First principle automatic calculation program
Template Oriented Atomic Simulation Toolkit (TOAST)
User's Manual

Contents

1. Outline of the program

The first principle automatic calculation program is a program that executes first principles calculation for a crystal structure (CIF file) prepared by a user. The first principle calculation program assumes that the program available to the user is used. The outline of the first principle automatic calculation program is shown in Fig. 1.1.
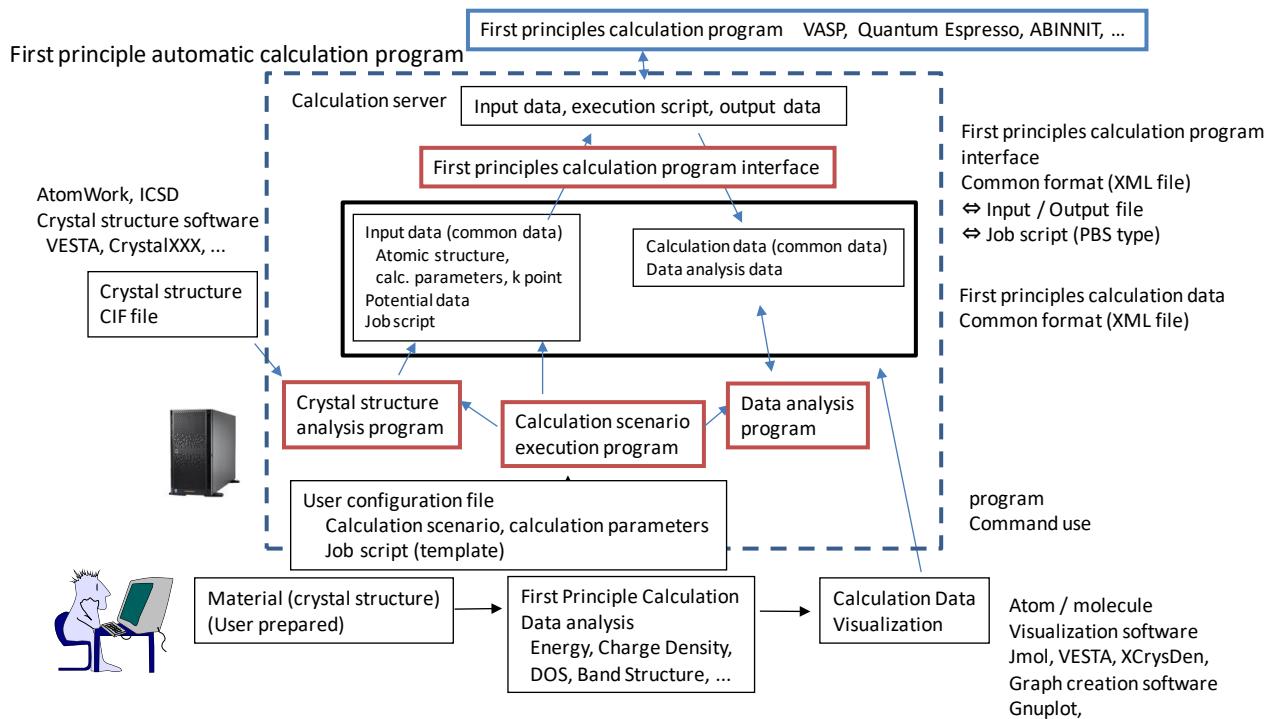
Fig.1.1   Outline of First Principle Automatic Calculation Program

Main features of the first principles calculation program are shown below.
- It consists of Python programs, and it runs on command basis in the Linux environment.
- he interface of the first principle automatic calculation program corresponds to the following first principle calculation program.
  - ・ The Vienna Abinitio Simulation Package (VASP)　　（http://www.vasp.at/）
  - ・ Quantum ESPRESSO　　（http://www.quantum-espresso.org/）
  - ・ ABINIT　　（http://www.abinit.org/）
- Execute first principles calculations sequentially based on the system or user prepared calculation scenario.
- By editing the configuration file, it can be used according to the user environment.

2. Installing programs, setting preferences

2.1 Operating Environment / Environment Setting

The first principle automatic calculation program is assumed to be used in the computer of the Linux environment.
Required applications are shown below.

Item	Application	Remarks
Python execution environment	Python 3.X	Standard package Needs numpy
First principles calculation program execution environment	First principles calculation program	VASP, Quantum Espresso , ABINIT
Calculation result visualization environment	Gnuplot Crystal structure visualization application	

2.1.1 Installing Python

The Python package can be installed as a distribution package for many Linux distributions. In addition to the standard package of Python package, installation of Python package numpy is necessary.
Or download the Python package and do the build. (https://www.python.org)

2.1.2 First principle calculation program

The first principle calculation program assumes that the program available to the user is used.
The interface of the first principles calculation program corresponds to the following first principle calculation program.

First principles calculation program

First principles calculation program	Operation confirmation version	Web site
The Vienna Abinitio Simulation Package (VASP)	VASP 5.4.4	http://www.vasp.at/
Quantum ESPRESSO	QE 6.4.1	http://www.quantum-espresso.org/
ABINIT	ABINIT 8.10.3	http://www.abinit.org/

For compiling and using the first principles calculation program, please refer to the manual of each program, website.

2.1.3 Visualization of calculation results

The visualization of the calculation result of the first principles calculation program can be carried out by a commercially available application or public use the application.

Item	Data Format	Applications
Crystal Structure	CIF file Input / output data of first principles	VESTA, Jmol, XCrysDen et al

	calculation program	
Brillouin Zone	Gnuplot script	Gnuplot
	Jmol script	Jmol
Charge Density	Gaussian Cube	VESTA, Jmol, Xcrysden, 他
Density of State		Gnuplot 他
Band Structure		Gnuplot 他

2.2 Installation

Deploy archive toast-X.X.X.tar.gz of the first principle automatic calculation program in the directory to install.

Structure of the first principle automatic calculation program

Install Directory	Subdirectory	Contents
toast-X.X.X	config	Configuration file
	calc	Python programs
	test	Sample data for test

2.3 Environment setting

The first principle automatic calculation program edits the setting file in toast / config according to the user's computing environment. The configuration file is in the Config File format (RFC 822 format), it is divided into sections by the header [sectioin], parameters and values are described in the form of name = value in each section.
* Details of the configuration file are described in Chapter 3.

Configuration file list

Item	File	Contents
Common configuration file	toast.cfg	Common configuration file Job management, Calculation scenario
Calculation scenario configuration file	vasp.para.cfg espresso..para.cfg abinit.para.cfg	Configuration file for VASP Configuration file for Quantum ESPRESSO Configuration file for ABINIT
Pseudopotential configuration file	vasp.pp.XXX.txt espresso.pp.XXX.txt abinit.pp.XXX.txt	Potential list for VASP Potential list for QE Potential list for ABINIT
Job execution configuration file	jobmanage.cfg jobtemplate/XXX.tmpl	Configuration of Job management system

2.3.1 Editing a calculation scenario configuration file

Describe the following items of the calculation scenario setting file of each calculation program according to the execution environment of the user's first principle calculation program.

Calculation scenario configuration file [general] section

Item	Contents	Description example

ppdir	Directory of pseudopotential file	ppdir = /opt/app/vasp/potpaw_PBE
		ppdir = /opt/app/espresso/SSSP_eff_PBE
		ppdir = /opt/app/abinit/JTH-PBE-atomicdata-1.0
cmd	Execution command of calculation program	cmd = /opt/app/vasp/vasp.5.3.5/vasp
		cmd = /opt/app/espresso/espresso-5.4.0/bin/pw.x
		cmd = /opt/app/abinit/abinit-8.0.8/bin/abinit

2.3.2 Editing of job execution configuration file

When using the job management system, edit the job execution setting file and create a template of the job execution script. In the first principle automatic calculation program, a template of a PBS based job management system is prepared.

Job execution configuration file [general] section

Item	Contents	Description example
jobmanage_type	Specify the type of job execution interactive　interactive execution section-name　Use job management system	jobmanage_type = interactive jobmanage_type = pbs
[section-name]	Specify job execution script template Specify variables in the template Specify job submission command Specify job status command	[pbs] template = job_template/pbs.tmpl core = 8 np = 8 queue = L ncpus = 1 nodes = 1 ppn = 8 walltime = 24:00:00 job_name = submit = qsub stat = qstat

3. Usage of the program

3.1 Overview

The first principle automatic calculation program is a program that executes first principles calculation for a crystal structure (CIF file) prepared by a user.
- It consists of Python programs, and it runs on command basis in the Linux environment.
- The interface of the first principle automatic calculation program corresponds to the following first principle calculation program.
  - ・ The Vienna Abinitio Simulation Package (VASP)　　(http://www.vasp.at/)
  - ・ Quantum ESPRESSO　　(http://www.quantum-espresso.org/)
  - ・ ABINIT　　(http://www.abinit.org/)
- Execute first principles calculations sequentially based on the system or user prepared calculation scenario.
- By editing the configuration file, it can be used according to the user environment.

The processing outline of the first principle automatic calculation program is as follows.
- Read multiple crystal structures (CIF File) easy for the user
- Create a calculation directory for each crystal structure (Material ID)
- Generate input data and generate a job execution script based on the calculation scenario (calculation scenario setting file) and execute calculation。
- Calculated data is extracted and output to an automatic calculation data file.
- Analyze calculation results such as band gap.
- Output the crystal structure, charge density, state density distribution, band structure in a data format that can be visualized by commercially available / published applications。
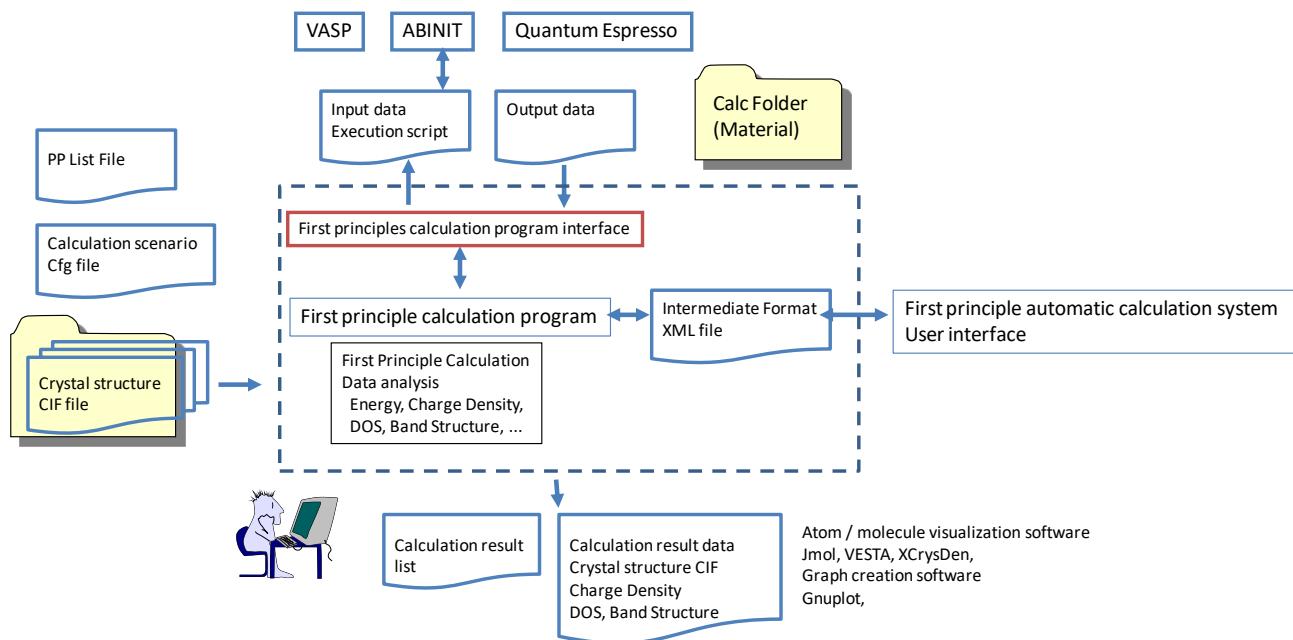

Fig.3.1 Outline of processing of automatic calculation program

3.2 Calculation parameters

Calculation parameters such as energy cutoff, exchange correlation term, SCF calculation iteration method, structure optimization method, convergence judgment value, etc. of the first principle calculation program are described in the calculation scenario setting file.

The unit cell (Primitive Cell) of calculation dependent on the crystal structure, the relative coordinates of atoms, the k point mesh, the k point route of the band structure calculation, the number of bands depending on the pseudopotential, etc. are calculated in the automatic calculation program.

Item	Calculation method
Crystal structure Atom list (atom coordinates)	Calculate Conventional Cell, Primitive Cell, atom list (atomic coordinates) from crystal_system, spacegroup, cell_length, cell_angle, symmetry, atom of CIF File
K point mesh	In calculation scenario setting file, length l is specified with _kpoints_length and calculated. bi, Reciprocal Lattice Vector $Nkx = max(4, l * |b1|+0.5)$ $Nky = max(4, l * |b2|+0.5)$ $Nkz = max(4, l * |b3|+0.5)$ In the calculation scenario setting file, spacing s is specified with _kpoints_spacing and calculated. $Nkx = max(4, |b1| / s +0.5)$ $Nky = max(4, |b2| / s +0.5)$ $Nkz = max(4, |b3| / s +0.5)$
Number of bands	Extract the value of Z Valence of the pseudopotential of each element. Calculate Electron number Nelect from Z Valence and the number of atoms of each element. $Nbands = int(Nelect*0.6+0.5) + max(4, Natom*2)$
k point path for the band calculation	Find the Brillouin Zone from crystal_system, spacegroup, cell_length, cell_angle, symmetry of CIF File and calculate k point path.

k point path for the band calculation

分類	System	Center	Type	Condition	K points Path,	K Points	
Simple cubic lattice	cubic	simple		A=B=C $\alpha=\beta=\gamma=90$	Delta Z Sigma Lambda T S	G(0.0 0.0 0.0) X(0.5 0.0 0.0) M(0.5 0.5 0.0) G(0.0 0.0 0.0) R(0.5 0.5 0.5) X(0.5 0.0 0.0)	X(0.5 0.0 0.0) M(0.5 0.5 0.0) G(0.0 0.0 0.0) R(0.5 0.5 0.5) M(0.5 0.5 0.0) R(0.5 0.5 0.5))
Face centered cubic lattice	cubic	face		A=B=C $\alpha=\beta=\gamma=90$	Delta Z Q Lambda Sigma S	G(0.0 0.0 0.0) X(1.0 0.0 0.0) W(1.0 0.5 0.0) L(0.5 0.5 0.5) G(0.0 0.0 0.0) U(1.0 0.5 0.5)	X(1.0 0.0 0.0) W(1.0 0.5 0.0) L(0.5 0.5 0.5) G(0.0 0.0 0.0) K(0.75 0.75 0.0) X(1.0 0.0 0.0)
Body centered cubic lattice	cubic	body		A=B=C $\alpha=\beta=\gamma=90$	Delta G	G(0.0 0.0 0.0) H(1.0 0.0 0.0)	H(1.0 0.0 0.0) N(0.5 0.5 0.0)

					Sigma	N(0.5 0.5 0.0)	G(0.0 0.0 0.0)
					Lambda	G(0.0 0.0 0.0)	P(0.5 0.5 0.5)
					D	P(0.5 0.5 0.5)	N(0.5 0.5 0.0)
					F	H(1.0 0.0 0.0)	P(0.5 0.5 0.5)
Hexagonal lattice	hexagonal	simple		$A=B\neq C$ $\alpha=\beta=90$ $\gamma=120$	Sigma	G(0.0 0.0 0.0)	M(0.5 0.0 0.0)
					T'	M(0.5 0.0 0.0)	K(1.0/3 1.0/3 0.0)
					T	K(1.0/3 1.0/3 0.0)	G(0.0 0.0 0.0)
					Lambda	G(0.0 0.0 0.0)	A(0.0 0.0 0.5)
					R	A(0.0 0.0 0.5)	L(0.5 0.0 0.5)
					S'	L(0.5 0.0 0.5)	H(1.0/3 1.0/3 0.5)
					S	H(1.0/3 1.0/3 0.5)	A(0.0 0.0 0.5)
					U	L(0.5 0.0 0.5)	M(0.5 0.0 0.0)
					P	K(1.0/3 1.0/3 0.0)	H(1.0/3 1.0/3 0.5)
Trigonal lattice 1	trigonal	simple	type1	$A=B=C$ $\alpha=\beta=\gamma$ $\alpha<90$	Q	F(0.0 0.5 1.0)	n1(2eta 0.5-eta 1.0)
					Sigma	n1(eta eta 0.0)	G(0.0 0.0 0.0)
					Lambda	G(0.0 0.0 0.0)	Z(0.0 0.0 1.5)
					B	Z(0.0 0.0 1.5)	n2(-eta 2eta 1.5)
					Y	n2(0.5-eta 2eta 0.5)	L(0.5 0.0 0.5)
					l1	L(0.5 0.0 0.5)	G(0.0 0.0 0.0)
Trigonal lattice 2	trigonal	simple	type2	$A=B=C$ $\alpha=\beta=\gamma$ $\alpha\geqq90$	Sigma	F(0.5 0.5 0.0)	G(0.0 0.0 0.0)
					Lambda	G(0.0 0.0 0.0)	n1(0.0 0.0 eta)
					P	n1(1.0 0.0 eta)	Z(1.0 0.0 -0.5)
					Y	Z(0.0 1.0 0.5)	L(0.5 0.0 0.5)
					l1	L(0.5 0.0 0.5)	G(0.0 0.0 0.0)
Simple tetoragonal lattice	tetragonal	simple		$A=B\neq C$ $\alpha=\beta=\gamma=90$	Delta	G(0.0 0.0 0.0)	X(0.5 0.0 0.0)
					Y	X(0.5 0.0 0.0)	M(0.5 0.5 0.0)
					Sigma	M(0.5 0.5 0.0)	G(0.0 0.0 0.0)
					Lambda	G(0.0 0.0 0.0)	Z(0.0 0.0 0.5)
					U	Z(0.0 0.0 0.5)	R(0.5 0.0 0.5)
					T	R(0.5 0.0 0.5)	A(0.5 0.5 0.5)
					S	A(0.5 0.5 0.5)	Z(0.0 0.0 0.5)
					W	R(0.5 0.0 0.5)	X(0.5 0.0 0.0)
					V	M(0.5 0.5 0.0)	A(0.5 0.5 0.5)
Body centered tetragonal lattice 1	tetragonal	body	type1	$A=B\neq C$ $\alpha=\beta=\gamma=90$ $A=B<C$	Lambda	Z(0.0 0.0 1.0)	G(0.0 0.0 0.0)
					Sigma	G(0.0 0.0 0.0)	n1(eta 0.0 0.0)
					F	n1(eta 0.0 1.0)	Z(0.0 0.0 1.0)
					U	Z(0.0 0.0 1.0)	n2(eta eta 1.0)
					Y	n2(eta 1.0-eta 0.0)	X(0.5 0.5 0.0)
					Delta	X(0.5 0.5 0.0)	G(0.0 0.0 0.0)
					W	X(0.5 0.5 0.0)	P(0.5 0.5 0.5)
					Q	P(0.5 0.5 0.5)	N(0.5 0.0 0.5)
Body centered tetragonal	tetragonal	body	type2	$A=B\neq C$ $\alpha=\beta=\gamma=90$	V	Z(1.0 0.0 0.0)	n1(1.0 0.0 eta)
					Lambda	n1(0.0 0.0 eta)	G(0.0 0.0 0.0)

lattice 2				A=B>C	Sigma	G(0.0 0.0 0.0)	Z(1.0 0.0 0.0)
					Y	Z(1.0 0.0 0.0)	X(0.5 0.5 0.0)
					Delta	X(0.5 0.5 0.0)	G(0.0 0.0 0.0)
					W	X(0.5 0.5 0.0)	P(0.5 0.5 0.5)
					Q	P(0.5 0.5 0.5)	N(0.5 0.0 0.5)
Simple orthorombic lattice	orthorhombic	simple		A≠B≠C $\alpha=\beta=\gamma=90$	Sigma	G(0.0 0.0 0.0)	X(0.5 0.0 0.0)
					D	X(0.5 0.0 0.0)	S(0.5 0.5 0.0)
					C	S(0.5 0.5 0.0)	Y(0.0 0.5 0.0)
					Delta	Y(0.0 0.5 0.0)	G(0.0 0.0 0.0)
					Lambda	G(0.0 0.0 0.0)	Z(0.0 0.0 0.5)
					A	Z(0.0 0.0 0.5)	U(0.5 0.0 0.5)
					P	U(0.5 0.0 0.5)	R(0.5 0.5 0.5)
					E	R(0.5 0.5 0.5)	T(0.0 0.5 0.5)
					B	T(0.0 0.5 0.5)	Z(0.0 0.0 0.5)
					G	U(0.5 0.0 0.5)	X(0.5 0.0 0.0)
					Q	S(0.5 0.5 0.0)	R(0.5 0.5 0.5)
					H	T(0.0 0.5 0.5)	Y(0.0 0.5 0.0)
Face centered orthorombic lattice 1	orthorhombic	face	type1	A≠B≠C $\alpha=\beta=\gamma=90$ $ka^2 < kb^2+kc^2$ $kb^2 < kc^2+ka^2$ $kc^2 < ka^2+kb^2$	Lambda	Z(0.0 0.0 1.0)	G(0.0 0.0 0.0)
					Sigma	G(0.0 0.0 0.0)	X(1.0 0.0 0.0)
					D	X(1.0 0.0 0.0)	n1(1.0 eta 0.0)
					B	n1(0.0 eta 1.0)	Z(0.0 0.0 1.0)
					A	Z(0.0 0.0 1.0)	n2(eta 0.0 1.0)
					C	n2(eta 1.0 0.0)	Y(0.0 1.0 0.0)
					Delta	Y(0.0 1.0 0.0)	G(0.0 0.0 0.0)
					H	Y(0.0 1.0 0.0)	n3(0.0 1.0 eta)
					G	n3(1.0 0.0 eta)	X(1.0 0.0 0.0)
Face centered orthorombic lattice 2	orthorhombic	face	type2	A≠B≠C $\alpha=\beta=\gamma=90$ $ka^2 > kb^2+kc^2$	Lambda	Z(0.0 0.0 1.0)	G(0.0 0.0 0.0)
					Sigma	G(0.0 0.0 0.0)	n1(eta 0.0 0.0)
					U	n1(eta 1.0 1.0)	X(0.0 1.0 1.0)
					B	X(0.0 1.0 1.0)	Z(0.0 0.0 1.0)
					A	Z(0.0 0.0 1.0)	n2(eta 0.0 1.0)
					C	n2(eta 1.0 0.0)	Y(0.0 1.0 0.0)
					Delta	Y(0.0 1.0 0.0)	G(0.0 0.0 0.0)
					H	Y(0.0 1.0 0.0)	X(0.0 1.0 1.0)
Face centered orthorombic lattice 3	orthorhombic	face	type3	A≠B≠C $\alpha=\beta=\gamma=90$ $kb^2 > kc^2+ka^2$	Lambda	Z(0.0 0.0 1.0)	G(0.0 0.0 0.0)
					Sigma	G(0.0 0.0 0.0)	X(1.0 0.0 0.0)
					D	X(1.0 0.0 0.0)	n2(1.0 eta 0.0)
					B	n2(0.0 eta 1.0)	Z(0.0 0.0 1.0)
					A	Z(0.0 0.0 1.0)	Y(1.0 0.0 1.0)
					R	Y(1.0 0.0 1.0)	n1(1.0 eta 1.0)
					Delta	n1(0.0 eta 0.0)	G(0.0 0.0 0.0)
					G	Y(1.0 0.0 1.0)	X(1.0 0.0 0.0)

Face centered orthorombic lattice 4	orthorhombic	face	type4	$A\neq B\neq C$ $\alpha=\beta=\gamma=90$ kc^2 > ka^2 + kb^2	Q Lambda Sigma D C Delta H G	Z(1.0 1.0 0.0) n1(0.0 0.0 eta) G(0.0 0.0 0.0) X(1.0 0.0 0.0) Z(1.0 1.0 0.0) Y(0.0 1.0 0.0) Y(0.0 1.0 0.0) n2(1.0 0.0 eta)	n1(1.0 1.0 eta) G(0.0 0.0 0.0) X(1.0 0.0 0.0) Z(1.0 1.0 0.0) Y(0.0 1.0 0.0) G(0.0 0.0 0.0) n2(0.0 1.0 eta) X(1.0 0.0 0.0)
Body centered orthorombic lattice 1	orthorhombic	body	type1	$A\neq B\neq C$ $\alpha=\beta=\gamma=90$ A>B A>C	Sigma U Delta Lambda G Q D P	G(0.0 0.0 0.0) X(1.0 0.0 0.0) n1(0.0 eta 0.0) G(0.0 0.0 0.0) n2(1.0 0.0 eta) R(0.5 0.0 0.5) W(0.5 0.5 0.5) T(0.5 0.5 0.0)	X(1.0 0.0 0.0) n1(1.0 eta 0.0) G(0.0 0.0 0.0) n2(0.0 0.0 eta) X(1.0 0.0 0.0) W(0.5 0.5 0.5) S(0.0 0.5 0.5) W(0.5 0.5 0.5)
Body centered orthorombic lattice 2	orthorhombic	body	type2	$A\neq B\neq C$ $\alpha=\beta=\gamma=90$ B>C B>A	Sigma F Delta Lambda G Q D P	G(0.0 0.0 0.0) n2(eta 1.0 0.0) X(0.0 1.0 0.0) G(0.0 0.0 0.0) n1(0.0 1.0 eta) R(0.5 0.0 0.5) W(0.5 0.5 0.5) T(0.5 0.5 0.0)	n2(eta 0.0 0.0) X(0.0 1.0 0.0) G(0.0 0.0 0.0) n1(0.0 0.0 eta) X(0.0 1.0 0.0) W(0.5 0.5 0.5) S(0.0 0.5 0.5) W(0.5 0.5 0.5)
Body centered orthorombic lattice 3	orthorhombic	body	type3	$A\neq B\neq C$ $\alpha=\beta=\gamma=90$ C>A C>B	Sigma F U Delta Lambda Q D P	G(0.0 0.0 0.0) n1(eta 0.0 1.0) X(0.0 0.0 1.0) n2(0.0 eta 0.0) G(0.0 0.0 0.0) R(0.5 0.0 0.5) W(0.5 0.5 0.5) T(0.5 0.5 0.0)	n1(eta 0.0 0.0) X(0.0 0.0 1.0) n2(0.0 eta 1.0) G(0.0 0.0 0.0) X(0.0 0.0 1.0) W(0.5 0.5 0.5) S(0.0 0.5 0.5) W(0.5 0.5 0.5)
Base centered orthorombic lattice 1	orthorhombic	base	type1	$A\neq B\neq C$ $\alpha=\beta=\gamma=90$ A<B	Sigma C Delta Lambda A E B H	G(0.0 0.0 0.0) n1(eta 1.0 0.0) Y(0.0 1.0 0.0) G(0.0 0.0 0.0) Z(0.0 0.0 0.5) n2(eta 1.0 0.5) T(0.0 0.0 0.5) Y(0.0 1.0 0.0)	n1(eta 0.0 0.0) Y(0.0 1.0 0.0) G(0.0 0.0 0.0) Z(0.0 0.0 0.5) n2(eta 0.0 0.5) T(0.0 1.0 0.5) Z(0.0 1.0 0.5) T(0.0 1.0 0.5)

					D	S(0.5 0.5 0.0)	R(0.5 0.5 0.5)
Base centered orthorombic lattice 2	orthorhombic	base	type2	A≠B≠C α＝β＝γ＝90 A＞B	Sigma	G(0.0 0.0 0.0)	Y(1.0 0.0 0.0)
					F	Y(1.0 0.0 0.0)	n1(1.0 eta 0.0)
					Delta	n1(0.0 eta 0.0)	G(0.0 0.0 0.0)
					Lambda	G(0.0 0.0 0.0)	Z(0.0 0.0 0.5)
					A	Z(0.0 0.0 0.5)	T(1.0 0.0 0.5)
					G	T(1.0 0.0 0.5)	n2(1.0 eta 0.5)
					B	n2(0.0 eta 0.5)	Z(0.0 0.0 0.5)
					H	Y(1.0 0.0 0.0)	T(1.0 0.0 0.5)
					D	S(0.5 0.5 0.0)	R(0.5 0.5 0.5)
Simple monoclinic lattice	monoclinic	simple		A≠B≠C α＝γ＝90 β＞90	Lambda	G(0.0 0.0 0.0)	Y(0.0 0.5 0.0)
					l1	Y(0.0 0.5 0.0)	C(0.0 0.5 0.5)
					W	C(0.0 0.5 0.5)	Z(0.0 0.0 0.5)
					l2	Z(0.0 0.0 0.5)	G(0.0 0.0 0.0)
					l3	G(0.0 0.0 0.0)	X(0.5 0.0 0.0)
					V	X(0.5 0.0 0.0)	A(0.5 0.5 0.0)
					l4	A(0.5 0.5 0.0)	Y(0.0 0.5 0.0)
					l5	Y(0.0 0.5 0.0)	E(0.5 0.5 -0.5)
					U	E(0.5 0.5 -0.5)	D(0.5 0.0 -0.5)
					l6	D(0.5 0.0 -0.5)	G(0.0 0.0 0.0)
Base monoclinic lattice 1	monoclinic	base	type1	A≠B≠C α＝γ＝90 β＞90 A＜B	Lambda	G(0.0 0.0 0.0)	Y(0.0 1.0 0.0)
					l1	Y(0.0 1.0 0.0)	n1(eta 1.0 0.0)
					l2	n1(eta 0.0 0.0)	G(0.0 0.0 0.0)
					l3	G(0.0 0.0 0.0)	Z(0.0 0.0 0.5)
					U	Z(0.0 0.0 0.5)	M(0.0 1.0 0.5)
					l4	M(0.0 1.0 0.5)	Y(0.0 1.0 0.0)
Base monoclinic lattice 2	monoclinic	base	type2	A≠B≠C α＝γ＝90 β＞90 A＞B	Lambda	G(0.0 0.0 0.0)	n1(0.0 eta 0.0)
					C	n1(1.0 eta 0.0)	Y(1.0 0.0 0.0)
					l1	Y(1.0 0.0 0.0)	G(0.0 0.0 0.0)
					l2	G(0.0 0.0 0.0)	Z(0.0 0.0 0.5)
					U	Z(0.0 0.0 0.5)	n2(0.0 eta 0.5)
					E	n2(1.0 eta -0.5)	M(1.0 0.0 -0.5)
					l3	M(1.0 0.0 -0.5)	Y(1.0 0.0 0.0)

3.3 Configuration file

3.3.1 Common configuration file (toast.cfg)

Common setting file toast.cfg sets common settings for job management and calculation scenarios for each program.
The settings in the common settings file take precedence over the calculation scenario settings file and job management settings file.

Section	name	value	
[job]	jobmanage_type	interactive	Interactive execution
		[section-name]	Generate job script using template and variable specified in [section]
	mpi_cmd		Specify a job script template
	nproc		Number of MPI execution processes
[vasp]	program		Specify the calculation program
	version		Program version
	ppdir		Specify the directory of the potential file
	pplist		Specify the potential list file
	cmd		Specify execution command of calculation program
	scenario		Specify Calculation scenario
[espresso]	program		Specify the calculation program
	version		Program version
	ppdir		Specify the directory of the potential file
	pplist		Specify the potential list file
	cmd		Specify execution command of calculation program
	scenario		Specify Calculation scenario
[abinit]	program		Specify the calculation program
	version		Program version
	ppdir		Specify the directory of the potential file
	pplist		Specify the potential list file
	cmd		Specify execution command of calculation program
	scenario		Specify Calculation scenario

3.3.2 Calculation scenario configuration file

The first principle automatic calculation program edits the configuration file in toast / config according to the user's computing environment. The configuration file is in the Config File format (RFC 822 format), it is divided into sections by the header [sectioin], parameters and values are described in the form of name = value in each section. Lines beginning with # are comment lines.
* Using the Python ConfigParser module.

● Execute multiple tasks in order according to the scenario specified by the user for the prepared CIF file.
● Configuration file is divided into sections with header [section-name].
● [general] section, [default] section The following sections set tasks to be executed sequentially.
● Each task consists of a unique parameter (_name) and a parameter (name) of the calculation program.
● The parameters of the calculation program are the keywords themselves of the input data of the first principles calculation program.

Section	name	value	
[geneal]	program		Specify the calculation program
		vasp	VASP
		espresso	Quantum ESPRESSO
		abinit	ABINIT
	version		Program version
	ppdir		Specify the directory of the potential file
	pplist		Specify the potential list file
	cmd		Specify execution command of calculation program
[default]	_kpoints_length	30	Specify length in K point mesh generation
	_kpoints_spacing	0.3	Specify spacing in K point mesh generation
	_spin		Specify spin calculation
		nomag	nomag calculatiion
		ferro	ferro calculatiion
	name	value	Common calculation program parameters in each [task] section In each [task] section, if _input = default is specified, these calculation parameters are added
[task]	_calc_dir		Specify subdirectory to execute [task]
	_structure	cif	Crystal structure of CIF file
		task 名	Crystal structure of calculation result of [task]
	_input	default	In each [task] section, the calculation parameter of [default] is added
	_spin_criteion	0.1	Spin determination value in spin determination calculation Valid when Task name is [check_spin]
	_mkdir_X		Specify subdirectory to generate
	_copy_X	[src] [dist]	Copy files
	_name_list_X	control system electrons	Namalist of input data (for QE)

	name	value	Calculation program parameters

3.3.3 Pseudopotential configuration file

In the calculation of the first principle calculation program, the potential of each element to be used is set. The first principle automatic calculation program prepares a pseudopotential setting file for each first principles calculation program.

Program	Configuration file	Pseudopotential	Remarks
VASP	potpaw_PBE.rec.txt	Potpaw_PBE	Recommended potential of VASP
QE	espresso.pp.pbe.sssp.eff.txt	SSSP_eff_PBE	Standard Solid State Pseudopotentials (SSSP) http://materialscloud.org/sssp/
	espresso.pp.pbe.gbrv.txt	GBRV pbe_UPF	GBRV pseudopotential http://www.physics.rutgers.edu/gbrv/
ABINIT	abinit.pp.pbe.jth.txt	JTH PAW	JTH PAW atomic datasets http://www.abinit.org/

Description of pseudopotential setting file

[Atomic number] [element name] [potential file / directory] …

3.3.4 Example of configuration file (default)

3.3.4.1 Example of configuration file (VASP)

An example configuration file for VASP is shown below.

(1) Calculation scenario configuration file
Spin determination calculation, structure optimization calculation, SCF calculation, DOS calculation, BAND calculation are sequentially calculated scenarios.

```
[general]
program = vasp
version = 5.3.5
ppdir = /opt/app/vasp/potpaw_PBE
pplist = vasp.pp.pbe.rec.txt
cmd = /opt/app/vasp/vasp.5.3.5/vasp
#mpi_cmd = mpijob -mpi
nproc = 1

[default]
_kpoints_length = 30
#_kpoints_spacing = 0.03
#_spin = nonmag
#_spin = ferro
NPAR = 1
SYSTEM =
ISTART = 0
```

```
PREC = high
ENCUT = 550
ALGO = fast
#ALGO = normal
EDIFF = 1E-6
NELM = 100  # default 60
#NELMIN = 8
#NELMDL = -5
ISPIN =
NBANDS =
ISMEAR = 0  # default 1
SIGMA = 0.1  # default 0.2
ISYM =

[check_spin]
_calc_dir = spin
_structure = cif
_input = default
_spin_criterion = 0.1
ISPIN = 2
LWAVE = .FALSE.
LCHARG = .FALSE.
IBRION = 2
ISIF = 3
NSW = 100
EDIFFG = 1e-5
POTIM = 0.05

[opt1]
_calc_dir = opt.1
_structure = cif
_input = default
NELMIN = 8
LWAVE =.FALSE.
LCHARG =.FALSE.
IBRION =2
ISIF = 3
NSW = 200
EDIFFG = 1e-5
POTIM = 0.05

[opt2]
_calc_dir = opt.2
_structure = opt1
_input = default
NELMIN = 8
LWAVE =.FALSE.
LCHARG =.FALSE.
IBRION =2
```

```
ISIF = 3
NSW = 200
EDIFFG = -0.01
POTIM = 0.05


[scf]
_calc_dir = scf
_structure = opt2
_input = default
NELMIN = 8
ISMEAR = -5
LAECHG = .TRUE.


[dos]
_calc_dir = dos
_structure = scf
_input = default
_copy_2 = ../scf/WAVECAR WAVECAR
_copy_3 = ../scf/CHGCAR CHGCAR
NELMIN = 8
ISMEAR = -5
ICHARG = 11
LORBIT = 11
_emin_ef = -20
_emax_ef = +20
EMIN = -20
EMAX = 30
NEDOS = 2501
LWAVE = .FALSE.


[band]
_calc_dir = band
_structure = scf
_input = default
_copy_2 = ../scf/WAVECAR WAVECAR
_copy_3 = ../scf/CHGCAR CHGCAR
ISMEAR =
SIGMA =
ICHARG = 11
LWAVE = .FALSE.
```

(2) Pseudopotential configuration file

```
1  H  H
2  He  He
3  Li  Li_sv
4  Be  Be
5  B  B
6  C  C
```

```
7  N  N
8  O  O
9  F  F
10  Ne  Ne
11  Na  Na_pv
12  Mg  Mg
13  Al  Al
14  Si  Si
15  P  P
16  S  S
17  Cl  Cl
18  Ar  Ar
19  K  K_sv
20  Ca  Ca_sv
21  Sc  Sc_sv
22  Ti  Ti_sv
23  V  V_sv
24  Cr  Cr_sv_GW
25  Mn  Mn_pv
26  Fe  Fe
27  Co  Co
28  Ni  Ni
29  Cu  Cu
30  Zn  Zn
31  Ga  Ga_d
32  Ge  Ge_d
33  As  As
34  Se  Se
35  Br  Br
36  Kr  Kr
37  Rb  Rb_sv
38  Sr  Sr_sv
39  Y  Y_sv
40  Zr  Zr_sv
41  Nb  Nb_sv
42  Mo  Mo_sv
43  Tc  Tc_pv
44  Ru  Ru_sv_GW
45  Rh  Rh_sv_GW
46  Pd  Pd
47  Ag  Ag
48  Cd  Cd
49  In  In_d
50  Sn  Sn_d
51  Sb  Sb
52  Te  Te
53  I  I
54  Xe  Xe
55  Cs  Cs_sv
```

```
56  Ba  Ba_sv
57  La  La
58  Ce  Ce
59  Pr  Pr_3
60  Nd  Nd_3
61  Pm  Pm_3
62  Sm  Sm_3
63  Eu  Eu_2
64  Gd  Gd_3
65  Tb  Tb_3
66  Dy  Dy_3
67  Ho  Ho_3
68  Er  Er_3
69  Tm  Tm_3
70  Yb  Yb_2
71  Lu  Lu_3
72  Hf  Hf_pv
73  Ta  Ta_sv_GW
74  W  W_sv
75  Re  Re
76  Os  Os
77  Ir  Ir
78  Pt  Pt
79  Au  Au
80  Hg  Hg
81  Tl  Tl_d
82  Pb  Pb_d
83  Bi  Bi_d
84  Po  Po_d
85  At  At_d_GW
86  Rn  Rn
87  Fr  Fr_sv
88  Ra  Ra_sv
89  Ac  Ac
90  Th  Th
91  Pa  Pa
92  U  U
93  Np  Np
94  Pu  Pu
95  Am  Am
96  Cm  Cm
```

3.3.4.1 Example of configuration file (Quantum ESPRESSO)

An example configuration file for Quantum ESPRESSO is shown below.

(1) Calculation scenario configuration file
Spin determination calculation, structure optimization calculation, SCF calculation, DOS calculation, BAND

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calculation are sequentially calculated scenarios.

```
[general]
program = espresso
version = 5.4.0
#ppdir = /opt/app/espresso/upf_files
ppdir = /opt/app/espresso/SSSP_eff_PBE
pplist = espresso.pp.pbe.sssp.eff.txt
#ppdir = /opt/app/espresso/gbrv
#pplist = espresso.pp.pbe.gbrv.txt
cmd = /opt/app/espresso/espresso-5.4.0/bin/pw.x
nproc = 1

[default]
_kpoints_length = 30
#_kpoints_spacing = 0.03
#_spin = nonmag
#_spin = ferro

_namelist_1 = control
calculation =
prefix =
tstress = .true.
tprnfor = .true.
pseudo_dir = '../'
outdir = './'
wfcdir =
etot_conv_thr = 1.0e-5
forc_conv_thr = 1.0e-4
disk_io = 'low'
wf_collect =

_namelist_2 = system
ibrav = 0
nat =
ntyp =
nbnd =
ecutwfc = 40.0
ecutrho = 200.0
occupations = 'smearing'
smearing = 'gaussian'
degauss = 0.1
nspin = 1

_namelist_3 = electrons
mixing_beta = 0.7
conv_thr = 1.0e-6
```

```
_namelist_4 = ions
_namelist_5 = cell


[check_spin]
_calc_dir = spin
_structure = cif
_input = default
calculation = 'vc-relax'
nspin = 2


[opt]
_calc_dir = opt
_structure = cif
_input = default
calculation = 'vc-relax'


[scf]
_calc_dir = scf
_structure = opt
_input = default
calculation = 'scf'
wfcdir = './'


[charge]
_calc_dir = scf
_cmd = /opt/app/espresso/espresso-5.4.0/bin/pp.x
_input_file = job2.in
_script_file = job2.sh
_log_file = log2
_namelist_1 = inputpp
prefix =
filplot = charge
plot_num = 0
spin_component = 0
#spin_component = 1  # spin up
#spin_component = 2  # spin down
_namelist_2 = plot
iflag = 3
output_format = 6
fileout = charge.cube


[nscf]
_calc_dir = dos
_structure = scf
_input = default
_mkdir = pwscf.save
_copy_1 = ../scf/pwscf.save/data-file.xml ./pwscf.save/data-file.xml
_copy_2 = ../scf/pwscf.save/charge-density.dat ./pwscf.save/charge-density.dat
_copy_3 = ../scf/pwscf.save/spin-polarization.dat ./pwscf.save/spin-polarization.dat
```

```
_copy_4 = ../scf/pwscf.paw ./pwscf.paw
calculation = 'nscf'
wf_collect = .true.
occupations = 'tetrahedra'
smearing =
degauss =


[tdos]
_calc_dir = dos
_cmd = /opt/app/espresso/espresso-5.4.0/bin/dos.x
_input_file = job2.in
_script_file = job2.sh
_log_file = log2
_namelist = dos
prefix =
fildos = dos
emin =
emax =


[pdos]
_calc_dir = dos
_cmd = /opt/app/espresso/espresso-5.4.0/bin/projwfc.x
_input_file = job3.in
_script_file = job3.sh
_log_file = log3
_namelist = projwfc
prefix =
filpdos = pdos
emin =
emax =


[dos_band]
_calc_dir = dos
_cmd = /opt/app/espresso/espresso-5.4.0/bin/bands.x
_input_file = job4.in
_script_file = job4.sh
_log_file = log4
_namelist = bands
prefix =
filband = band
#lsym = .true.


[dos_band2]
_calc_dir = dos
_cmd = /opt/app/espresso/espresso-5.4.0/bin/bands.x
_input_file = job5.in
_script_file = job5.sh
_log_file = log5
_namelist = bands
```

```
prefix =
filband = band2
#lsym = .true.
spin_component = 2


[band]
_calc_dir = band
_structure = scf
_input = default
_mkdir = pwscf.save
_copy_1 = ../scf/pwscf.save/data-file.xml ./pwscf.save/data-file.xml
_copy_2 = ../scf/pwscf.save/charge-density.dat ./pwscf.save/charge-density.dat
_copy_3 = ../scf/pwscf.save/spin-polarization.dat ./pwscf.save/spin-polarization.dat
_copy_4 = ../scf/pwscf.paw ./pwscf.paw
calculation = 'bands'
prefix =
occupations = 'smearing'
smearing = 'gaussian'
degauss = 0.01
#K_POINTS = {crystal_b}


[band_plot]
_calc_dir = band
_cmd = /opt/app/espresso/espresso-5.4.0/bin/bands.x
_input_file = job2.in
_script_file = job2.sh
_log_file = log2
_namelist = bands
prefix =
filband = band
#lsym = .true.


[band_plot2]
_calc_dir = band
_cmd = /opt/app/espresso/espresso-5.4.0/bin/bands.x
_input_file = job3.in
_script_file = job3.sh
_log_file = log3
_namelist = bands
prefix =
filband = band2
#lsym = .true.
spin_component = 2
```

(2) Pseudopotential configuration file

```
1 H H.pbe-rrkjus_psl.0.1.UPF
2 He He_ONCV_PBE-1.0.upf
3 Li li_pbe_v1.4.uspp.F.UPF
```

```
4 Be Be_ONCV_PBE-1.0.upf

4 Be be_pbe_v1.4.uspp.F.UPF

5 B B.pbe-n-kjpaw_psl.0.1.UPF

6 C C_pbe_v1.2.uspp.F.UPF

7 N N.pbe.theos.UPF

8 O O_pbe_v1.2.uspp.F.UPF

9 F f_pbe_v1.4.uspp.F.UPF

10 Ne Ne.pbe-n-kjpaw_psl.1.0.0.UPF

11 Na Na_pbe_v1.uspp.F.UPF

12 Mg mg_pbe_v1.4.uspp.F.UPF

13 Al Al.pbe-n-kjpaw_psl.1.0.0.UPF

14 Si Si.pbe-n-rrkjus_psl.1.0.0.UPF

15 P P.pbe-n-rrkjus_psl.1.0.0.UPF

16 S S_pbe_v1.2.uspp.F.UPF

17 Cl cl_pbe_v1.4.uspp.F.UPF

18 Ar Ar.pbe-n-rrkjus_psl.1.0.0.UPF

19 K K.pbe-spn-rrkjus_psl.1.0.0.UPF

20 Ca Ca_pbe_v1.uspp.F.UPF

21 Sc Sc_pbe_v1.uspp.F.UPF

22 Ti ti_pbe_v1.4.uspp.F.UPF

23 V V_pbe_v1.uspp.F.UPF

24 Cr cr_pbe_v1.5.uspp.F.UPF

25 Mn Mn.pbe-spn-kjpaw_psl.0.3.1.UPF

26 Fe Fe.pbe-spn-kjpaw_psl.0.2.1.UPF

27 Co Co_pbe_v1.2.uspp.F.UPF

28 Ni ni_pbe_v1.4.uspp.F.UPF

29 Cu Cu_pbe_v1.2.uspp.F.UPF

30 Zn Zn_pbe_v1.uspp.F.UPF

31 Ga Ga.pbe-dn-rrkjus_psl.0.2.UPF

32 Ge Ge.pbe-dn-kjpaw_psl.1.0.0.UPF

33 As As.pbe-n-rrkjus_psl.0.2.UPF

34 Se Se_pbe_v1.uspp.F.UPF

35 Br br_pbe_v1.4.uspp.F.UPF

36 Kr Kr.pbe-n-rrkjus_psl.0.2.3.UPF

37 Rb Rb_ONCV_PBE-1.0.upf

38 Sr Sr.pbe-spn-rrkjus_psl.1.0.0.UPF

39 Y Y_pbe_v1.uspp.F.UPF

40 Zr Zr_pbe_v1.uspp.F.UPF

41 Nb Nb.pbe-spn-kjpaw_psl.0.3.0.UPF

42 Mo Mo_ONCV_PBE-1.0.upf

43 Tc Tc_ONCV_PBE-1.0.upf

44 Ru Ru_ONCV_PBE-1.0.upf

45 Rh Rh.pbe-spn-kjpaw_psl.1.0.0.UPF

46 Pd Pd.pbe-spn-kjpaw_psl.1.0.0.UPF

47 Ag ag_pbe_v1.4.uspp.F.UPF

48 Cd Cd.pbe-dn-rrkjus_psl.0.3.1.UPF

49 In In.pbe-dn-rrkjus_psl.0.2.2.UPF

50 Sn Sn_pbe_v1.uspp.F.UPF

51 Sb sb_pbe_v1.4.uspp.F.UPF
```

```
52 Te Te_pbe_v1.uspp.F.UPF

53 I I_pbe_v1.uspp.F.UPF

54 Xe Xe.pbe-dn-rrkjus_psl.1.0.0.UPF

55 Cs Cs_pbe_v1.uspp.F.UPF

56 Ba Ba_ONCV_PBE-1.0.upf

57 La La.GGA-PBE-paw-v1.0.UPF

58 Ce Ce.GGA-PBE-paw-v1.0.UPF

59 Pr Pr.GGA-PBE-paw-v1.0.UPF

60 Nd Nd.GGA-PBE-paw-v1.0.UPF

61 Pm Pm.GGA-PBE-paw-v1.0.UPF

62 Sm Sm.GGA-PBE-paw-v1.0.UPF

63 Eu Eu.GGA-PBE-paw-v1.0.UPF

64 Gd Gd.GGA-PBE-paw-v1.0.UPF

65 Tb Tb.GGA-PBE-paw-v1.0.UPF

66 Dy Dy.GGA-PBE-paw-v1.0.UPF

67 Ho Ho.GGA-PBE-paw-v1.0.UPF

68 Er Er.GGA-PBE-paw-v1.0.UPF

69 Tm Tm.GGA-PBE-paw-v1.0.UPF

70 Yb Yb.GGA-PBE-paw-v1.0.UPF

71 Lu Lu.GGA-PBE-paw-v1.0.UPF

72 Hf Hf.pbe-spn-rrkjus_psl.0.2.UPF

73 Ta Ta_pbe_v1.uspp.F.UPF

74 W W_pbe_v1.2.uspp.F.UPF

75 Re Re_pbe_v1.2.uspp.F.UPF

76 Os Os_pbe_v1.2.uspp.F.UPF

77 Ir Ir_pbe_v1.2.uspp.F.UPF

78 Pt pt_pbe_v1.4.uspp.F.UPF

79 Au Au_ONCV_PBE-1.0.upf

80 Hg Hg_pbe_v1.uspp.F.UPF

81 Tl Tl.pbe-dn-rrkjus_psl.0.2.3.UPF

82 Pb Pb.pbe-dn-kjpaw_psl.0.2.2.UPF

83 Bi Bi.pbe-dn-kjpaw_psl.0.2.2.UPF

84 Po Po.pbe-dn-rrkjus_psl.1.0.0.UPF

86 Rn Rn.pbe-dn-rrkjus_psl.1.0.0.UPF
```

3.3.4.1 Example of configuration file （ABINIT）

An example configuration file for ABINIT is shown below.

(1) Calculation scenario configuration file

Spin determination calculation, structure optimization calculation, SCF calculation, DOS calculation, BAND calculation are sequentially calculated scenarios.

```
[general]
program = abinit
version = 8.0.7
ppdir = /opt/app/abinit/JTH-PBE-atomicdata-1.0
pplist = abinit.pp.pbe.jth.txt
```

```
#ppdir = /opt/app/abinit/gbrv
#pplist = abinit.pp.pbe.gbrv.txt
cmd = /opt/app/abinit/abinit-8.0.8/bin/abinit
#cmd = /opt/app/abinit/abinit-7.10.5/bin/abinit
nproc = 1

[default]
_kpoints_length = 30
#_kpoints_spacing = 0.03
#_spin = nonmag
#_spin = ferro
acell =
rprim =
ntypat = 0
znucl =
natom = 0
typat =
xred =
nband =
ecut = 30
pawecutdg = 40
iscf = 17
#ixc = 11
nstep = 100
occopt = 7
nsppol =
enunit = 1
prtxml = 1
kptopt = 1
ngkpt =
nshiftk =
shiftk =
prtcif = 1
autoparal = 1

[check_spin]
_calc_dir = spin
_structure = cif
_input = default
#_spin_criterion = 0.1
_spin_criterion = 0.0001
nsppol = 2
toldfe = 1.0e-6
#tolmxf = 0.5e-4
optcell = 1
ionmov = 2
dilatmx = 1.05
ecutsm = 0.5
ntime = 50
```

```
[opt1]
_calc_dir = opt.1
_structure = cif
_input = default
toldfe = 1.0e-6
#tolmxf = 1.0e-4
optcell = 1
ionmov = 2
dilatmx = 1.05
ecutsm = 0.5
ntime = 50


[opt2]
_calc_dir = opt.2
_structure = opt1
_input = default
toldfe = 1.0e-6
#toldff = 1.0e-4
#tolmxf = 1.0e-4
optcell = 1
ionmov = 2
#dilatmx = 1.05
dilatmx = 1.1
ecutsm = 0.5
ntime = 50


[scf]
_calc_dir = scf
_structure = opt2
_input = default
toldfe = 1.0e-6


[dos]
_calc_dir = dos
_structure = scf
_input = default
_copy = ../scf/jobxo_DEN jobxi_DEN
iscf = -2
tolwfr = 1.0e-10
prtdos = 2
#prtdos = 3


[pdos]
_calc_dir = pdos
_structure = scf
_input = default
_copy = ../scf/jobxo_DEN jobxi_DEN
iscf = -2
```

```
tolwfr = 1.0e-10
#prtdos = 2
prtdos = 3


[band]
_calc_dir = band
_structure = scf
_input = default
_copy = ../scf/jobxo_DEN jobxi_DEN
iscf = -2
tolwfr = 1.0e-10
kptopt = 0
```

(2) Pseudopotential configuration file

```
1 H H.GGA_PBE-JTH.xml
2 He He.GGA_PBE-JTH.xml
3 Li Li.GGA_PBE-JTH.xml
4 Be Be.GGA_PBE-JTH.xml
5 B B.GGA_PBE-JTH.xml
6 C C.GGA_PBE-JTH.xml
7 N N.GGA_PBE-JTH.xml
8 O O.GGA_PBE-JTH.xml
9 F F.GGA_PBE-JTH.xml
10 Ne Ne.GGA_PBE-JTH.xml
11 Na Na.GGA_PBE-JTH.xml
12 Mg Mg.GGA_PBE-JTH.xml
13 Al Al.GGA_PBE-JTH.xml
14 Si Si.GGA_PBE-JTH.xml
15 P P.GGA_PBE-JTH.xml
16 S S.GGA_PBE-JTH.xml
17 Cl Cl.GGA_PBE-JTH.xml
18 Ar Ar.GGA_PBE-JTH.xml
19 K K.GGA_PBE-JTH.xml
20 Ca Ca.GGA_PBE-JTH.xml
21 Sc Sc.GGA_PBE-JTH.xml
22 Ti Ti.GGA_PBE-JTH.xml
23 V V.GGA_PBE-JTH.xml
24 Cr Cr.GGA_PBE-JTH.xml
25 Mn Mn.GGA_PBE-JTH.xml
26 Fe Fe.GGA_PBE-JTH.xml
27 Co Co.GGA_PBE-JTH.xml
28 Ni Ni.GGA_PBE-JTH.xml
29 Cu Cu.GGA_PBE-JTH.xml
30 Zn Zn.GGA_PBE-JTH.xml
31 Ga Ga.GGA_PBE-JTH.xml
32 Ge Ge.GGA_PBE-JTH.xml
#33 As As.GGA_PBE-JTH_sp.xml
33 As As.GGA_PBE-JTH.xml
```

```
34 Se Se.GGA_PBE-JTH.xml

35 Br Br.GGA_PBE-JTH.xml

36 Kr Kr.GGA_PBE-JTH.xml

37 Rb Rb.GGA_PBE-JTH.xml

38 Sr Sr.GGA_PBE-JTH.xml

39 Y Y.GGA_PBE-JTH.xml

40 Zr Zr.GGA_PBE-JTH.xml

41 Nb Nb.GGA_PBE-JTH.xml

42 Mo Mo.GGA_PBE-JTH.xml

43 Tc Tc.GGA_PBE-JTH.xml

44 Ru Ru.GGA_PBE-JTH.xml

45 Rh Rh.GGA_PBE-JTH.xml

46 Pd Pd.GGA_PBE-JTH.xml

47 Ag Ag.GGA_PBE-JTH.xml

48 Cd Cd.GGA_PBE-JTH.xml

#49 In In.GGA_PBE-JTH_sp.xml

49 In In.GGA_PBE-JTH.xml

#50 Sn Sn.GGA_PBE-JTH_sp.xml

50 Sn Sn.GGA_PBE-JTH.xml

#51 Sb Sb.GGA_PBE-JTH_sp.xml

51 Sb Sb.GGA_PBE-JTH.xml

52 Te Te.GGA_PBE-JTH.xml

53 I I.GGA_PBE-JTH.xml

54 Xe Xe.GGA_PBE-JTH.xml

55 Cs Cs.GGA_PBE-JTH.xml

56 Ba Ba.GGA_PBE-JTH.xml

57 La La.GGA_PBE-JTH.xml

58 Ce Ce.GGA_PBE-JTH.xml

59 Pr Pr.GGA_PBE-JTH.xml

60 Nd Nd.GGA_PBE-JTH.xml

61 Pm Pm.GGA_PBE-JTH.xml

62 Sm Sm.GGA_PBE-JTH.xml

63 Eu Eu.GGA_PBE-JTH.xml

64 Gd Gd.GGA_PBE-JTH.xml

65 Tb Tb.GGA_PBE-JTH.xml

66 Dy Dy.GGA_PBE-JTH.xml

67 Ho Ho.GGA_PBE-JTH.xml

68 Er Er.GGA_PBE-JTH.xml

69 Tm Tm.GGA_PBE-JTH.xml

70 Yb Yb.GGA_PBE-JTH.xml

71 Lu Lu.GGA_PBE-JTH.xml

72 Hf Hf.GGA_PBE-JTH.xml

73 Ta Ta.GGA_PBE-JTH.xml

74 W W.GGA_PBE-JTH.xml

75 Re Re.GGA_PBE-JTH.xml

76 Os Os.GGA_PBE-JTH.xml

77 Ir Ir.GGA_PBE-JTH.xml

78 Pt Pt.GGA_PBE-JTH.xml

79 Au Au.GGA_PBE-JTH.xml
```

```
80 Hg Hg.GGA_PBE-JTH.xml
#81 Tl Tl.GGA_PBE-JTH_sp.xml
81 Tl Tl.GGA_PBE-JTH.xml
#82 Pb Pb.GGA_PBE-JTH_sp.xml
82 Pb Pb.GGA_PBE-JTH.xml
#83 Bi Bi.GGA_PBE-JTH_sp.xml
83 Bi Bi.GGA_PBE-JTH.xml
84 Po Po.GGA_PBE-JTH.xml
85 At At.GGA_PBE-JTH.xml
86 Rn Rn.GGA_PBE-JTH.xml
```

3.3.5 Job execution configuration file

Job execution setting file jobmanage.cfg sets the format of job submission command and job script according to the user's job execution environment (job management system). For the job script format, use the template in the config / job_template directory.

Section	name	value	
[general]	jobmanage_type	interactive [section-name]	Interactive execution Generate job script using template and variable specified in [section]
[type]	template		Specify a job script template
	np		Number of MPI execution processes
	name	value	Specify variables in job script template

3.3.6 Example of job execution configuration file

3.3.6.1 Example of configuration file (PBS)

An example job execution setting file using Torque as the PBS job management system is shown below.

(1) Job execution configuration file   jobmanage.cfg

```
[general]
#jobmanage_type = interactive
jobmanage_type = pbs

[interactive]
submit = sh
stat = ps

[pbs]
template = job_template/pbs.tmpl
core = 8
np = 8
queue = L
ncpus = 1
nodes = 1
```

```
ppn = 8
walltime = 24:00:00
job_name =
submit = qsub
stat = qstat
```

(2) Job script template　pbs.tmpl

```
#!/bin/csh
#PBS -q $queue
#PBS -l ncpus=$ncpus
#PBS -l nodes=$nodes:ppn=$ppn
#PBS -l walltime=$walltime

#PBS -N $job_name
cd $$PBS_O_WORKDIR
```

3.4 Execution of program

3.4.1 Automatic calculation of multiple materials

Read the crystal structure (CIF File) of multiple materials easier for the user, and execute sequential calculation based on the calculation scenario.

- Crystal structure files are prepared by users in one directory.
- Calculation data is calculated in a subdirectory for each crystal structure in the specified directory.
- Material ID is set from the CIF filename. (CIF File minus the extension. Cif)

Python Script	Option		
calc/ac-setup.py	-m, --matdir	Directory with crystal structure (CIF File)	
	-c, --caldir	Directory where calculation is performed	
	-p, --program	Specify first principles calculation program	vasp (default) espresso abinit
	-s, --scenario	Specify calculation scenario configuration file	Default System provides User scenario
	-n, --nproc	Number of MPI execution processes	

Example of execution

%python　[INSTALLDIR]/toast/calc/ac-setup.py -m matdir -c caldir -p vasp -s vasp.para.opt.checkspin.cfg -n 8

3.4.2 Automatic calculation of multiple materials (Job status update / Add submit)

Read the crystal structure (CIF File) of multiple materials easier for the user, and execute sequential calculation based on the calculation scenario.

- Job status update / Add submit)
- Submit new job

Python Script	Option		
calc/ac-update.py	joblist	joblist file	joblist.txt
	-c, --caldir	Directory where calculation is performed	
	-n, --dry-run	Status Update only	No new Job submit
	-q, --qstat	Check job management system status and update job status	
	-v, --verbose		

Example of execution

%python　[INSTALLDIR]/toast/calc/ac-update.py –c caldir -v joblist.txt

3.4.3 First principle automatic calculation of one crystal structure

Execute the calculation based on the calculation scenario in the directory with the crystal structure (CIF File).

It is a Python script called from Python script ac-setup.py, ac-update.py which performs first principles calculation of multiple crystal structures (CIF File).

Python Script	Option		
calc/ac-calc.py	-m, --mat	Material ID Crystal structure (CIF File) excluding extension. Cif	For AtomWork CIF files, excluding -1-2.cif
	-p, --program	Specify first principles calculation program	vasp (default) espresso abinit
	-s, --scenario	Specify calculation scenario configuration file	Default System provides User scenario
	-n, --nproc	Number of MPI execution processes	

Example of execution

%python   [INSTALLDIR]/toast/calc/ac-calc.py -m 4295272247 -p vasp -s vasp.para.opt.checkspin.cfg -n 8

3.4.4 Calculated data list

For a plurality of crystal structures (CIF File) easy for the user, part of calculation result of first principle automatic calculation is outputted to a text file in list format.

Python Script	Option		
calc/ac-summary.py	-c, --cal	Directory where calculation was performed	
	-o, --output	Output file	caldata.txt

Example of execution

%python　[INSTALLDIR]/toast/calc/ac-summary.py -c caldir

Contents of Output

Item	Contents	Remarks
Material ID		Information on CIF File
Chemical Formula		Information on CIF File
Spacegroup		Information on CIF File
Spacegroup No		Information on CIF File
Lattice Parameter (original)	Cell Length a, b, c Cell Angle　alpha, beta, gamma	Information on CIF File
Lattice Parameter (relaxed)	Cell Length a, b, c Cell Angle　alpha, beta, gamma	
Total Energy (eV)		
Fermi Energy (eV)		
Bandgap Type	metal, direct, indirect	
Bandgap (eV)		

Output example

```
material chemica_formula spacegroup_name spacegroup_no lattice_parameter(original) lattice_parameter(relaxed)
total_energy(eV/atom) fermi_energy(eV) bandgaptype bandgap(eV)
4295272247 Si cubic Fd-3m 227 5.429 5.429 5.429 90.0 90.0 90.0 5.4688472 5.4688472 5.4688472 90.0 90.0 90.0 -5.42460796
5.65437076 indirect 0.618
4295278799 Fe cubic Im-3m 229 2.862 2.862 2.862 90.0 90.0 90.0 2.83553114 2.83553114 2.83553114 90.0 90.0 90.0
-8.23692267 5.75646479 metal -
4295349454 O Si cubic F-43m 216 5.45 5.45 5.45 90.0 90.0 90.0 4.87188342 4.87188342 4.87188342 90.0 90.0 90.0
-5.506395975 6.30502700 metal -
```

3.4.5 Calculation status

For the plurality of crystal structures (CIF File) easy for the user, the calculation status of the first principle automatic calculation is outputted to the text file in the list format.

Python Script	Option		
calc/ac-stat.py	-c, --caldir	Directory where calculation was performed	
	-o, --output	Output file	Default calstat.txt

Example of execution

%python [INSTALLDIR]/toast/calc/ac-stat.py -c caldir

Contents of Output

項目	内容	備考
Material ID		Information on CIF File
Chemical Formula		Information on CIF File
Spacegroup		Information on CIF File
Spacegroup No		Information on CIF File
CIF File		Information on CIF File
Calculation Status	Calculation status o End calculation E Abnormal termination / (Calculating) - Unexecuted	Calculation status of each task in calculation scenario

Determination of calculation status

計算状況	VASP	Quantum ESPRESSO	ABINIT
o End calculation	vasprun.xml is normal output OUTCAR is normal output	JOB DONE. Outputs to the log file (standard output)	Calculation Completed is output to job.out
E Abnormal termination / (Calculating)	vasprun.xml is abnormal OUTCAR is abnormal	JOB DONE. Is not output to log file (standard output)	Calculation Completed is not output to job.out
- Unexecuted	vasprun.xml, OUTCAR does not exist	Log file (standard output) does not exist	Job.out does not exist

Output example

```
material chemica_formula spacegroup_name spacegroup_no calculation_status
4295272247 Si cubic Fd-3m 227 4295272247-1-2.cif o o o o o o
4295278799 Fe cubic Im-3m 229 4295278799-1-2.cif o o o o o o
4295349454 O Si cubic F-43m 216 4295349454-1-2.cif o o o o o o
```

3.4.6 Visualization Data

The visualization data of the calculation result of the first principle calculation is output to the HTML file of the list display and the detailed display.
To visualize the crystal structure, it is necessary to change the browser settings.
Reference: http://wiki.jmol.org/index.php/Troubleshooting/Local_Files

Python Script	Option		
calc/ac-vis.py	-c, --caldir	Directory where calculation was performed	
	-o, --output	Output file	default caldata.html
	-j, --jsdir	Java Script Library Path	cdn / None　(default) Local User define
	-a, --archive	Visualization data (zip file)	

Example of execution

%python　[INSTALLDIR]/toast/calc/ac-vis.py -c [caldir] -a caldata.zip

Contents of Output (List)

項目	内容	備考
Material ID		Information about CIF File
Chemical Formula		Information about CIF File
Spacegroup		Information about CIF File
Spacegroup No		Information about CIF File
Lattice Parameter (original)	Cell Length a, b, c Cell Angle　alpha, beta, gamma	Information about CIF File
Lattice Parameter (relaxed)	Cell Length a, b, c Cell Angle　alpha, beta, gamma	
Total Energy (eV)		
Fermi Energy (eV)		
Bandgap Type	metal, direct, indirect	
Bandgap (eV)		

Contents of Output (Detail)

項目	内容	備考
Material Information		
Crystal Structure	Crystal System Space Group Space Group Number Cell Parameter Atom Sites	
Structure	Conventional Cell (Initial) Primitive Cell (Initial) Primitive Cell (Relaxed) Brillouin Zone	
Energy	Total Energy	

	Fermi Energy	
Band Structure		
Density of State		
Electronic Property	Band Gap Band Gap Type	

Example of Output (List)

Example of Output (Detail)

3.5 Calculation data

3.5.1 Outline of calculation data

 A sub-directory of each task (task) of the calculation scenario is created in the calculation execution directory for each crystal, and the first principle calculation is executed. The input / output data for calculation of each task (task) is stored in the subdirectory.

The main calculation data are summarized in the first principle automatic calculation data file calculations.xml. In addition, a part of the calculation data is output in a data structure that can be visualized by Gnuplot visualization application or crystal structure.

項目	データファイル	内容	備考
Crystal structure	[maid].cif [maid].relaxed.cif [maid].relaxed.p1cif	User prepared CIF File CIF File after structure optimization CIF File after structure optimization (P1)	Update lattice constant of original CIF File CIF File of P1 structure
Automatic calculation data	calculations.xml	First principle automatic calculation data file	
	calculations.txt	Output part of calculation data	
Brillouin Zone	[matid].bz.plt [matid].bz.spt	Brillouin Zone + K point Path Gnuplot script Jmol script	
Charge Density	[matid].charge.cube	Gaussian Cube Format	Visualized with VESTA, Jmol, XCrysDen etc.
DOS	dos.plt dos.dat	Gnuplot script	Simple display for check
	band.plt band.dat	Gnuplot script	Simple display for check

3.5.2 First principle automatic calculation data file　calculations.xml

The main calculation data are summarized in the first principle automatic calculation data file calculations.xml.

The structure (hierarchical structure, tags, attributes) of the data file calculations.xml is shown below.

データファイル calculations.xml の構成

Tag 1	Tag 2	Tag 3	Tag 4	Tag 5	Tag 6	Tag 7	
calculations							
	materials	material_id chemical_formulla crystal_system spacegroup spacegroup_no cif					
	structuire [@name=initial)						Initial structure
		lattice [@name=conventional]	a, b, c alpha,beta,gamma a1,a2,a3				Cell length Cell Angle Lat vector
		lattice [@name=primitive]	a, b, c alpha,beta,gamma a1,a2,a3				
		atom	i[@name=name]				coordinate
	structuire [@name=relaxed)						Optimization structure (Structure of SCF calculation)
	calculation [@name=task]						Task calculation data
		inputs	i[@name=value]				
		kpoint[@type=kmesh]					nkx nky nkz
		kpoint[@type=kpath]	i[@name=KP]				kx ky kz
		property	i[@name=prop.@unit]				
			dos	spin	i		DOS　ene dos
			pdos	atom	spin	i	PDOS　ene pdos
			band	spin	kpoint	i	Band Struc　ene occ

Example of the data file　calculations.xml

```
<?xml version="1.0"?>
<calculations>
  <material>
    <material_id>4295272247</material_id>
    <chemical_formula>Si</chemical_formula>
    <crystal_system>cubic</crystal_system>
    <spacegroup>Fd-3m</spacegroup>
    <spacegroup_no>227</spacegroup_no>
    <cif>4295272247-1-2.cif</cif>
  </material>
  <structure name="original">
```

```xml
  <lattice type="conventional">
    <a>5.429</a>
    <b>5.429</b>
    <c>5.429</c>
    <alpha>90.0</alpha>
    <beta>90.0</beta>
    <gamma>90.0</gamma>
  </lattice>
  <lattice type="conventional">
    <a1>5.429 0.0 0.0</a1>
    <a2>0.0 5.429 0.0</a2>
    <a3>0.0 0.0 5.429</a3>
  </lattice>
  <lattice type="primitive">
    <a1>0.0 2.7145 2.7145</a1>
    <a2>2.7145 0.0 2.7145</a2>
    <a3>2.7145 2.7145 0.0</a3>
  </lattice>
  <lattice/>
  <atom>
    <i name="Si">  0.12500   0.12500   0.12500</i>
    <i name="Si">  0.87500   0.87500   0.87500</i>
  </atom>
</structure>
<structure name="relaxed">
  <lattice type="conventional">
    <a>5.4688472</a>
    <b>5.4688472</b>
    <c>5.4688472</c>
    <alpha>90.0</alpha>
    <beta>90.0</beta>
    <gamma>90.0</gamma>
  </lattice>
  <lattice type="conventional">
    <a1>5.4688472 0.0 0.0</a1>
    <a2>0.0 5.4688472 0.0</a2>
    <a3>0.0 0.0 5.4688472</a3>
  </lattice>
  <lattice type="primitive">
    <a1>0.0 2.7344236 2.7344236</a1>
    <a2>2.7344236 0.0 2.7344236</a2>
    <a3>2.7344236 2.7344236 0.0</a3>
  </lattice>
  <atom>
    <i name="Si">0.12500000 0.12500000 0.12500000</i>
    <i name="Si">0.87500000 0.87500000 0.87500000</i>
  </atom>
</structure>
<calculation name="check_spin">
```

```
…
  <calculation name="opt1">
…
  <calculation name="opt2">
…
  <calculation name="scf">
   <inputs>
     <i name="_calc_dir">scf</i>
     <i name="_structure">opt2</i>
     <i name="_input">default</i>
     <i name="npar">1</i>
     <i name="system"/>
     <i name="istart">0</i>
     <i name="prec">high</i>
     <i name="encut">550</i>
     <i name="algo">fast</i>
     <i name="ediff">1E-6</i>
     <i name="nelm">100  # default 60</i>
     <i name="ispin"/>
     <i name="nbands"/>
     <i name="ismear">-5</i>
     <i name="sigma">0.1  # default 0.2</i>
     <i name="isym"/>
     <i name="nelmin">8</i>
     <i name="laechg">.TRUE.</i>
   </inputs>
   <structure name="initial">
     <lattice type="primitive">
       <a1>0.00000000 2.73442360 2.73442360</a1>
       <a2>2.73442360 0.00000000 2.73442360</a2>
       <a3>2.73442360 2.73442360 0.00000000</a3>
     </lattice>
     <atom>
       <i name="Si">0.12500000 0.12500000 0.12500000</i>
       <i name="Si">0.87500000 0.87500000 0.87500000</i>
     </atom>
   </structure>
   <structure name="final">
     <lattice type="primitive">
       <a1>0.00000000 2.73442360 2.73442360</a1>
       <a2>2.73442360 0.00000000 2.73442360</a2>
       <a3>2.73442360 2.73442360 0.00000000</a3>
     </lattice>
     <atom>
       <i name="Si">0.12500000 0.12500000 0.12500000</i>
       <i name="Si">0.87500000 0.87500000 0.87500000</i>
     </atom>
   </structure>
   <kpoints type="kmesh">10 10 10</kpoints>
```

```xml
    <parameters>
      <i name="ispin">1</i>
      <i name="nbands">10</i>
      <i name="nelect">8.00000000</i>
      <i name="nkpoints">47</i>
      <kpoints>
      </kpoints>
    </parameters>
    <properties>
      <i name="etotal" unit="eV">-10.84921592</i>
      <i name="etotal_per_atom" unit="eV/atom">-5.42460796</i>
      <i name="efermi" unit="eV">5.65437076</i>
    </properties>
  </calculation>
  <calculation name="dos">
    <inputs>
…
    <properties>
      <i name="etotal" unit="eV">-10.84994683</i>
      <i name="etotal_per_atom" unit="eV/atom">-5.424973415</i>
      <i name="efermi" unit="eV">5.62480381</i>
      <dos>
        <spin spin="1">
          <i>-14.0000 0.0000 0.0000</i>
          <i>-13.9844 0.0000 0.0000</i>
          <i>-13.9688 0.0000 0.0000</i>
          <i>-13.9532 0.0000 0.0000</i>
…
    <pdos>
      <i name="value">energy s py pz px dxy dyz dz2 dxz dx2</i>
      <atom atom="">
        <spin spin="1">
          <i> -14.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000 </i>
          <i> -13.9844  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000 </i>
          <i> -13.9688  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000 </i>
          <i> -13.9532  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000 </i>
          <i> -13.9376  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000 </i>
…
    <i name="bandgap_type">indirect</i>
    <i name="bandgap" unit="eV">0.618</i>
    <band>
      <spin spin="1">
        <kpoint kpoint="1">
          <i>-6.1986 1.0000</i>
          <i>5.6156 1.0000</i>
          <i>5.6156 1.0000</i>
…
        </kpoint>
  <calculation name="band">
```

```
    <inputs>
…
    <kpoints type="kpath">
     <i name="Gamma">  0.00000   0.00000   0.00000</i>
     <i>  0.00000   0.02174   0.02174</i>
     <i>  0.00000   0.04348   0.04348</i>
     <i>  0.00000   0.06522   0.06522</i>
     <i>  0.00000   0.08696   0.08696</i>
…
    <properties>
     <i name="etotal" unit="eV">-7.97993391</i>
     <i name="etotal_per_atom" unit="eV/atom">-3.989966955</i>
     <i name="efermi" unit="eV">5.74667513</i>
     <band>
      <spin spin="1">
       <kpoint kpoint="1">
         <i>-6.1986 1.0000</i>
         <i>5.6156 0.9434</i>
         <i>5.6156 0.9433</i>
         <i>5.6156 0.9433</i>
         <i>8.1724 -0.0000</i>
         <i>8.1724 -0.0000</i>
         <i>8.1724 -0.0000</i>
         <i>8.7488 -0.0000</i>
         <i>13.3247 0.0000</i>
         <i>13.4902 0.0000</i>
…
      </band>
     </properties>
    </calculation>
  </calculations>
```

4. Details of the program

4.1 Structure of program

The first principle automatic calculation program is composed of Python program group. The outline of the first principle automatic calculation program structure is shown below.

Install Directory	Subdirectory	Pyhthon Program	
toast/calc		ac-setup.py	First principle automatic calculation of multiple crystal structures
		ac-update.py	First principle automatic calculation of multiple crystal structures (Job status update / Add submit)
		ac-calc.py	First principles calculation based on calculation scenario
		ac-summary.py	Calculation data list output
		ac-stat.py	Calculation status output
	calculation	autocalc.py	Class of First principle automatic calculation for multiple crystal structures
		calc.py	Class of First principle calculation based on calculation scenario
		calculator.py	Abstract class of processing of first principles calculation program
		vasp.py	Class for VASP
		esprsso.py	Class for QE
		abinit.py	Class for ABINIT
	structure	crystal.py	Class of crystal structure analysis
	jobmanage	job.py	Class of job execution
toast/config			Configuration file
	job_template		job script template

4.2 Functions of main class

4.2.1 calculation./autocalc.py

Class of first principle automatic calculation for multiple crystal structures

Class	Function	
autocalc	calculate	First principle automatic calculation of multiple crystal structures
	calc_prep	Pre-processing for automatic calculation
	calc	Execution of automatic calculation
	caldata	Output of calculation data list
	calstat	Output of calculation status

4.2.2 calculation./calc.py

Class of first principles calculation based on calculation scenario

Class	Function	
calc	calculate	First principles calculation based on calculation scenario
	read_config	Read calculation scenario configuration file
	structure	Generation of unit cell
	calc_prep	Preprocessing
	write_parameter	Generation of first principle automatic calculation data file calculations.xml
	calc_task	Execution of each task
	calc_post	Post-processing, calculation result analysis Update of automatic calculation data file calculations.xml
	kpoints	Calculation of K point mesh
	ispin	Spin decision
	execute	Execution of first principles calculation program
	calstat	Output of calculation status

4.2.3 calculation./calculator.py

Abstract class of processing of first principles calculation program

Class	Function	
calculator	calc	First principles calculation based on calculation scenario
	potentials	Generate and copy a pseudo potential file
	inputs	Generate input data
	nbands	Calculate number of bands
	structure	Generation of crystal structure, atomic coordinates from calculation result of CIF File or other Task
	mag	Extraction of magnetization for spin determination
	efermi	Extraction of Fermi Energy for Emin, Emax in DOS calculation
	results	Extraction of calculation result data Update of automatic calculation data file calculations.xml
	calstat	Output of calculation status

4.2.4 calculation./vasp.py

Class for VASP

Class	Function	
calculator	calc	First principles calculation based on calculation scenario
	potentials	Generate and copy a pseudo potential file
	inputs	Generate input data
	nbands	Calculate number of bands
	structure	Generation of crystal structure, atomic coordinates from calculation result of CIF File or other Task
	mag	Extraction of magnetization for spin determination
	efermi	Extraction of Fermi Energy for Emin, Emax in DOS calculation
	results	Extraction of calculation result data Update of automatic calculation data file calculations.xml
	calstat	Output of calculation status

4.2.5 calculation./espresso.py

Class for Quantum ESPRESSO

Class	Function	
calculator	calc	First principles calculation based on calculation scenario
	potentials	Generate and copy a pseudo potential file
	inputs	Generate input data
	nbands	Calculate number of bands
	structure	Generation of crystal structure, atomic coordinates from calculation result of CIF File or other Task
	mag	Extraction of magnetization for spin determination
	efermi	Extraction of Fermi Energy for Emin, Emax in DOS calculation
	results	Extraction of calculation result data Update of automatic calculation data file calculations.xml
	calstat	Output of calculation status

4.2.6 calculation./abinit.py

Class for ABINIT

Class	Function	
calculator	calc	First principles calculation based on calculation scenario
	potentials	Generate and copy a pseudo potential file
	inputs	Generate input data
	nbands	Calculate number of bands
	structure	Generation of crystal structure, atomic coordinates from calculation result of CIF File or other Task
	mag	Extraction of magnetization for spin determination
	efermi	Extraction of Fermi Energy for Emin, Emax in DOS calculation

	results	Extraction of calculation result data
		Update of automatic calculation data file calculations.xml
	calstat	Output of calculation status

4.2.7 structure/crystal.py

Class of crystal structure analysis

Class	Function	
calculator	loadCIF	Read CIF File
	checkCIF	Check CIF File
	convertCIF2VASP	Cell (Conventional Cell, Primitive Cell), calculation of the internal coordinates of atoms
	saveKPoints	Calculation of k point path for band calculation
	saveBrillouin	Output Brillouin Zone visualization script
	printLog	Log output

4.2.8 jobmanage/job.py

Class of job execution

Class	Function	
job	read_config	Read job execution configuration file
	jobscript	Generate job execution script
	jobscript_interactive	Generate execution script for Interactive calculation
	jobscript_template	Generation of job script using template of job script of job management system

4.2.9 calculation/calprop.py

計算結果解析

Class	Function	
	cellparameter	Calculate Cell parameter
	bandgap	Calculate Bandgap
	fermisurf	Generation of Fermi surface visualization data
	dosplot	Generation of DOS plot data
	pdosplot	Generation of PDOS plot data
	bandplot	Generation of band structure plot data
	caldata	Output Calculation data

4.2.10 calculation/calvis.py

可視化データ

Class	Function	
	visdata	Generate visualization data