`HiLAPW`
`Version 1.4`
— 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].

To remove a possible appearance of the so-called ghost band, the radial energy-derivative function $\dot{R}_l$ is forced to be exactly orthogonalized to the highest core state R_{cl} with keeping the orthogonalization to the corresponding radial function R_l [7] as

$$\tilde{\dot{R}}_l = \dot{R}_l + \alpha R_{cl} + \beta R_l \tag{1}$$

where the coefficients α and β are determined by the orthogonal conditions

$$\alpha = -\frac{\langle R_{cl}|\dot{R}_l\rangle}{\langle R_{cl}|R_{cl}\rangle - |\langle R_{cl}|R_l\rangle|^2} \tag{2}$$

$$\beta = -\alpha\langle R_{cl}|R_l\rangle \tag{3}$$

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) [8]. 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 [9] can be employed depending on the SCF convergency 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 [10] 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 [11] 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 basic executables and related data files are summarized in Table 1.

Table 1: Basic executables and related data files in `HiLAPW`.

executable (parallel ver.)	role	input files	output files
`xsets`	generation of initial data	`atomdata`* `atomdens`* `spgrdata_alt`* `sets.in`	`wavout` `sets.out`

`xlapw`
 `(xplapw)`
	SCF FLAPW calculation	`wavin`
		 `lapw.in`
		 `lapwadv.in`**
			`wavout`
			 `ekn`
			 `dis`
			 `foa`
			 `tau`
			 `ten`
			 `lapw.out`

`xdoss`
 `(xpdoss)`
	DOS calculation	`wavin`
		 `doss.in`
			`pdos`
			 `pdos.index`
			 `doss.out`

`xnewa`	k-point update	`wavin`	`wavout` `newa.out`
`xspin`	addition of spin degree	`wavin`	`wavout` `spin.out`

`xsymm`	symmetry calculation	`wavin`	`ekl`
			 `cml`
			 `symm.out`

`xrept`	reorder of the eigenstates	`ekl`
		 `cml`
			`eig1`
			 `eig2`
			 `rept.out`

*: Files on $HOME/hilapw/data are used unless provided in $CWD.

**: Default values are assumed unless provided in $CWD.

4 Installation

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

```
# tar zxvf hilapw.tar.gz
```

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

```
hilapw/
      1.4
      bin@ -> current/bin
      bz@ -> current/bz
      configure.sh
      current@ -> 1.4
      data@ -> current/data
```

Some of the tool commands and all of the executables after the proper compilation 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 data and some example data are placed. To configure the information of the installed directory, type

```
# cd hilapw
# ./configure.sh
```

Before compilation, check the `FORTRAN90` compiler name and its appropriate options available on your computer and modify `Makefile` in `hilapw/current`, if necessary. (If you wish to compile the parallel version of the package, compiler and option information in `pMakefile` are also properly set.) 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` (and also `pMakefile`), one can compile by typing `make` to install.

```
# cd hilapw/current
# make all
```

The same process is needed if you wish to compile the parallel version.

```
# make -f pMakefile all
```

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

```
# cd
# mkdir hilapw1
```

5 Examples: Basic

5.1 Cu with FCC Structure

5.1.1 SCF Calculation

Under the directory `hilapw1` just made above, another new directory `Cu` is created for calculations of fcc Cu.

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

To perform example calculations for fcc Cu, extract files from the directory `$HOME/hilapw/data` like

```
# tar xvf $HOME/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.

5.1.2 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

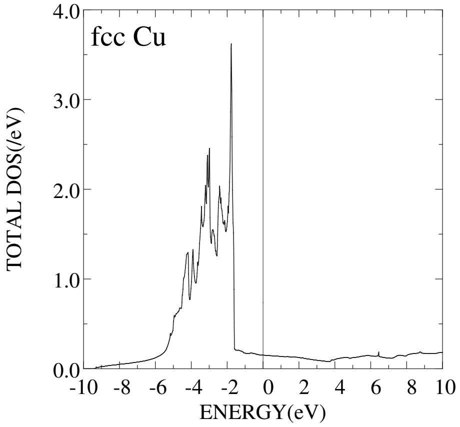

Fig. 1: Total density of states in fcc Cu. The origin of energy is taken at the Fermi energy.

```
# 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.

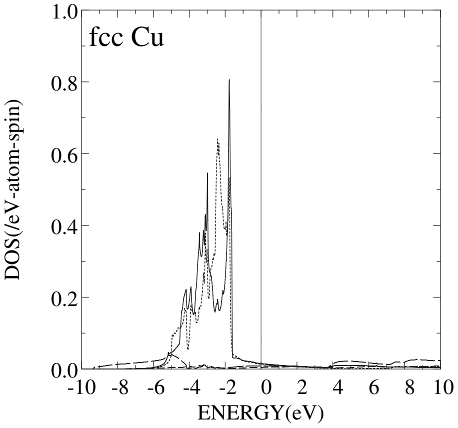

Fig. 2: Partial density of states in fcc Cu. The origin of energy is taken at the Fermi energy. Long broken, short broken, dotted and solid lines denote components of the partial DOS of s, p, $d(e_g)$ and $d(t_{2g})$, respectively.

5.1.3 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
```

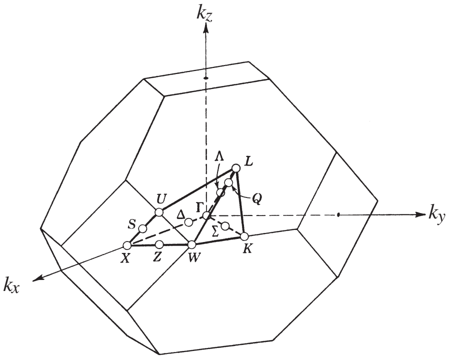

Fig. 3: Brillouin zone of the fcc structure.

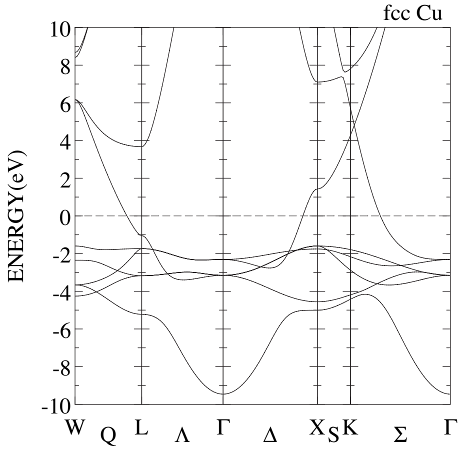

Fig. 4: Band structure of fcc Cu. The origin of energy is taken at the Fermi energy.

5.2 Si with Diamond Structure

5.2.1 SCF Total-Energy Calculations

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

```
# cd $HOME/hilapw1
# mkdir Si
# cd Si
# tar xvf $HOME/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
```

SCF calculations at eleven lattice constants between $a = 5.20$Å and $a = 5.60$Å are performed. Using calculated results, total energies as a function of the unitcell volume are fitted to Murnaghan's equation of state[12].

```
# ./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
 B'    =       4.0200000000
 B0    =       0.0066414363       97.6955282824 GPa
```

where `V0` is the equilibrium unitcell volume in atomic units, `B0` 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.

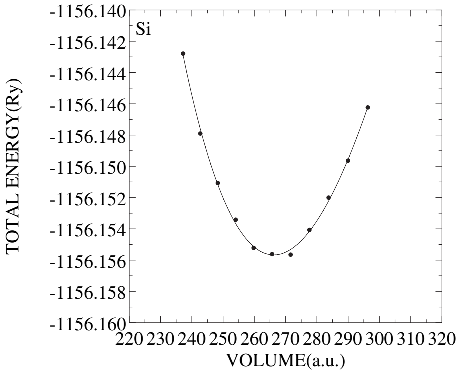

Fig. 5: Volume dependence of calculated total energy in diamond Si. Dots represent calculated data points and solid line is the fitted equation of state.

5.3 Ferromagnetic Fe with BCC Structure

5.3.1 SCF Calculation

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

```
# cd $HOME/hilapw1
# mkdir Fe
# cd Fe
# tar xvf $HOME/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

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

Detailed scripts in `JOB-SCF` should be checked carefully.

5.3.2 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

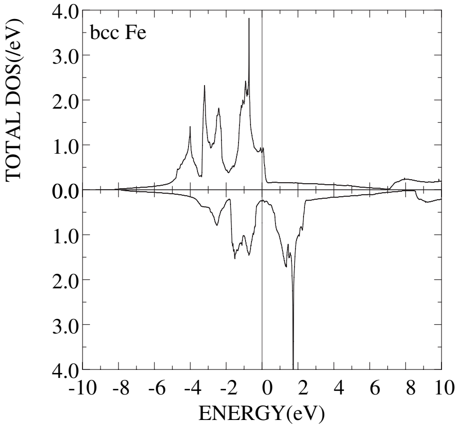

Fig. 6: Total density of states in ferromagnetic bcc Fe. Upper and lower panels show density of states for up and down spin bands, respectively. The origin of energy is taken at the Fermi energy.

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

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

5.3.3 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
```

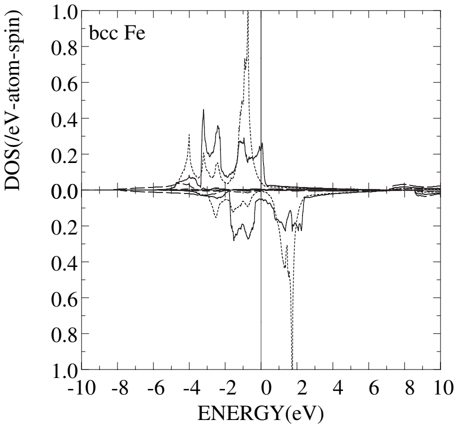

Fig. 7: Partial density of states in ferromagnetic bcc Fe. Long broken, short broken, doted and solid lines denote components of the density of states projected on cubic harmonics s, p, $d(e_g)$, $d(t_{2g})$. Upper and lower panels show density of states for up and down spin bands, respectively. The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

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 (1Å) 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
                UP-SPIN                                 DOWN-SPIN
BAND     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.

5.3.4 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.

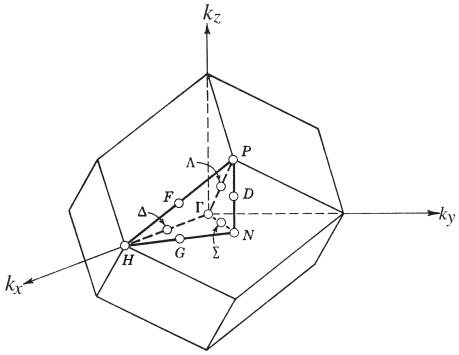

Fig. 8: Brillouin zone of bcc lattice.

6 Input Data

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

6.1 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
```

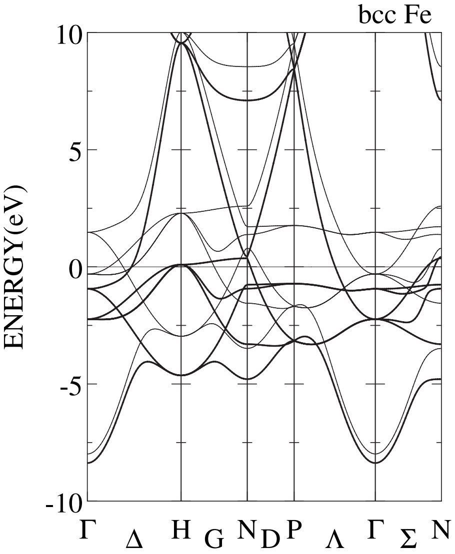

Fig. 9: Band structure of ferromagnetic bcc Fe. The majority-spin and minority-spin bands are plotted with thick and thin lines, respectively. The origin of energy is taken at the Fermi energy.

```
06: 3.61 3.61 3.61
07: 90.0 90.0 90.0
08:-----atoms
09:1
10:Cu 0
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_alt` 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` 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

Table 2: Crystal system, lattice constants a, b, c, α, β, γ, lattice type. The b axis in monoclinic lattice is taken as the unique axis here and the other choices may be allowed in a wider definition of space group.

crystal system (lattice)	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 (hexagonal)	a	a	c	90	90	120	P
trigonal (rhombohedral)	a	a	a	α	α	α	R
monoclinic	a	b	c	90	β	90	P, B
triclinic	a	b	c	α	β	γ	P

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.

6.2 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:     160.0                     egmax
04:        -1                     lbroad
05:     0.005                     deltae
06:         0                     ne
07:        -1                     atomic_loop_mode
08:      loop  dta  scf cmix smix field
09:        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 with 0 for the input. An integer number in line `07` 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 `08` is a comment. Input data in line `09` 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.

6.3 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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