ used as a basis set can be represented efficiently. This is well understood from its Taylor expansion

$$R_l(r, E) = R_l(r, E_l) + (E - E_l)\dot{R}_l(r, E_l) + \dots \quad (1)$$

with use of the radial and energy-derivative functions $\dot{R}_l(r, E_l) = (dR_l(r, E)/dE)_{E_l}$ solved at a particular energy E_l . Alternatively, the energy-derivative function is orthogonalized with the corresponding radial function normalized inside the MT sphere

$$\int_0^S r^2 dr R_l(r, E_l)\dot{R}_l(r, E_l) = 0 \quad (2)$$

and the radial and energy-derivative functions provide a minimal basis for a given orbital angular momentum component l .

In linear augmented plane wave method, the plane waves are augmented with the radial and energy-derivative functions and the radial function with any logarithmic derivative D can be constructed with their linear combination such as

$$R_l(r, D) = R_l(r, E_l) + \omega(D)\dot{R}_l(r, E_l) \quad (3)$$

This is quite convenient for the connectivity to the plane wave on the sphere. Especially, the expectation value inside the sphere with respect to the radial function with the logarithmic derivative D is shown to be correct up to the third order.

$$\langle R_l(D)|\mathcal{H} - E|R_l(D)\rangle_S = \mathcal{O}(E - E_l)^4 \quad (4)$$

However, in linear method, the so-called ghost band may happen to appear and become very serious problem, particularly in the case of systems with a shallow core state. To eliminate the ghost band, the energy parameter E_l must be set to a higher energy value and the energy representation of the radial function may be worse in the valence band region.

One of the reasons of the ghost band originates in the fact that the energy-derivative function in the valence band region may be a possible bound state similar to the shallow core state. Figure 1 shows the logarithmic derivatives of the s and p channels in the

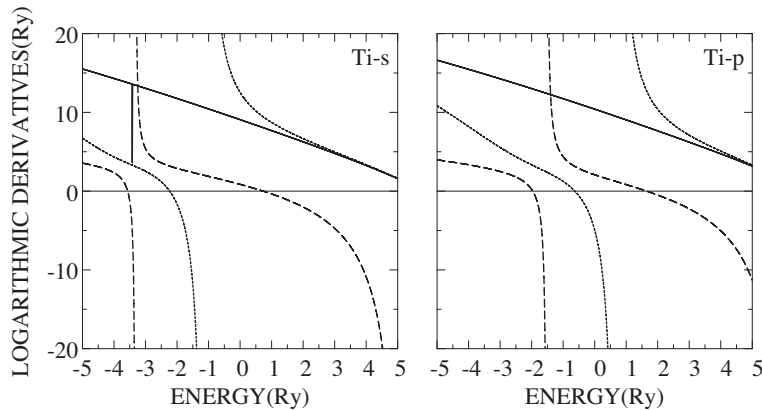


Figure 1: The logarithmic derivative of the s and p channels in Ti. Broken and dotted lines denote that for the radial and energy-derivative functions. Solid lines indicate that for the orthogonalized energy-derivative function.

valence band region in Ti, which has shallow core $3s$ and $3p$ states. A possible bound state may appear in the energy region where the logarithmic derivative is negative. The energy-derivative functions with s and p waves become negative in the valence band region.

Let us consider to correct the energy-derivative function to prevent the appearance of the ghost band. Well localized core states with no amplitude on the MT sphere are rigorously orthogonalized to the radial and energy-derivative functions. However, the orthogonality is broken when a core state has finite amplitude penetrating outside the MT sphere, which actually happens for shallow core systems. If this is the case, the energy-derivative function has a negative logarithmic derivative in the valence band region and might give rise to a bound state (ghost band) similar to the shallow core state. So, the orthogonality to the core state should be recovered to eliminate the ghost band. Suppose the following new energy-derivative function \tilde{R}_l orthogonalized not only to the shallow core state R_{cl} but also to the corresponding radial function.

$$\tilde{R}_l = \dot{R}_l + \alpha R_{cl} + \beta R_l \quad (5)$$

where coefficients α and β are determined by the orthogonal conditions

$$\alpha = -\frac{\langle R_{cl} | \dot{R}_l \rangle}{\langle R_{cl} | R_{cl} \rangle - |\langle R_{cl} | R_l \rangle|^2} \quad (6)$$

$$\beta = -\alpha \langle R_{cl} | R_l \rangle \quad (7)$$

As expected, this orthogonalized energy-derivative function \tilde{R}_l has a non-negative value of the logarithmic derivative in the valence band region and shows very smooth behavior as a function of energy (see solid lines in Fig. 1). In an actual band structure calculation with the new energy-derivative function, the energy parameters are always chosen within the valence band region without any appearance of the ghost band.

4 Installation

Downloaded the complete set of HiLAPW version `xx.xxx`, `hilapw_xx.xxx_tar.gz`, is placed on the home directory, unzipped and extracted by typing

```
# cd ~
# gunzip hilapw_xx.xxx_tar
# tar xvf hilapw_xx.xxx_tar
```

to get the following directory structure under the home directory:

```
hilapw/
  xx.xxx/
    bin/
    bz/
    data/
    lib/
    ps/
    sources/
    sources_fermi/
  bin/
  bz/
  current/
  data/
```

The directory `current` is symbolically linked to that with the latest version name (`xx.xxx` in the present case). The directories `bin`, `bz` and `data` are also symbolically linked to the corresponding directories under `current`. Compilation by typing `make` is just in a similar manner to the previous version.

```
# cd hilapw/current/sources/
# make clean
# make all
# make install
```

The codes for band fitting described in the advanced edition of HiLAPW document are located in the directory `hilapw/current/sources_fermi/`. After completion of the compilation above, the band-fitting codes can be compiled as follows:

```
# cd hilapw/current/sources_fermi/
# make clean
# make all
# make install
```

The setting for path is just the same as before. For example, if you use `cs` new setting in `.cshrc` is given as

```
set path = ( . $home/hilapw/bin $path)
```

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