BURAI Documentation

Release 1.2

BURAI-team

Jun 12, 2017

Contents

BURAI is a GUI system of Quantum ESPRESSO. You can download and use it freely.
This system is developed as JavaFX application, and requires Java Runtime Environment (JRE).

CHAPTER 1

Version

The latest version is 1.2.

CHAPTER 2

License

GNU-GPL v3

CHAPTER 3

Runtime Environment

- Windows 10 (recommended) or Mac OS X 10.12
- JRE1.8 or later version

CHAPTER 4

Web Page

http://nisihara.wixsite.com/burai

CHAPTER 5

Documentation

Install

In the following, it is shown how to install BURAI: to download and set it.

Optionally, it may be possible to install Quantum ESPRESSO.

Download

You can download executables from here:

- Windows
- Mac OSX

Note: These zip-files contain precompiled executable files of Quantum ESPRESSO.

Setting

1. unzip the downloaded file
2. copy it to any directory on your computer e.g.:
   - for Windows, C:¥BURAI1.2_Windows¥
   - for MacOSX, /Applications/BURAI1.2.app
3. install JRE1.8 or later version, if your computer does not have it.

Quantum ESPRESSO (optionally)

Although BURAI contains executables of Quantum ESPRESSO,

it is allowed to install other executables optionally from here.

Note: However, the other executalbes are not recommened.

Usage

In the following, it is shown how to use BURAI.

Layout of Window

This page shows the initial window of BURAI as

Header bar

Header bar has two items:

1. Main menu.
2. Materials API

- Main menu

Main menu, which is symbolized ">" icon, has eight items.

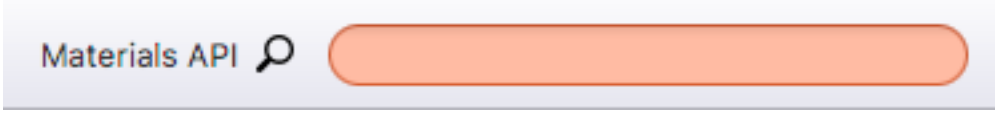
Table 5.1: Items of main menu

Item	Explanation
About BURAI	BURAI information, where version and license are shown.
Documents	This documantation is shown.
Links (Web)	Some links (QE web page, psudopotential page ...)
Path of QE	Set and Show QE and MPI paths.
Proxy server	Set proxy system.
Full screen	BURAI windows size are changed full screen.
Quit [Ctr + Q]	Quit the system of BURAI.

- Materials API

You can get crystal structure through Materials API.

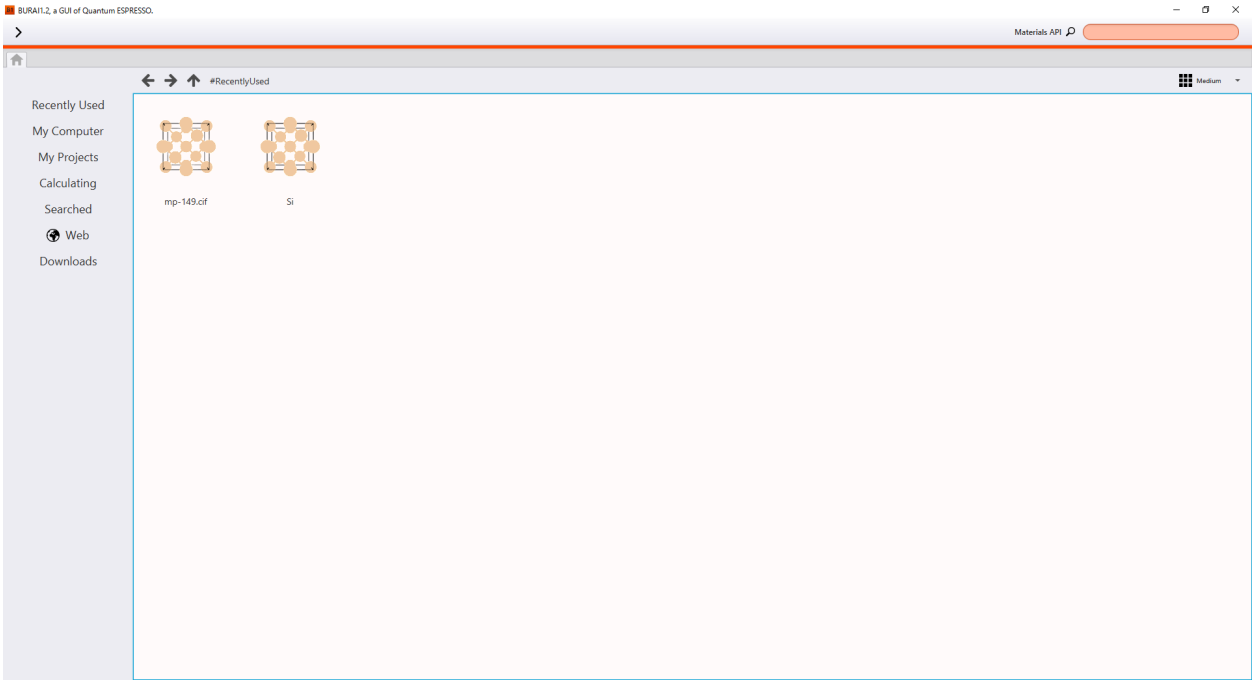
Please see here for the details.



Home tab

Home tab, which is located under header bar, has explorer system.

Please see here for the details of the explorer.



Explorer

Following items control states of the explorer.

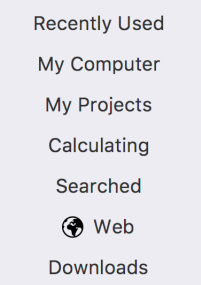


Table 5.2: Item of left sidebar

Item	Explanation
Recently Used	Recently used files.
My Computer	The root directory (Windows: C¥, MacOSX: /).
My Projects	The directory where projects are saved. ($HOME/.burai/).
Calculating	Calculating projects.
Web	Bookmarks of web sites.
Downloads	Downloaded files form web sites.

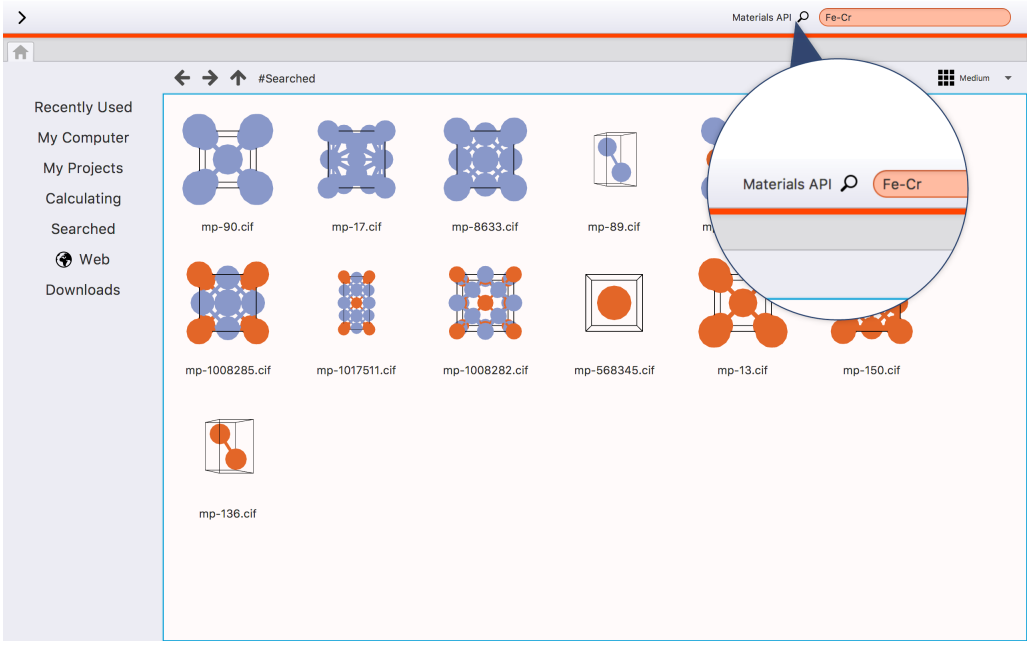
Size of icons in the explorer can be changed as:

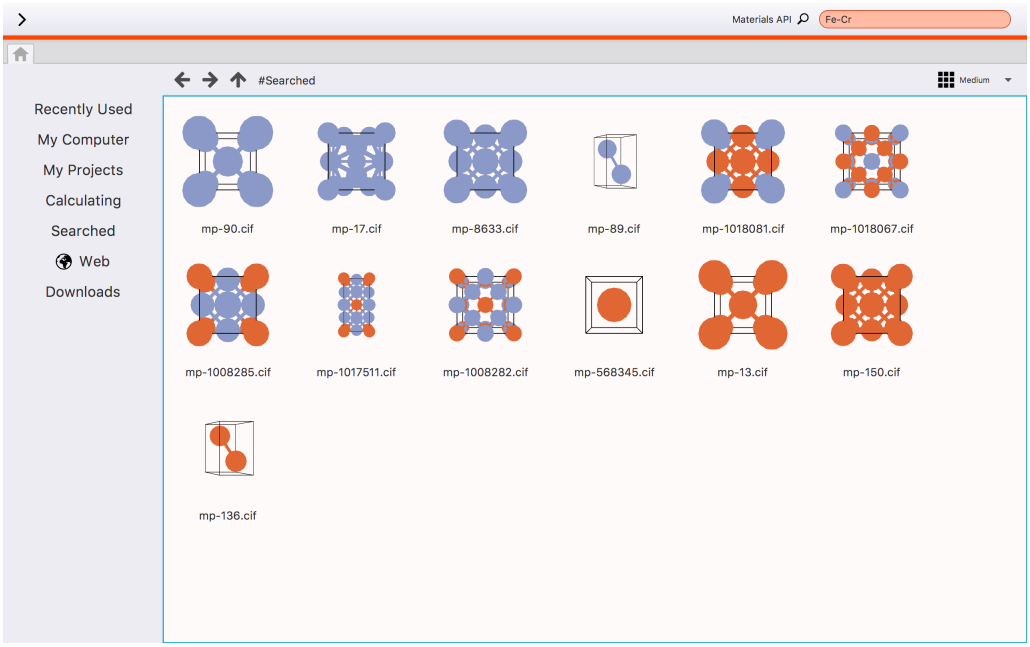
File System

The explorer shows file system. Especially, crystal structures are shown as 3D models, if their file formats are .cif (Crystallographic Information Framework) or .xyz (XYZ chemical file format) or .in (QE input file).

Materials API

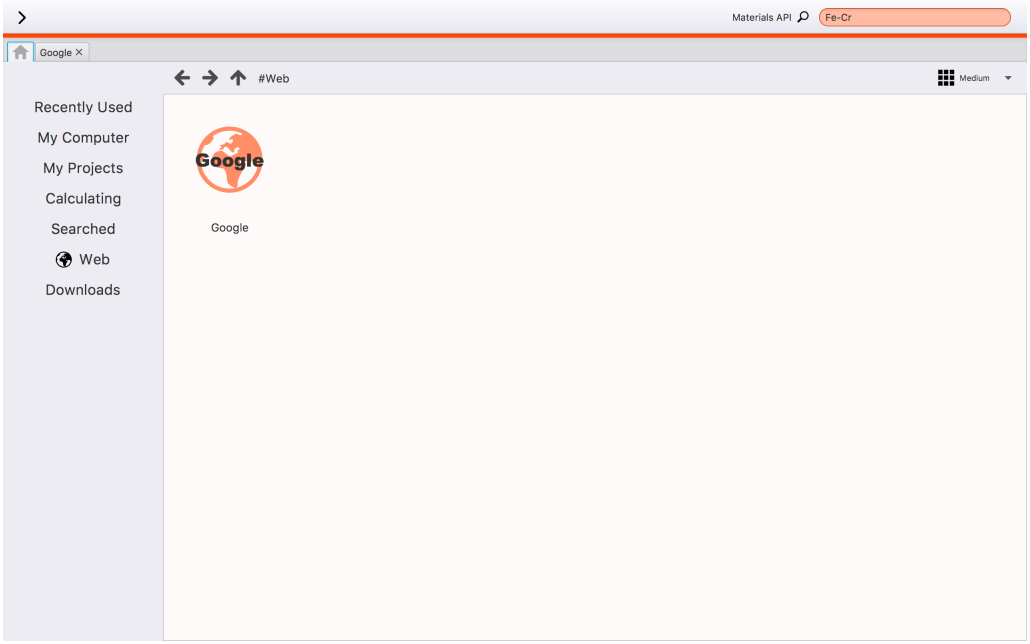
You can get crystal structure through Materials API . Entering element symbols or chemical formulas in the field of Materials API causes that crystal structures are searched. For example, if "Fe-Cr" system is entered, the crystal structures of compound with Fe and/or Cr are shown.





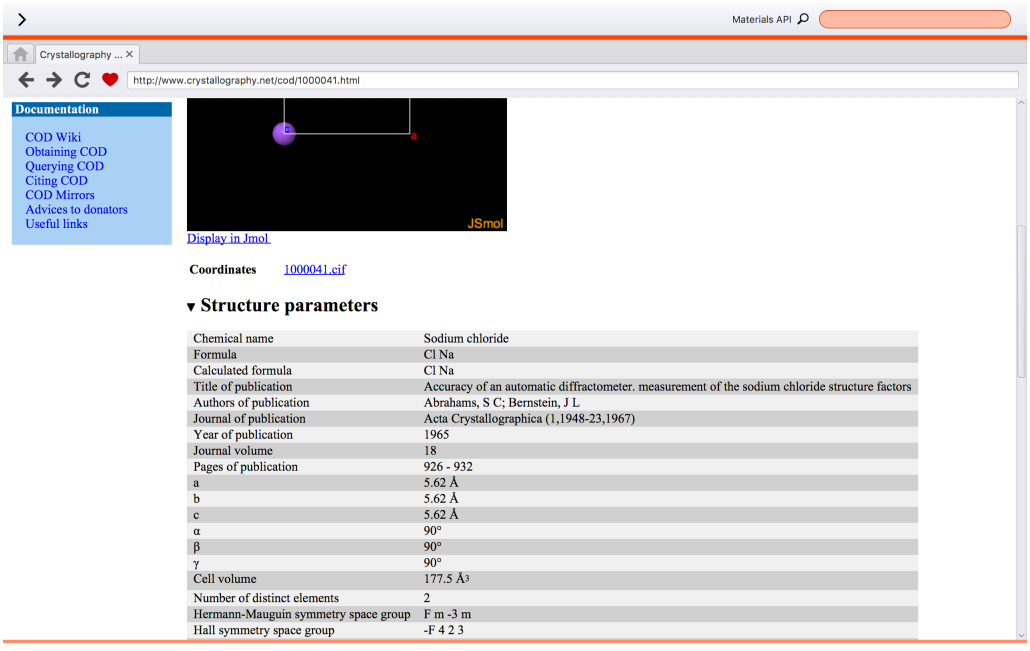
Web Browser

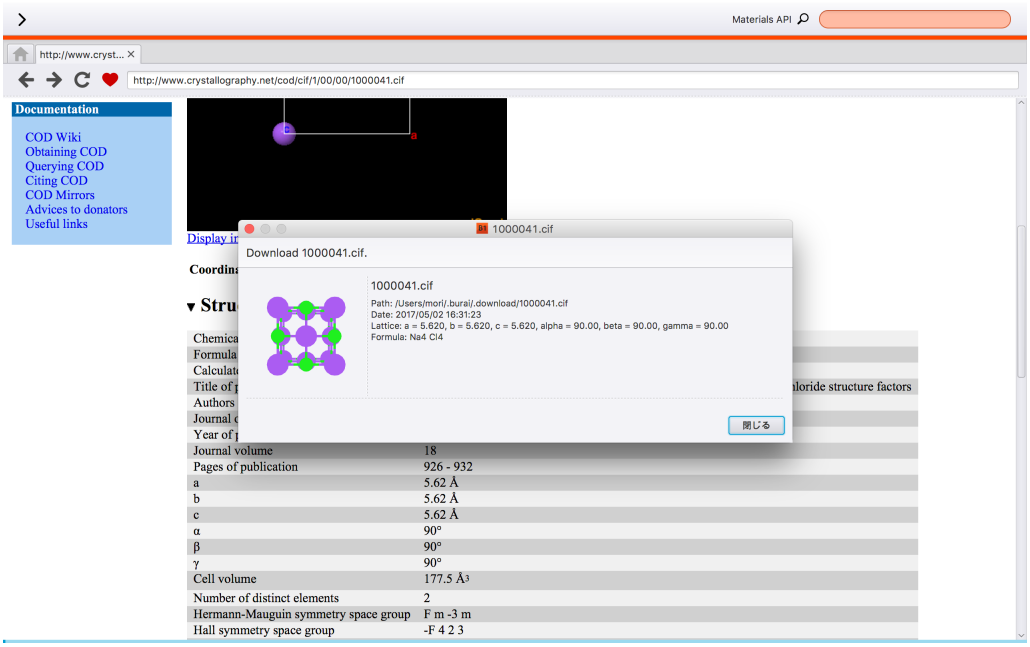
BURAI has *build-in* web browser. if you want to search something at the internet, you should select “Web” from menu.

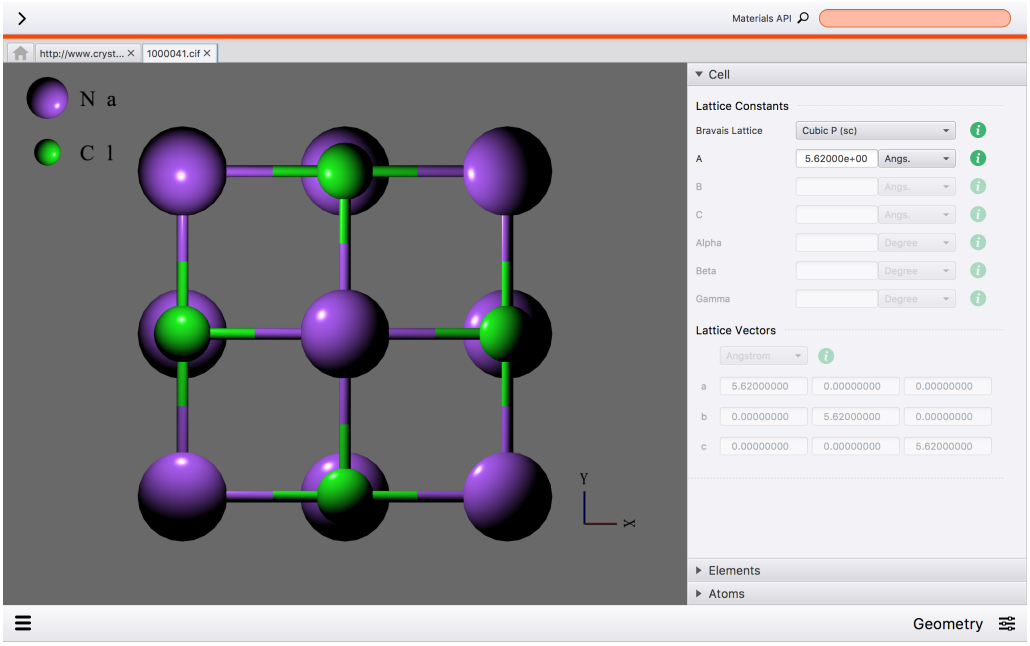


Getting Crystal Structures

This chapter illustrate to get the crystal structure from some web site. You search the crystal data from *build-in* web browser. Opening the link of the crystal structure pops up the window with 3D model. Clicking the model shows the new project tab.

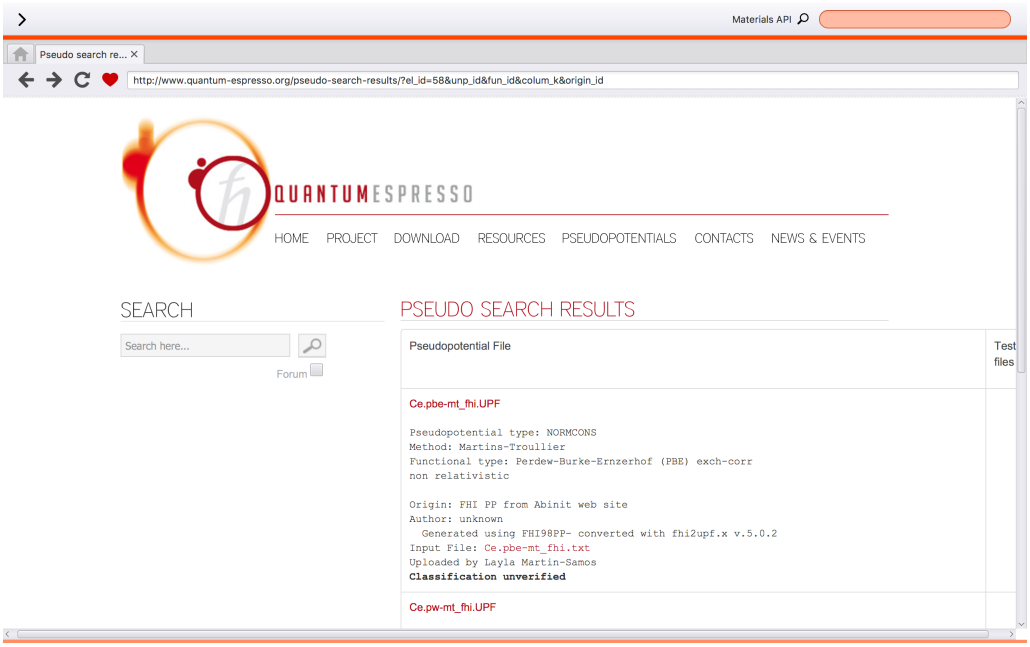


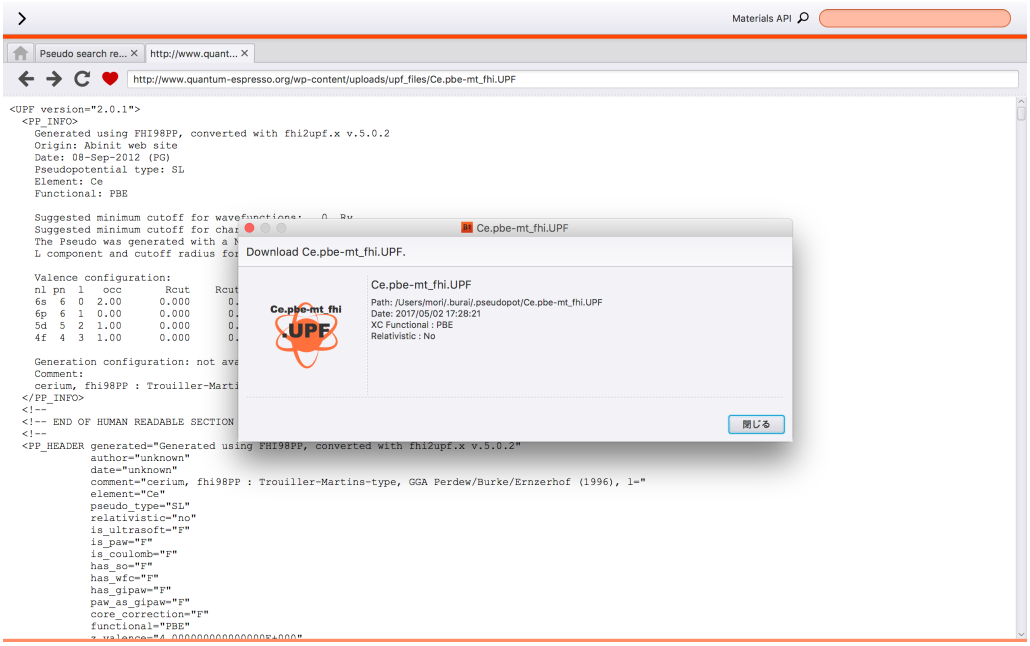


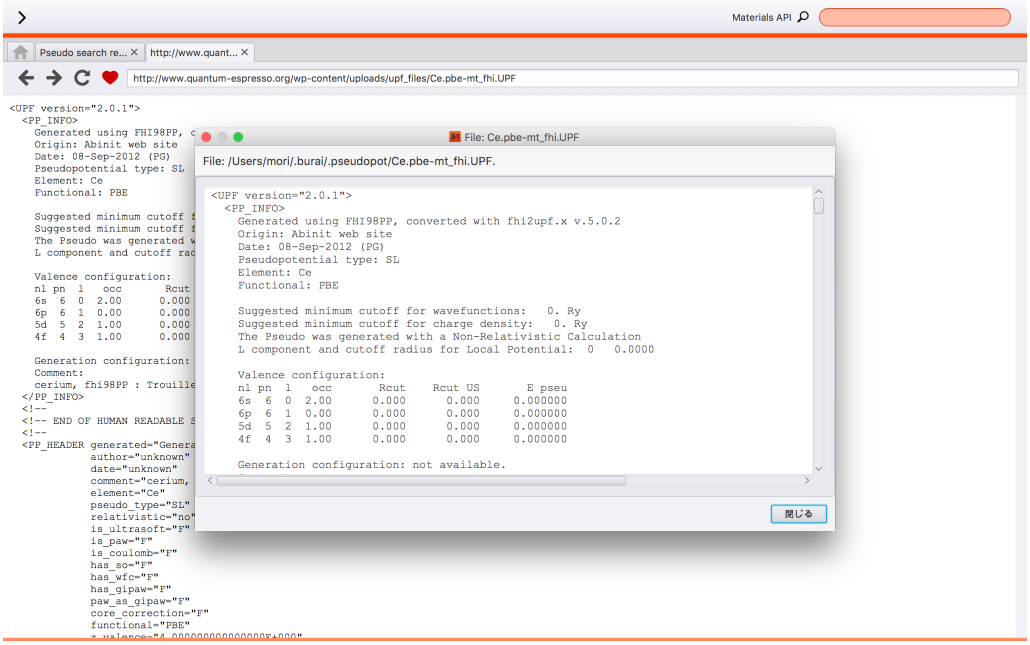


Getting Pseudopotentials

You can get pseudopotentials from the web site of QE.


Materials API
Pseudo search re...
http://www.quantum-espresso.org/pseudo-search-results/?el_id=58&unp_id&fun_id&colum_k&origin_id
QUANTUMESPRESSO
HOME PROJECT DOWNLOAD RESOURCES PSEUDOPOTENTIALS CONTACTS NEWS & EVENTS
SEARCH
Search here...
Forum
PSEUDO SEARCH RESULTS
Pseudopotential File
Test files
Ce.pbe-mt_fhi.UPF
Pseudopotential type: NORMCONS
Method: Martins-Troullier
Functional type: Perdew-Burke-Ernzerhof (PBE) exch-corr
non relativistic
Origin: FHI PP from Abinit web site
Author: unknown
Generated using FHI98PP- converted with fhi2upf.x v.5.0.2
Input File: Ce.pbe-mt_fhi.txt
Uploaded by Layla Martin-Samos
Classification unverified
Ce.pw-mt_fhi.UPF


Materials API
Pseudo search re...
http://www.quant...
http://www.quantum-espresso.org/wp-content/uploads/upf_files/Ce.pbe-mt_fhi.UPF
<UPF version="2.0.1">
<PP_INFO>
Generated using FHI98PP, converted with fhi2upf.x v.5.0.2
Origin: Abinit web site
Date: 08-Sep-2012 (PG)
Pseudopotential type: SL
Element: Ce
Functional: PBE
Valence configuration:
nl pn l occ Rcut
6s 6 0 2.00 0.000
6p 6 1 0.00 0.000
5d 5 2 1.00 0.000
4f 4 3 1.00 0.000
Comment:
cerium, fhi98PP : Trouiller-Marti
</PP_INFO>
<!--
<!-- END OF HUMAN READABLE SECTION
-->
<PP_HEADER generated="Generated using FHI98PP, converted with fhi2upf.x v.5.0.2"
author="unknown"
date="unknown"
comment="cerium, fhi98PP : Trouiller-Martins-type, GGA Perdew/Burke/Ernzerhof (1996), l="
element="Ce"
pseudo_type="SL"
relativistic="no"
is_ultrasoft="F"
is_paw="F"
is_coulomb="F"
has_so="F"
has_wfc="F"
has_gipaw="F"
paw_as_gipaw="F"
core_correction="F"
functional="PBE"
Ce.pbe-mt_fhi.UPF
Download Ce.pbe-mt_fhi.UPF.
Ce.pbe-mt_fhi.UPF
Path: /Users/mori/.burai/.pseudopot/Ce.pbe-mt_fhi.UPF
Date: 2017/05/02 17:28:21
XC Functional : PBE
Relativistic : No
閉じる



Project of Quantum ESPRESSO

Contents:

Creating Project

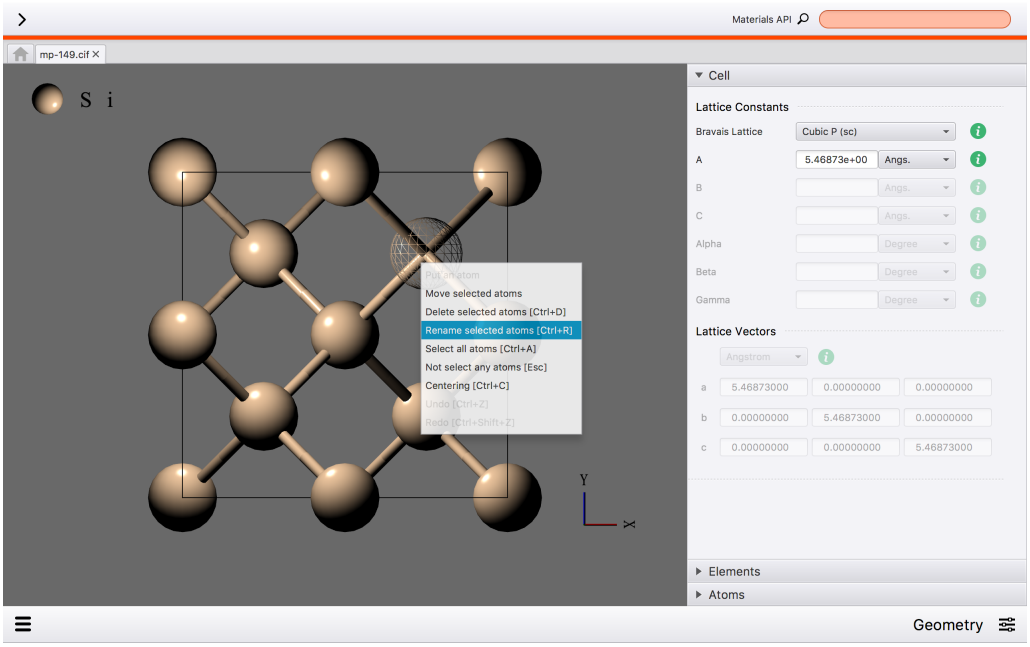
Clicking the 3D model in the explorer open a new tab. The tab contains a QE project.

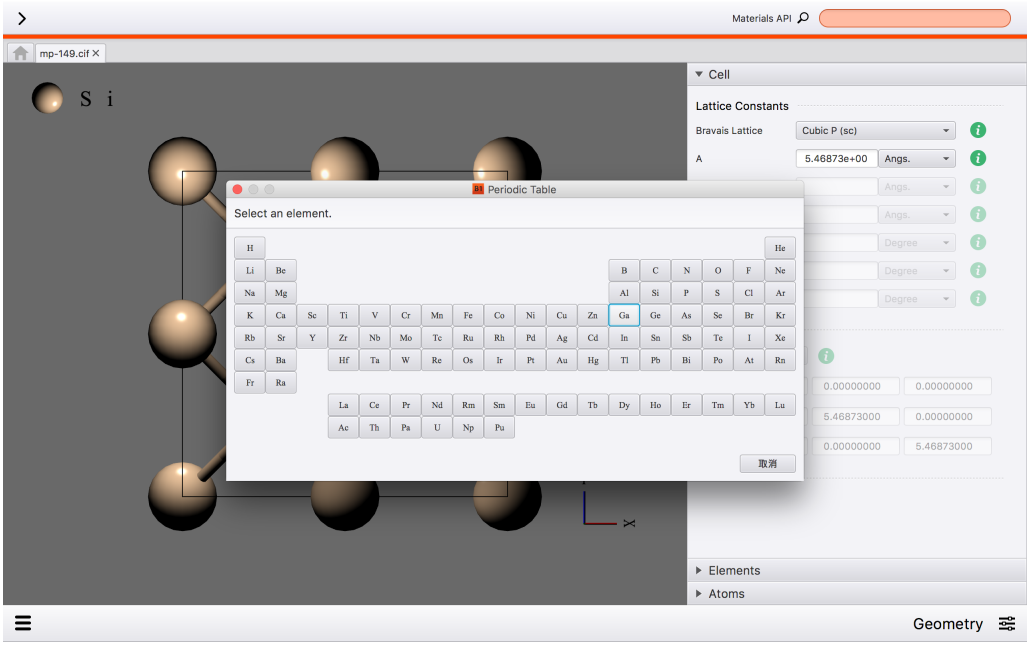
Atoms Viewer

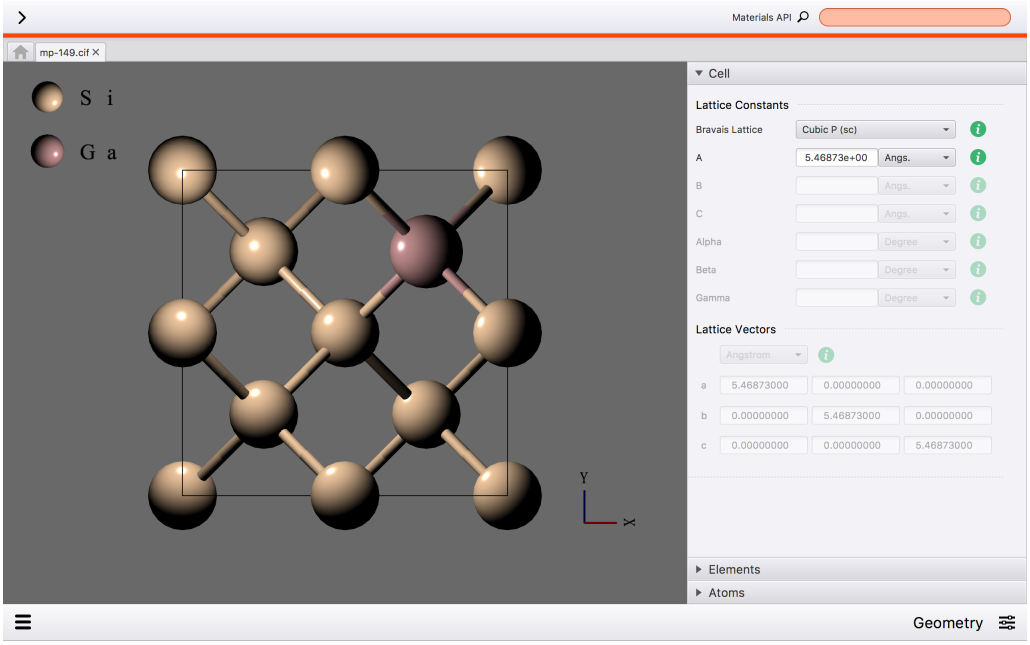
Project tab has the atoms viewer, which can edit atoms in the model. It has the following operations.

Rename Atom

You can rename an atom to another atom. The first step is selecting the atom with right click. Then, you select "Rename selected atoms" from menu.

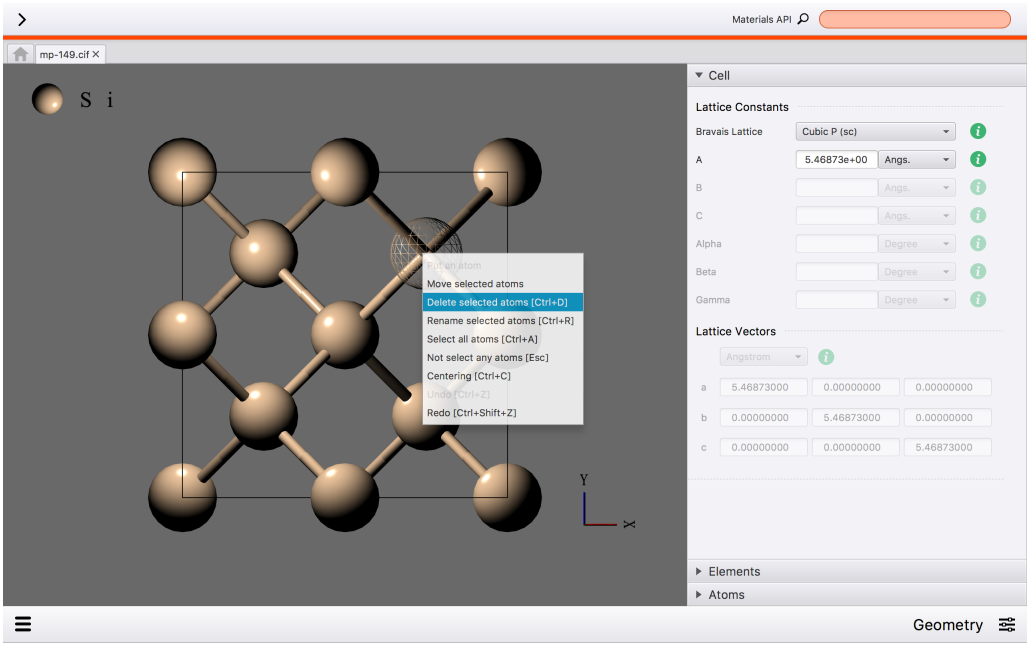

Materials API
mp-149.cif
S i
Put an atom
Move selected atoms
Delete selected atoms [Ctrl+D]
Rename selected atoms [Ctrl+R]
Select all atoms [Ctrl+A]
Not select any atoms [Esc]
Centering [Ctrl+C]
Undo [Ctrl+Z]
Redo [Ctrl+Shift+Z]
Y
X
Cell
Lattice Constants
Bravais Lattice
Cubic P (sc)
A
5.46873e+00
Angs.
B
C
Alpha
Beta
Gamma
Degree
Lattice Vectors
Angstrom
a
b
c
5.46873000
0.00000000
Elements
Atoms
Geometry

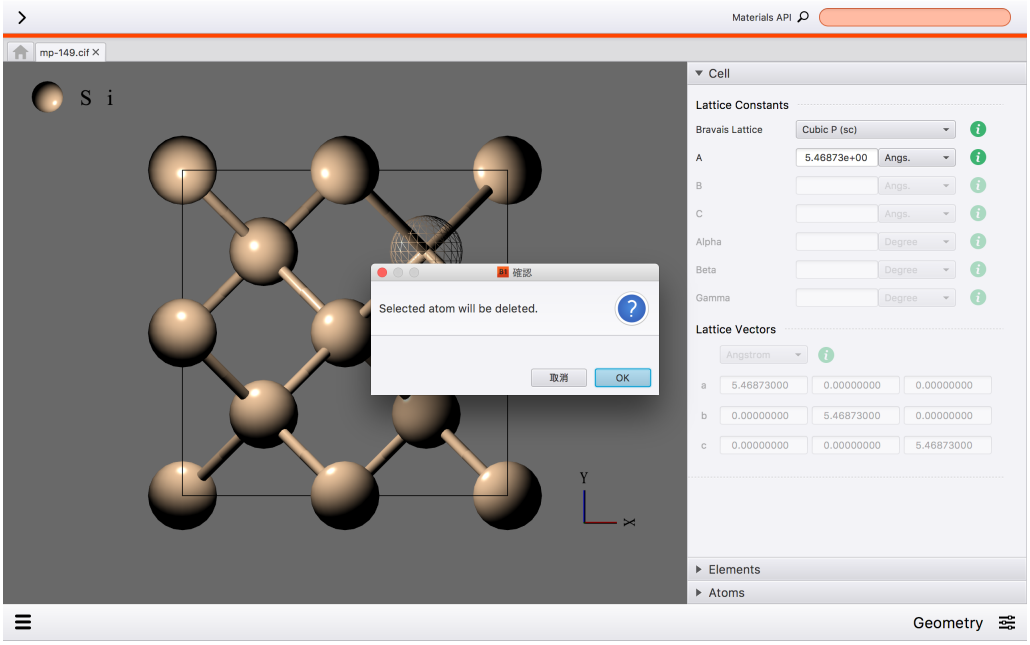

Materials API
mp-149.cif
S i
Periodic Table
Select an element.
取消
Cell
Lattice Constants
Bravais Lattice
Cubic P (sc)
A
5.46873e+00
Angs.
Degree
Elements
Atoms
Geometry

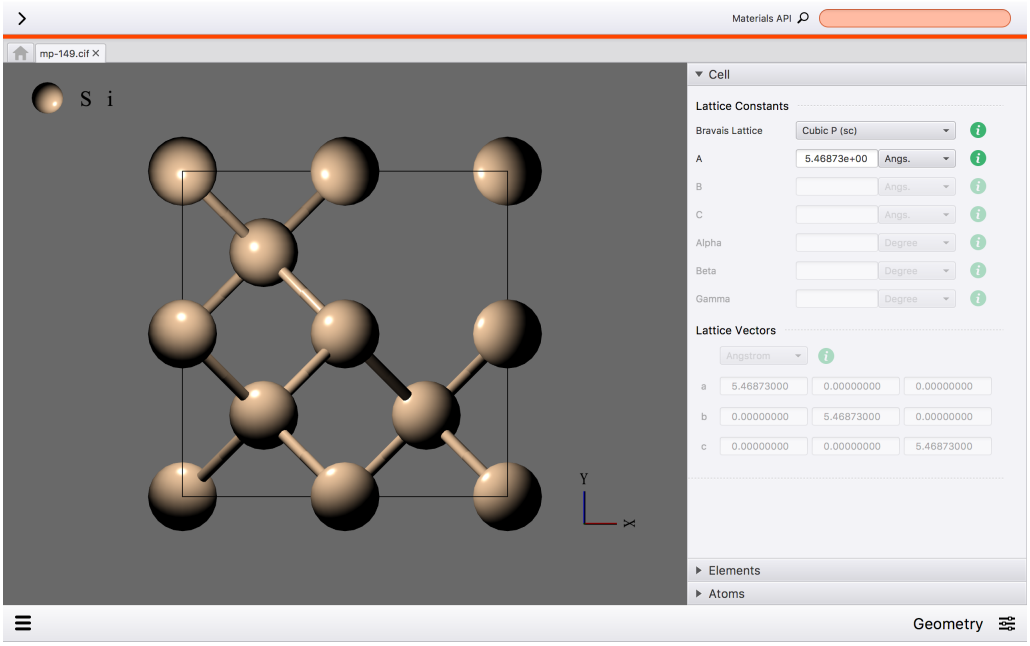


Delete Atom

You can delete an atom. The first step is selecting the atom with right click. Then, you select “Delete selected atoms” from menu.

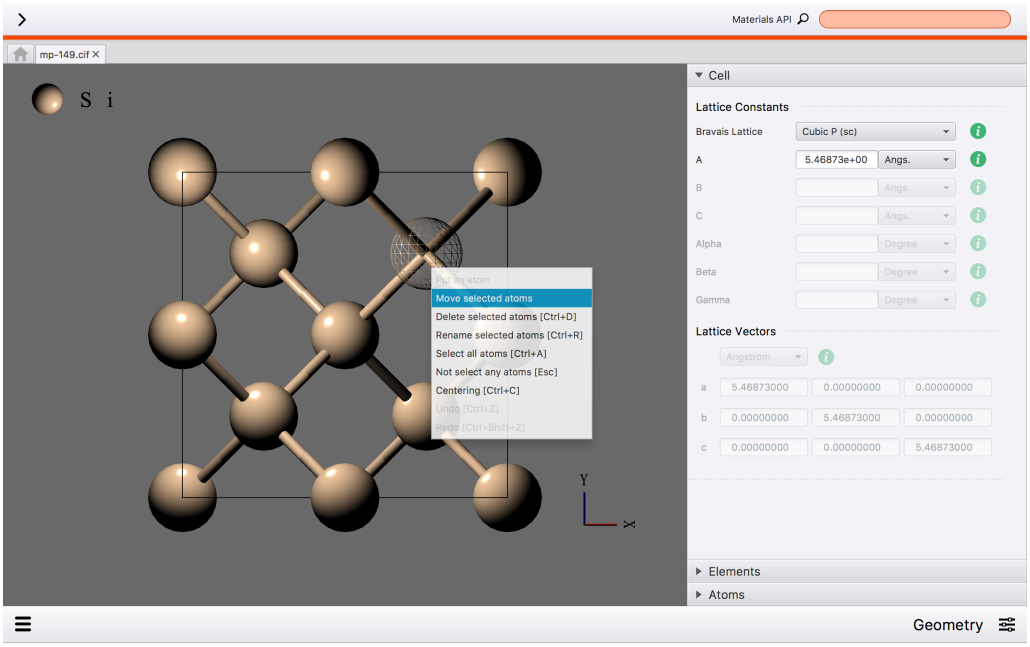


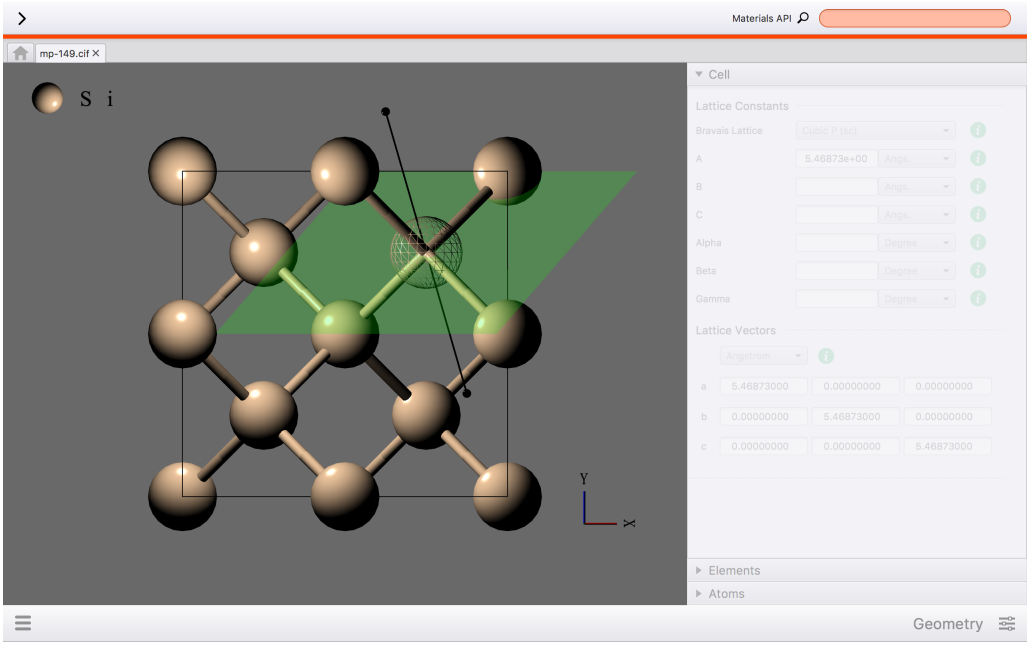


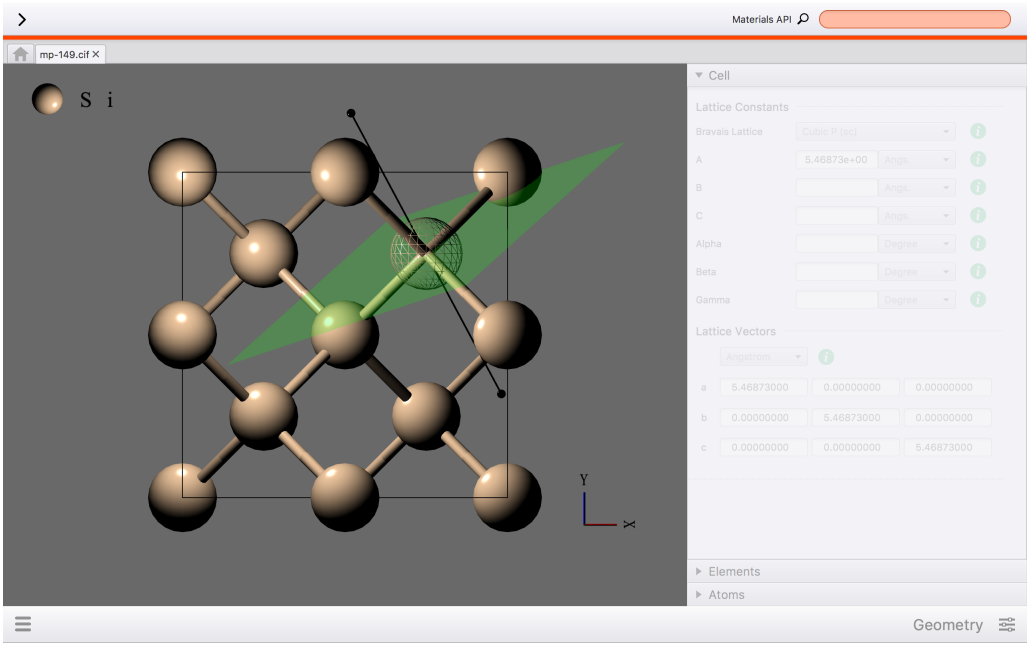


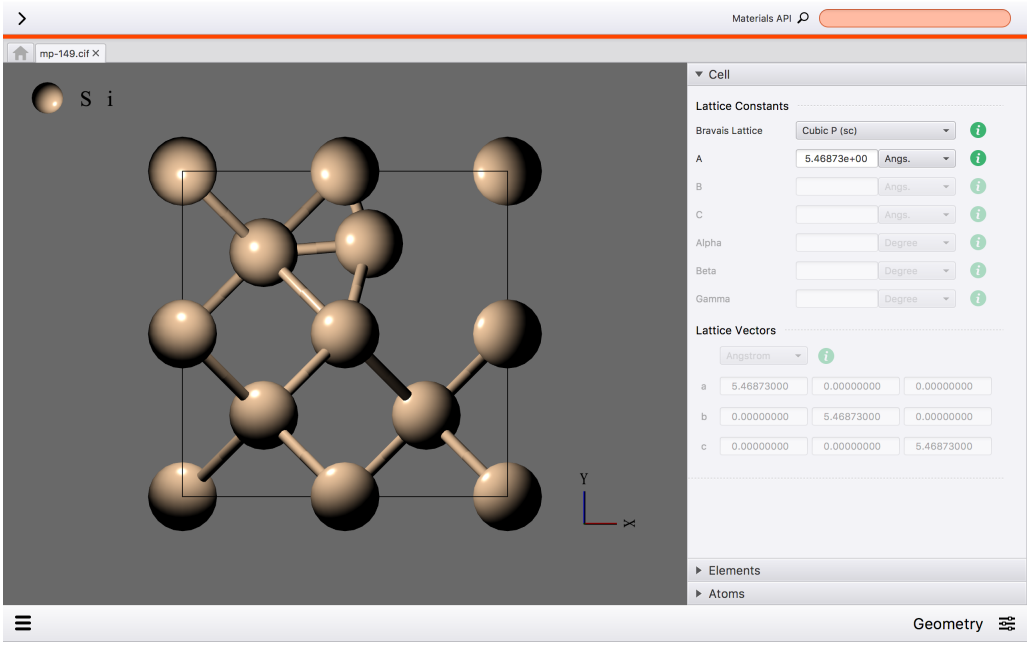
Move Atom

You can move an atom. The first step is selecting the atom with right click. Then, you select “Move selected atoms” from menu.


Materials API
mp-149.cif
S i
Cell
Lattice Constants
Bravais Lattice
Cubic P (sc)
A
5.46873e+00
Angs.
B
C
Alpha
Beta
Gamma
Degree
Lattice Vectors
Angstrom
a
b
c
5.46873000
0.00000000
Put an atom
Move selected atoms
Delete selected atoms [Ctrl+D]
Rename selected atoms [Ctrl+R]
Select all atoms [Ctrl+A]
Not select any atoms [Esc]
Centering [Ctrl+C]
Undo [Ctrl+Z]
Redo [Ctrl+Shift+Z]
Y
X
Elements
Atoms
Geometry

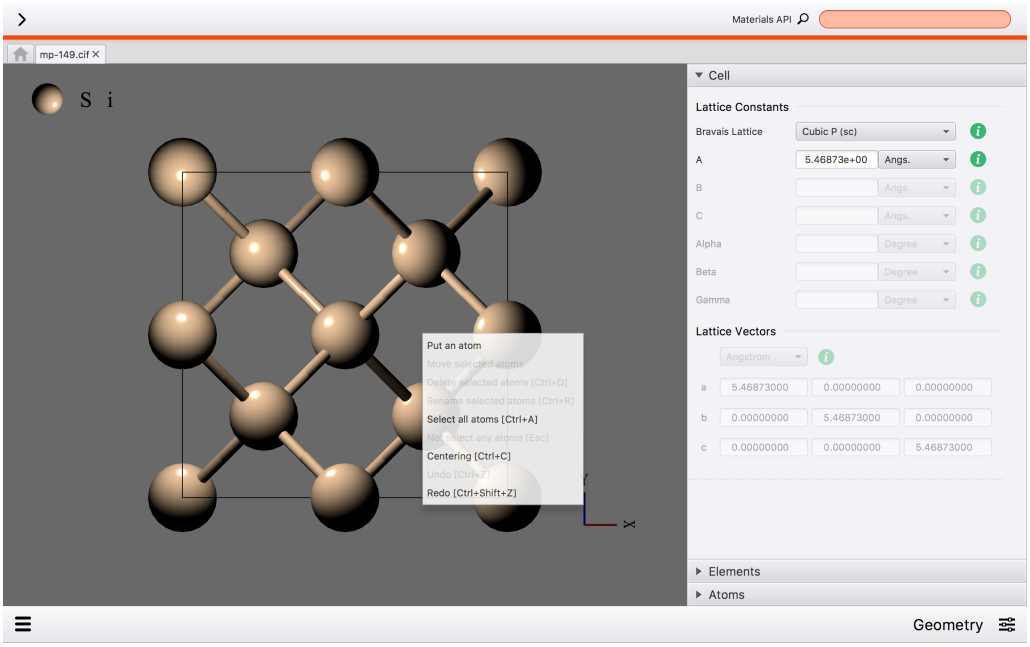

Materials API
mp-149.cif
S i
Cell
Lattice Constants
Bravais Lattice
Cubic P (sc)
A
5.46873e+00
Angs.
B
C
Alpha
Beta
Gamma
Degree
Lattice Vectors
Angstrom
a
b
c
5.46873000
0.00000000
Y
X
Elements
Atoms
Geometry

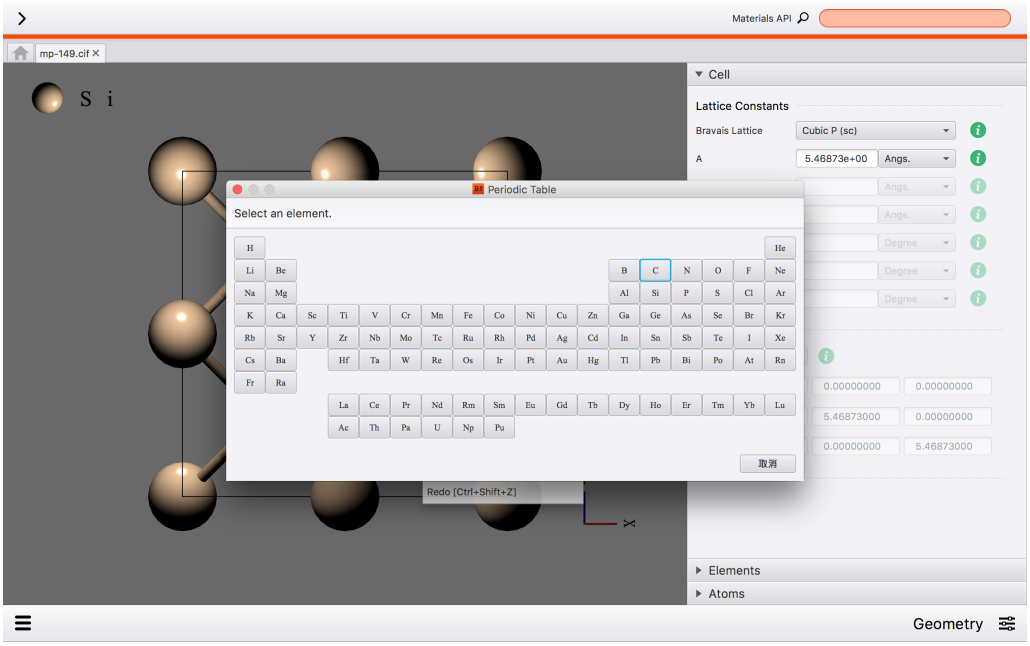


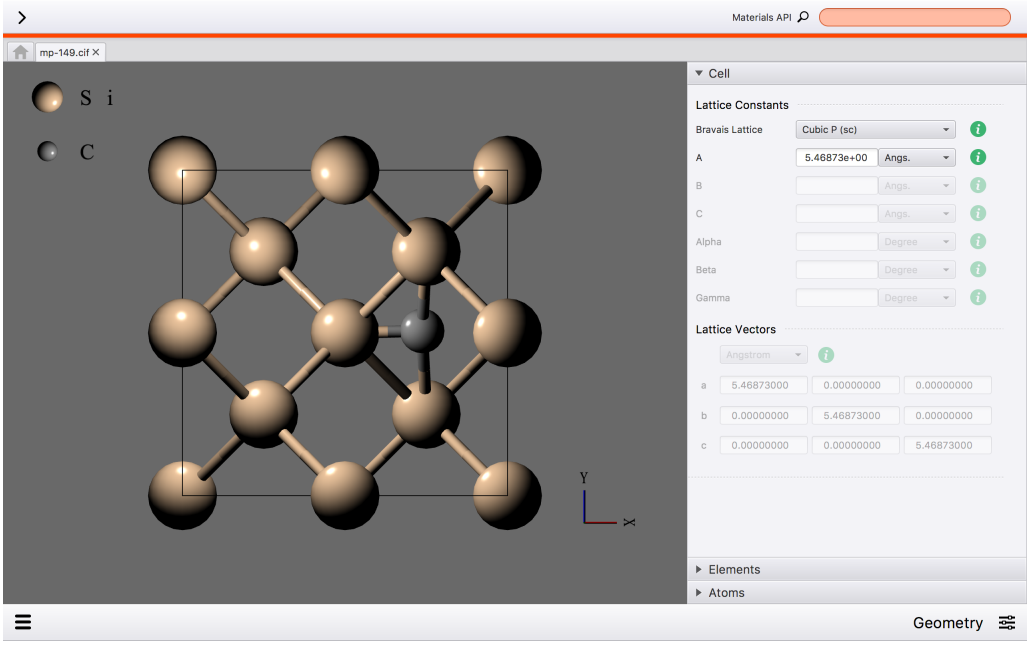


Put Atom

You can put an atom. The first step is selecting the atom with right click. Then, you select Put an atom" from menu.

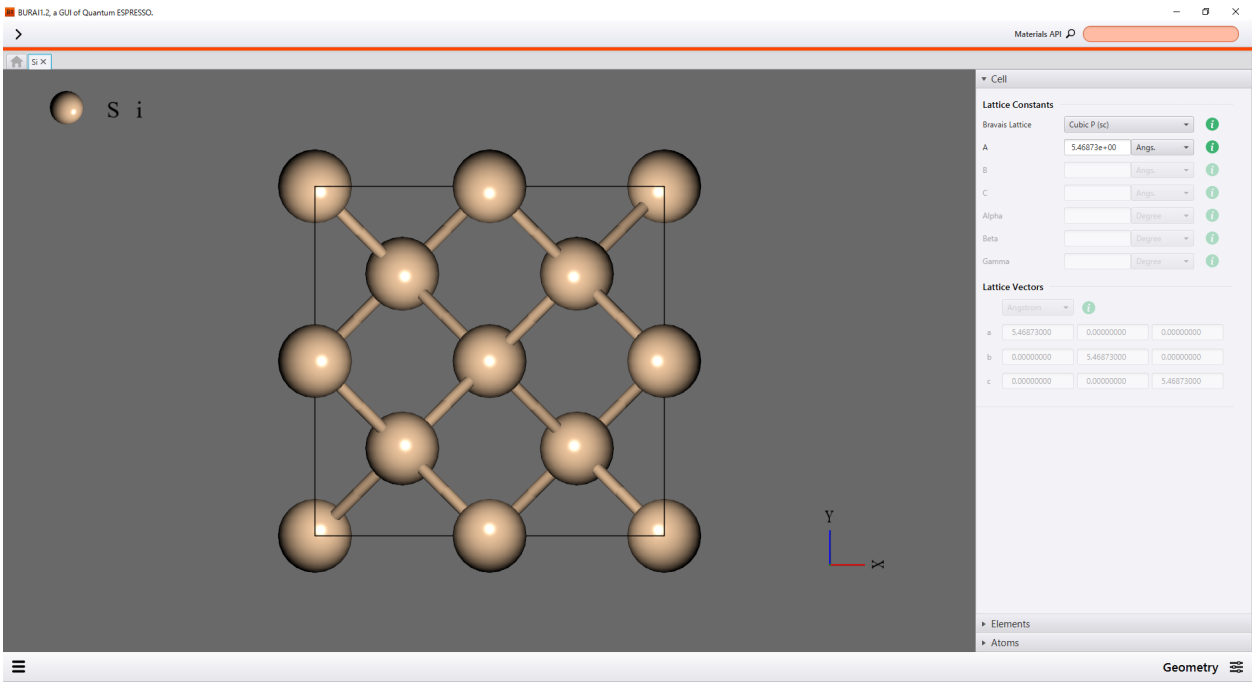

Materials API
mp-149.cif
Si
Cell
Lattice Constants
Bravais Lattice
Cubic P (sc)
A
5.46873e+00
Angs.
B
C
Alpha
Beta
Gamma
Degree
Lattice Vectors
Angstrom
a
b
c
5.46873000
0.00000000
Put an atom
Move selected atoms
Delete selected atoms [Ctrl+D]
Rename selected atoms [Ctrl+R]
Select all atoms [Ctrl+A]
Not Select any atoms [Esc]
Centering [Ctrl+C]
Undo [Ctrl+Z]
Redo [Ctrl+Shift+Z]
Elements
Atoms
Geometry


Materials API
mp-149.cif
Si
Cell
Lattice Constants
Bravais Lattice
Cubic P (sc)
A
5.46873e+00
Angs.
Periodic Table
Select an element.
H
He
Li
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Sc
Ti
V
Cr
Mn
Fe
Co
Ni
Cu
Zn
Ga
Ge
As
Se
Br
Kr
Rb
Sr
Y
Zr
Nb
Mo
Tc
Ru
Rh
Pd
Ag
Cd
In
Sn
Sb
Te
I
Xe
Cs
Ba
Hf
Ta
W
Re
Os
Ir
Pt
Au
Hg
Tl
Pb
Bi
Po
At
Rn
Fr
Ra
La
Ce
Pr
Nd
Rm
Sm
Eu
Gd
Tb
Dy
Ho
Er
Tm
Yb
Lu
Ac
Th
Pa
U
Np
Pu
取消
Redo [Ctrl+Shift+Z]
Elements
Atoms
Geometry

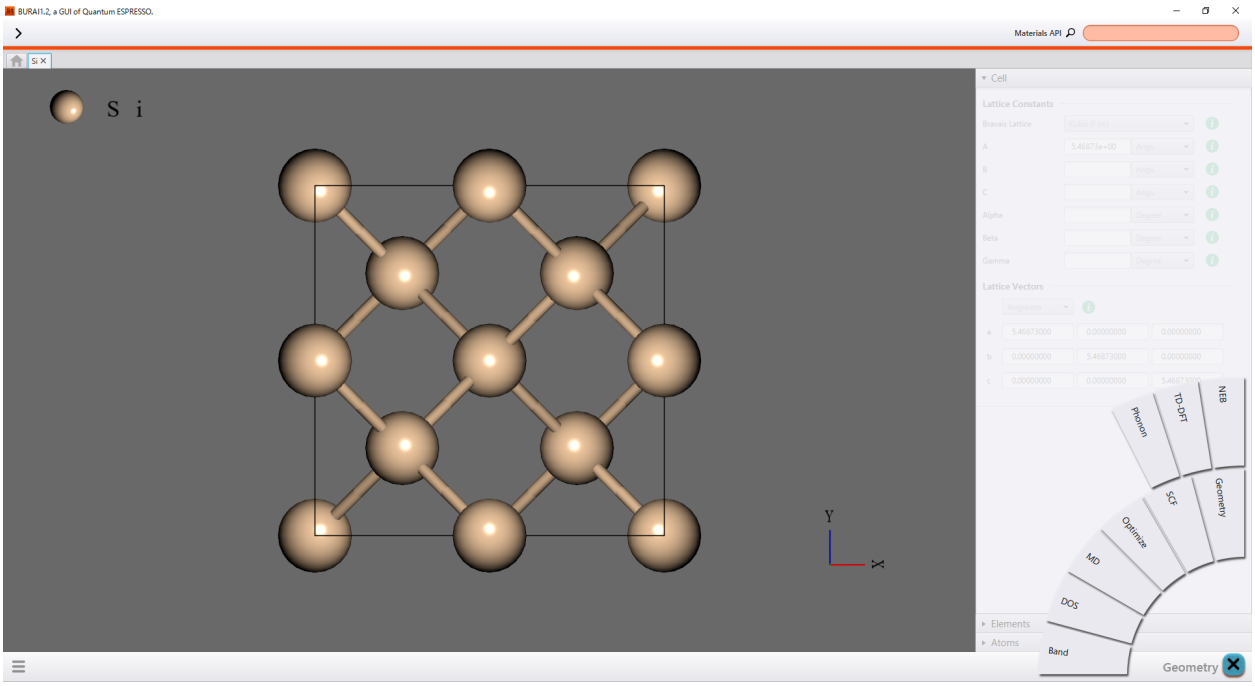


Input Editor

Project tab has the input editor, which can edit input file of QE. This is the input editor.



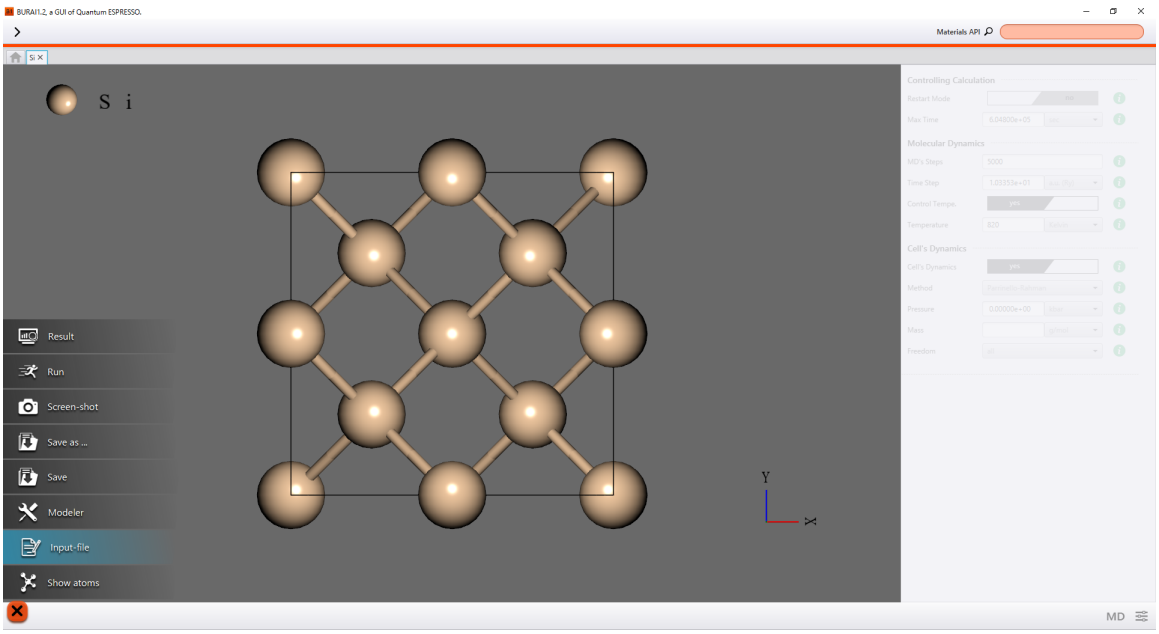
The input editor has several modes which can be selected by following menu.



Pleas see here for the details.

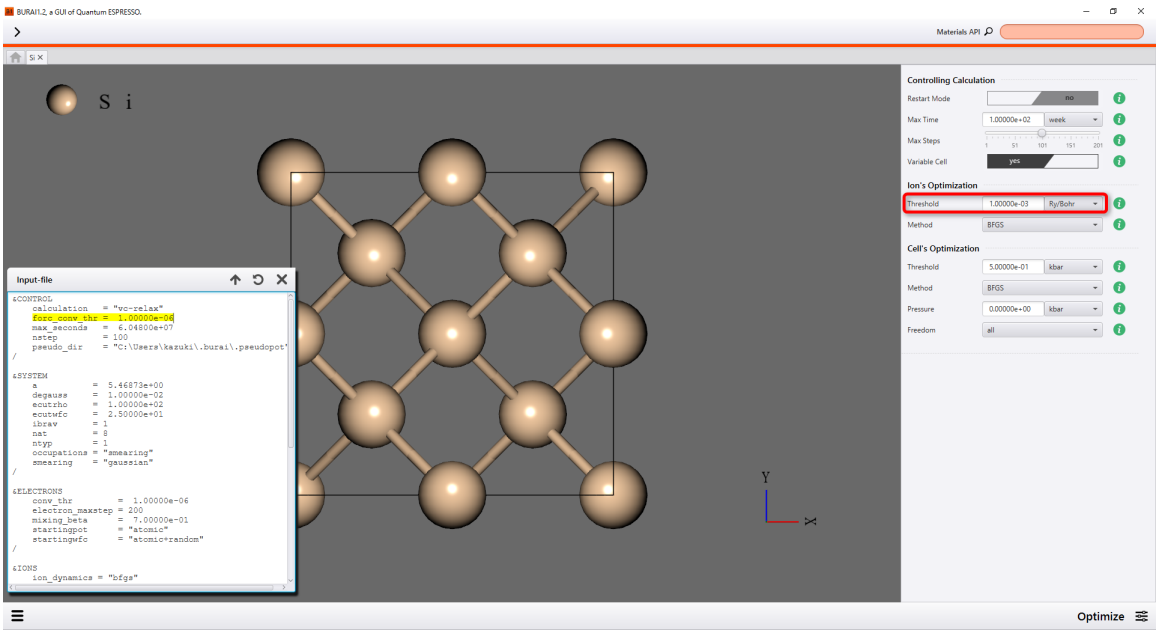
Input Editor (Build-in Text Editor)

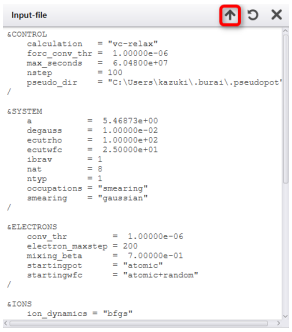
Project tab has *build-in* text editor, which can edit input file of QE. This editor can show and modify input file with *text*. You select "Input-file" from left menu, to display the editor.

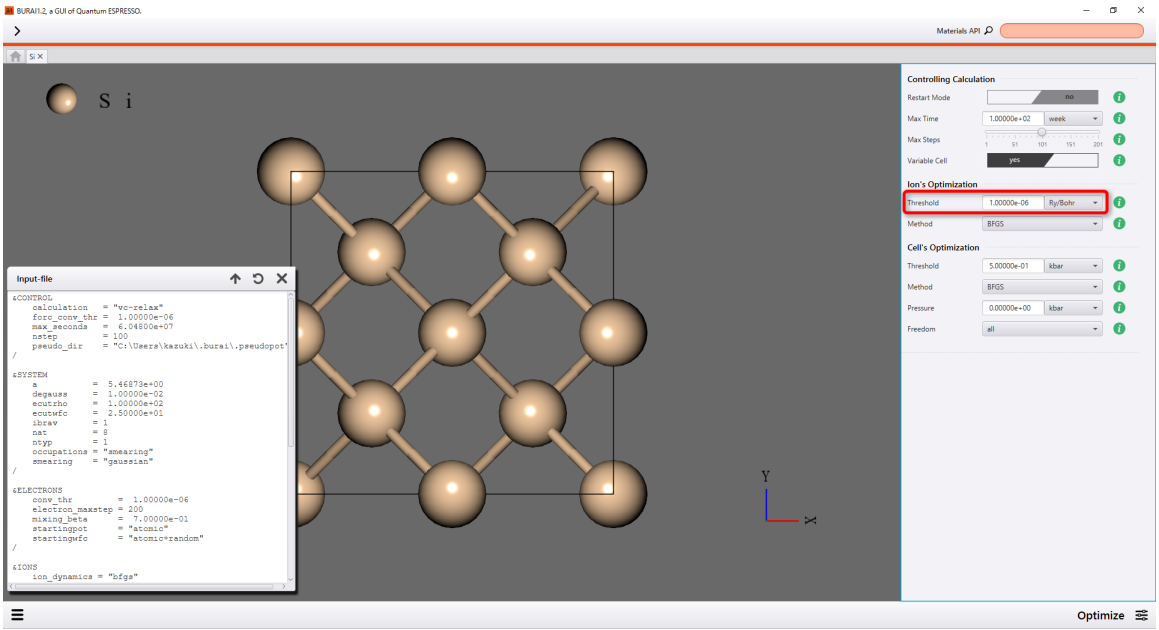


Upload

After the modification of text editor, pushing the upload button reflects it to project tab.

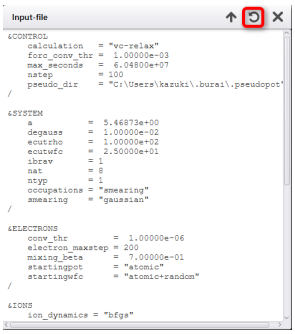

Materials API
Si
Controlling Calculation
Restart Mode
Max Time
Max Steps
Variable Cell
Ion's Optimization
Threshold
Method
Cell's Optimization
Threshold
Method
Pressure
Freedom
Input-file
&CONTROL
calculation = "vc-relax"
forc_conv_thr = 1.00000e-04
max_seconds = 6.04800e+07
nstep = 100
pseudo_dir = "C:\Users\kazuki\.burai\.pseudopot"
/
&SYSTEM
a = 5.46873e+00
degauss = 1.00000e-02
ecutrho = 1.00000e+02
ecutwfc = 2.50000e+01
ibrav = 1
nat = 8
ntyp = 1
occupations = "smearing"
smearing = "gaussian"
/
&ELECTRONS
conv_thr = 1.00000e-06
electron_maxstep = 200
mixing_beta = 7.00000e-01
startingpot = "atomic"
startingwfc = "atomic+random"
/
&IONS
ion_dynamics = "bfgs"
Optimize


Input-file
&CONTROL
calculation = "vc-relax"
forc_conv_thr = 1.00000e-06
max_seconds = 6.04800e+07
nstep = 100
pseudo_dir = "C:\Users\kazuki\.burai\.pseudopot"
/
&SYSTEM
a = 5.46873e+00
degauss = 1.00000e-02
ecutrho = 1.00000e+02
ecutwfc = 2.50000e+01
ibrav = 1
nat = 8
ntyp = 1
occupations = "smearing"
smearing = "gaussian"
/
&ELECTRONS
conv_thr = 1.00000e-06
electron_maxstep = 200
mixing_beta = 7.00000e-01
startingpot = "atomic"
startingwfc = "atomic+random"
/
&IONS
ion_dynamics = "bfgs"


Materials API
Si
Controlling Calculation
Restart Mode
Max Time
Max Steps
Variable Cell
Ion's Optimization
Threshold
Method
Cell's Optimization
Threshold
Method
Pressure
Freedom
Input-file
&CONTROL
calculation = "vc-relax"
forc_conv_thr = 1.00000e-06
max_seconds = 6.04800e+07
nstep = 100
pseudo_dir = "C:\Users\kazuki\.burai\.pseudopot"
/
&SYSTEM
a = 5.46873e+00
degauss = 1.00000e-02
ecutrho = 1.00000e+02
ecutwfc = 2.50000e+01
ibrav = 1
nat = 8
ntyp = 1
occupations = "smearing"
smearing = "gaussian"
/
&ELECTRONS
conv_thr = 1.00000e-06
electron_maxstep = 200
mixing_beta = 7.00000e-01
startingpot = "atomic"
startingwfc = "atomic+random"
/
&IONS
ion_dynamics = "bfgs"
Optimize

Reload

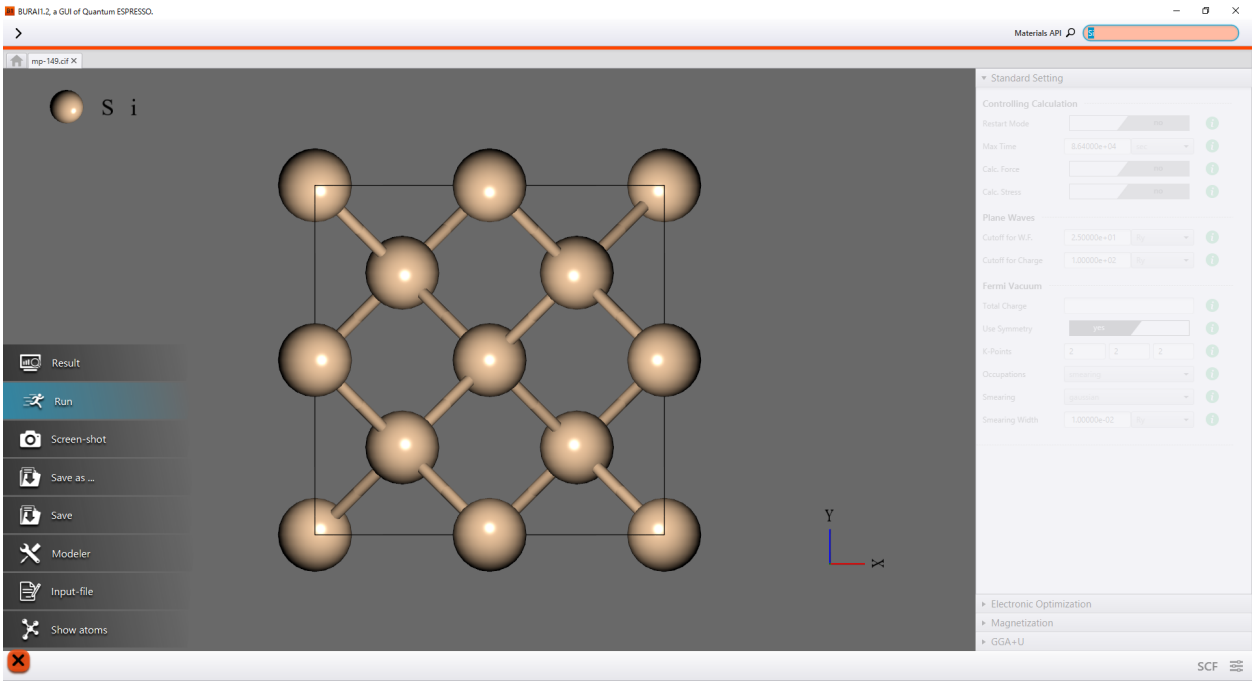
After the modification of project tab, pushing the reload button reflects it to text editor.



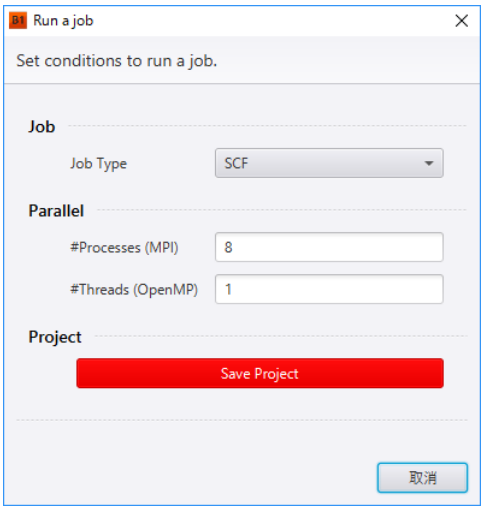
Running Calculation

Run jobs

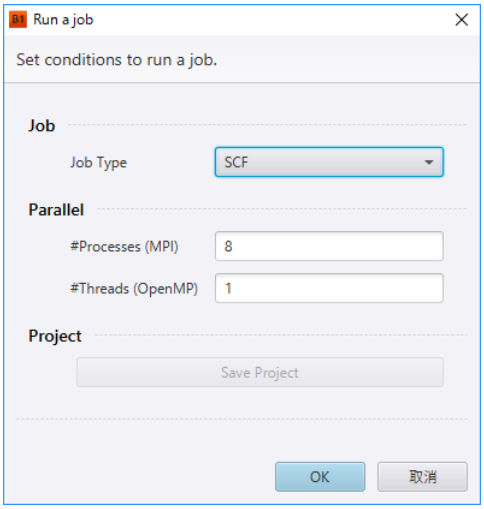
In case users start to the calculate, users select “Run” in the left menu.



However, users have to save a project before users calculate, if not saved, they have to push the “Save Project”.



Users save the project, then users push the OK button to run the calculation.



Moreover, BURAI platform has job controller. Jobs can be calculated in the order of waiting.

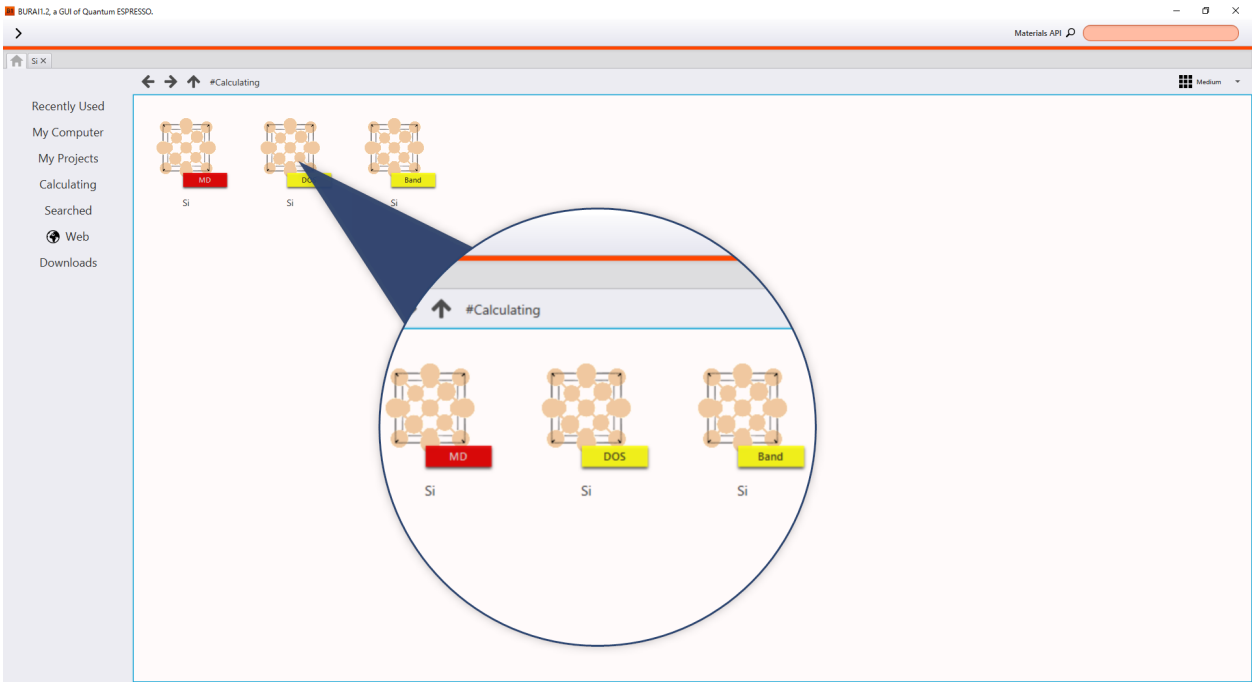
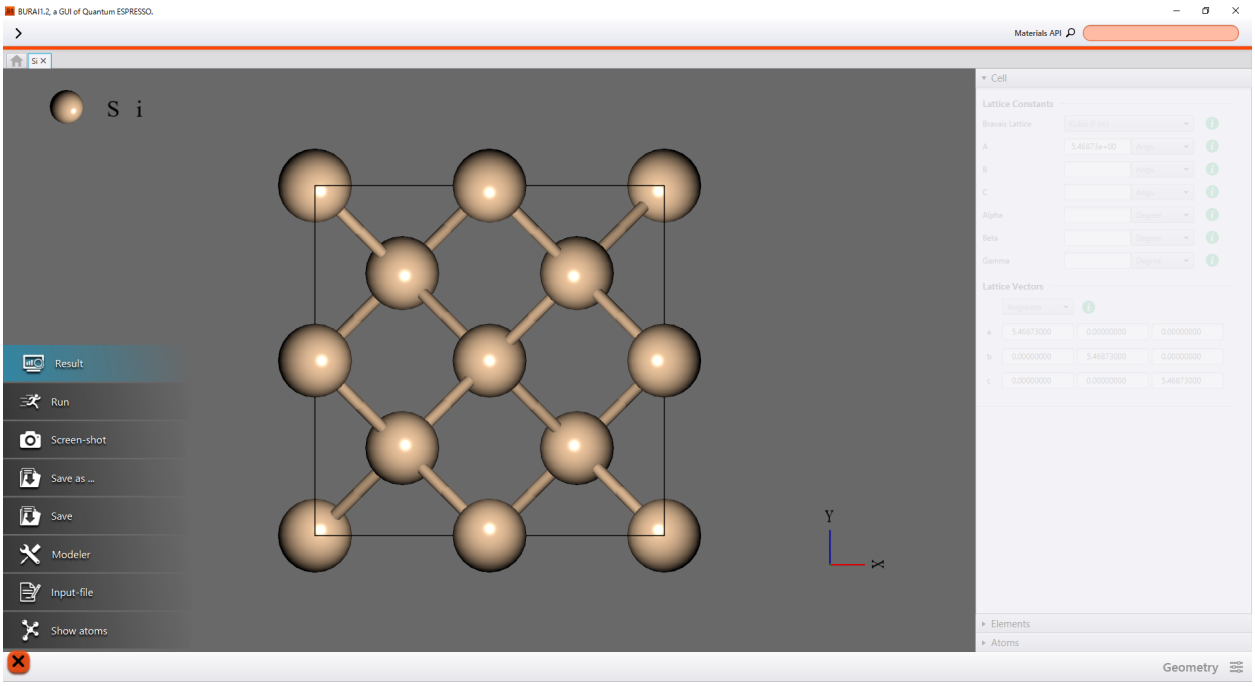


Table 5.3: jobs status

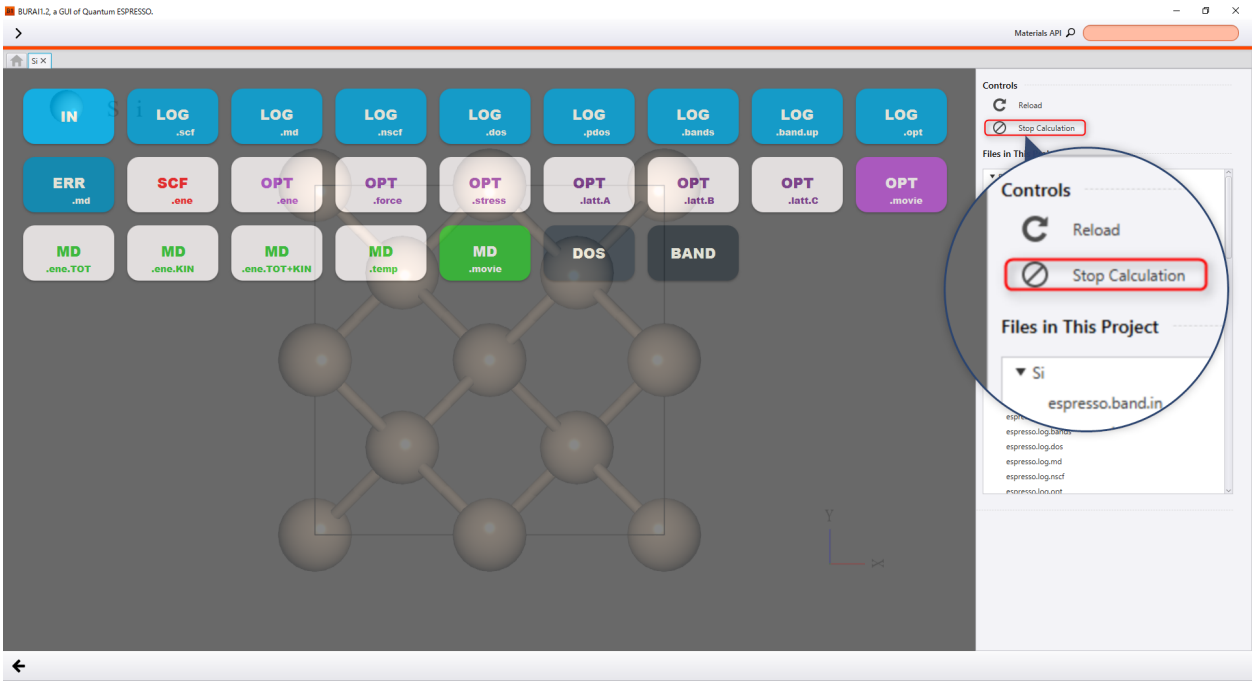
color.	Details
green	finished job
red	calculating job
yellow	waiting job

Stop jobs

In case users want to stop the calculating,

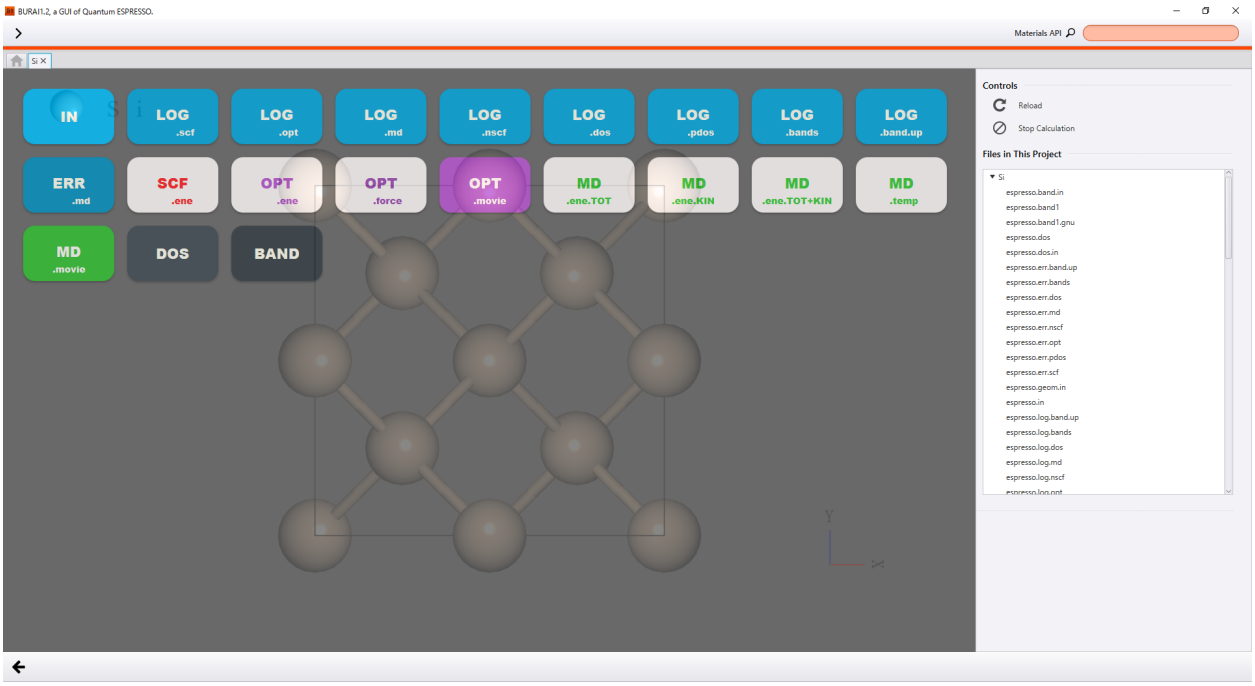


user should push “Stop Calculation”

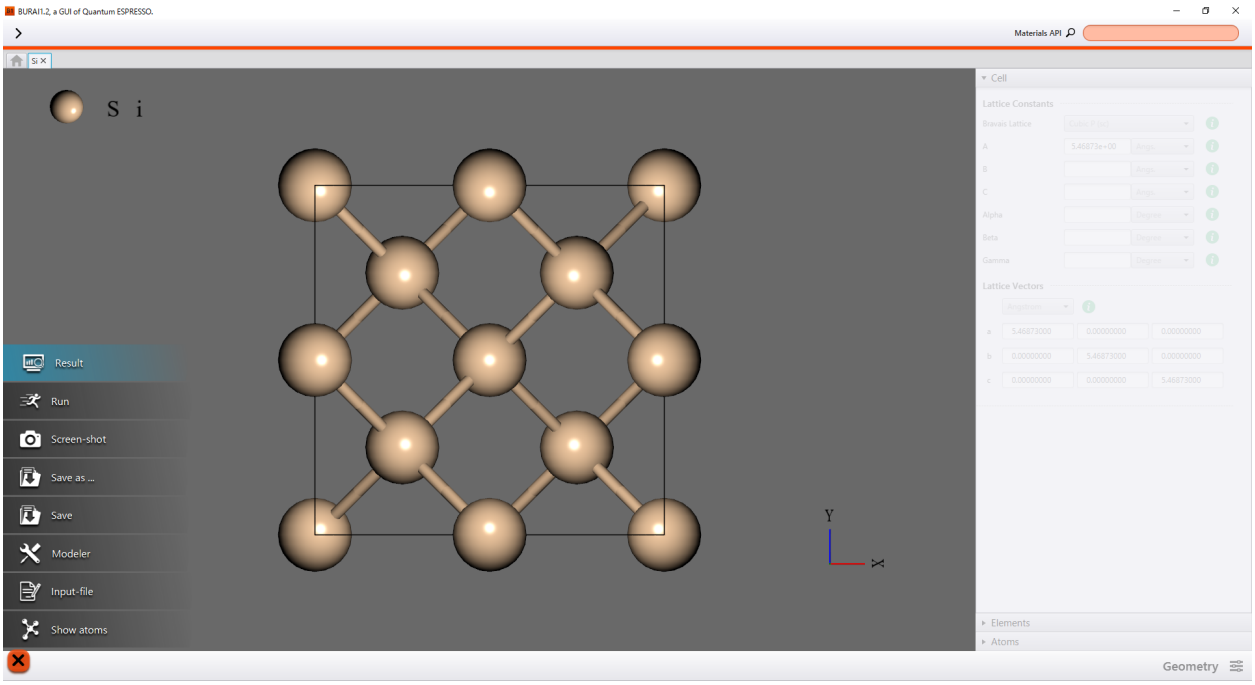


Result

BURAI manages the each calculation in the project directly as shown following figure.

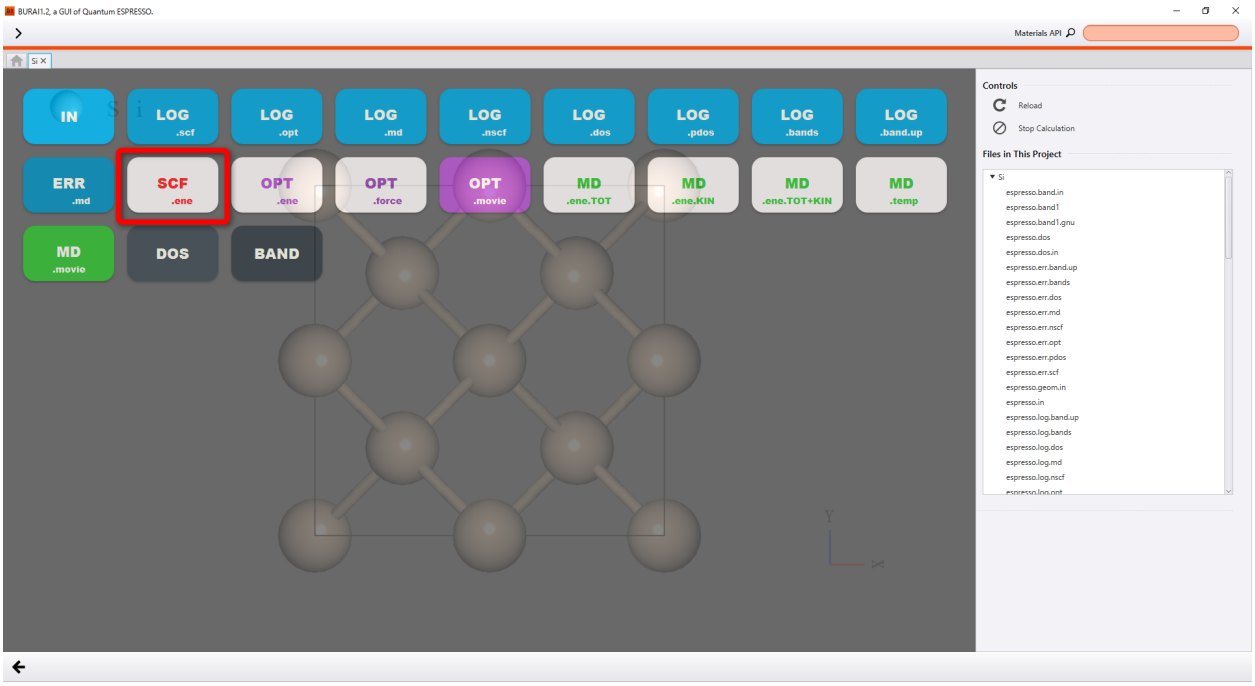


If users conform the result, users should select “Result” from the left menue.

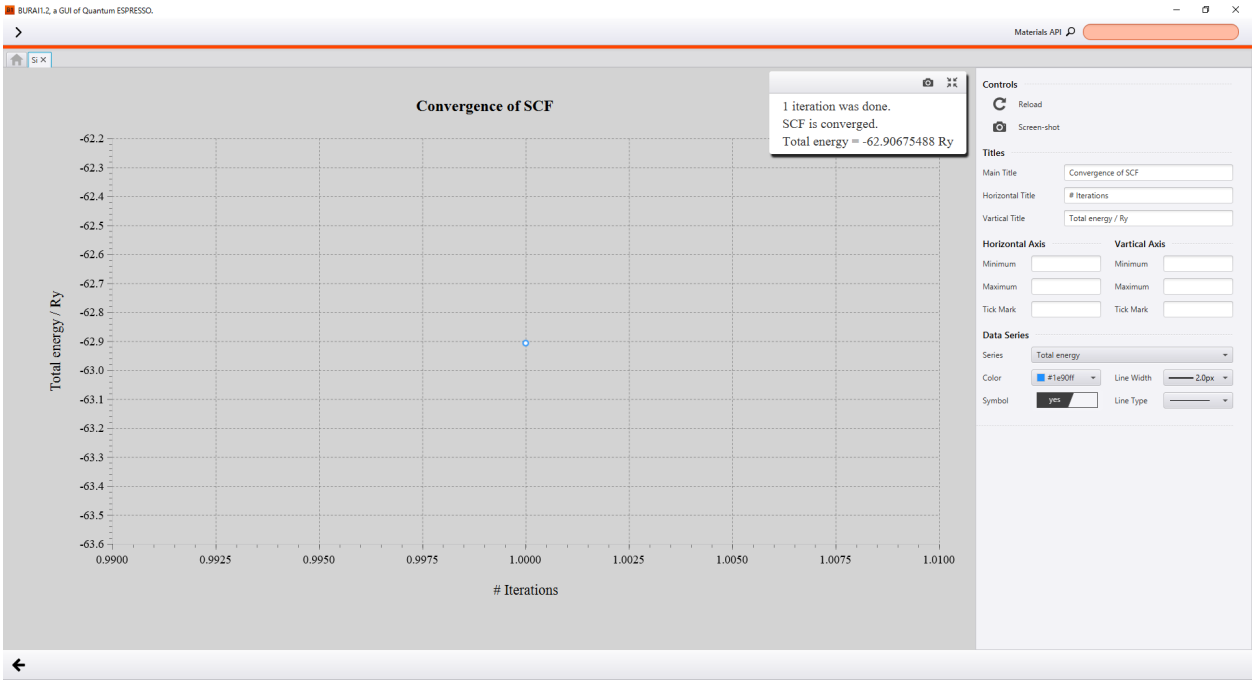


SCF

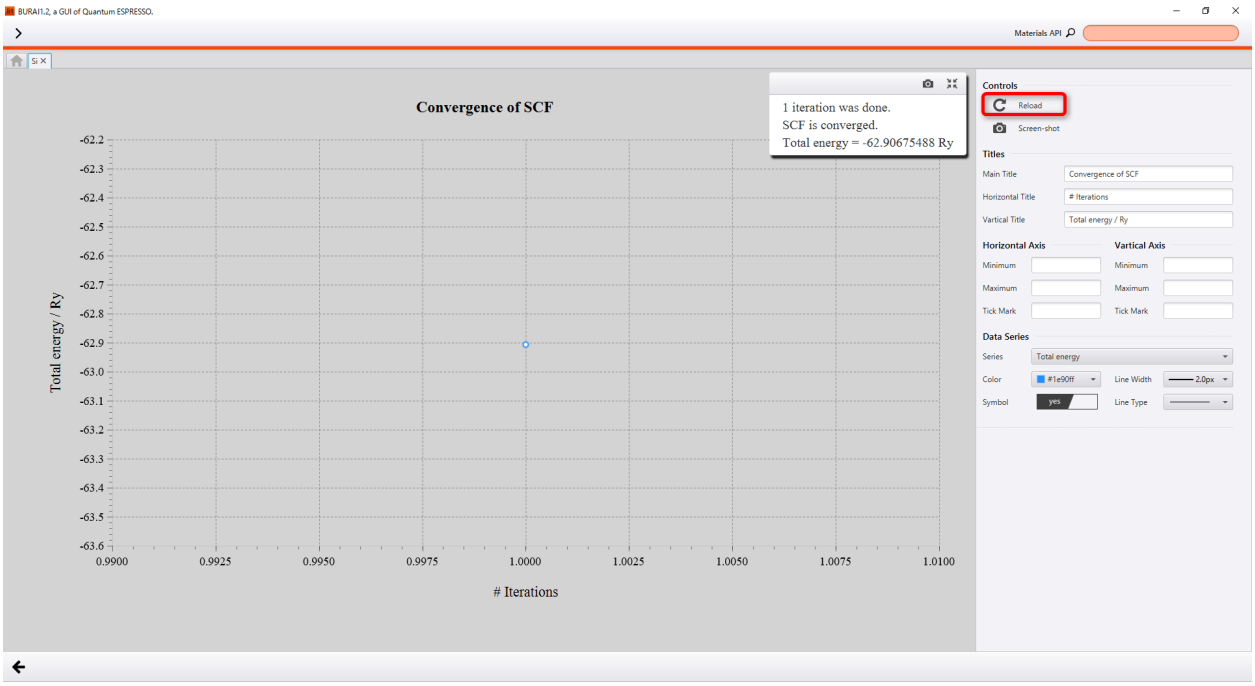
In case users estimate the SCF calculation, users select and push the “SCF.ene” icon in the result window.



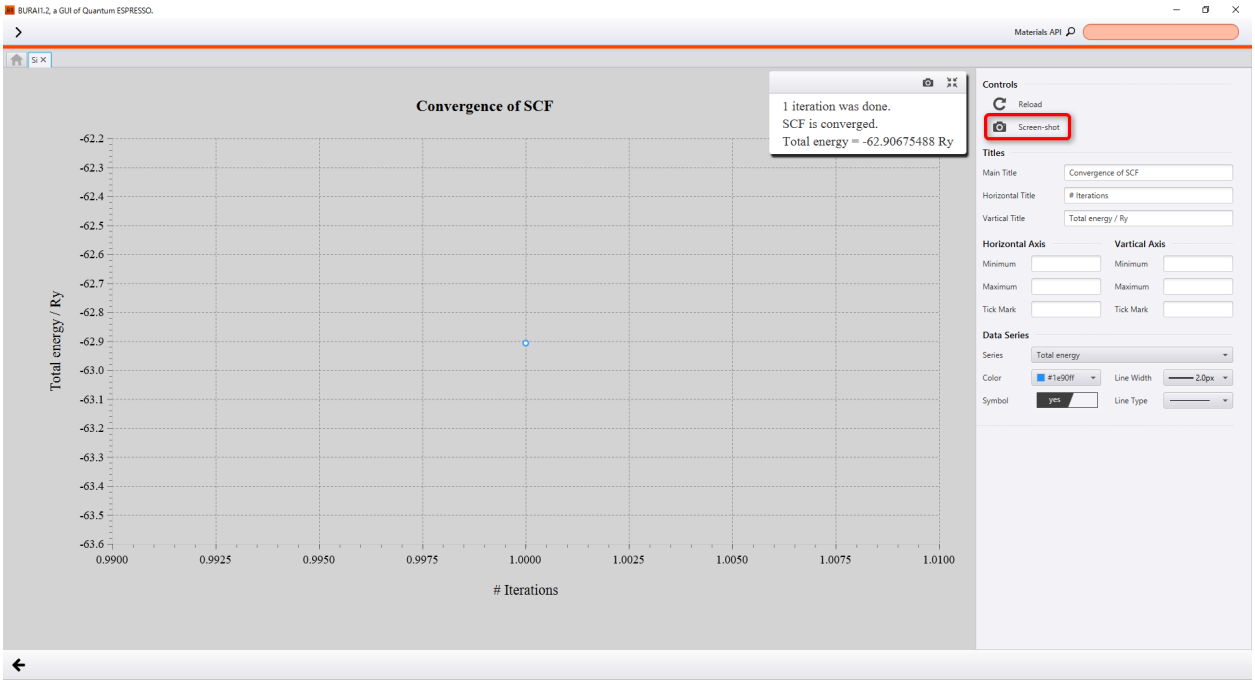
Users can adjust the figure of SCF plot by using right option.



If users show the result while calcurating, user push “Reload”. The present result is shown.

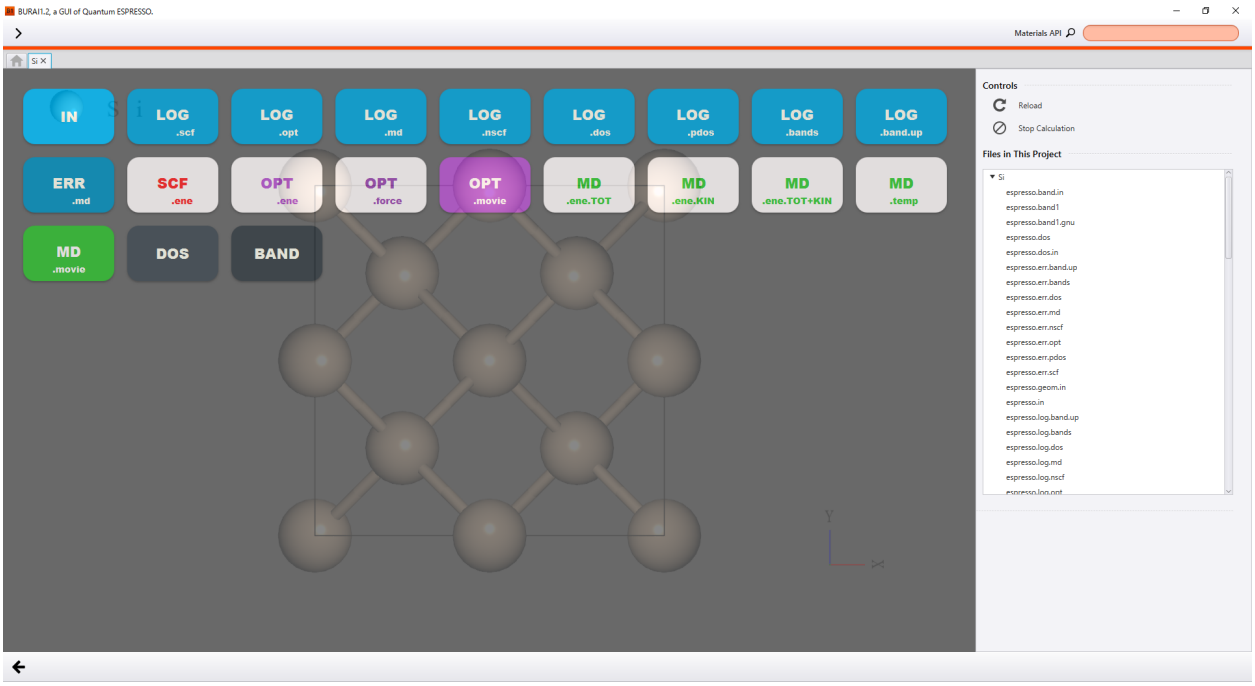


if users save as image files, users push “Screen-shot”

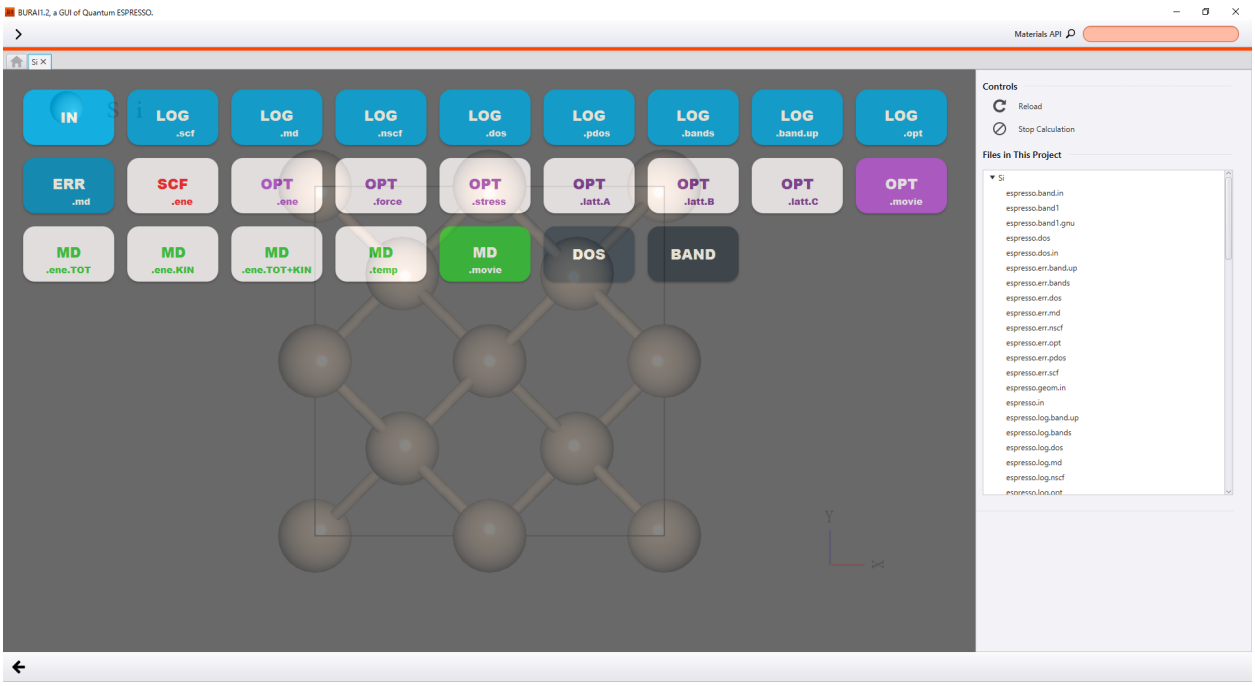


OPT

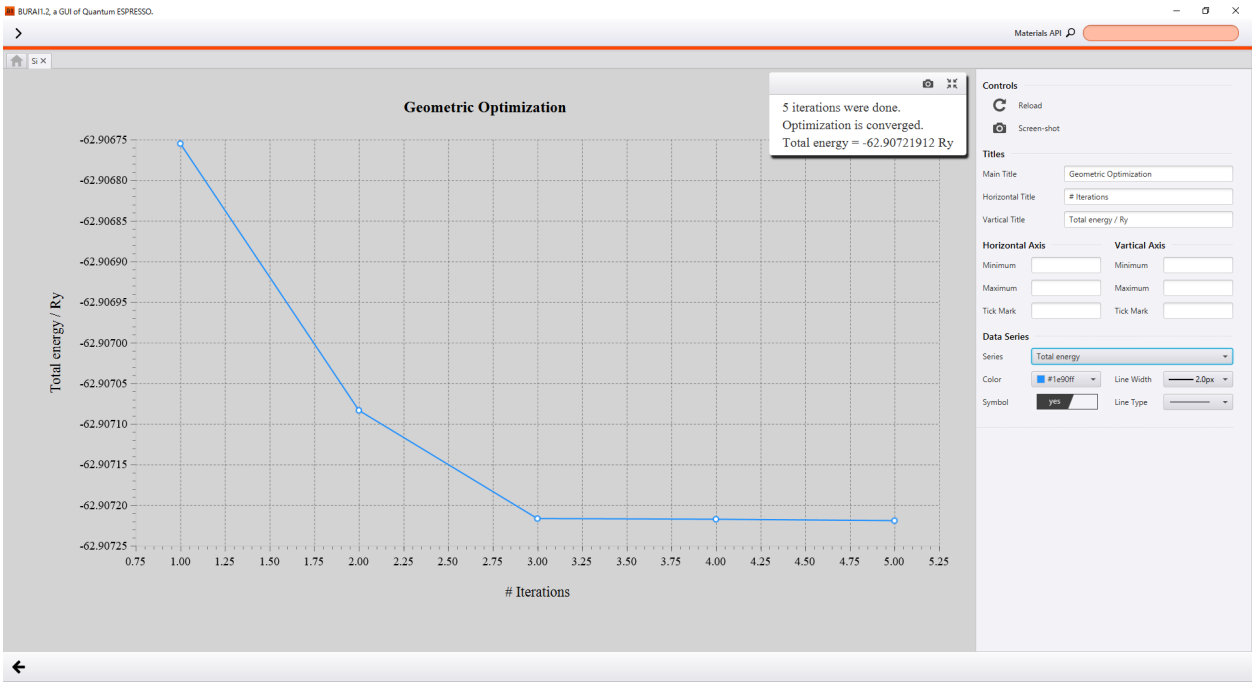
In case users calculated without variable cell, geometry optimization result is saved as OPT.ene, OPT.forec, and OPT.movie. OPT.ene include the energy result. OPT.forec has the force infomation. OPT.movie has the coordinates of each step.



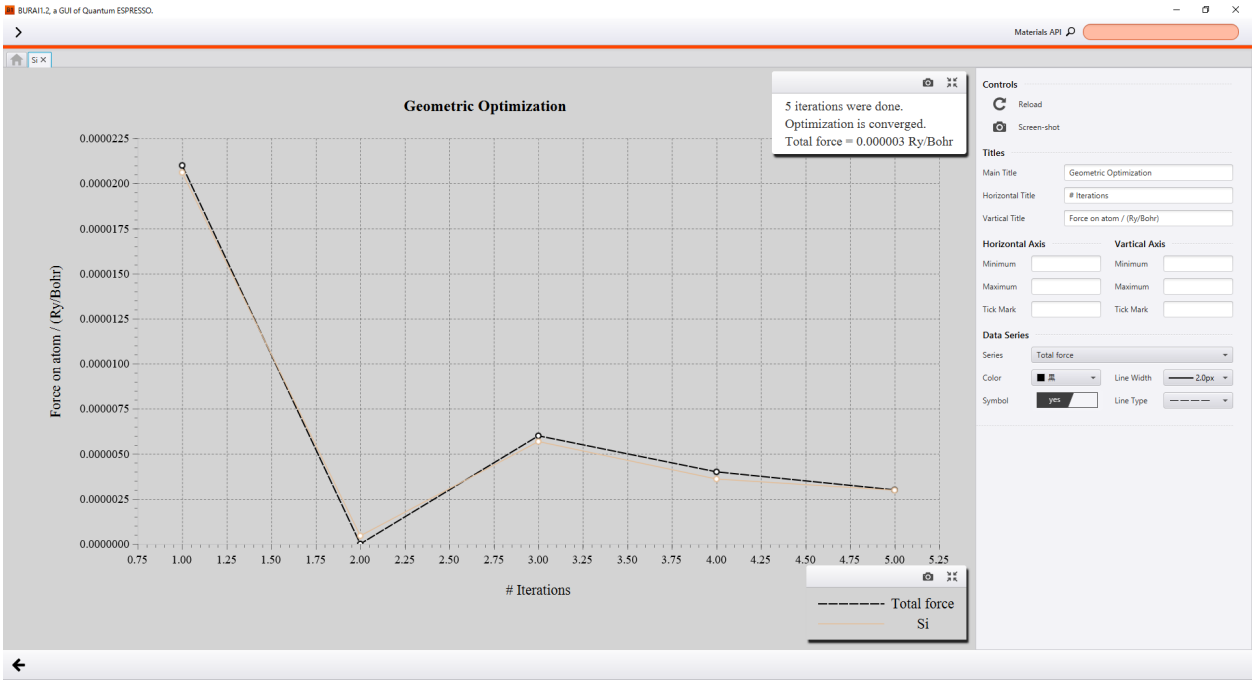
In case users calculated with variable cell, geometry optimization result is saved as OPT.ene, OPT.forec, OPT.stress, OPT.latt.A, OPT.latt.B, OPT.latt.C, and OPT.movie.



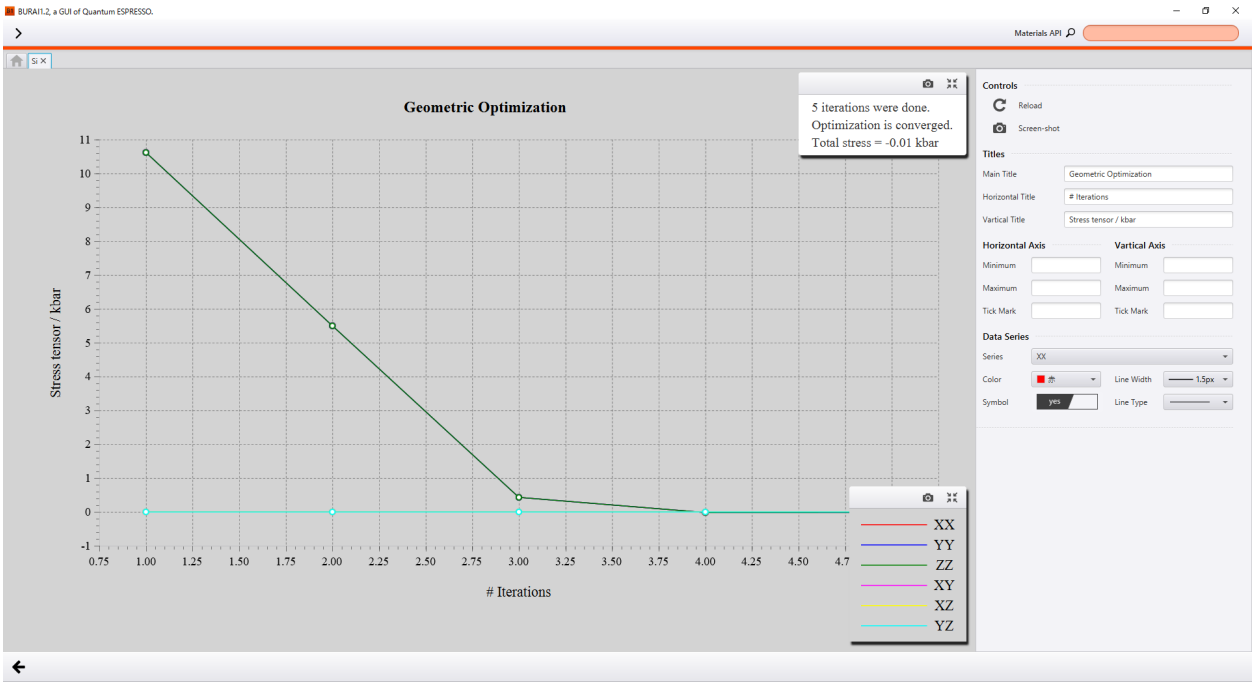
OPT.ene shows energy plots as folloing the figure.



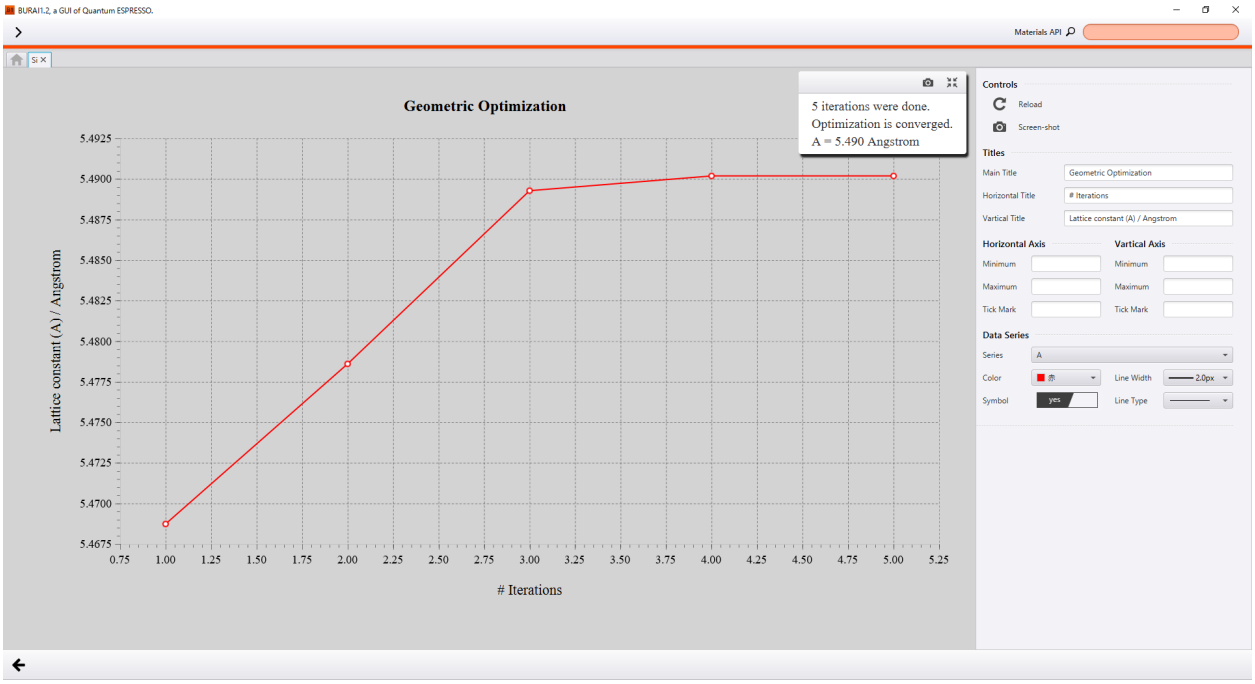
OPT.forec shows the force result.



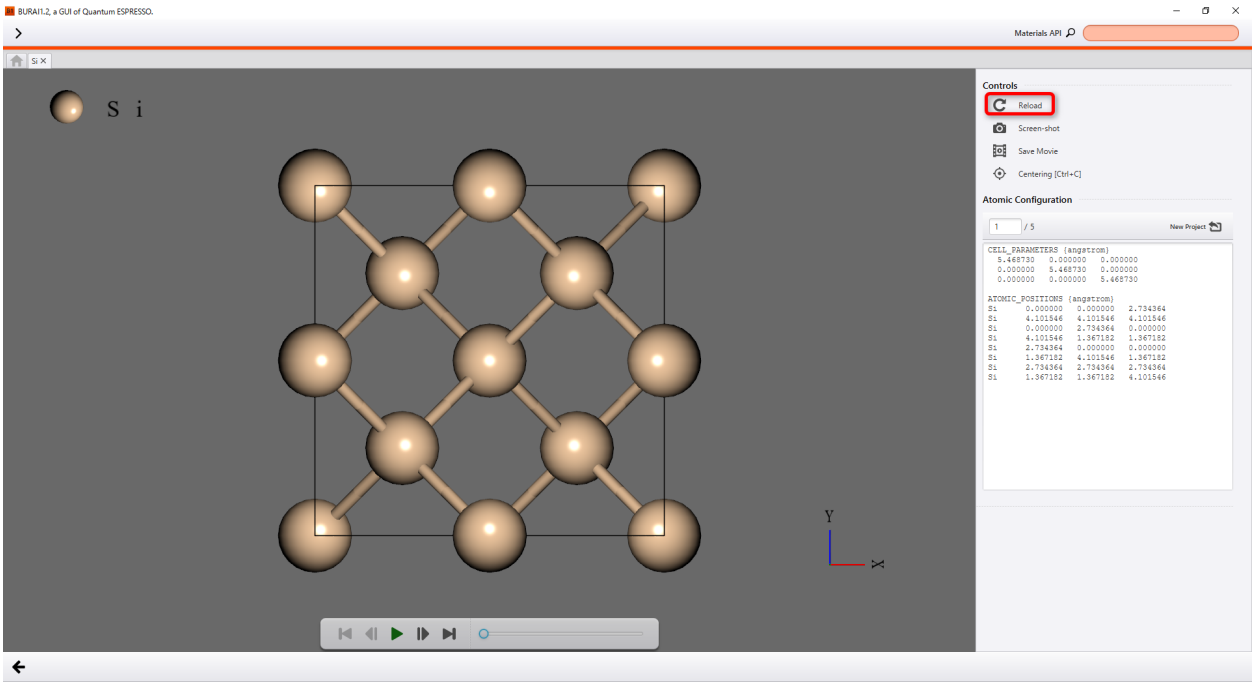
OPT.stress shows the stress tensors.



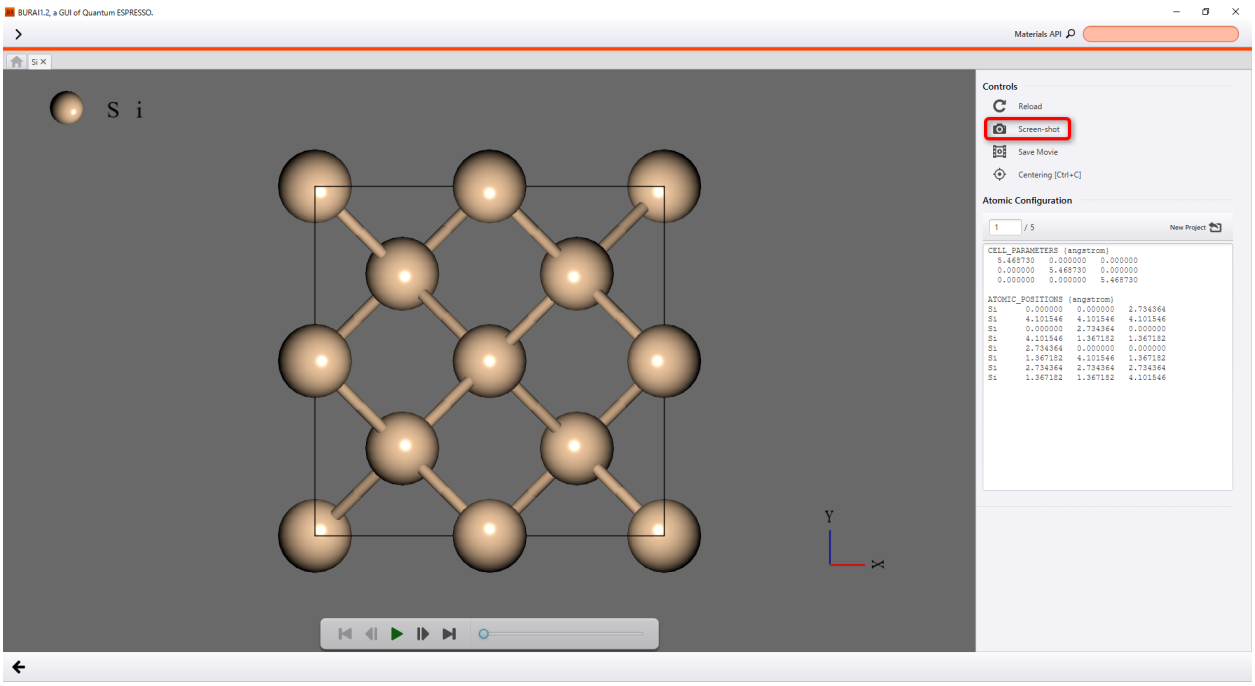
OPT.latt.A, OPT.latt.B, and OPT.latt.C shown result of each lattice constant. The following figure shows the result of lattice constant a.



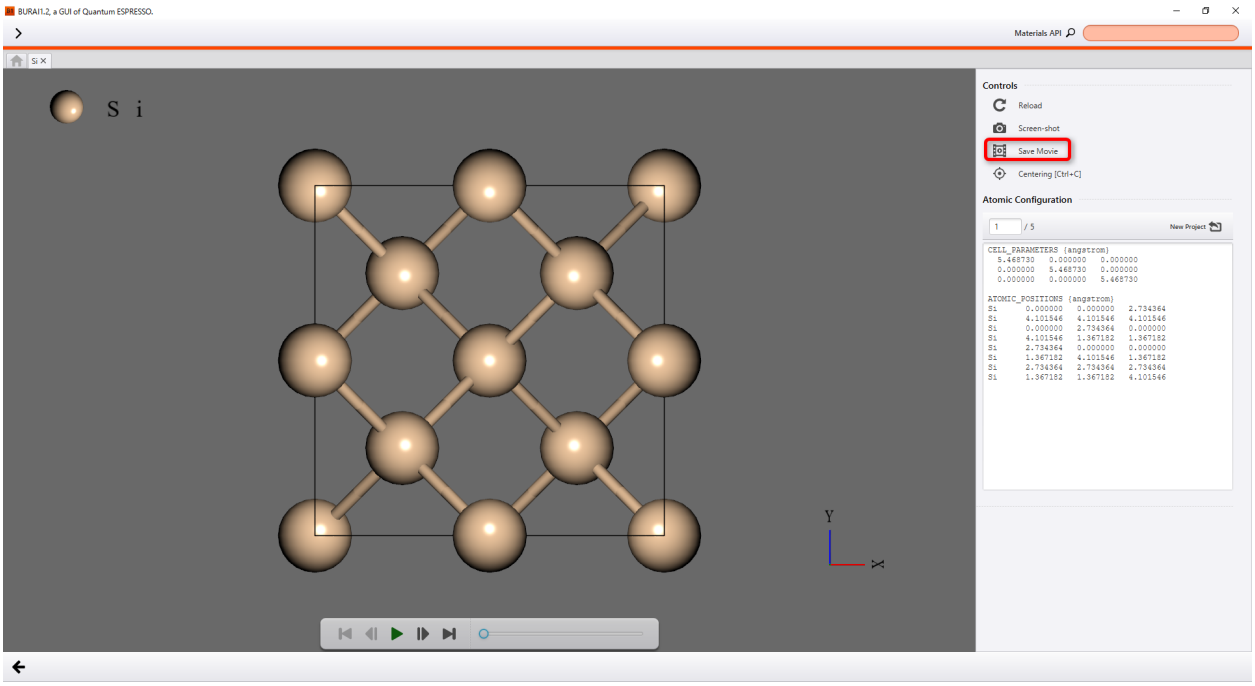
If users show the result while calcurating, user push “Reload”. The present result is shown.



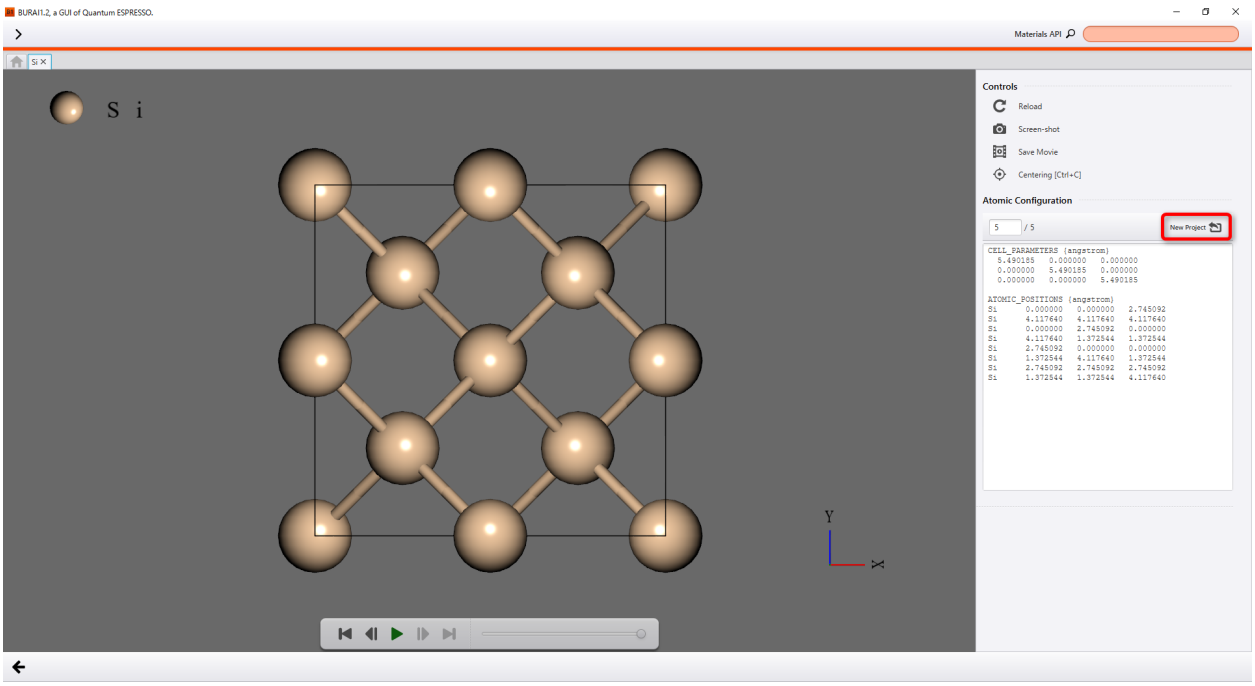
if users save as image files, users push “Screen-shot”



if users save as move files (MP4 format), users push “Save Movie”

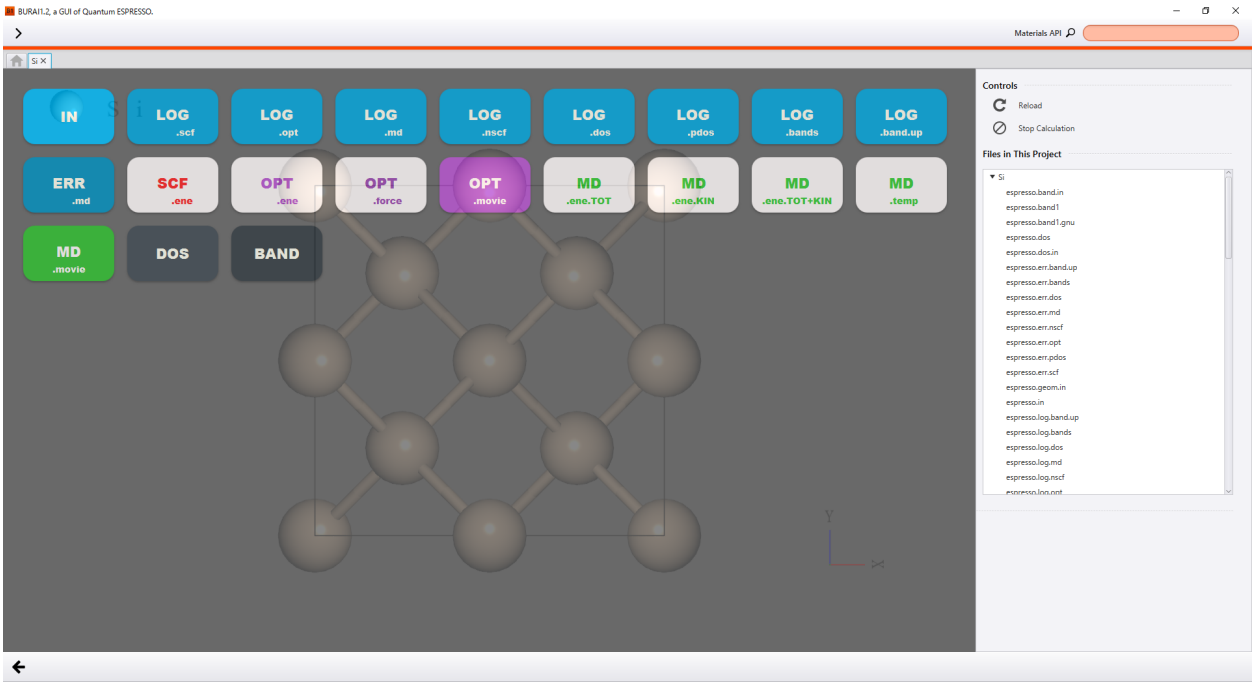


If users want to treat optimized structure for other project, users should push “New Pjoject”.



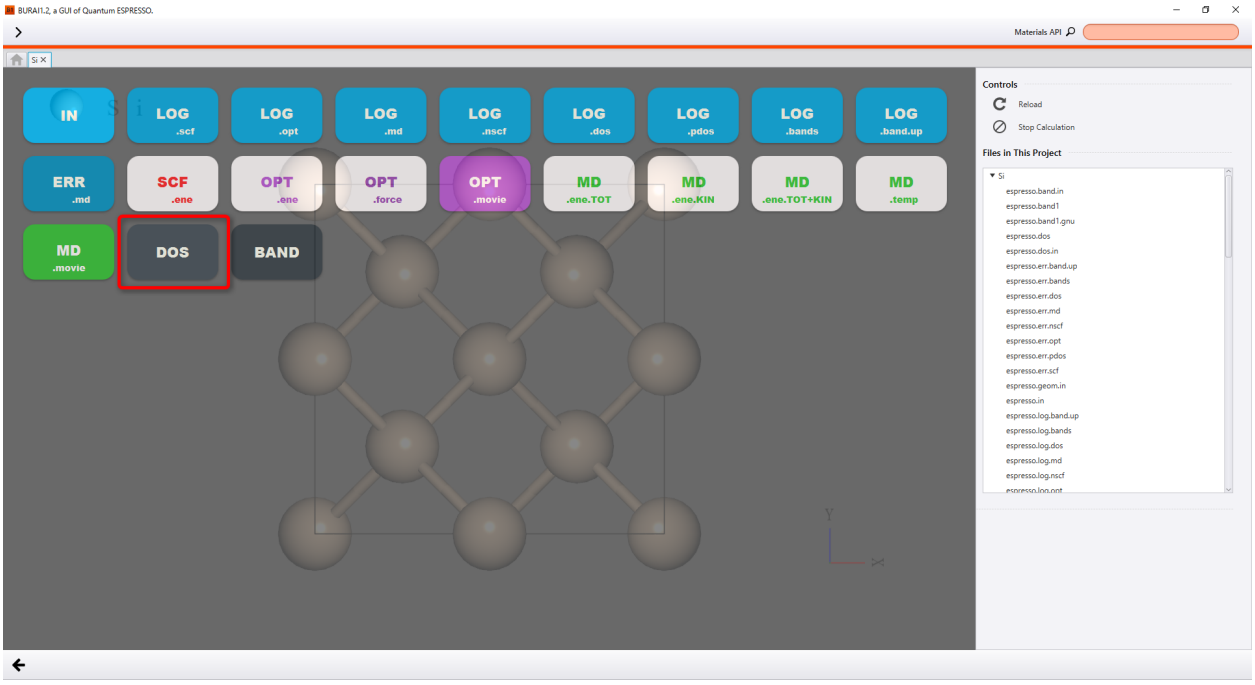
MD

In case users calculated without variable cell, molecular dynamics result is saved as MD.ene.TOT, MD.ene.KIN, and OPT.ene.TOT+KIN, and MD.temp, and MD.movie.

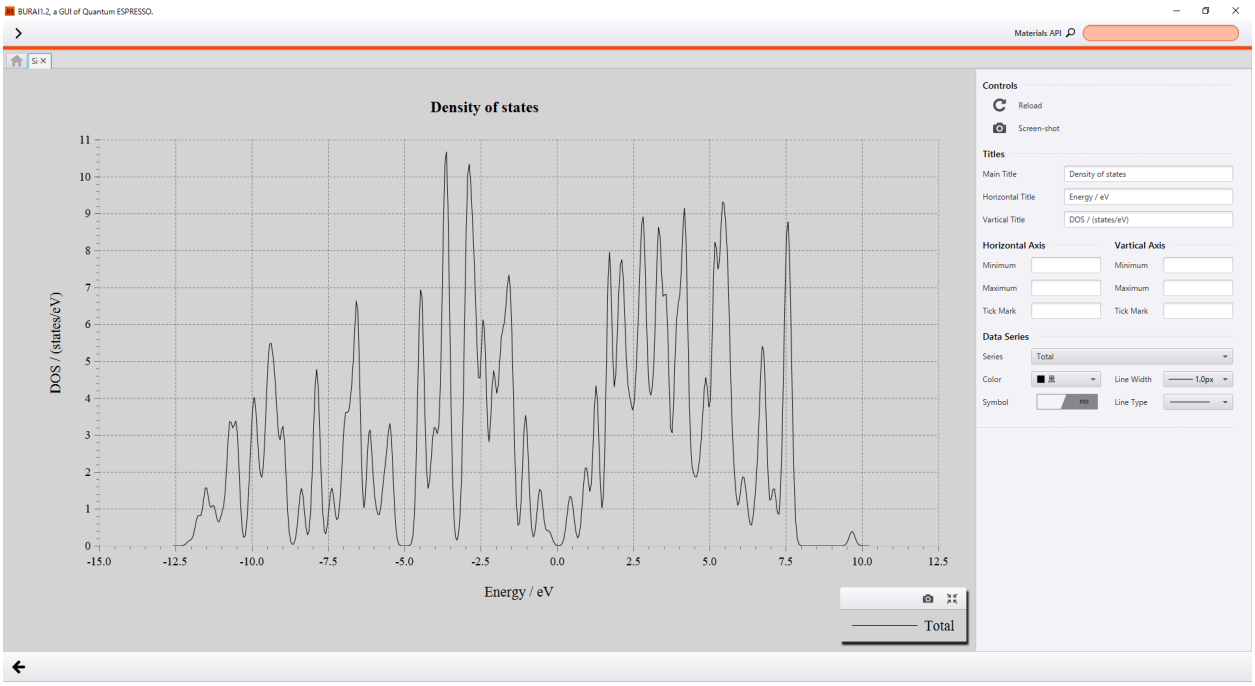


DOS

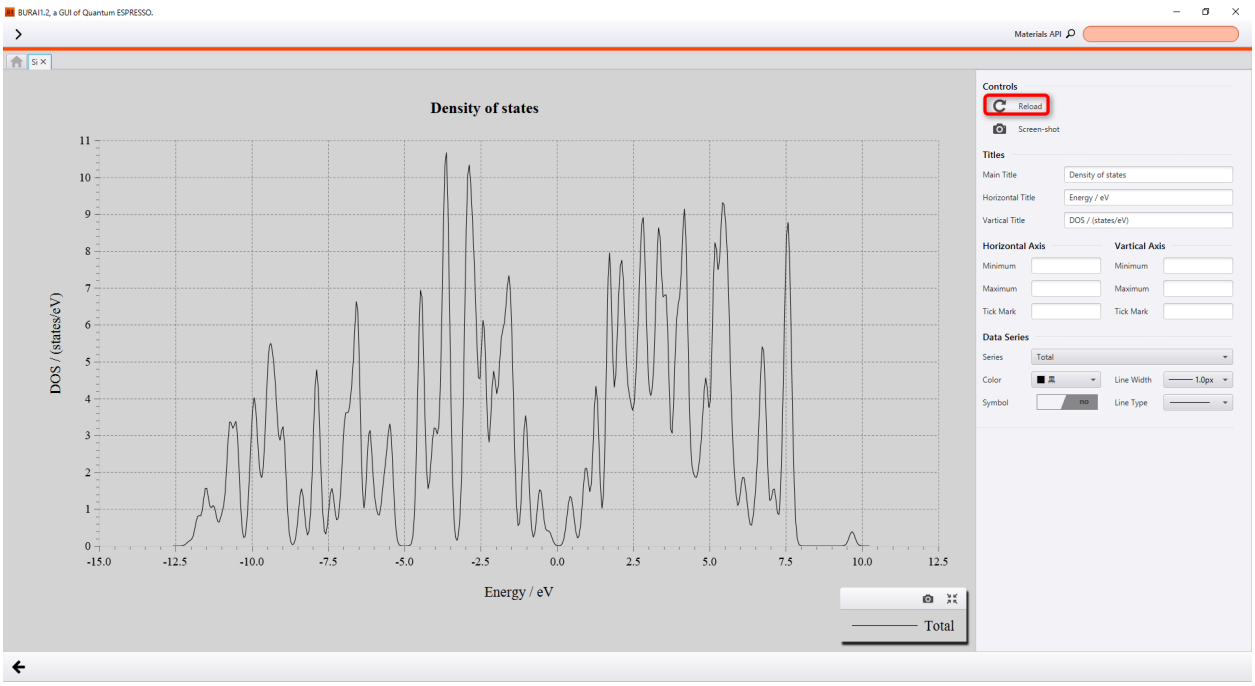
DOS result is saved as “DOS”.



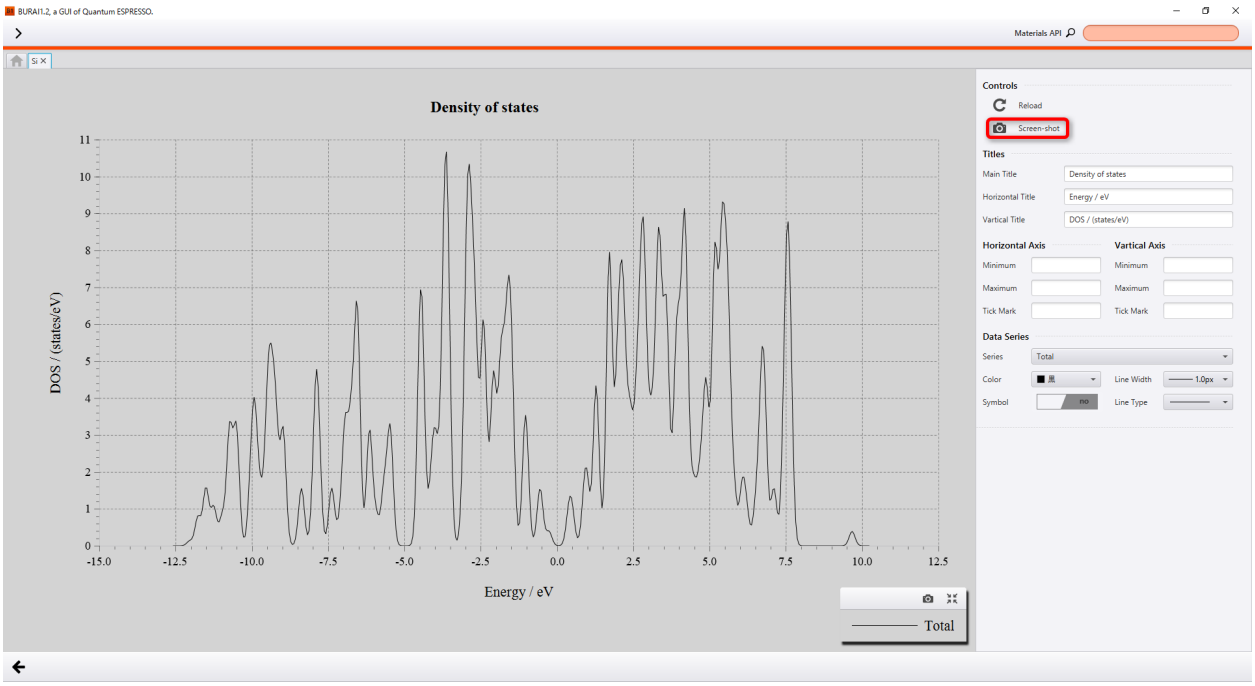
the DOS result is plotted as following figure.



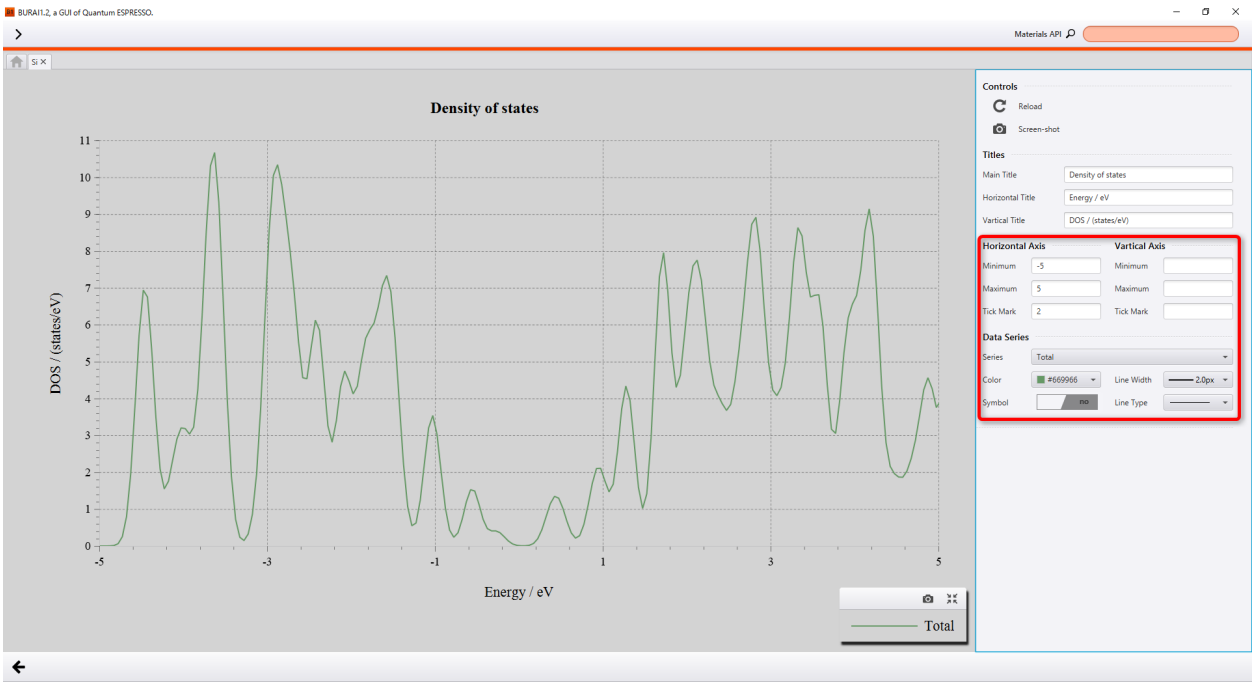
If users show the result while calcurating, user push “Reload”. The present result is shown.



if users save as image files, users push “Screen-shot”



Users can adjust the figure of DOS plot by using right option.



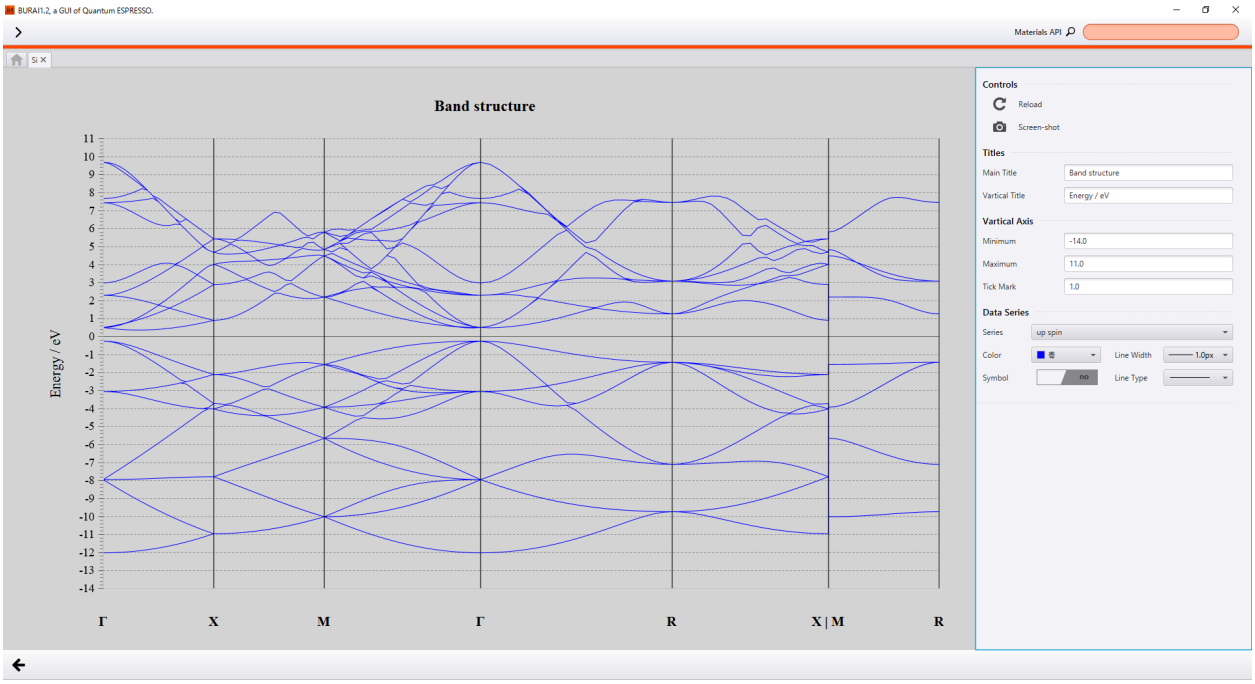
BAND

The band structure result is saved as “BAND”. | .. image:: ../../../img/projects/imgResultBAND00.png

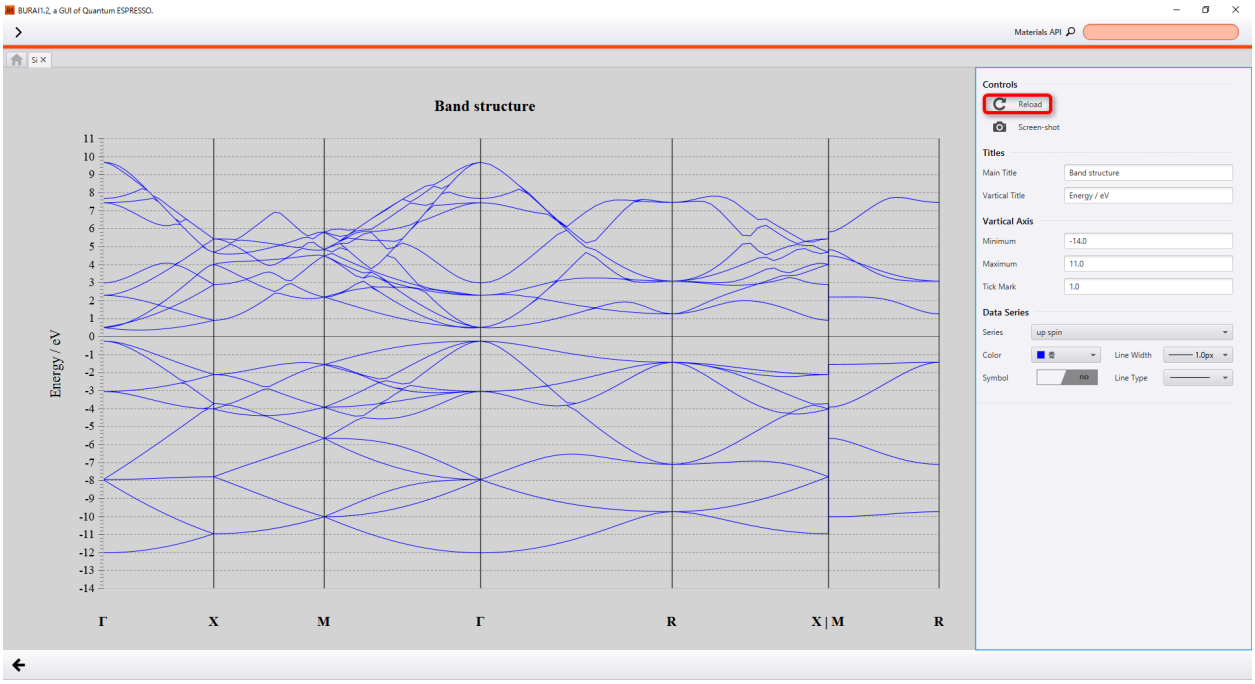
scale 50 %

align center

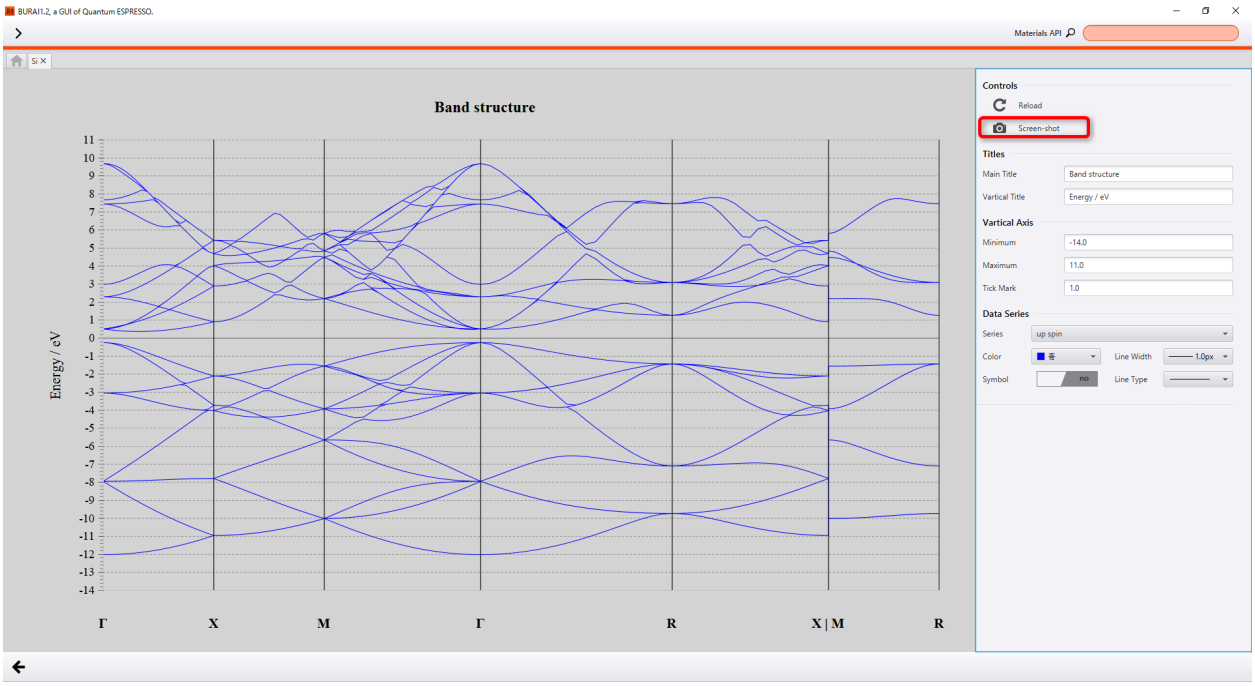
The band structure is plotted as as following figure.



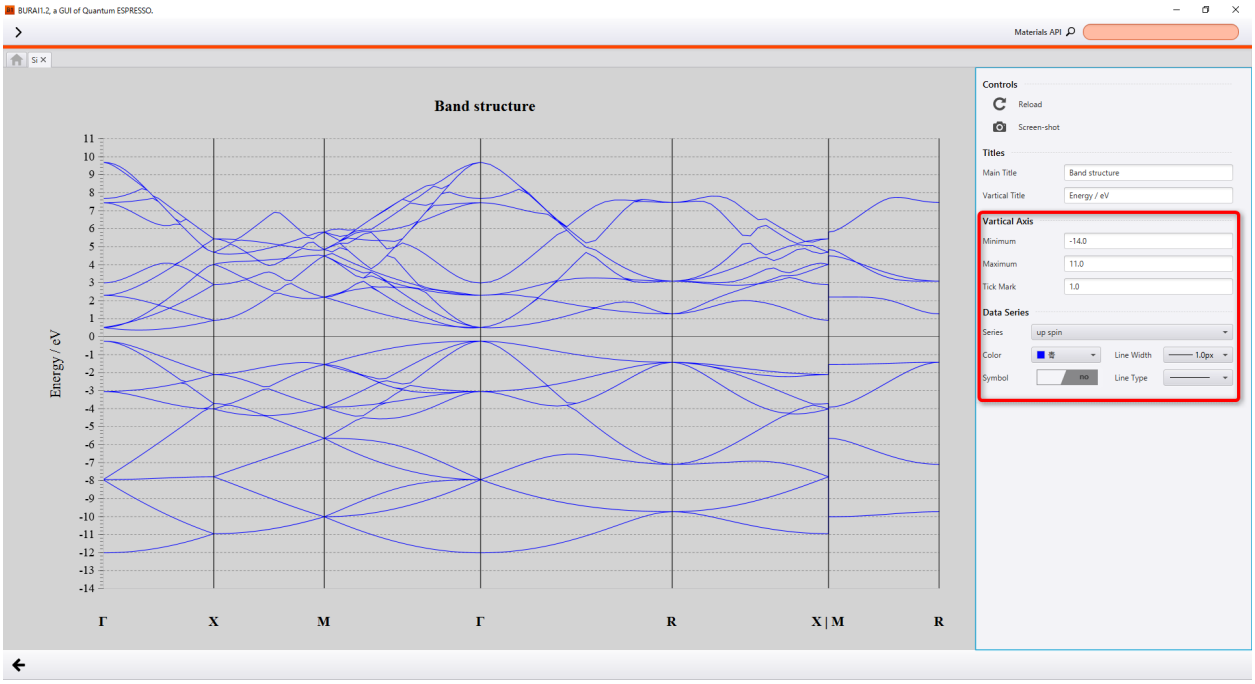
If users show the result while calcurating, user push “Reload”. The present result is shown.



if users save as image files, users push “Screen-shot”



Users can adjust the figure of DOS plot by using right option.



Input Editor in Project

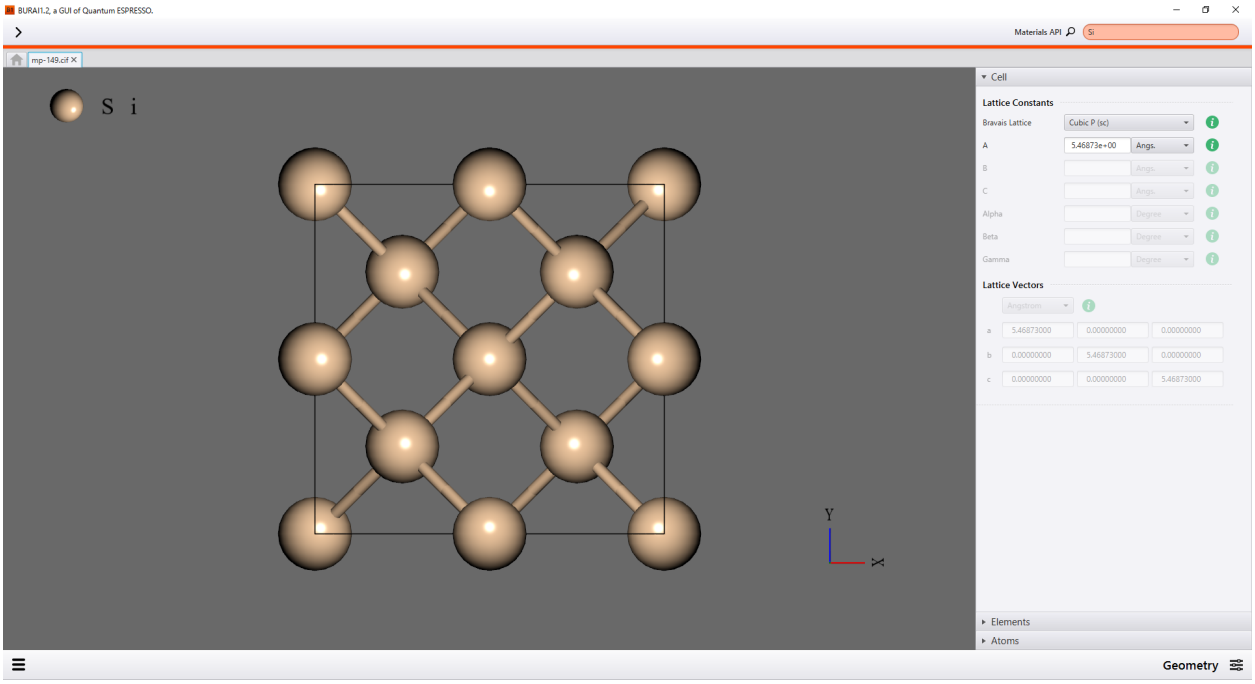
Contents:

Geometry

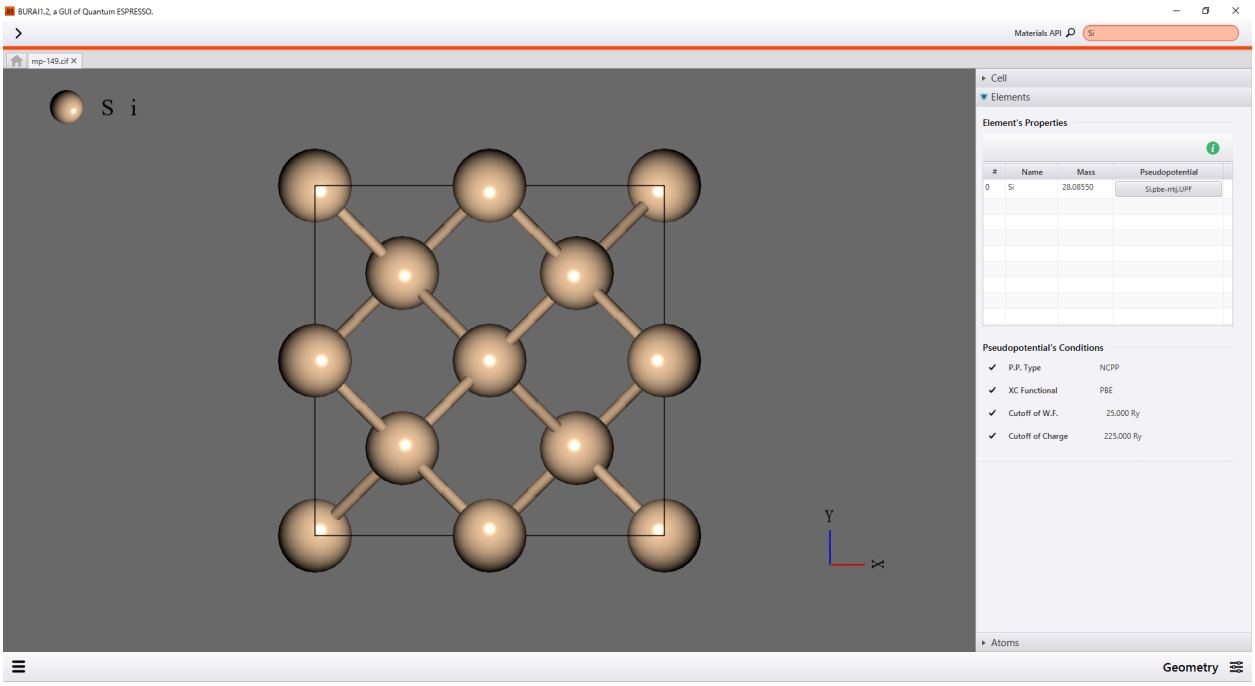
The geometry window is consist of three windows, “Cell”, “Elemant”, and “Atoms”. The geometry window shows the crystallographic information which user select. Also, the information of used psudopotential is shown.

Cell

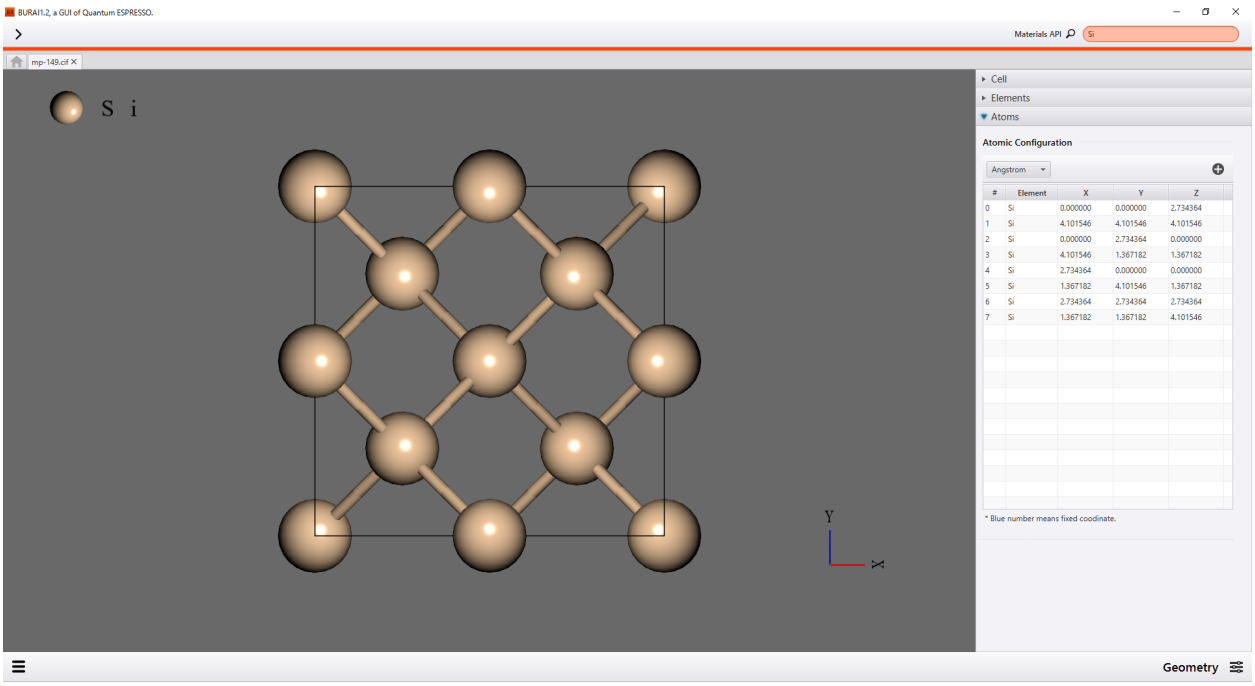
Cell window shows the lattice constants and lattice vectors. if users change the lattice constants, users directly enter volume into the lattice constant’s columns.



Elements window shows the element information of selected crystal structure. Also, in this window, users can select the pseudopotential for each element.



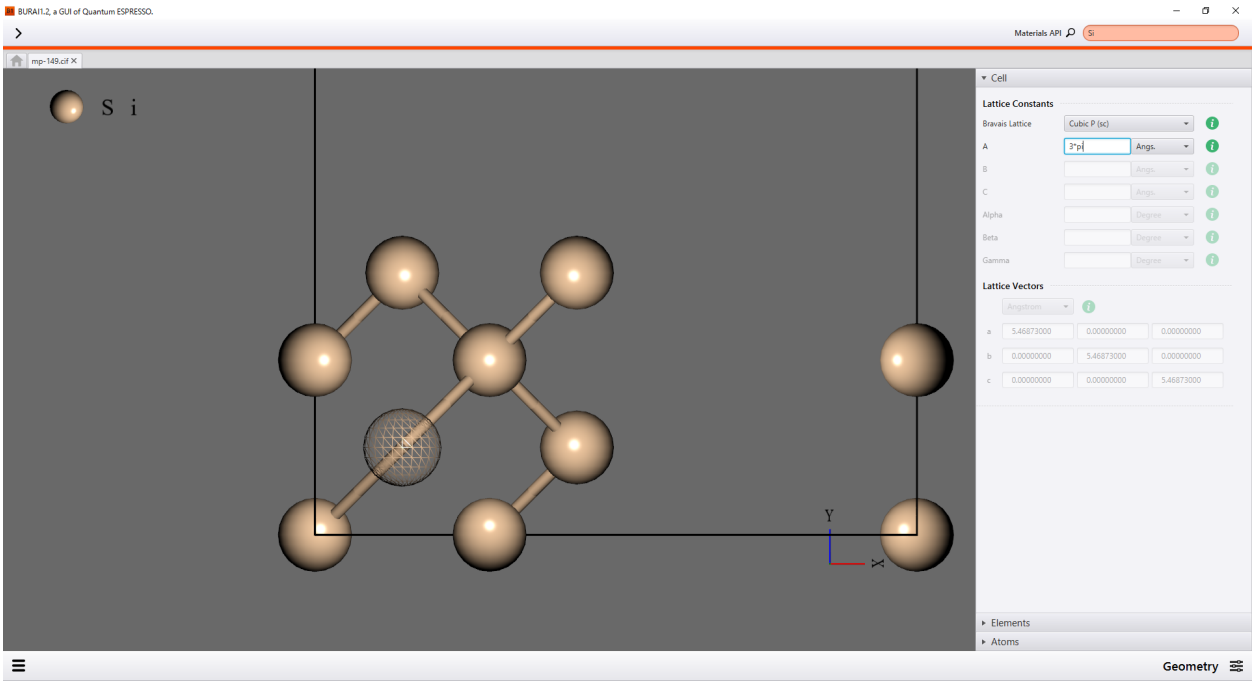
Atoms window shows the atomic positions of selected crystal structure in the table. Select the column of the table, the atom which are selected, becomes a mesh sphere.



In the case that users enter the volume into the column, it is possible to use a numerical expression and pi in BURAI system. | .. image:: ../../../img/input_editor/imgCreateJob_Geometry03.png

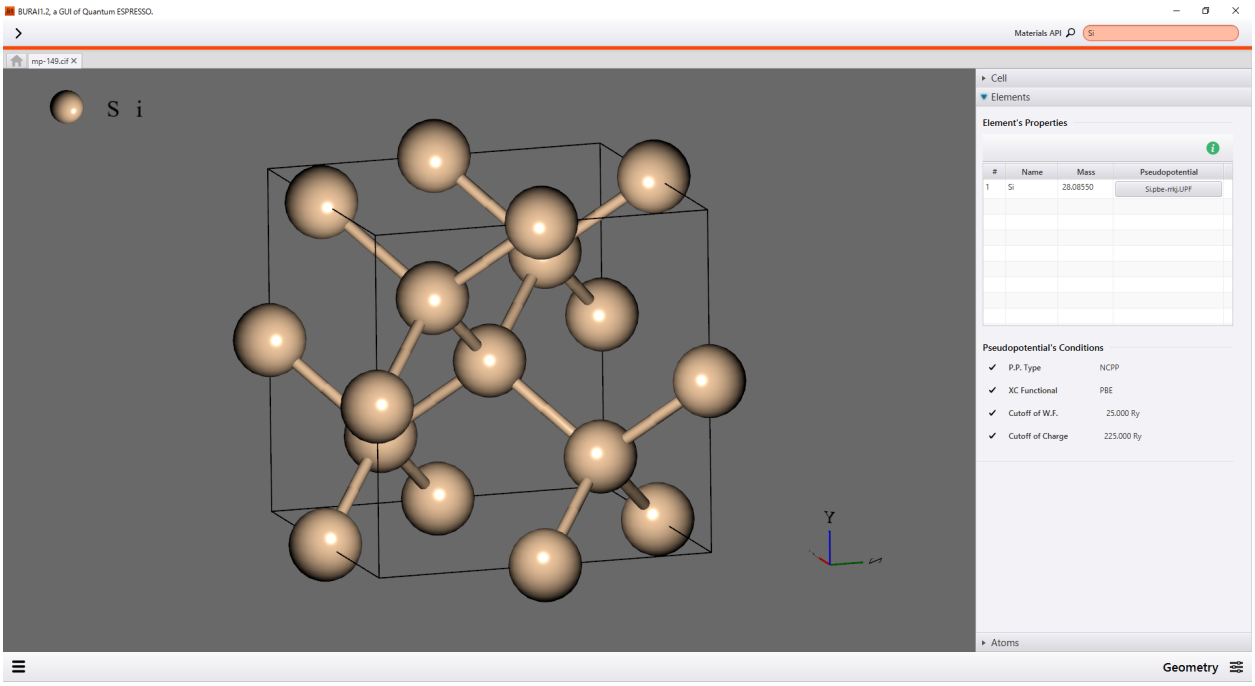
scale 50 %

align center

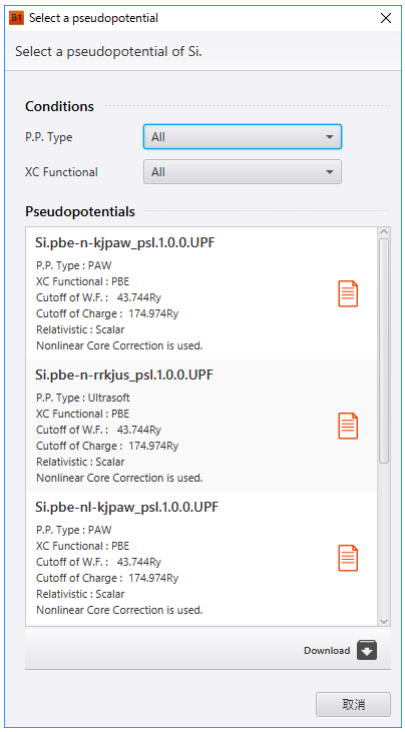


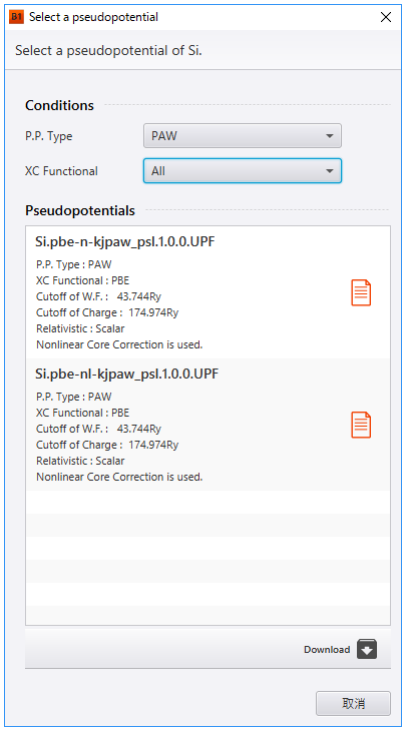
Elements

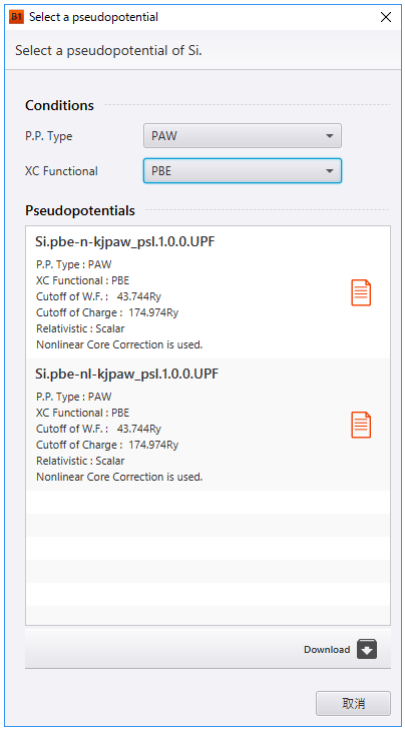
Elements window shows the kind of elements and psudopotential information. If users would like to change the psudopotential, users push the button of each element in the table of Element's Properties. Subsequently, users should select the psudopotential that users would like to use to calculate.



When users select psudopotential, by selecting conditions of P.P. Type or XC Functional, users can narrow down the psudopotential.



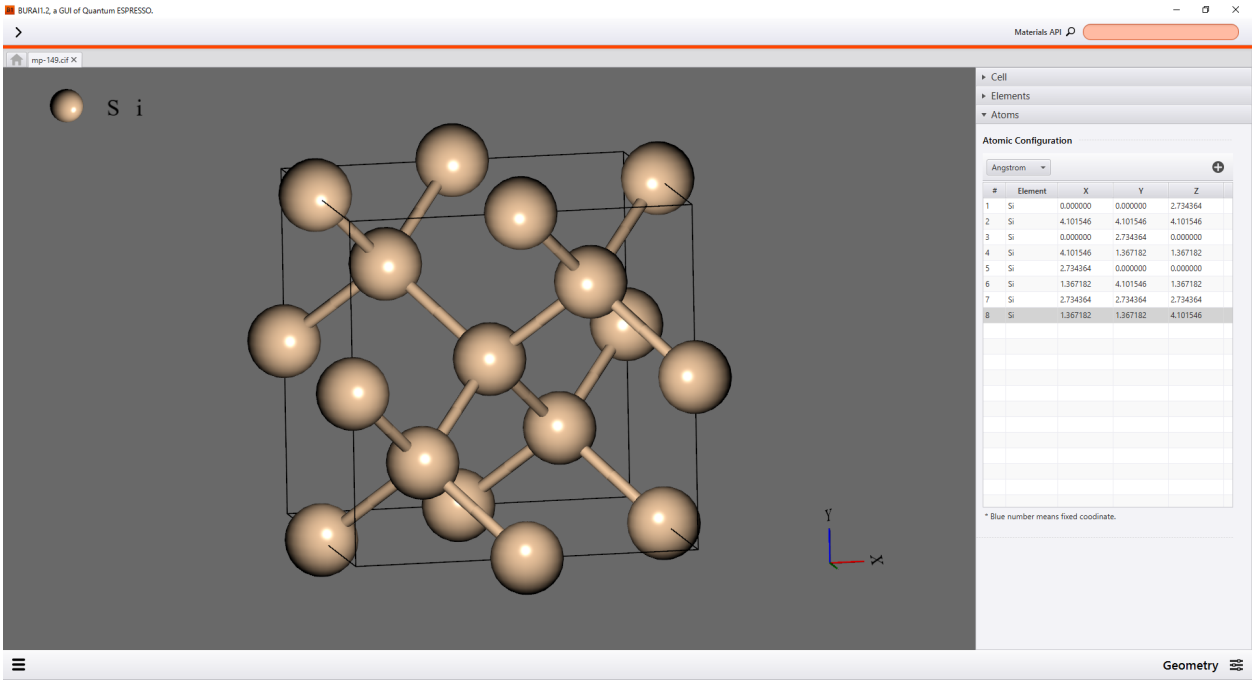




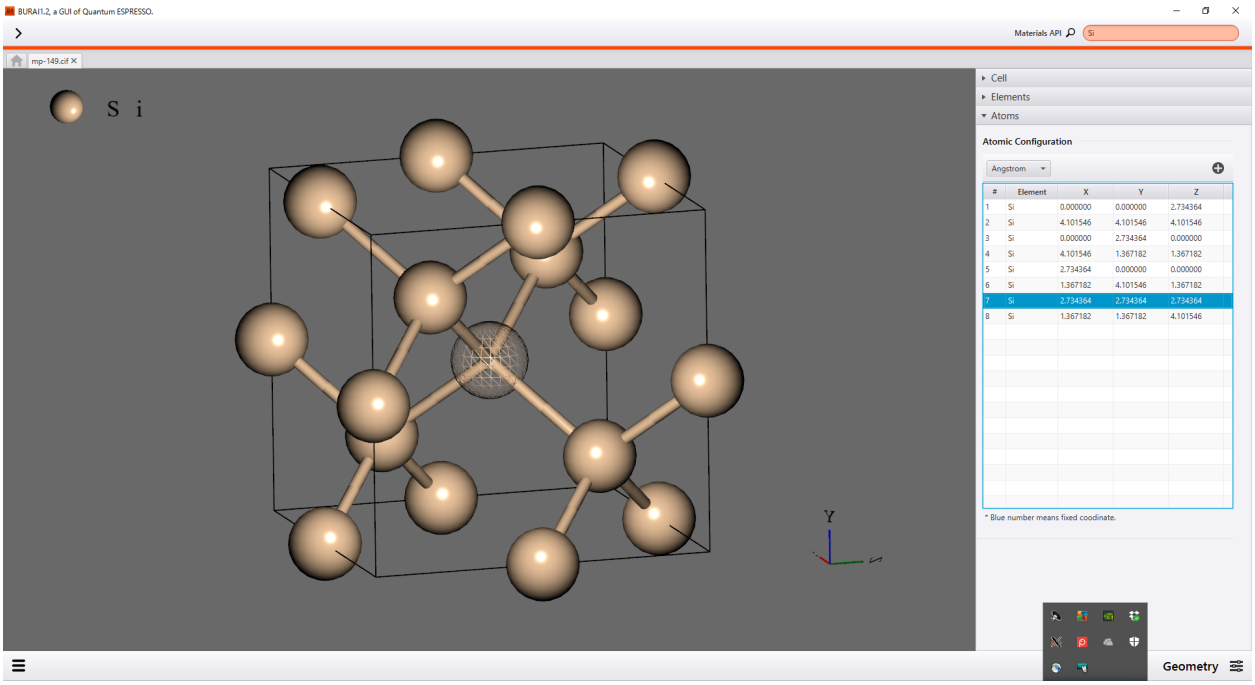
The psudopotential detail information was shown in the psudopotential conditions area.

Aroms

Atoms windows shows the coordinate and element of all atoms.

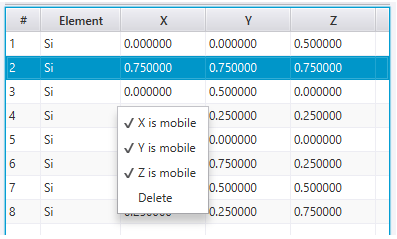


In the case that users select a column in the table of Atomic Configuration, the atom sphere that is selected, changes the sphere of grid mesh.

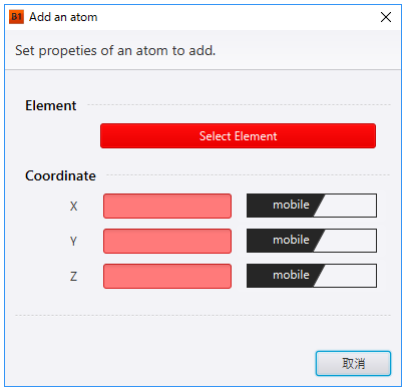


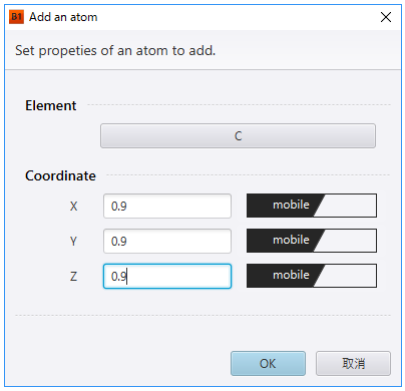
The notation of atomic coordinate can be selected in “Alat”, “Bohr”, “Angstrom”, and “Crystal”.

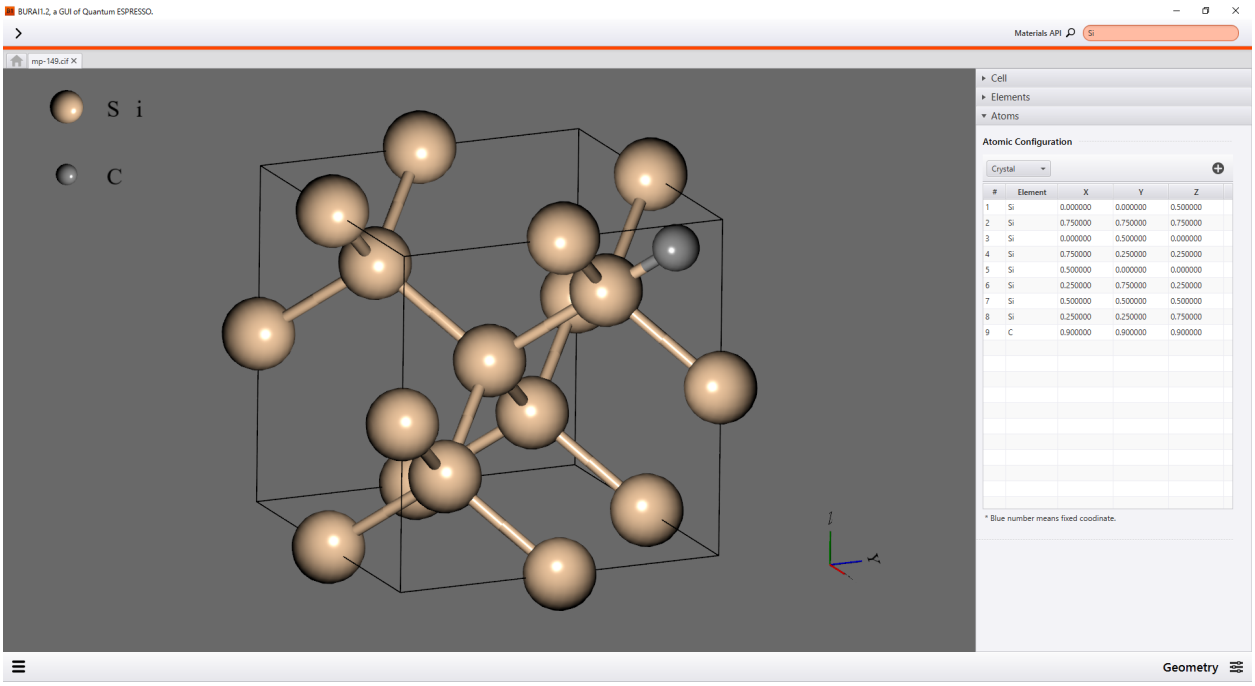
If users would like to delete or fix the atom, users should select atom in the table. Subsequently, users right-click and select delete or fix from menu.



If users would like to add atom in the calculation model, users should push + mark in the table. Subsequently, users select element that user would like to enter into the calculation model, and input its coordinate.







SCF

In case users set scf condition, users select “scf” from right menu. The scf window is consist of three windows, “Standard Setting”, “Electronic Optimization”, “Magnetization”, and “GGA+U”.

Standard Setting

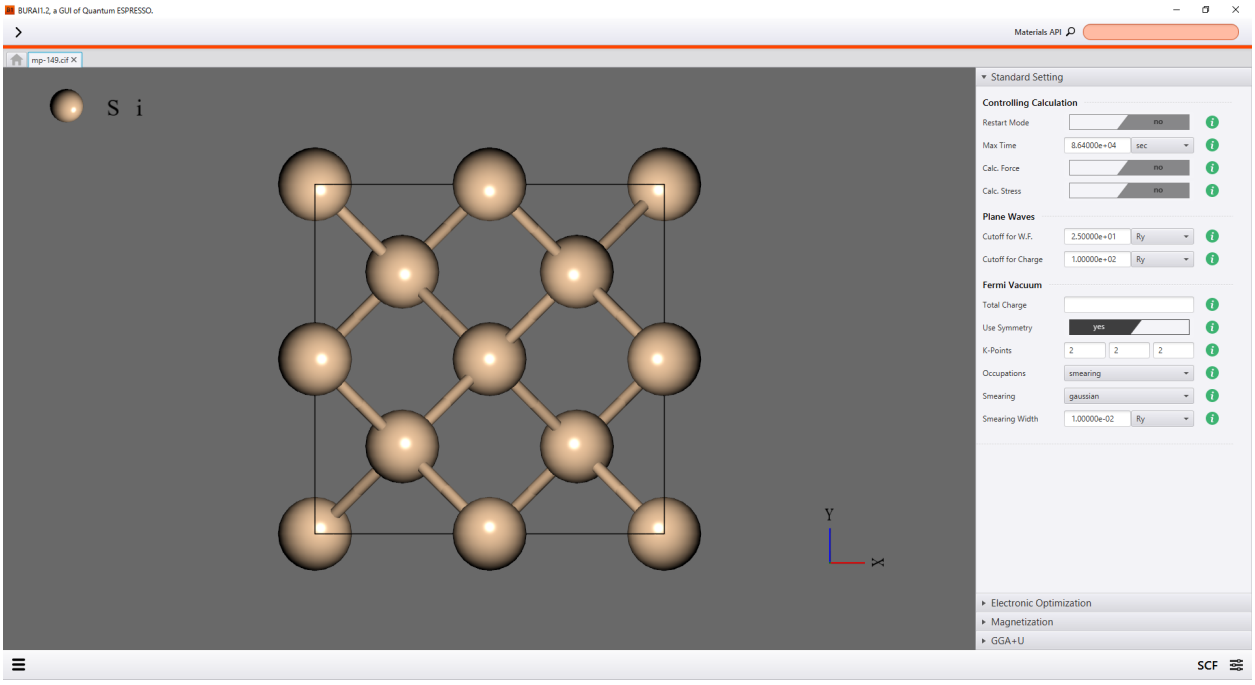


Table 5.4: Standard Setting

No.	Name	Details
1	Restart Mode	if users would like to to continue an interrupted calculation, users select yes.
2	Max Time	Job stops after users set CPU time.
3	Calc. Force	calculate forces
4	Calc. Stress	calculate stress.
5	Cutoff for W.F.	kinetic energy cutoff for wavefunctions
6	Cutoff for Charge	kinetic energy cutoff for charge density
7	Total Charge	Total charge of the system. +1 means one electron lost from calculation cell. -1 means one electron add to calculation cell.
8	Use Symmetry	Use Symmetry
9	K-Points	Monkhorst-Pack scheme
10	Occupations	
11	Smearing	select smearing method
12	Smearing Width	

Electronic Optimization

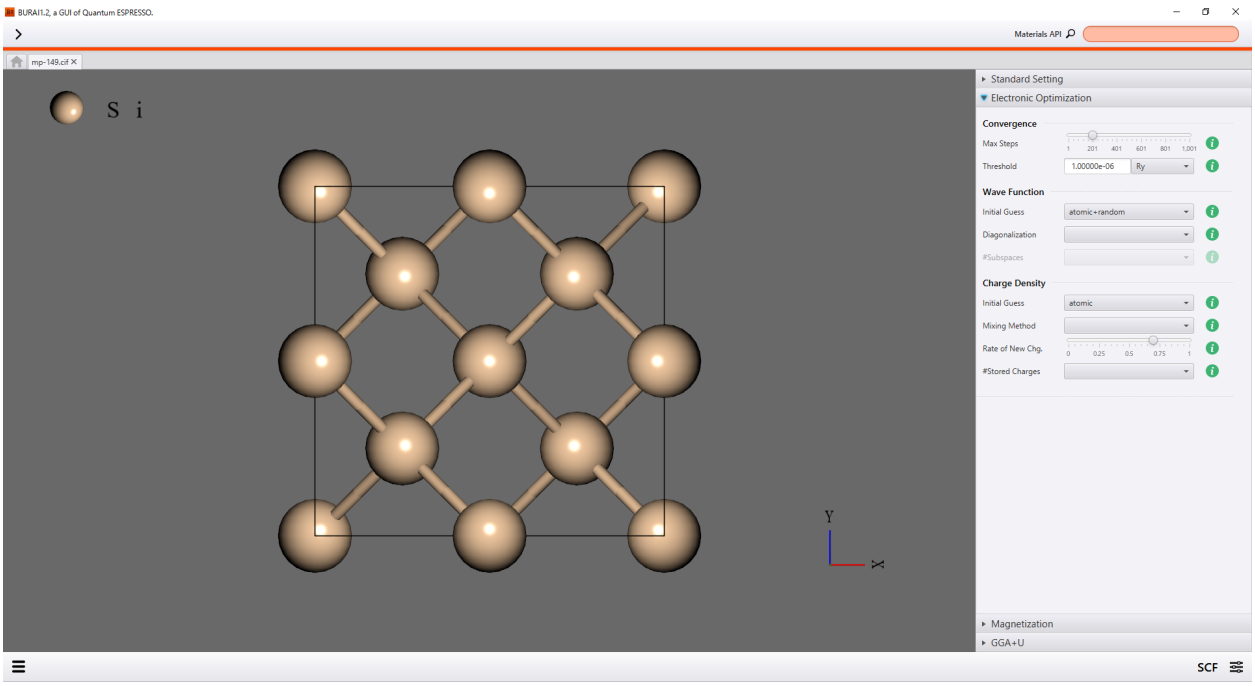
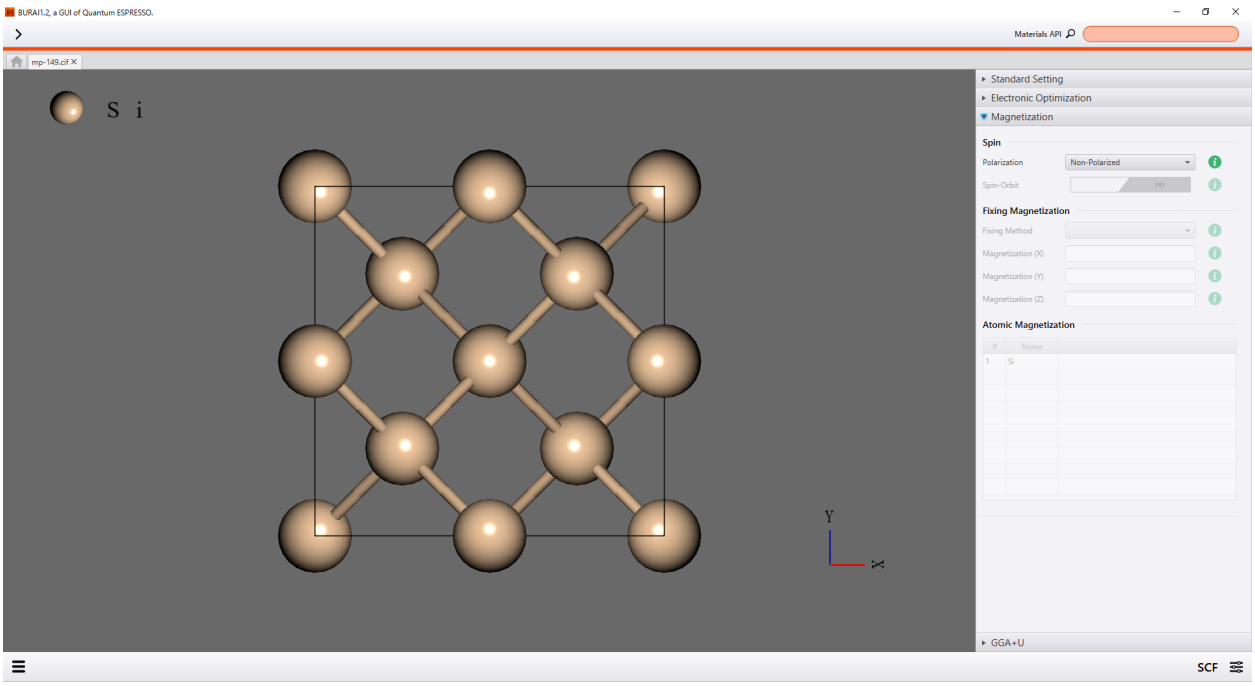


Table 5.5: Electronic Optimization

No.	group	name
1	Convergence	Max Steps
2	Convergence	Threshold
3	Wave Function	Initial Guess
4	Wave Function	Diagonalization
5	Wave Function	Initial Guess
6	Charge Density	Mixing Method
7	Charge Density	Rate of New Chg.
8	Charge Density	Stored Charges

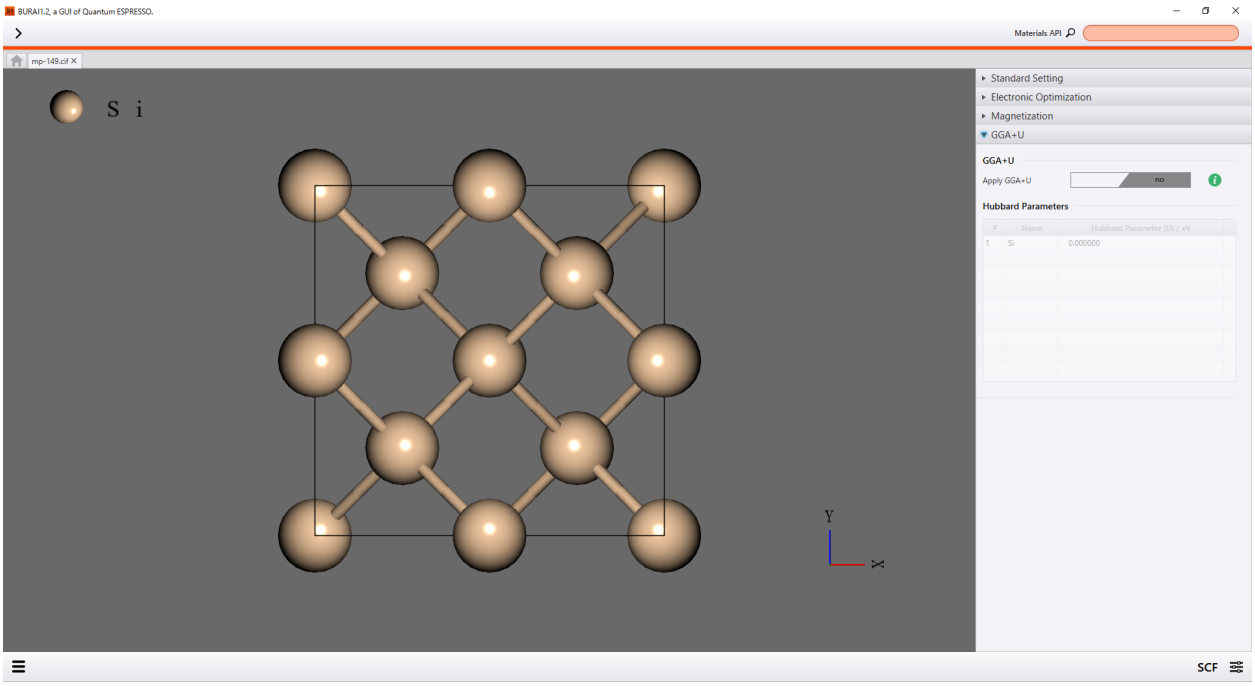
Magnetization

If users would like to consider the spin for system, user handles this window.

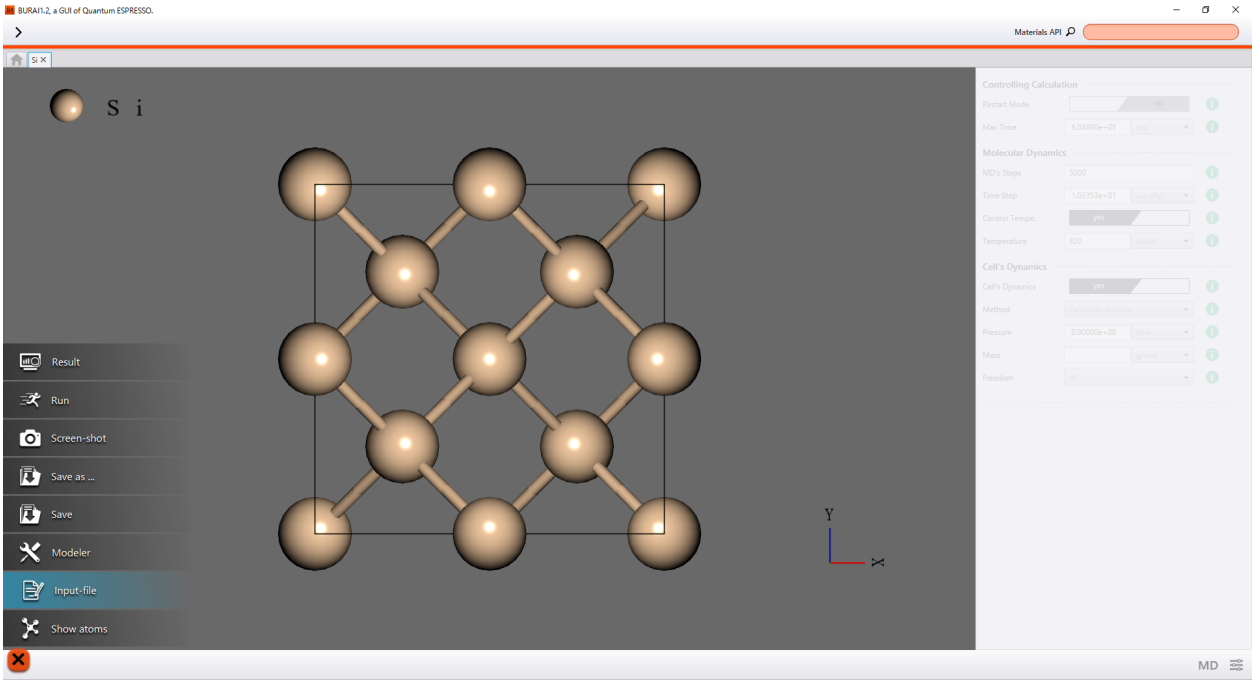


GGA+U

If users would like to consider the GGA+U for system, user handles this window.



In addition, users can conform input condition form input-file of left menue.



Optimize

In case users set the condition of optimization, users select “opt” from right menu. Also, users should set the condition after or before user set scf condition.

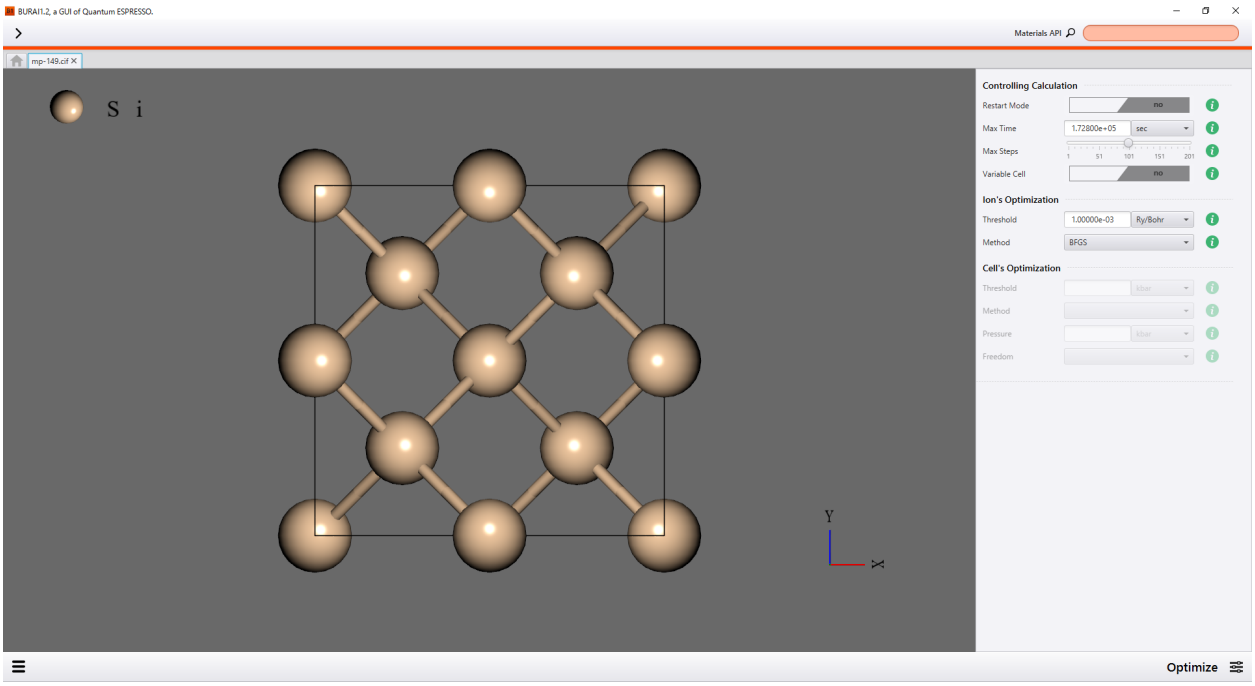
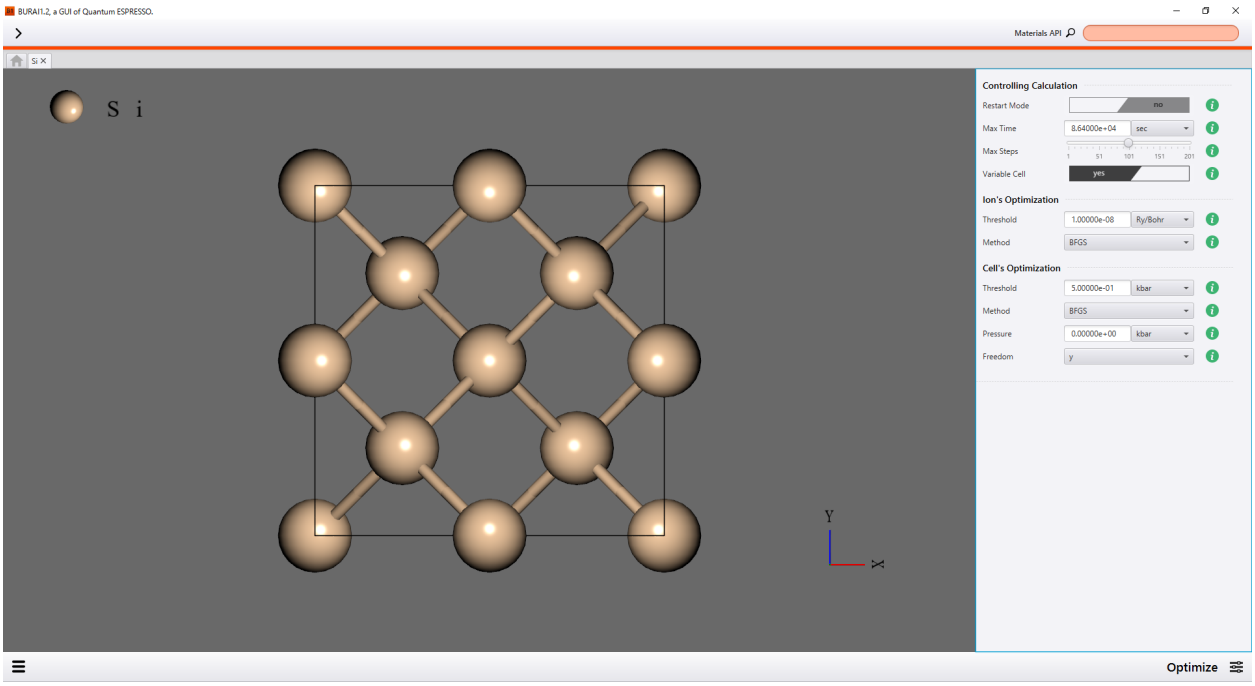


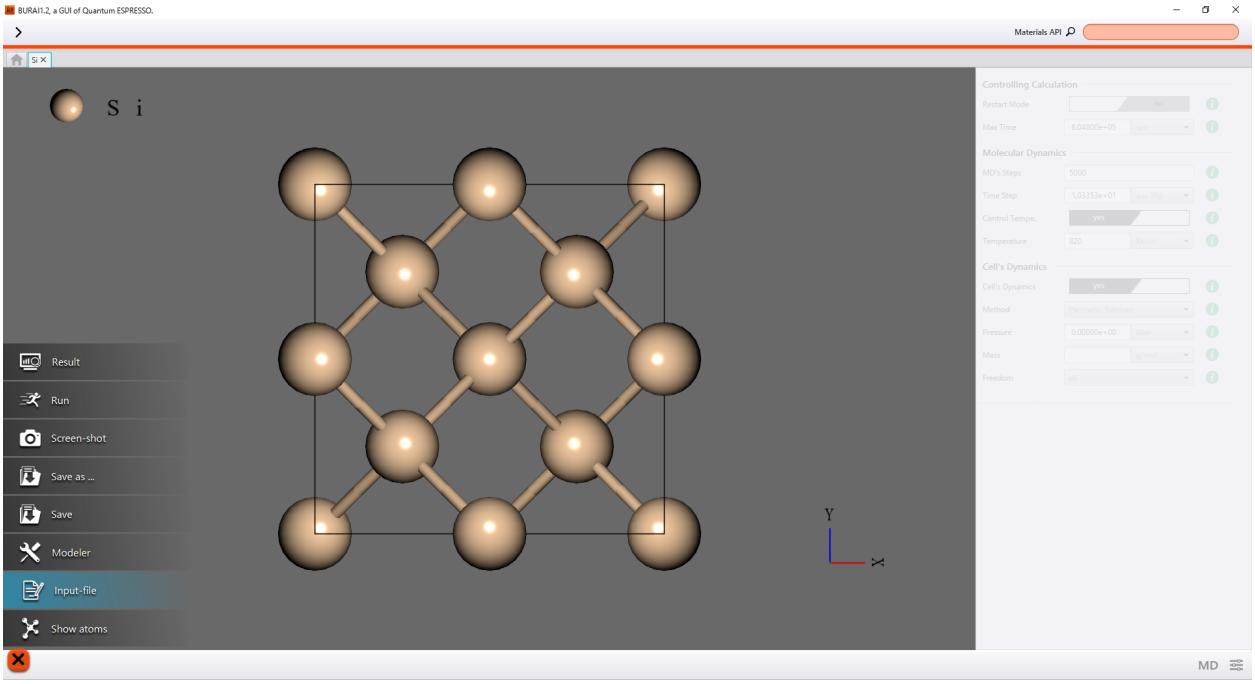
Table 5.6: Optimize

No.	Name	Details
1	Restart Mode	if users would like to to continue an interrupted calculation, users select yes.
2	Max Time	Job stops after users set CPU time.
3	Max Steps	number of structural optimization steps
4	Variable Cell	whether optimize cell size or not
5	Threshold	Convergence threshold on forces for ionic minimization
6	Method	the type of ionic dynamics
7	Pressure	Target pressure
8	Freegom	Select which of the cell parameters should be moved

if Variable Cell is “yes”, users can input Threshold, Method, Pressure, and Freedom.



In addition, users can conform input condition form input-file of left menue.



MD

In case users set the condition of first-principles molecular dynamics, users select “MD” from right menu. Also, users should set the condition after or before user set scf condition.

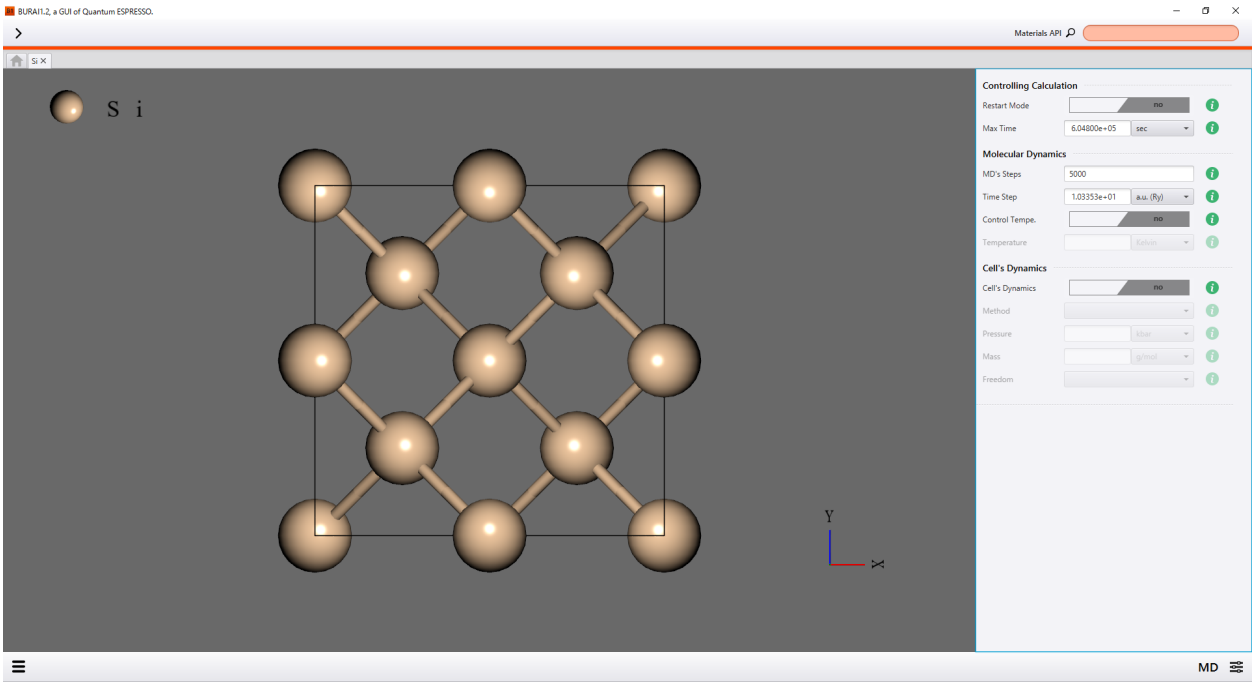
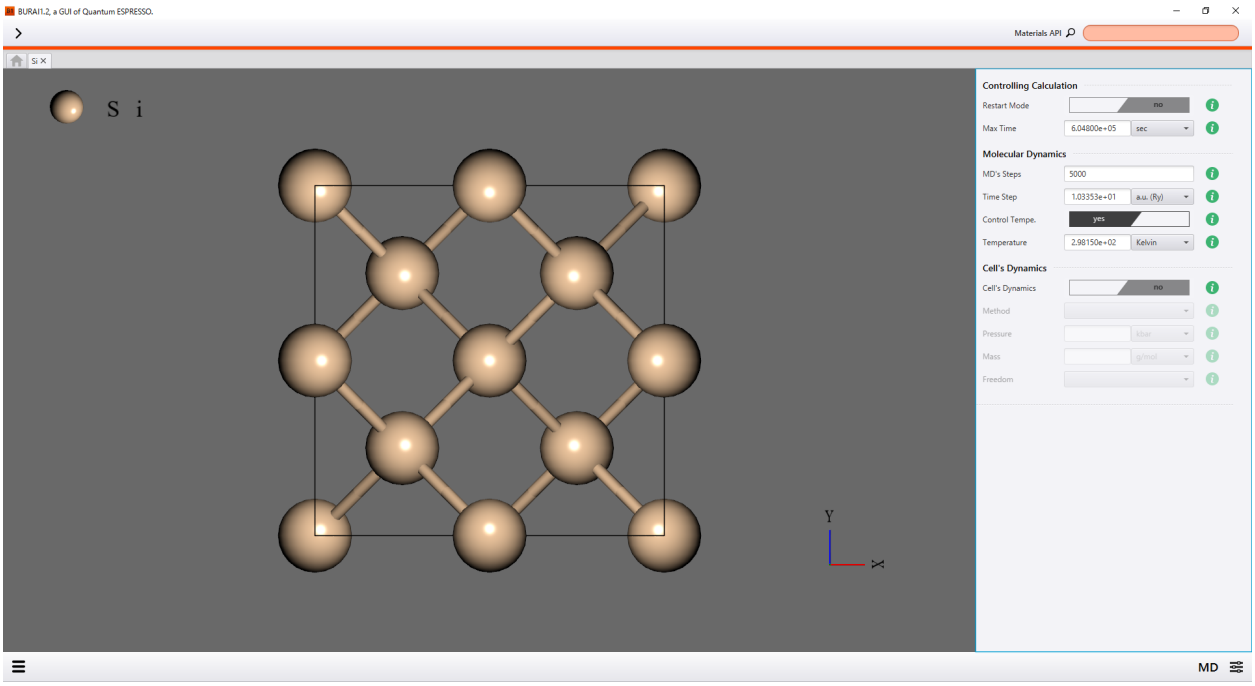


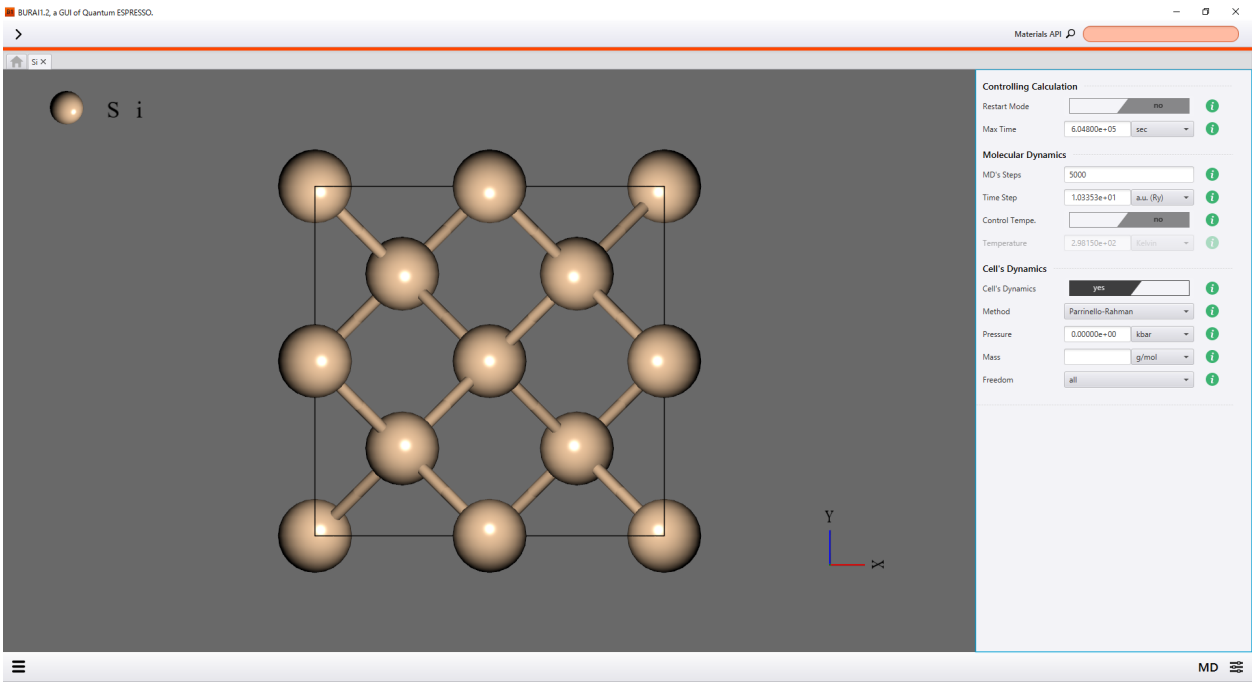
Table 5.7: MD

No.	Name	Details
1	Restart Mode	if users would like to to continue an interrupted calculation, users select yes.
2	Max Time	Job stops after users set CPU time.
3	MD's Step	number of molecular-dynamics steps
4	Ime Step	time step for molecular dynamics
5	Control Tempe.	select whether control ionic temperature or not.
6	Temperature	target temperature
7	Cell's Dynamics	select whether variable-cell or not.
8	Method	Select the extended lagrangian method
9	Pressure	Target pressure
10	Mass	Fictitious cell mass
11	Freedom	Select which of the cell parameters should be moveds

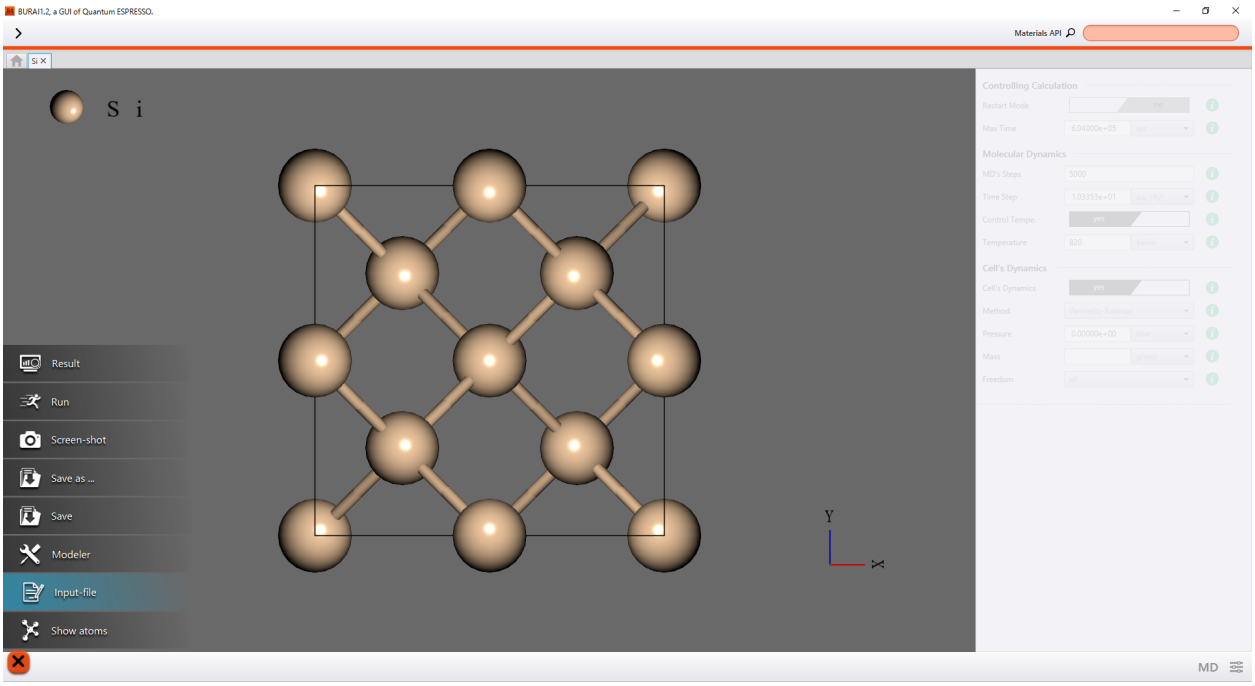
if Control Tempe. is "yes", users can input Temperature.



if Cell's Dynamics. is "yes", users can input Method, Pressure, Mass, and Freedom.



In addition, users can conform input condition form input-file of left menue.



DOS

If users calculate DOS, user should select “DOS” from right menu.

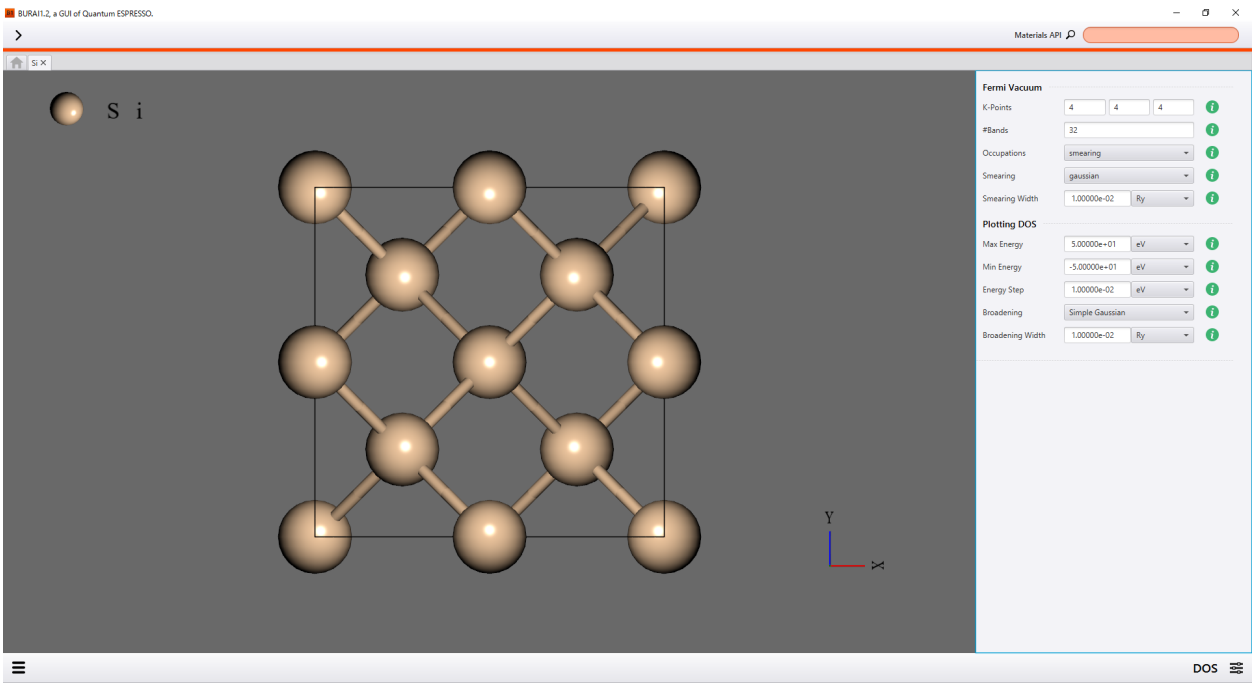
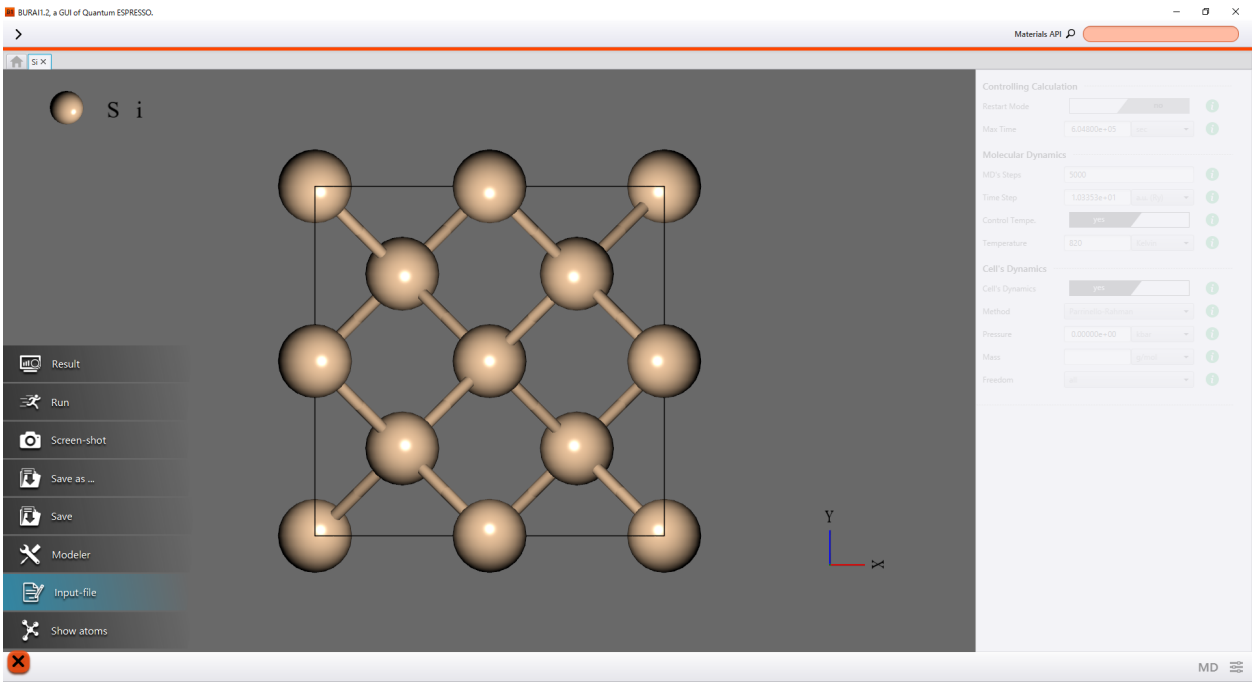


Table 5.8: DOS

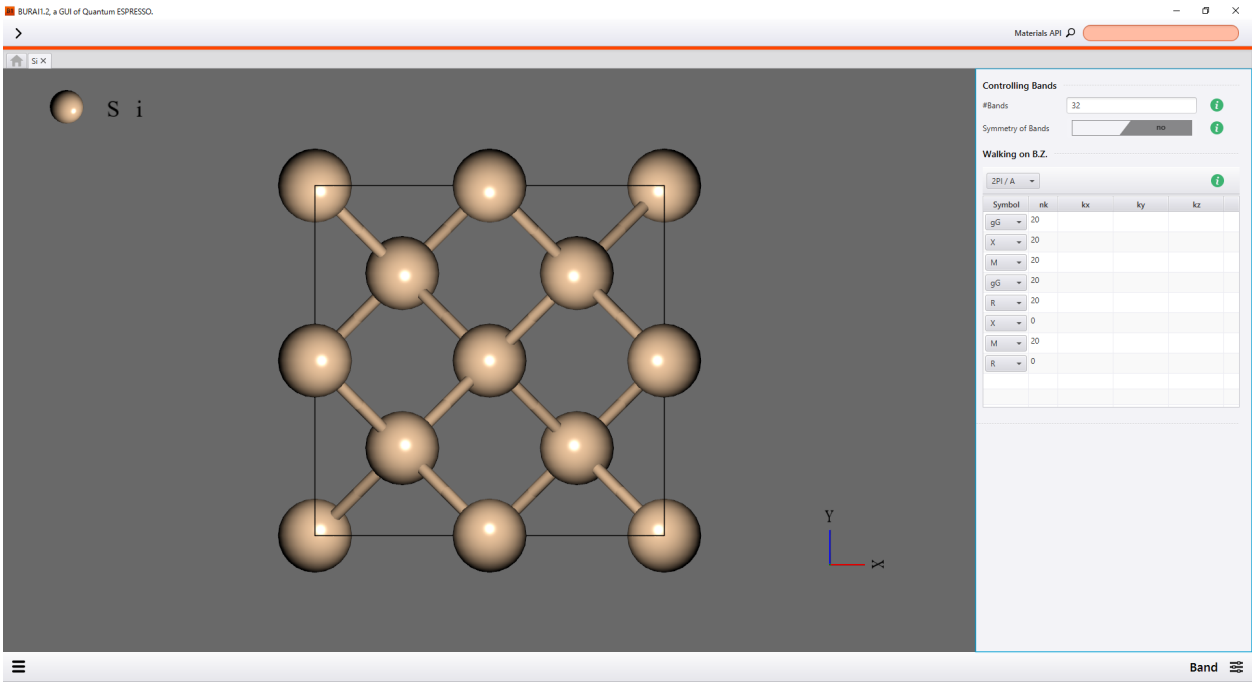
No.	Name	Details
1	K-Points	Monkhorst-Pack grids
2	#Bands	Number of electronic states to be calculated
3	Occupations	gaussian smearing for metals (recommended)
4	Smearing	Gaussian spreading (recommended)
5	Smearing Width	value of the gaussian spreading
6	Max Energy	max energy for DOS plot.
7	Mini Energy	min energy for DOS plot.
8	Energy Step	gaussian broadening
9	Broadening	Simple Gauusian (recommended)
10	Broadening Width	value of the gaussian spreading

In addition, users can conform input condition form input-file of left menue.



Band

If users calculate the band structure, user should select “Band” from right menu.



BURAI system automatically set just a recommendation k-path for the band structure plot. | In addition, users can conform input condition form input-file of left menue.