Device Studio Manual

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CONTENTS

Welcome to Device Studio. Device Studio is free for academic use. This tutorial provides detailed instructions for the **Windows version** of Device Studio.

Device Studio (DS for short) is a multi-scale materials design and simulation platform developed by Hongzhiwei Technology (Shanghai) Co., Ltd. It enables **atomic-level material modeling (million-scale)**, **high-performance scientific simulation computing**, **computation task monitoring and management**, and **data visualization** analysis in an integrated workflow. This integration of material design and scientific simulation significantly enhances research efficiency and helps researchers address important challenges in multi-scale materials design and simulation.

Device Studio integrates various scientific computing software to meet users'simulation needs across different fields. It includes DS-PAW for first-principles plane-wave calculations, BDF for quantum chemistry calculations.

Based on its powerful material design modeling and high-performance scientific simulation capabilities, Device Studio can be widely applied in quantum devices, artificial biology, advanced batteries, intelligent lighting, memory devices, and other industries. It assists in material research and development in electronic materials, alloys, biotechnology, and other fields, providing professional technical support for optoelectronics and integrated circuits industries.

CHAPTER

ONE

INTRODUCTION TO DEVICE STUDIO

Device Studio as a multi-scale materials design and simulation platform consists of four main modules: **Atomic-level Material Modeling (Million-scale)**, **High-performance Scientific Simulation Computing**, **Computation Task Monitoring and Management**, and **Data Visualization**.

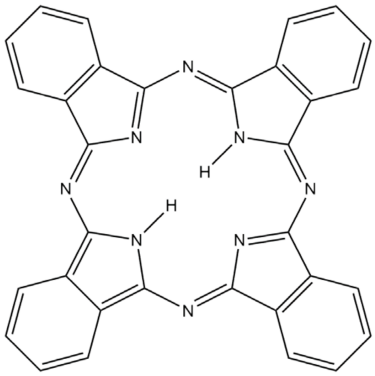
1.1 Atomic-level Material Modeling

1.1.1 Import and Export of Various Material Structure Files

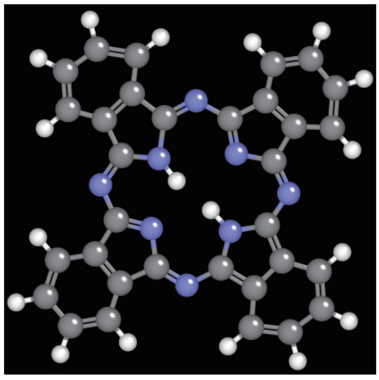
Device Studio platform supports importing structure files in formats such as `.hzw`, `.xyz`, `.cif`, `.xsd`, `scf.input`, `.py`, `POSCAR`, `CONTCAR`, `.mol`, and `.pdb`. It also supports exporting structure files in formats such as `.hzw`, `.xyz`, `.cif`, and `.png`.

1.1.2 Visualization of Molecules, Crystals, Devices, and Special Structures

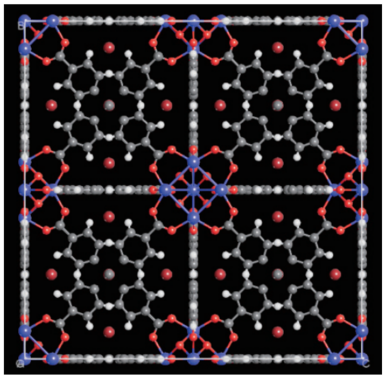
Once a material structure file is imported into Device Studio, users can view the structure's 3D visualization in real-time in the main window. Users can zoom in/out, rotate, or pan the 3D view; view the structure from any plane (ZY, XY, XZ, YZ, YX, ZX); and choose between orthographic or perspective view modes for the 3D visualization.



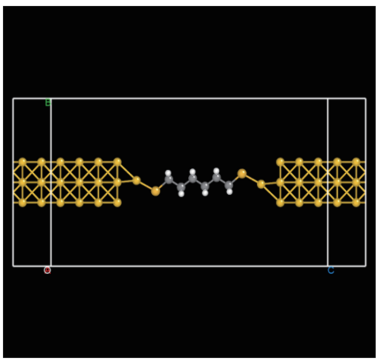
2D molecular structure: Phthalocyanine



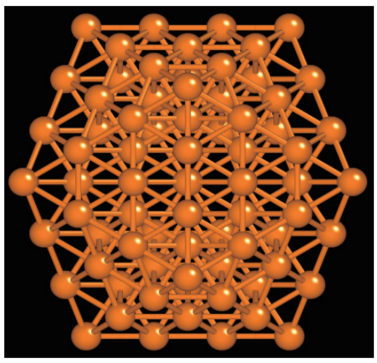
3D molecular structure: Phthalocyanine



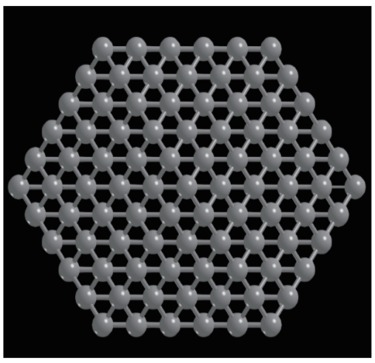
Crystal structure: UiO-67



Device structure: Au-Alkanethiol-Au



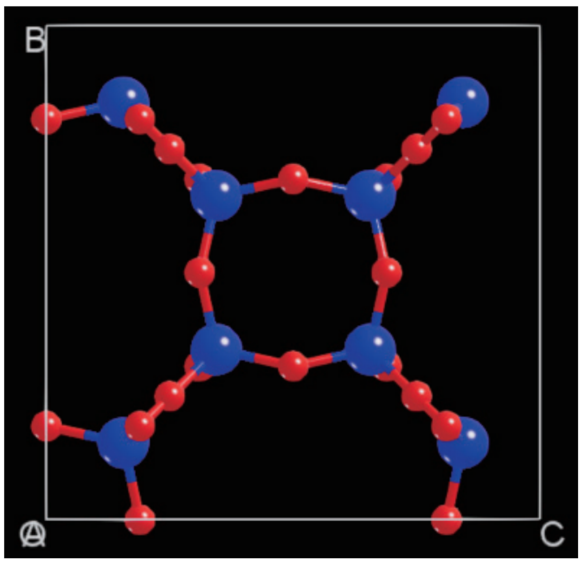
Cluster structure: Icosahedron



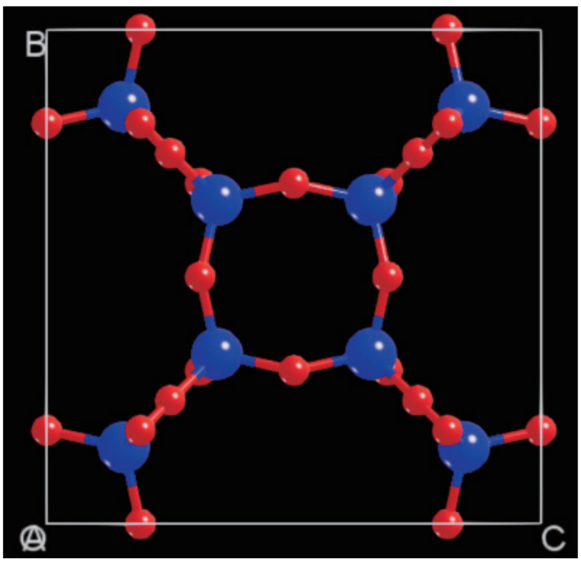
Cluster structure: Cubooctahedron

1.1.3 Support for Atomic Structure Refinement

- The Device Studio platform supports adding, deleting, and modifying atomic structures.
- Users can choose between ball-and-stick or polyhedral display modes for atomic structures; users can adjust the transparency of polyhedra.
- Users can modify the color, radius, and lighting of atoms of the same element, multiple atoms, or individual atoms in the structure.
- Users can select and apply Device Studio initial templates, and can customize colors, radii, lighting, and background parameters based on research needs or personal preferences to create and apply user-specific templates.

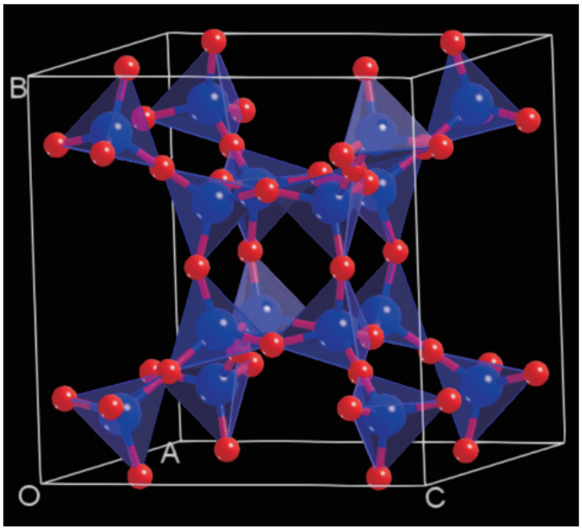


(a) Hide equivalent atoms

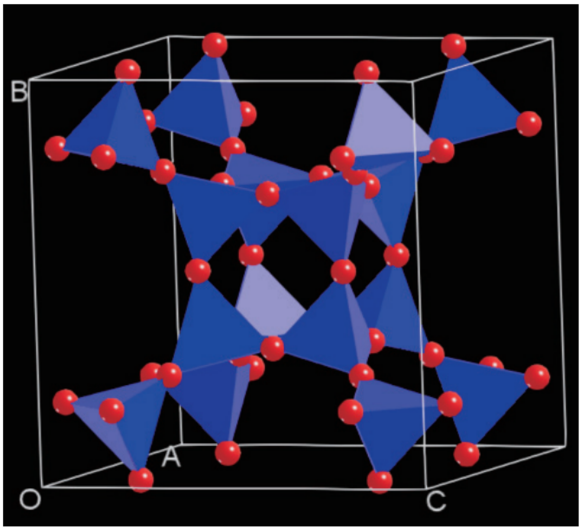


(b) Show equivalent atoms

3D view of the $Si_{16}O_{32}$ crystal structure in ball-and-stick mode

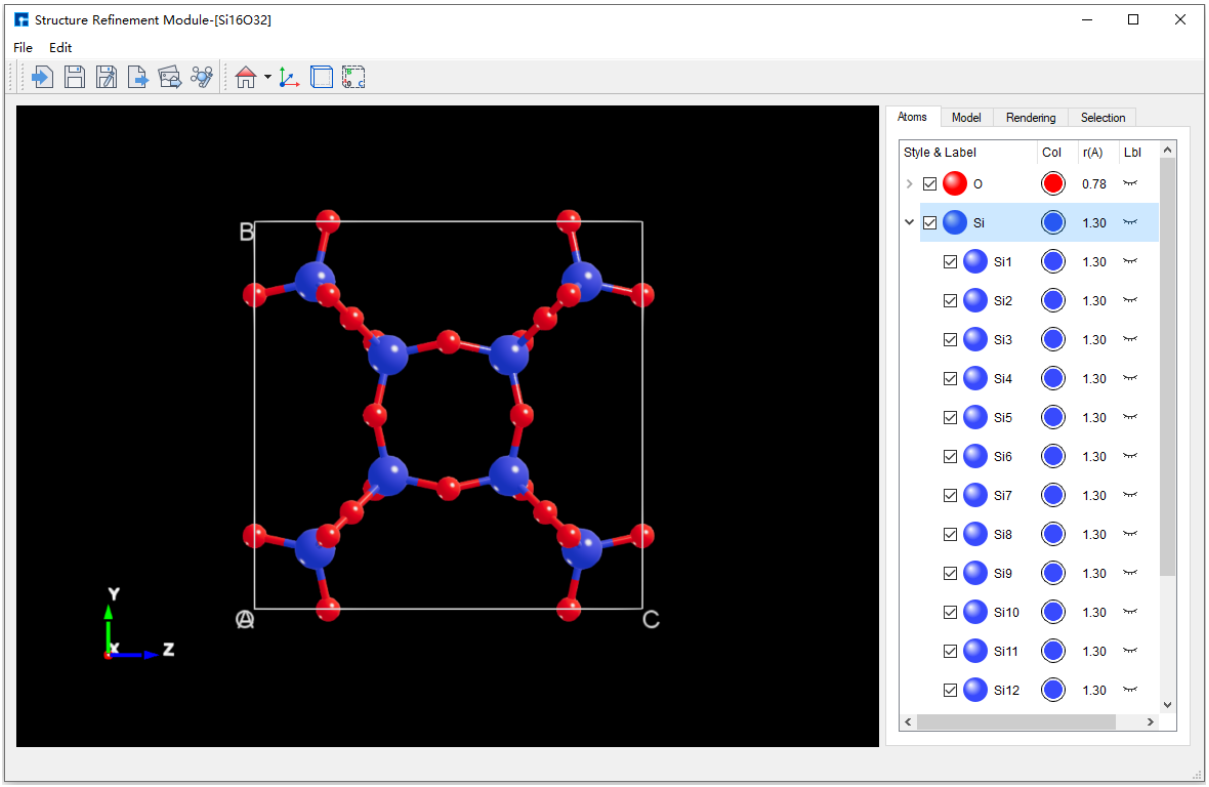


(a) transparent

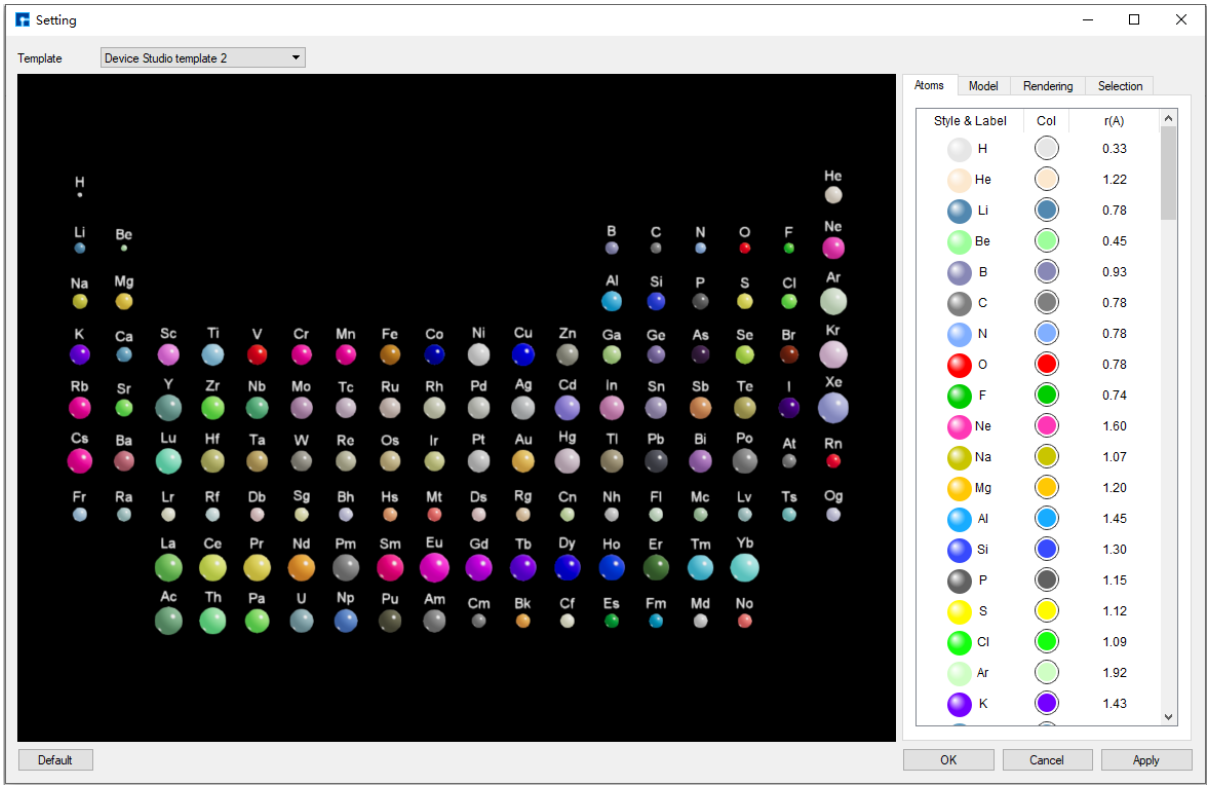


(b) opaque

3D view of the $Si_{16}O_{32}$ crystal structure in polyhedral mode



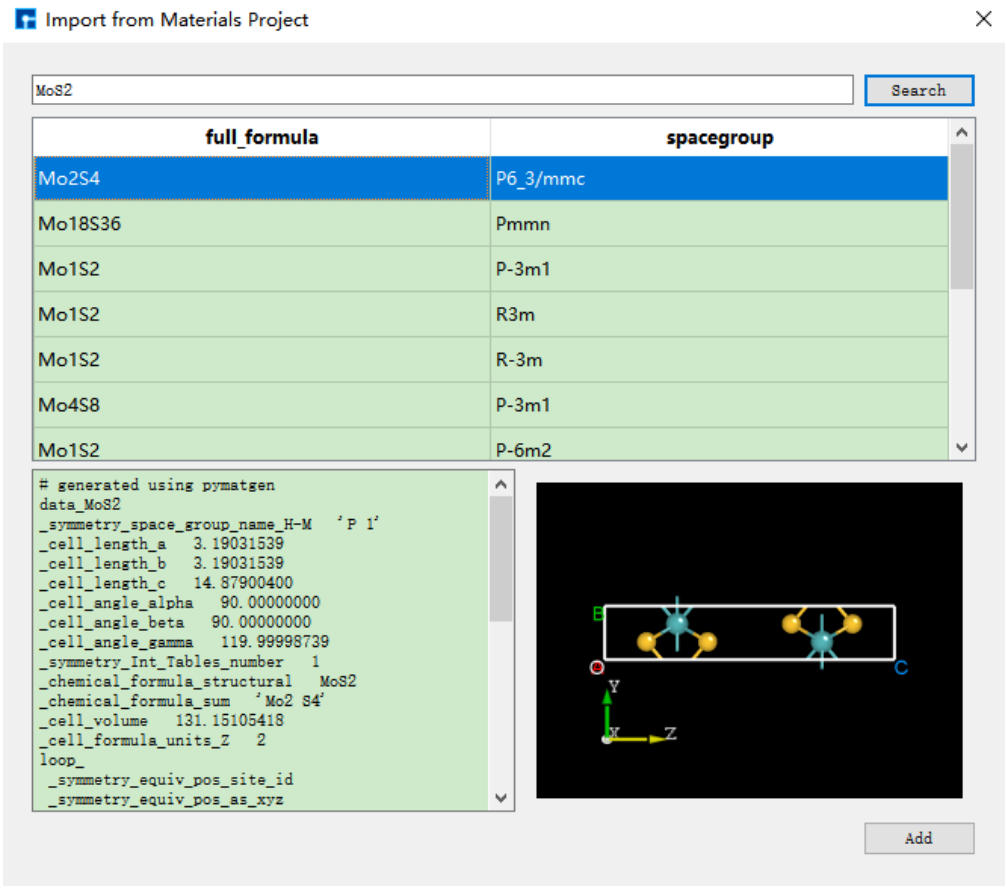
Device Studio Atomic Structure Refinement Interface



Device Studio Initial Template

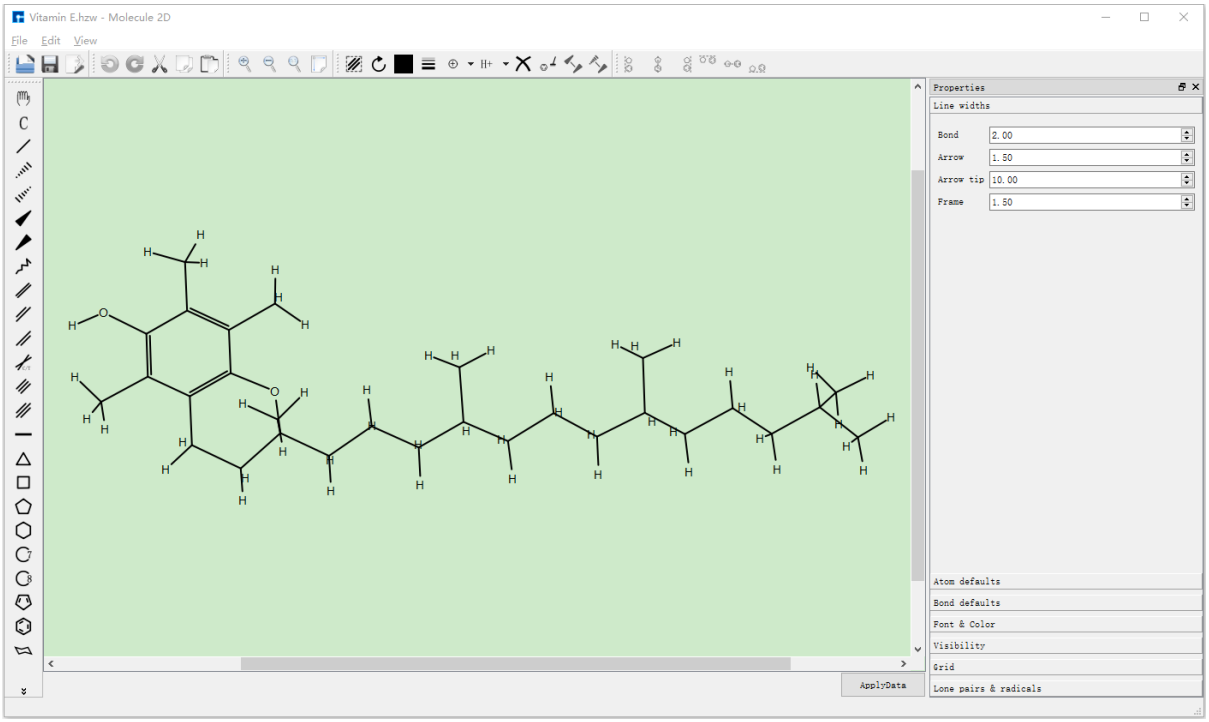
1.1.4 Rich Material Database

- Local Database: Currently contains over 500 commonly used or popular materials, with continuous updates and expansion planned.
- The Device Studio platform supports the online Materials Project database. Users can connect to this database through the platform to search and import structures, and view information such as space group symmetry and atomic coordinates.

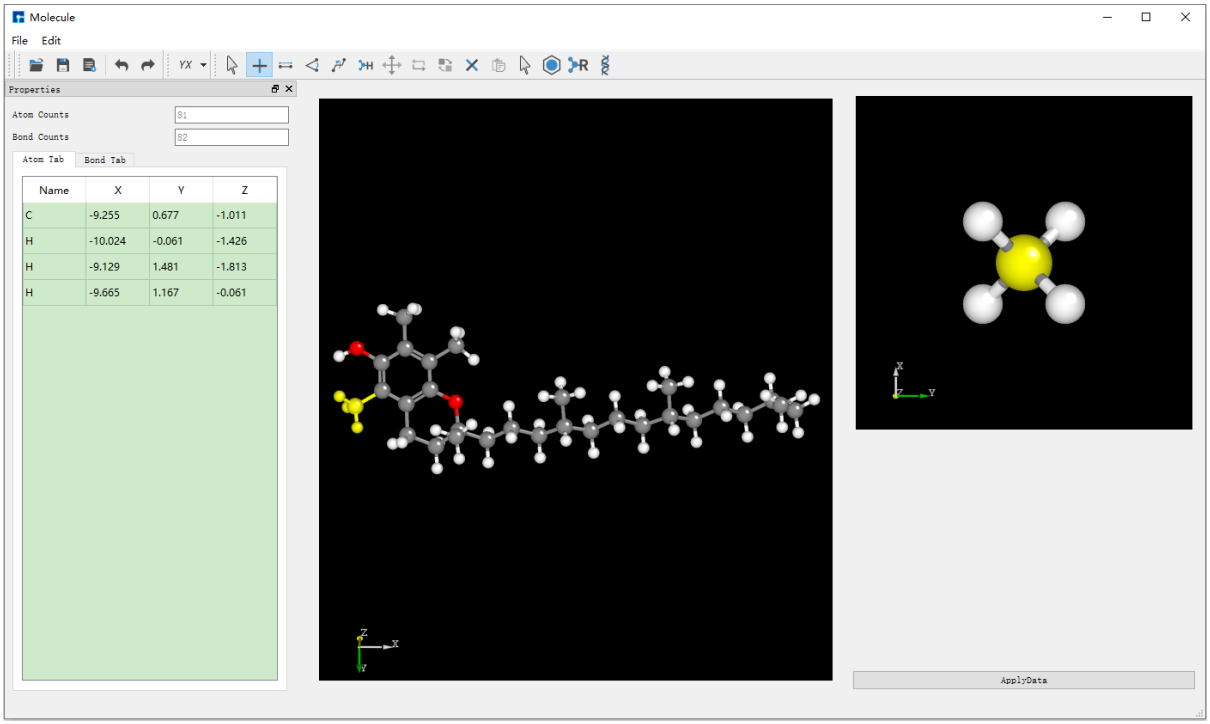


1.1.5 Creation of Molecules, Crystals, Devices, and Special Structures

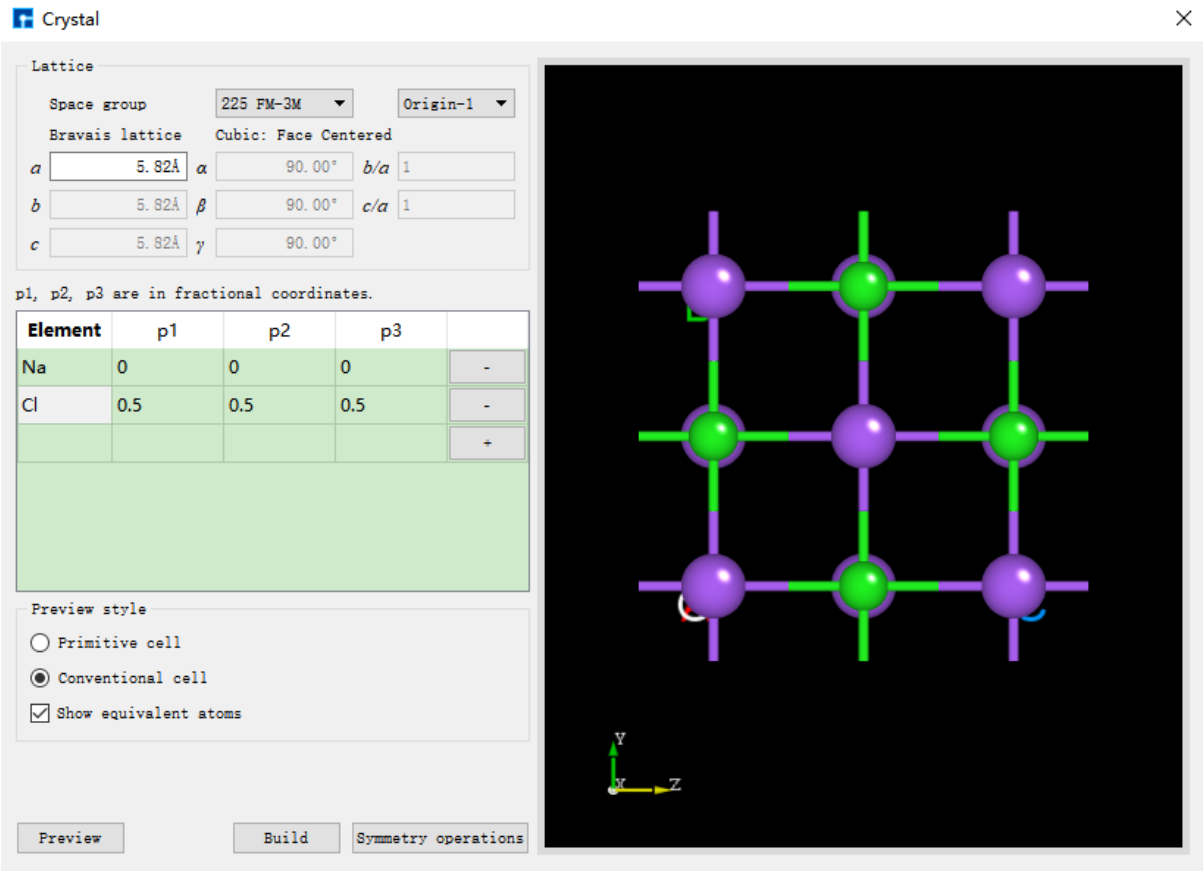
- The Device Studio platform has powerful modeling capabilities, supporting the creation of various molecules, crystals, devices, and special structures.
- It can automatically cleave crystal planes and match device structures based on matching precision; it can match and construct crystal and multilayer film structures.
- It can generate special structures such as Nanoribbons, Nanotubes, clusters, grain boundaries, and random doping.



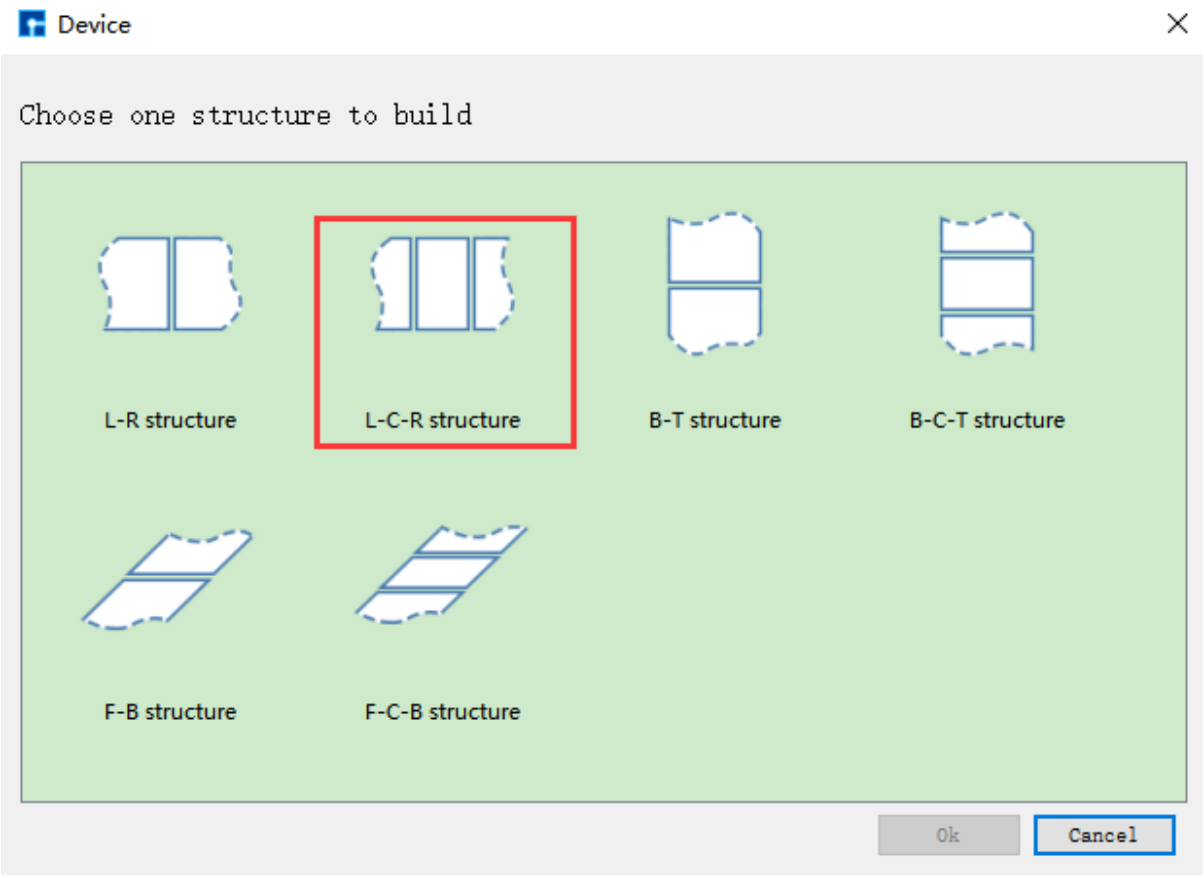
Device Studio Platform Building 2D Molecular Structure

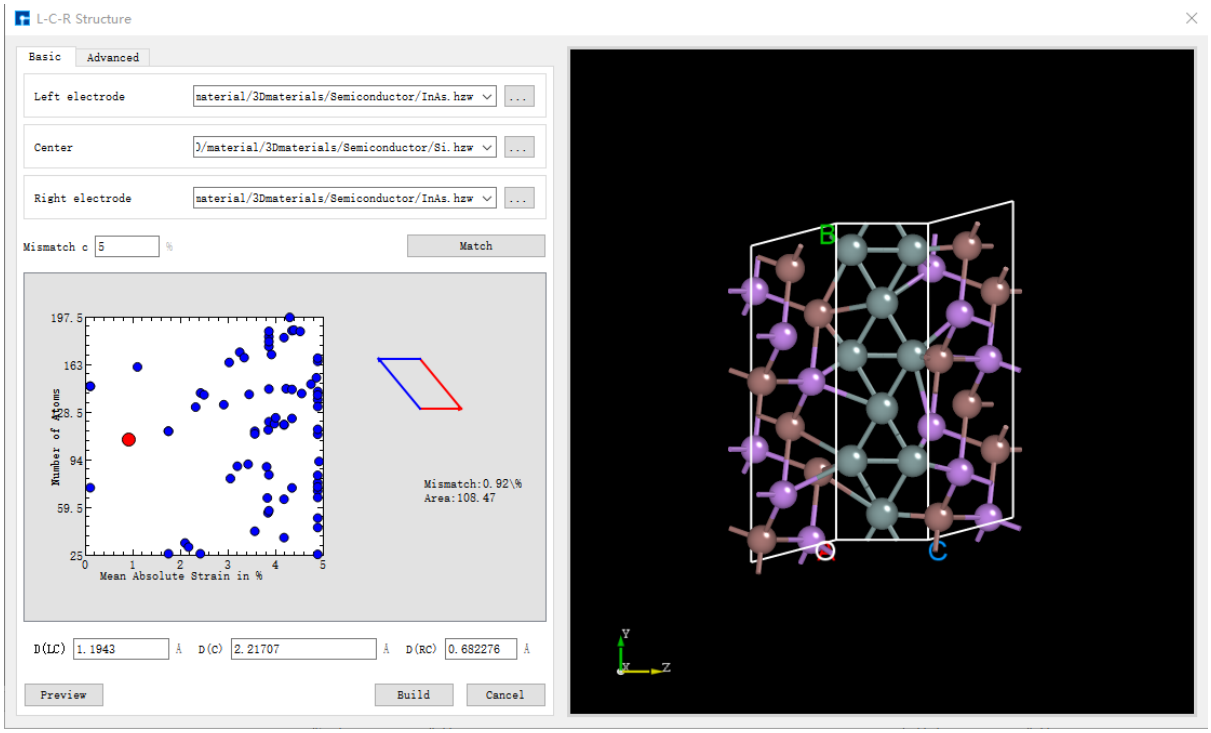


Device Studio Platform Building 3D Molecular Structure

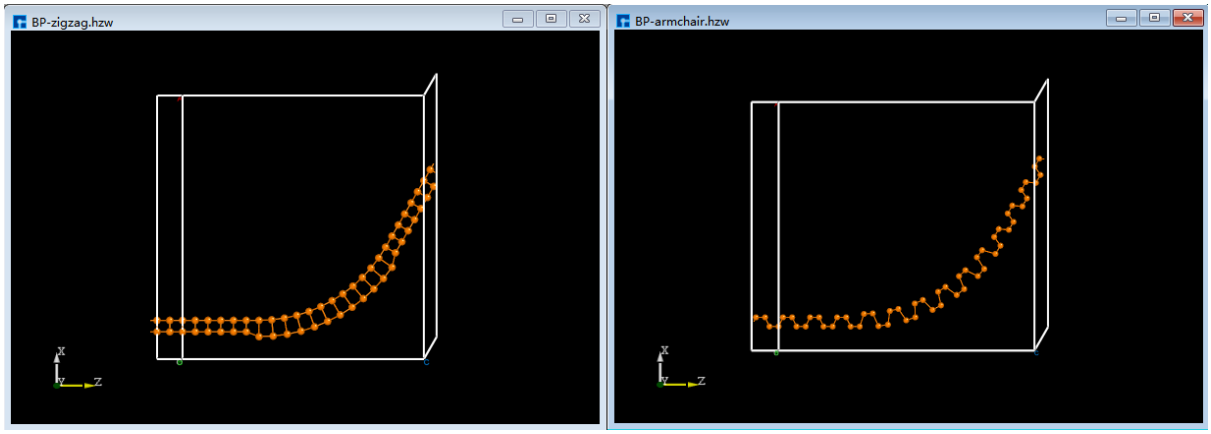


Device Studio Platform Building Crystal Structure





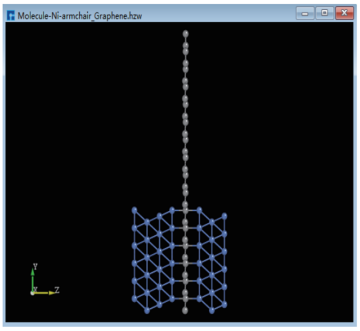
Device Studio Platform Building L-C-R Device Structure



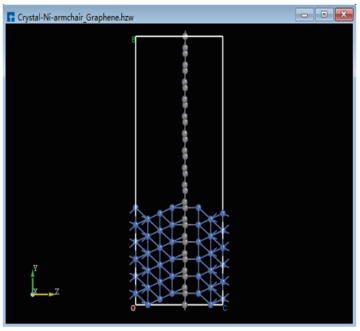
Device Studio Platform Building Flexible Device Structure

1.1.6 Interconversion of Molecular, Crystal, and Device Structures

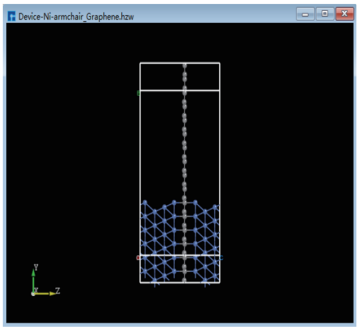
The Device Studio platform supports interconversion between molecular, crystal, and device structures.



molecular structure: Ni-armchair_graphene



crystal structure: Ni-armchair_graphene



device structure: Ni-armchair_graphene

1.2 High-performance Scientific Simulation Computing

- **Multiple Computing Software Ready to Use**.

Device Studio integrates various scientific computing software that are ready to use, meeting users'simulation needs across different fields. It includes DS-PAW for first-principles plane-wave calculations, BDF for quantum chemistry calculations.

1.3 Computation Task Monitoring and Management

- **Connection to Supercomputing Servers and Local Computers**.

Using the Device Studio platform, users can automatically connect to supercomputing servers and local computers, switching between server and local computer usage with one click based on computational needs.

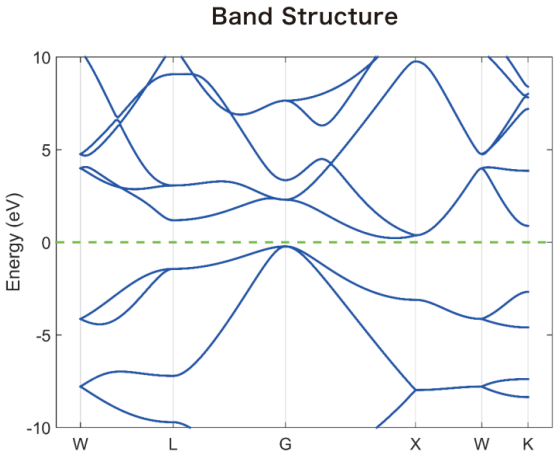
- **Computation Task Monitoring and Management**.

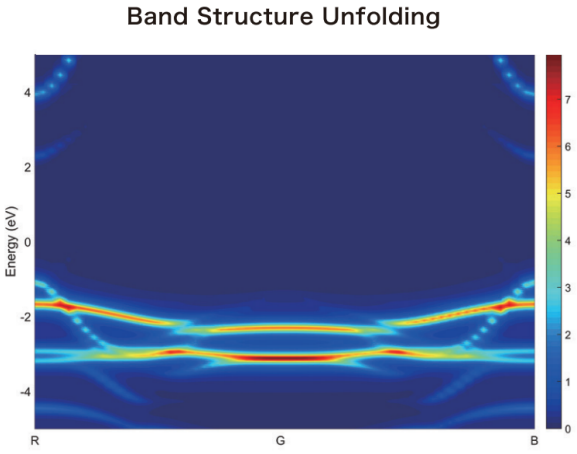
Through the Device Studio platform's graphical interface, users can submit various scientific simulation software computation tasks with mouse clicks, without needing to master Linux systems. Users can monitor computation task status in real-time (queued, computing, completed), and results are automatically retrieved locally upon completion, significantly reducing the learning curve and operational difficulty for beginners.

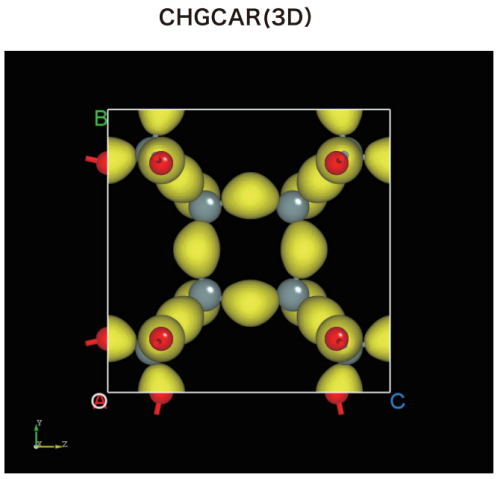
1.4 Data Visualization

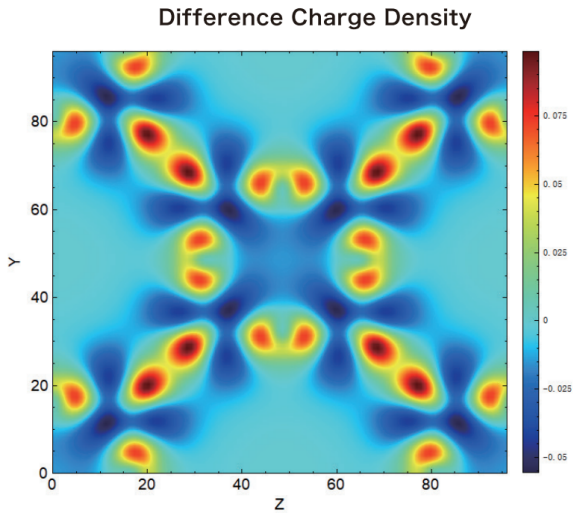
- **Data Visualization of Computation Results**.

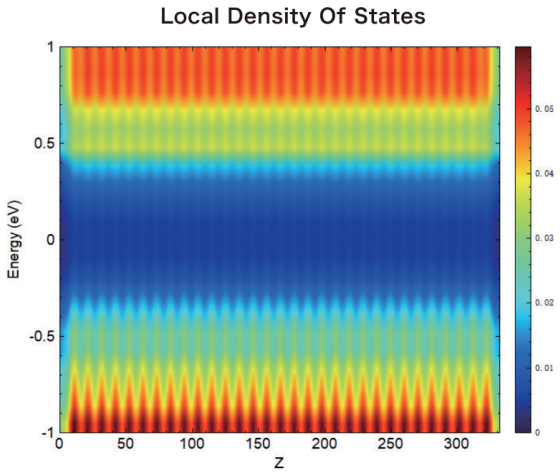
The Device Studio platform can automatically analyze scientific simulation computation results and generate data visualization graphics. Users can switch between 3D, 2D, or 1D data visualization graphics with one click, and can export visualizations in formats such as `.png`, `.jpg`, `.bmp`, `.pdf`, `.tif`, and `.eps`. For dynamic visualizations such as motion trajectories, users can export the visualization graphics as `.gif` animations.

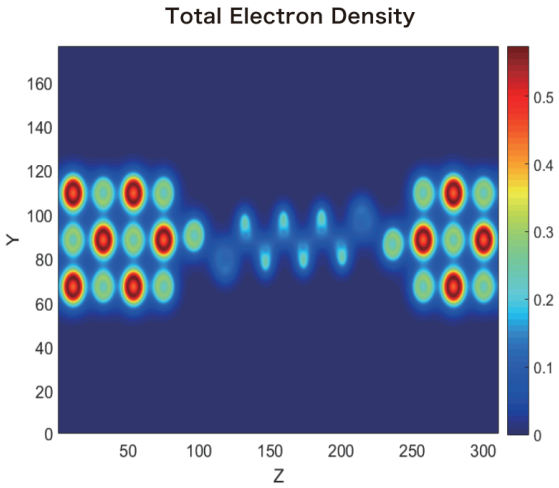


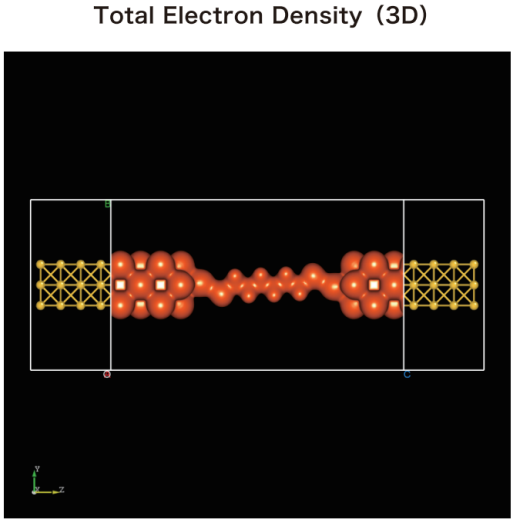


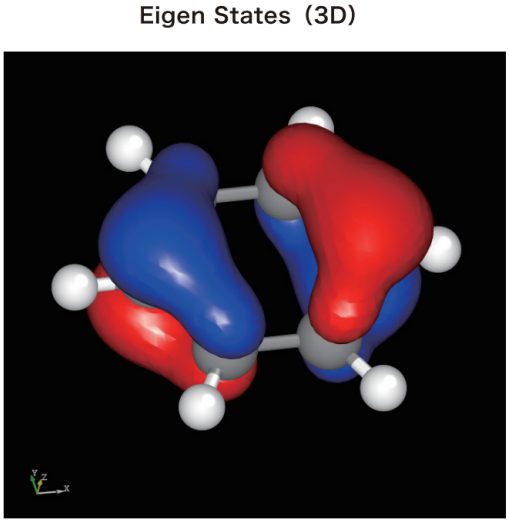












- **Visualization Graphics Editing**.

For visualization graphics, the Device Studio platform provides editing functions such as zoom in/out, rotation, Colorbar display options, Colormap selection, modification of axis ranges, and customization of title and axis font types, sizes, and bold settings.

CHAPTER

TWO

QUICK START GUIDE

This Quick Start Guide uses the **Self-consistent and Band Structure Calculation of Si Crystal Structure** in the first-principles quantum transport calculation software Nanodcal as an example. It is divided into several steps, including logging in and starting Device Studio, creating a Device Studio project, importing the Si crystal structure, generating self-consistent and band structure calculation input files, submitting self-consistent and band structure calculation tasks, data visualization of the Si crystal structure band structure, and exporting band structure visualization results.

2.1 Login and Start Device Studio

Double-click the *DeviceStudio.exe* file in the **bin** directory of the extracted Device Studio installation package or the **Device Studio shortcut** on your desktop. The login and startup process is shown in fig. 2.1.

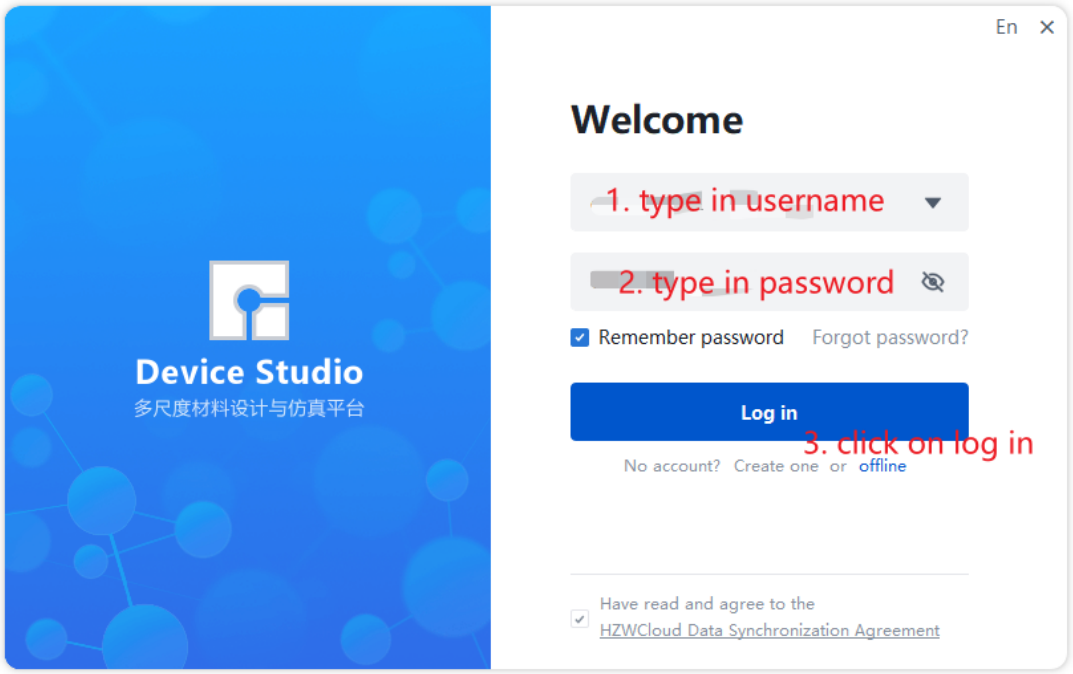


fig. 2.1: Login and Start Device Studio

2.2 Create a Device Studio Project

After logging in and starting Device Studio, you can create a Device Studio project. The project creation process is shown in fig. 2.2, fig. 2.3, and fig. 2.4.

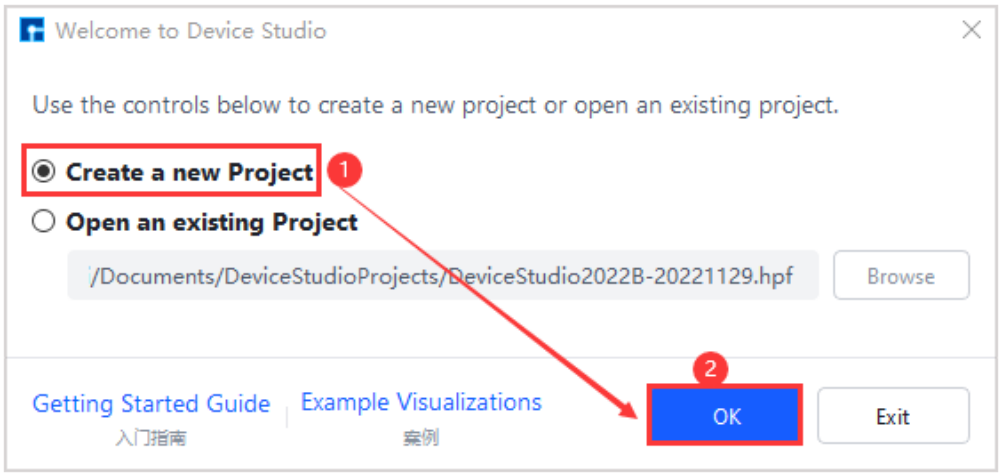


fig. 2.2: Create Project

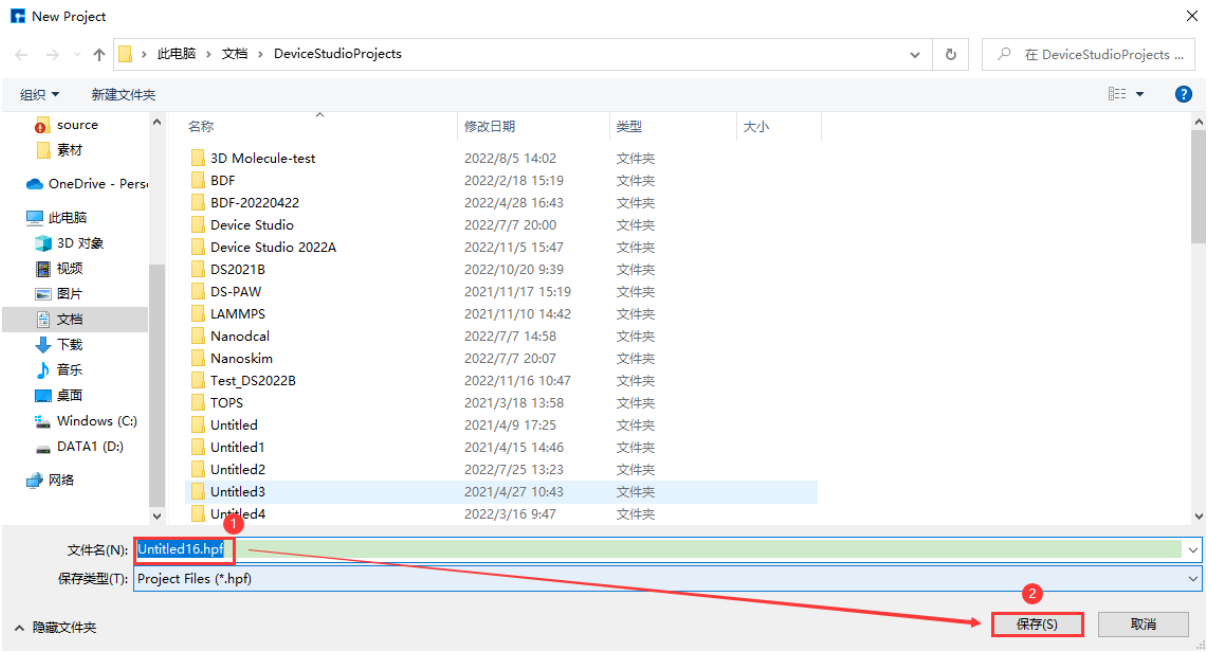


fig. 2.3: Name the Project

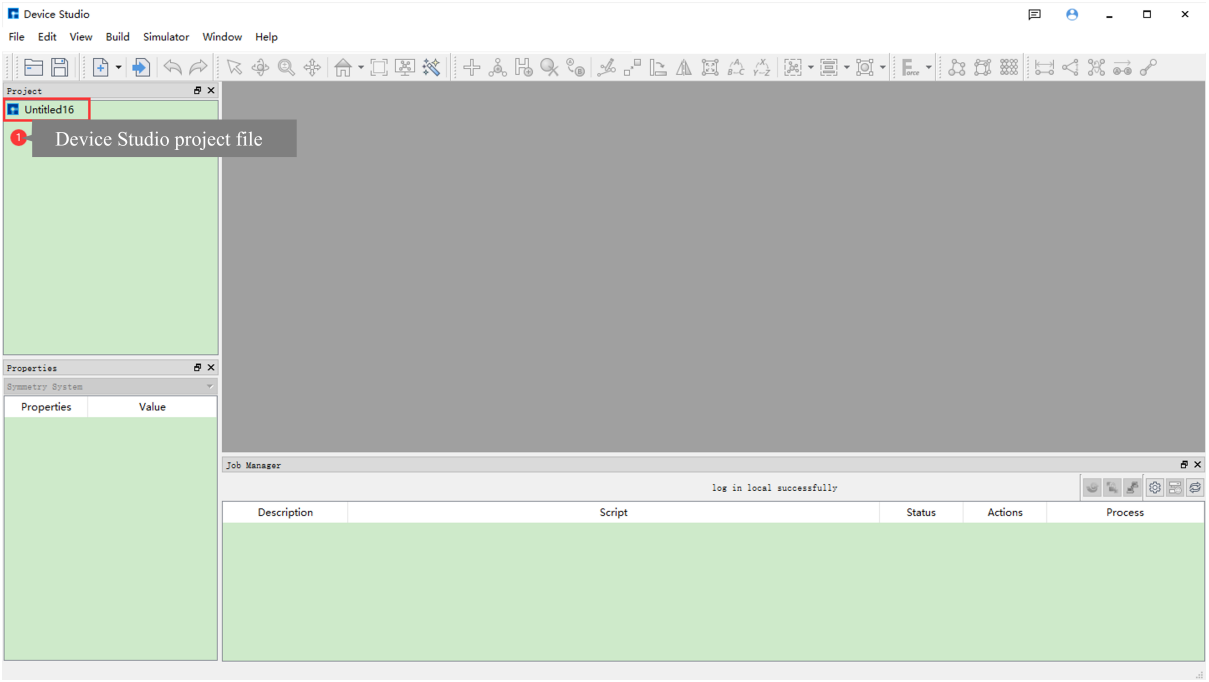


fig. 2.4: Device Studio Interface After Project Creation

2.3 Import Si Crystal Structure

The process of importing the Si crystal structure is shown in fig. 2.5, fig. 2.6, and fig. 2.7.

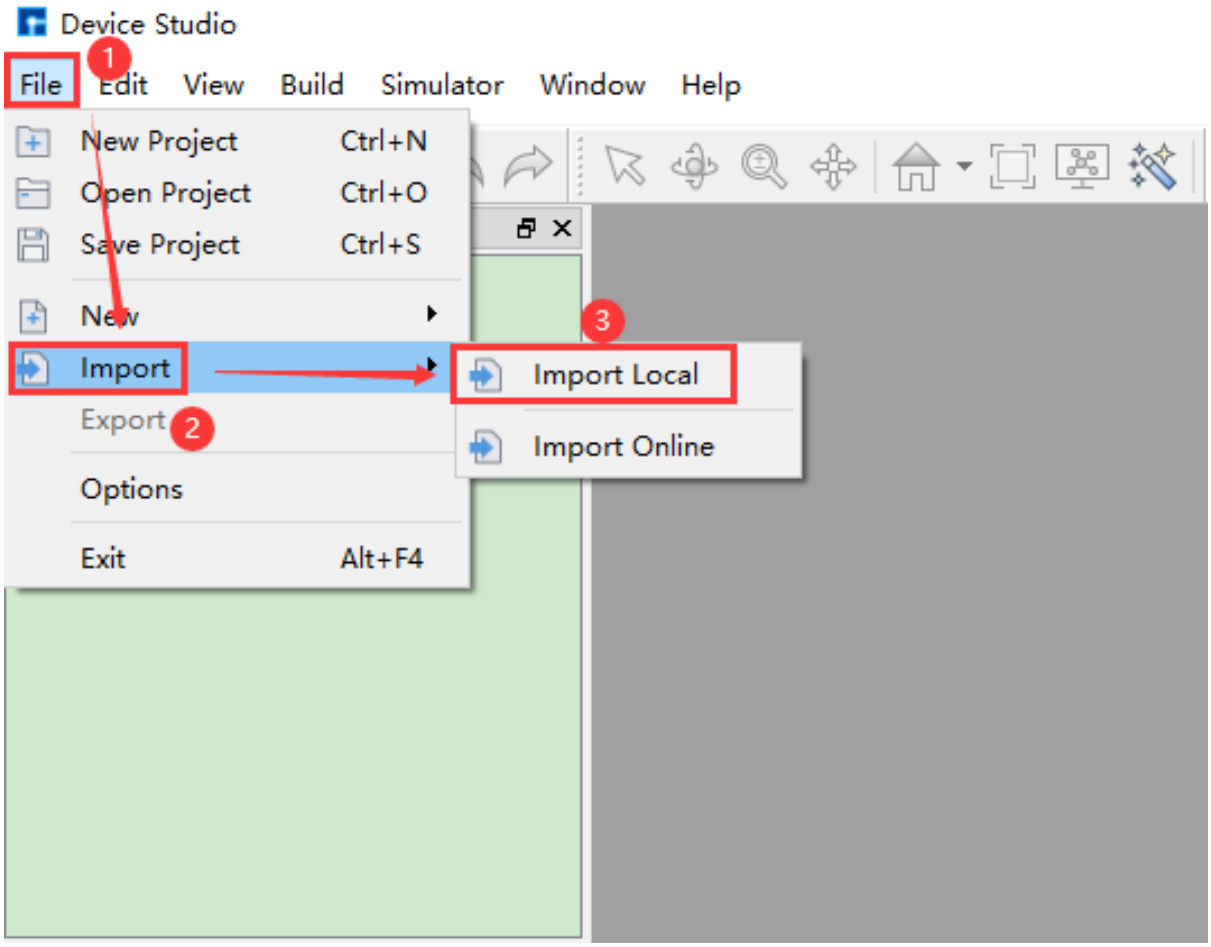


fig. 2.5: Open Import Structure Interface

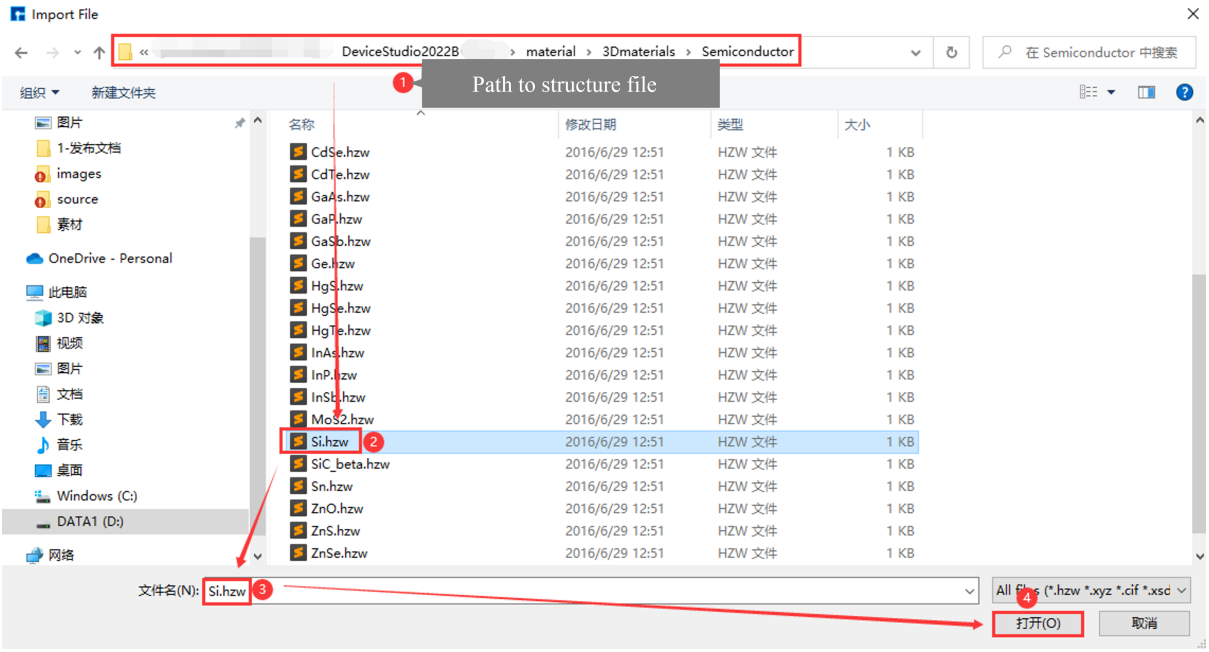


fig. 2.6: Import Si Crystal Structure

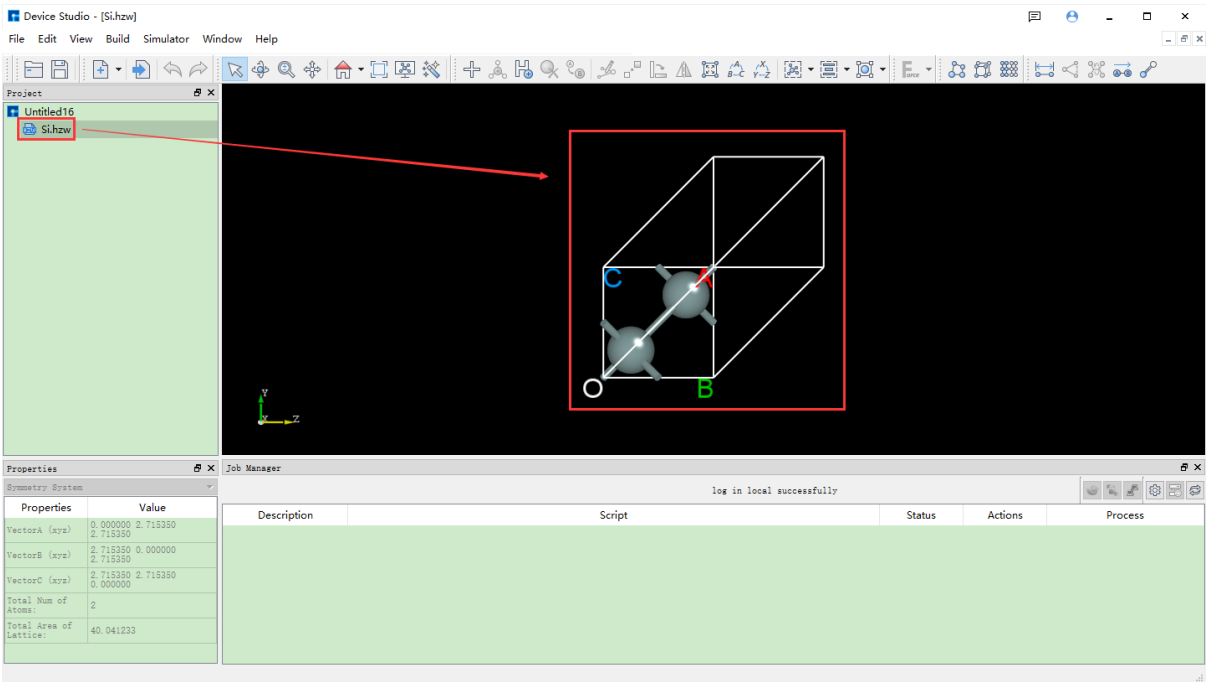


fig. 2.7: Device Studio Interface After Importing Si Crystal Structure

2.4 Generate Self-consistent and Band Structure Calculation Input Files

The process of generating the Si crystal structure self-consistent calculation input file is shown in fig. 2.8, fig. 2.9, and `StartedGuide_10`.

The process of generating the Si crystal structure band structure calculation input file is shown in `StartedGuide_11`, fig. 2.10, and fig. 2.11.

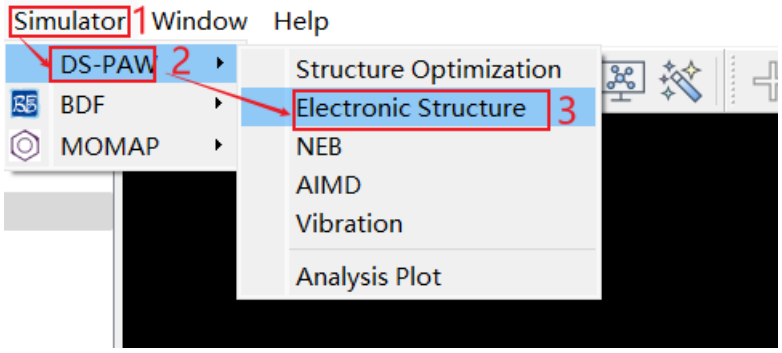


fig. 2.8: Open Generate Self-consistent Calculation Input File Interface

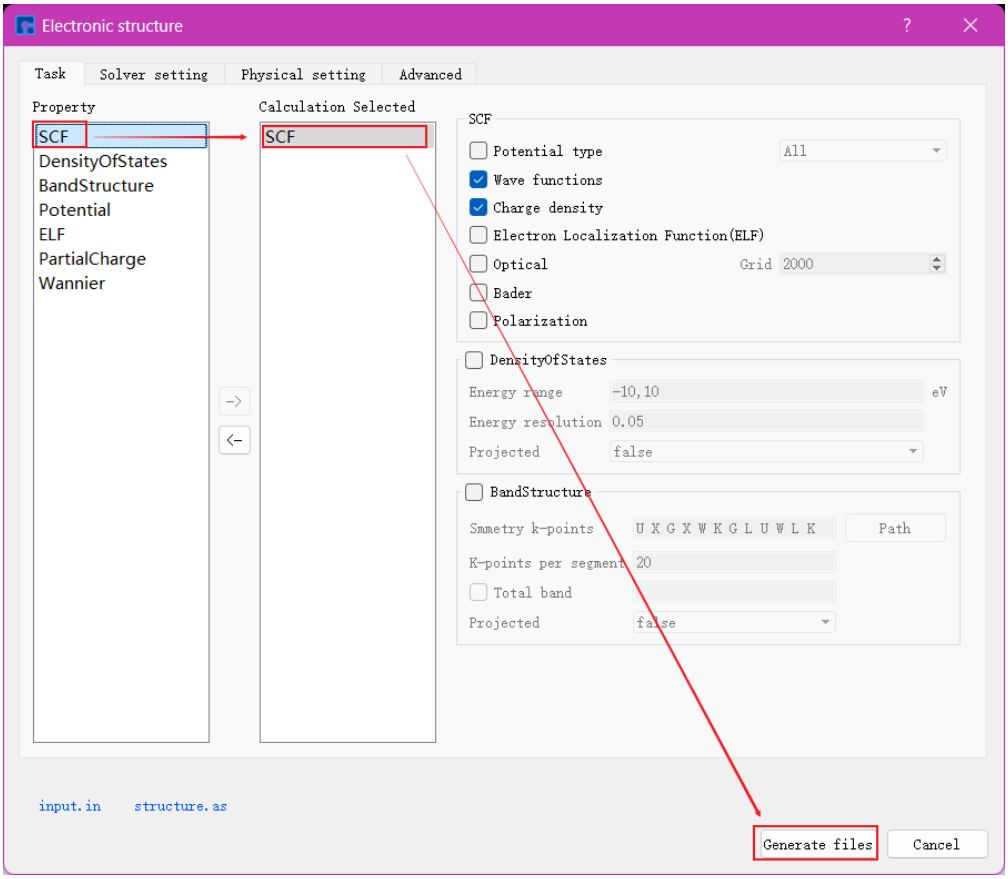


fig. 2.9: Set Parameters and Generate Self-consistent Calculation Input File

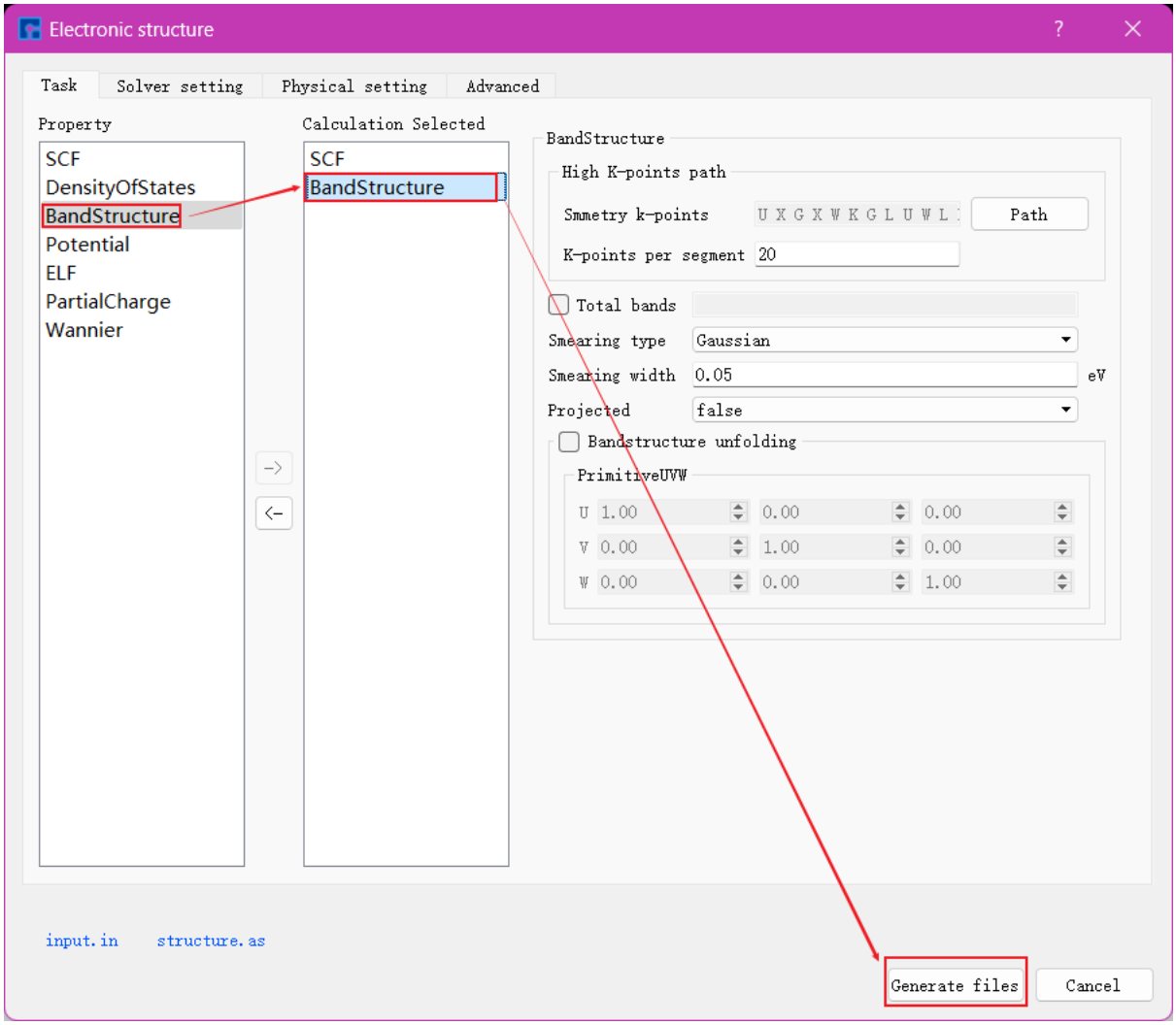


fig. 2.10: Set Parameters and Generate Band Structure Calculation Input File

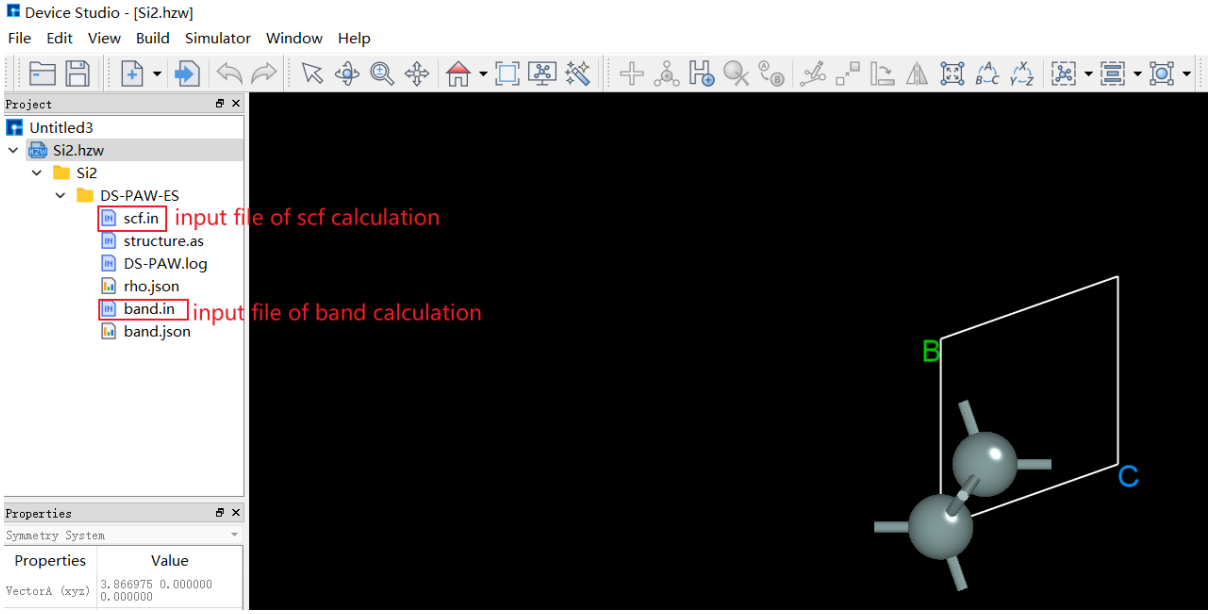


fig. 2.11: Device Studio Interface After Generating Band Structure Calculation Input File

2.5 Submit Self-consistent and Band Structure Calculation Tasks

First, perform the self-consistent calculation for the Si crystal structure. The process of submitting the Si crystal structure self-consistent calculation task is shown in fig. 2.12 and fig. 2.13.

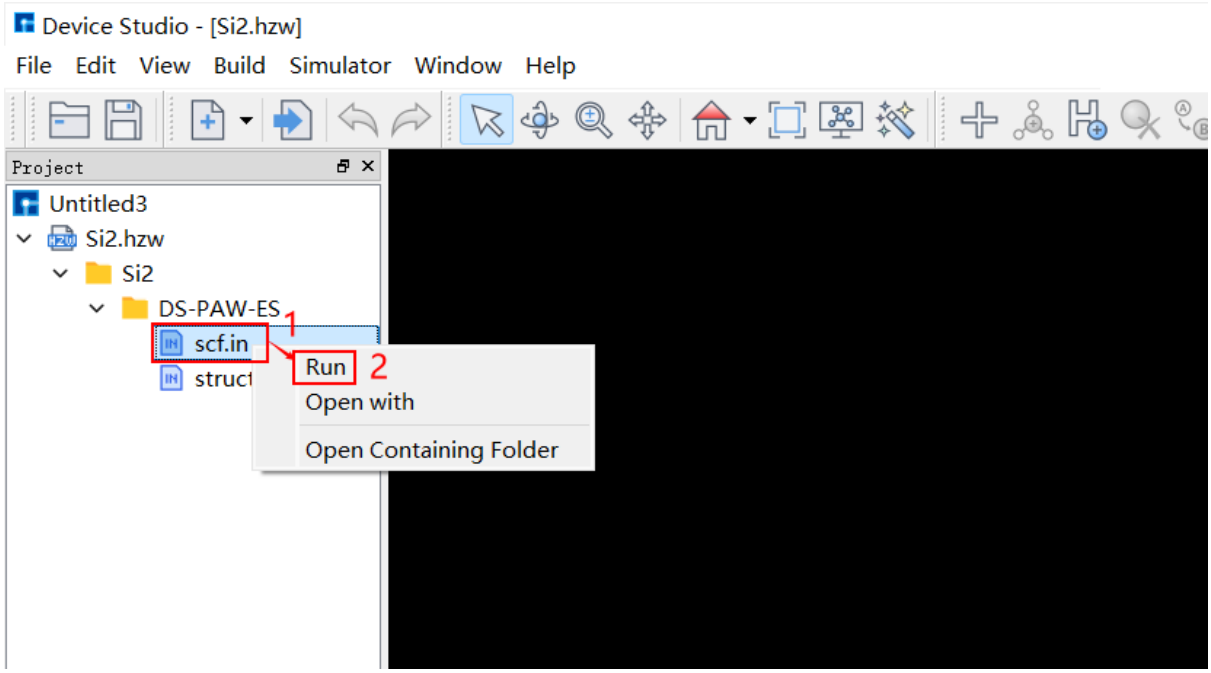


fig. 2.12: Submit Self-consistent Calculation Task Step 1

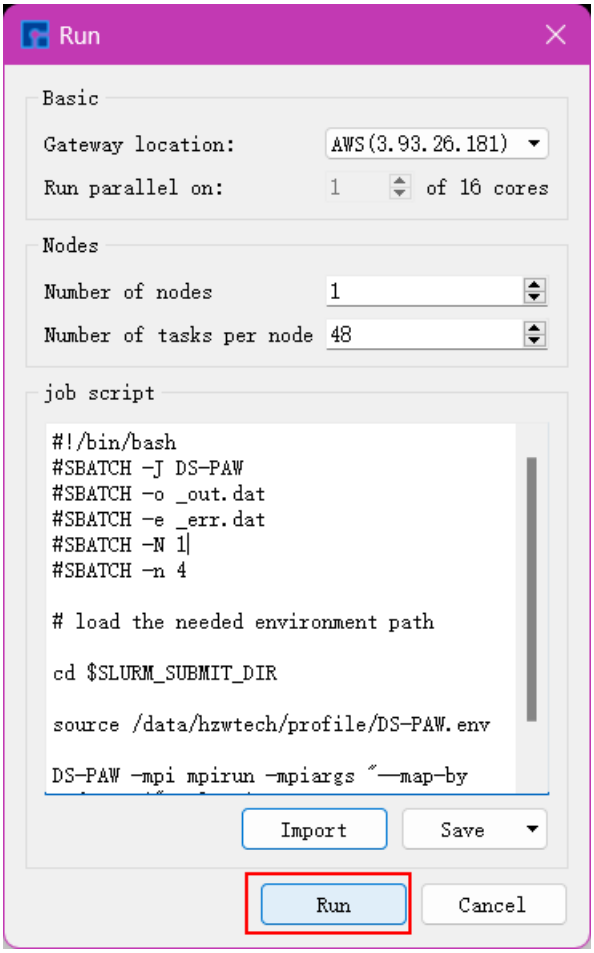


fig. 2.13: Submit Self-consistent Calculation Task Step 2

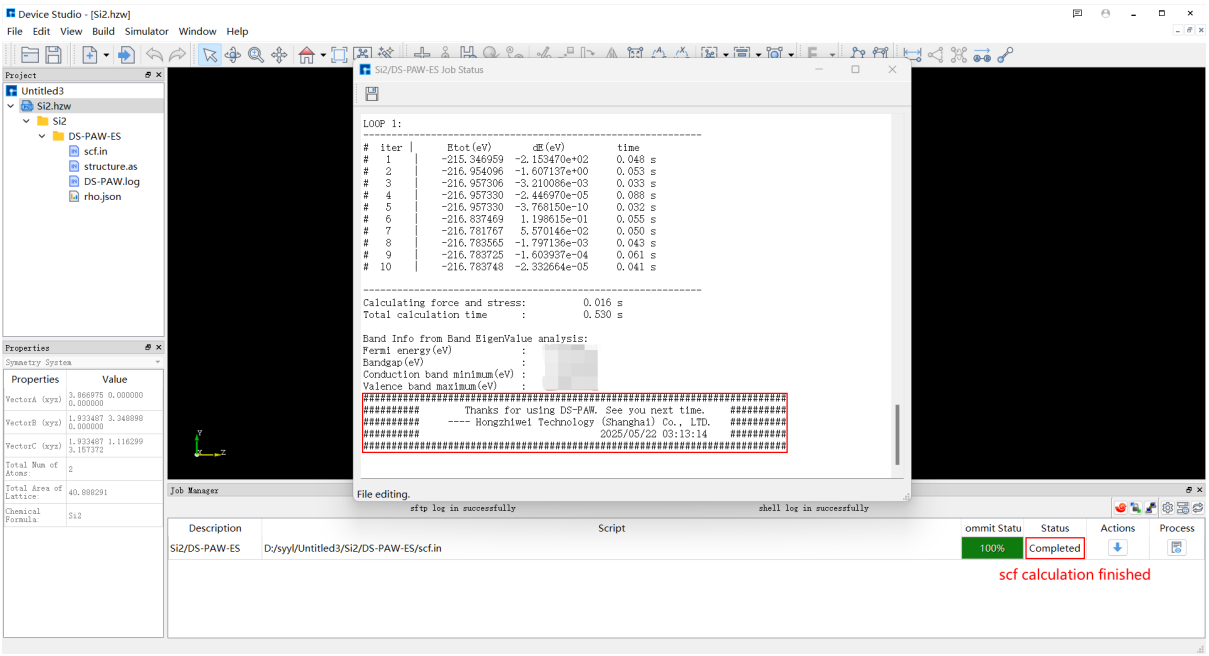


fig. 2.14: Device Studio Interface After Si Crystal Structure Self-consistent Calculation Completion

Only after the self-consistent calculation is completed can the band structure calculation of the Si crystal structure be performed. You can determine whether the self-consistent calculation task is completed through the **Computation Task Monitoring Management Area**. When the calculation task is queued, running, or completed, the *Status* will be Queued, Running, or Completed respectively. The Device Studio interface after the Si crystal structure self-consistent calculation is completed is shown in fig. 2.14. The process of submitting the Si crystal structure band structure calculation task is shown in fig. 2.15 and fig. 2.16. The Device Studio interface after the Si crystal structure band structure calculation is completed is shown in fig. 2.17.

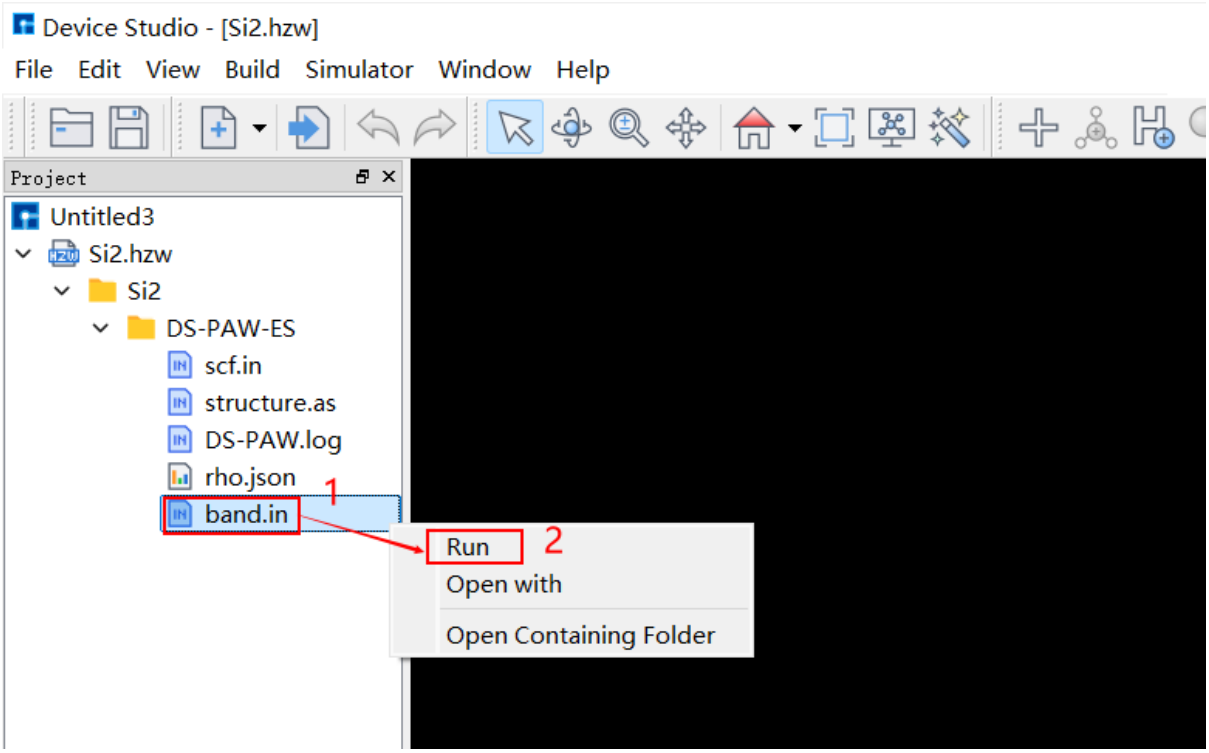


fig. 2.15: Submit Band Structure Calculation Task Step 1

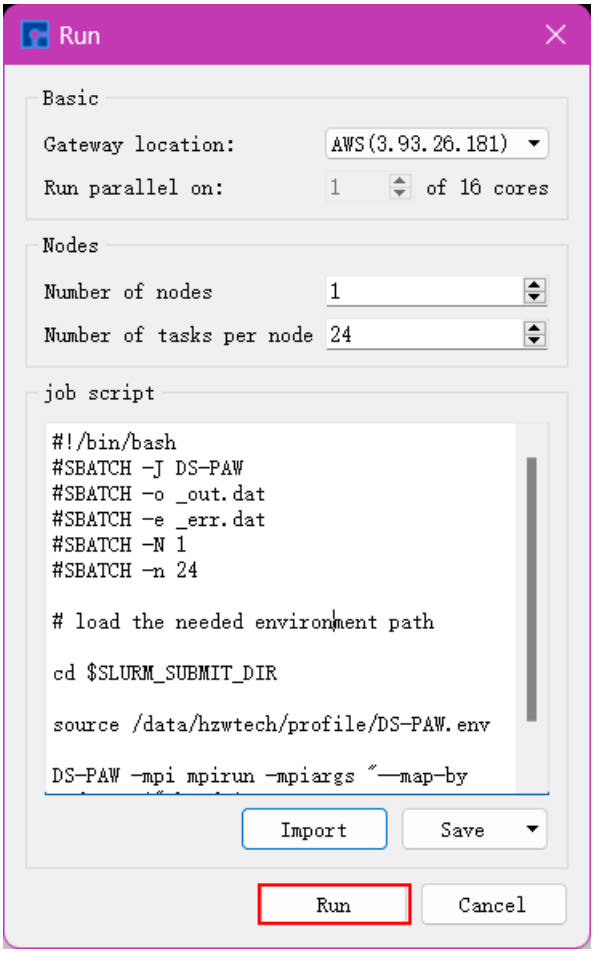


fig. 2.16: Submit Band Structure Calculation Task Step 2

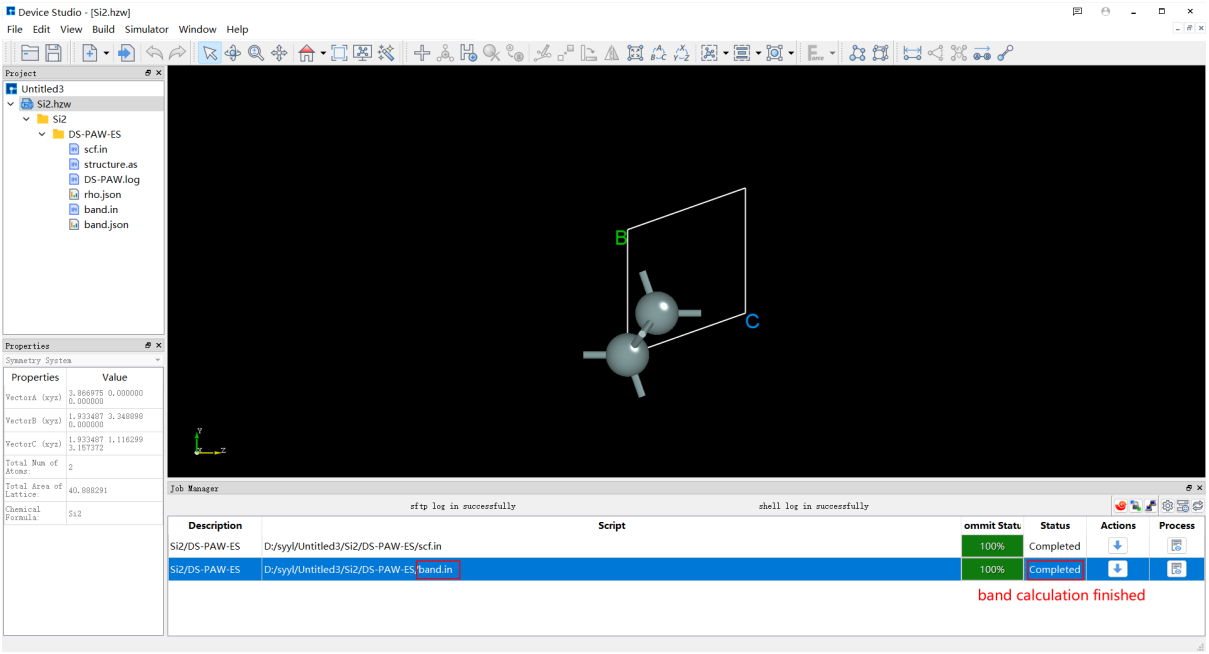


fig. 2.17: Device Studio Interface After Si Crystal Structure Band Structure Calculation Completion

2.6 Data Visualization of Si Crystal Structure Band Structure

After the Si crystal structure band structure calculation is completed, you can perform visualization analysis on the band structure calculation results. The process is shown in fig. 2.18.

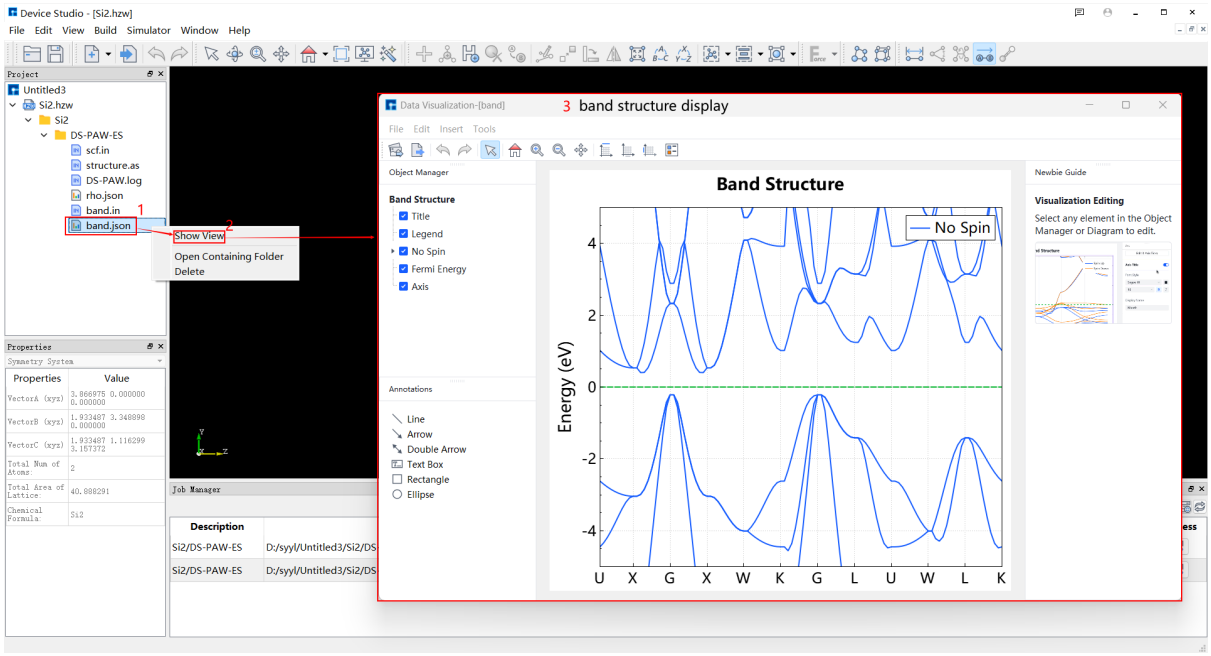


fig. 2.18: Device Studio Steps for Data Visualization of Si Crystal Structure Band Structure Calculation Results

2.7 Export Band Structure Data Visualization Results

After visualizing the Si crystal structure band structure calculation results, users can export the data visualization results as needed. The export process is shown in fig. 2.19.

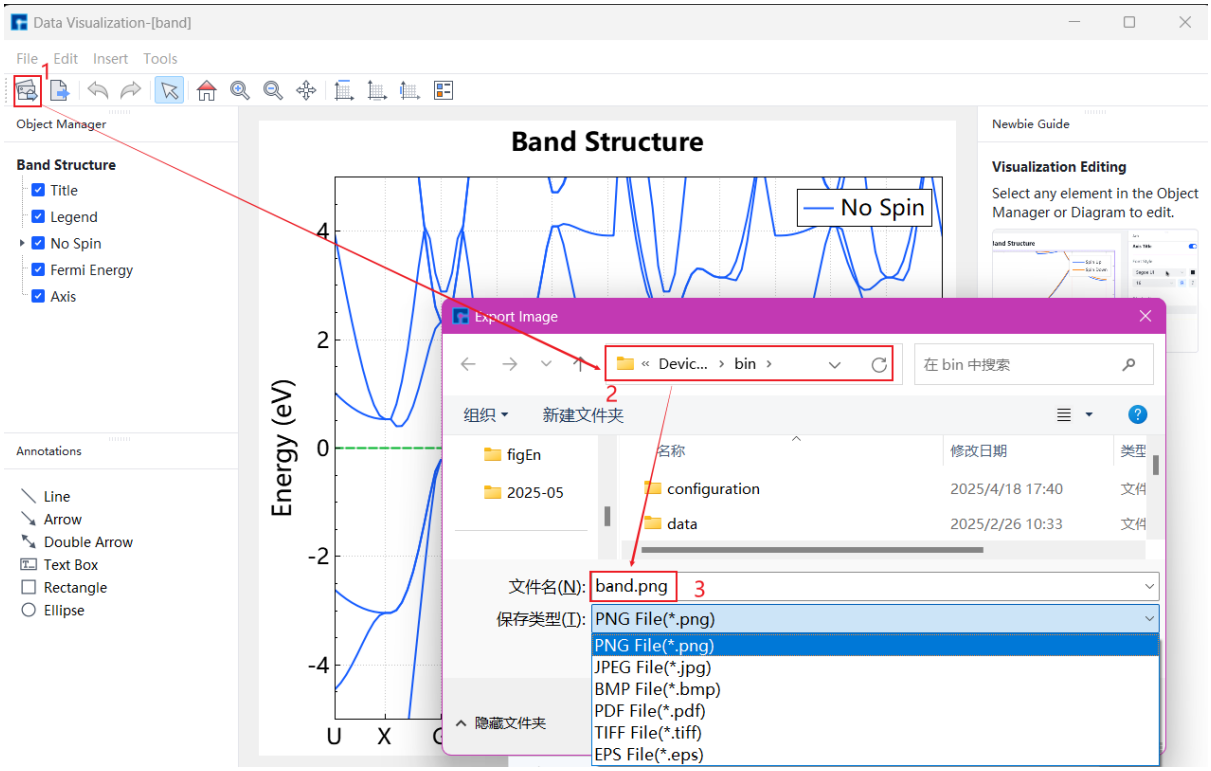


fig. 2.19: Device Studio Steps for Exporting Si Crystal Structure Band Structure Data Visualization Results

CHAPTER

THREE

GRAPHICAL INTERFACE INTRODUCTION

The Device Studio graphical interface is shown in fig. 3.1.

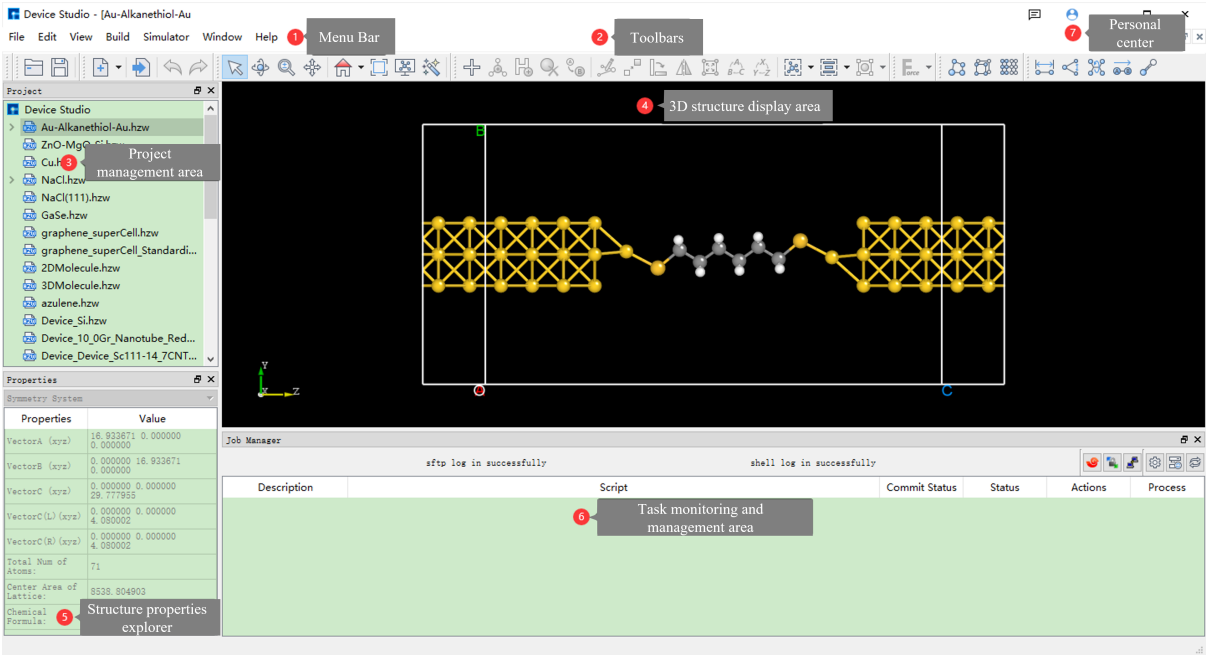


fig. 3.1: Device Studio Graphical Interface

3.1 Menu Bar

The Device Studio menu bar graphical interface is shown in fig. 3.2.

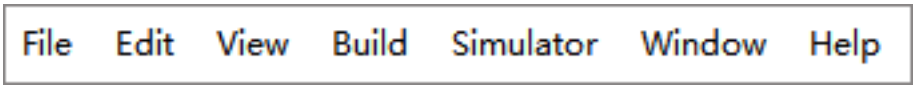


fig. 3.2: Menu Bar

3.1.1 File

Click on *File*, and the interface is shown in fig. 3.3.

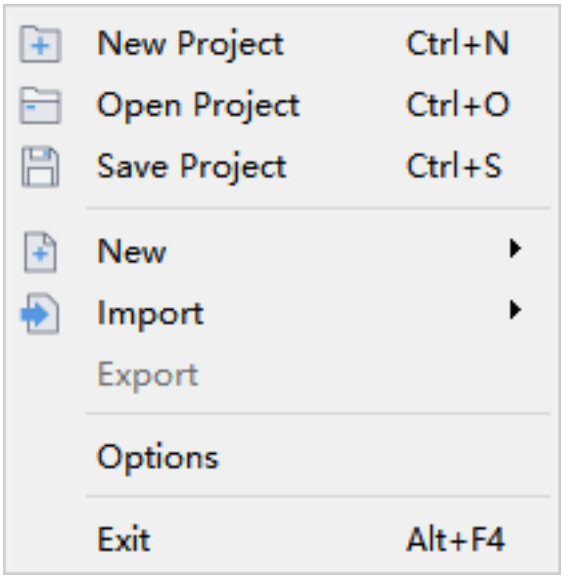


fig. 3.3: File

- *New Project*: Opens the new project interface where users can create a new project with the file extension `.hpf`. Users can name the project as needed, such as `DeviceStudio.hpf`, or use the default name, such as `Untitled.hpf`. After naming, click the "Save"button to create the project; otherwise, if you don't want to create a new project, click the "Cancel" button.
- *Open Project*: Opens the project interface where users can open an existing project, such as the `DeviceStudio.hpf` project. Find and select the project file, then click the "Open" button to open it; otherwise, if you don't want to open the project, click the "Cancel"button.
- *Save Project*: Saves the current project.
- *New*: Users can choose to build device, crystal, or molecular structures as needed.
- *Import*: Opens the structure file import interface where users can choose to import device, crystal, or molecular structures from local or online databases.
- *Export*: Opens the structure file export interface where users can name the structure file as needed or use the default name and choose the storage location.
- *Options*: Opens the options interface where users can choose the pseudopotential basis set file, set the **background color** of Device Studio, and refresh time.
- *Exit*: Closes the Device Studio software.

3.1.2 Edit

Click on *Edit*, and the interface is shown in fig. 3.4.

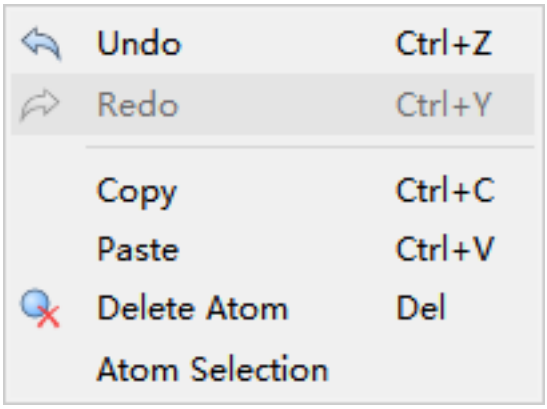


fig. 3.4: Edit

- *Undo*: Undoes.
- *Redo*: Redoes.
- *Copy*: Copies.
- *Paste*: Pastes.
- *Delete Atom*: Deletes the selected atom.
- *Atom Selection*: Selects specific atoms of a specific element in the selected atoms. Users can select specific atoms as needed. For example: First, select a part of the atoms, then select all C atoms in the selected part of the atoms.

3.1.3 View

Click on *View*, and the interface is shown in fig. 3.5.

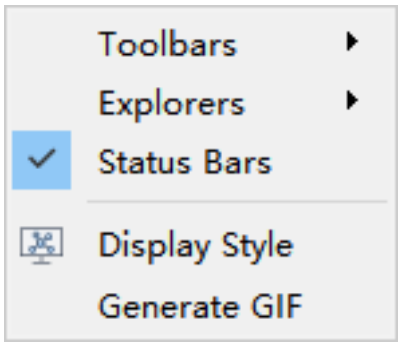


fig. 3.5: View

- *Toolbars*: Users can choose whether to display the Project, Standard, 3D View modules in the toolbar. If displayed, select the corresponding modules; otherwise, do not select.
- *Explorers*: Users can choose whether to display the Project Explorer, Properties Explorer, and Job Manager modules on the software. If displayed, select the corresponding modules; otherwise, do not select.
- *Status Bars*: Select to display the module on the software; otherwise, do not display.
- *Display Style*: Opens the DisplayStyle setting interface. For atoms, users can choose not to display, display in line form, or display in ball stick form. For lattice basis vectors, users can choose not to display, display in solid line, or display in dashed line. If displayed in solid line, users can set the line thickness as needed.
- *generate GIF*: Opens the generategif interface where users can import a series of existing pictures and generate a dynamic graph with the file extension `.gif`, then export the dynamic graph.

3.1.4 Build

Click on *Build*, and the interface is shown in fig. 3.6.

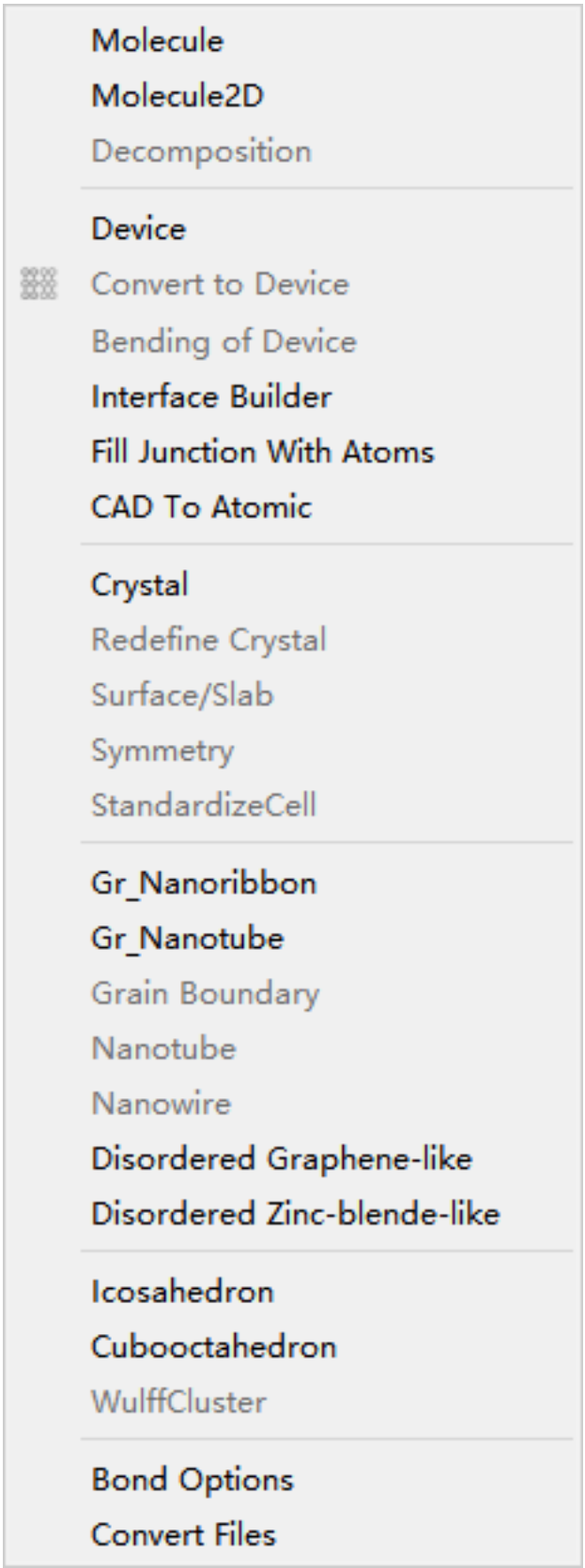


fig. 3.6: Build

- *Molecule*: Builds a 3D molecular structure.

- *Molecule2D*: Builds a 2D molecular structure.
- *Decomposition*: Decomposes a molecular structure.
- *Device*: Builds a device structure. Device types include L-R structure, L-C-R structure, B-T structure, etc. Users can choose to build according to their needs.
- *Convert to Device*: Builds a device structure on the basis of molecular or crystal structure.
- *Bending of Device*: Performs bending operation on two-port device structure.
- *Interface Builder*: Builds heterojunction structure.
- *Fill Junction With Atoms*: Builds multilayer membrane structure.
- *CAD to Atomic*: Builds multilayer membrane structure through 2D CAD.
- *Crystal*: Builds a crystal structure.
- *Redefine Crystal*: Crystal cell redefinition and expansion.
- *Surface/Slab*: Crystal structure cut surface/slice.
- *Symmetry*: Performs space group recognition on crystal structure.
- *StandardizeCell*: Super cell recognition primitive cell.
- *Gr_Nanoribbon*: Builds nanoribbon structure.
- *Gr_Nanotube*: Builds nanotube structure.
- *Grain Boundary*: Builds crystal boundary structure on basis of unit cell.
- *Nanotube*: Builds nanotube on basis of crystal structure.
- *Nanowire*: Builds nanowire on basis of crystal structure.
- *Disordered Graphene-like*: Builds disordered graphene-like structure.
- *Disordered Zinc-blende-like*: Builds disordered zinc-blende-like structure.
- *Icosahedron*: Builds regular icosahedron structure.
- *Cubooctahedron*: Builds regular cubooctahedron structure.
- *WulffCluster*: Builds WulffCluster structure on basis of unit cell.
- *Bond Options*: Bond setting.
- *Convert Files*: Structure file conversion.

3.1.5 Simulator

Click on *Simulator*, and the interface is shown in fig. 3.7. Users can choose the corresponding module according to their needs to generate input files for corresponding software, calculate, and visualize data.

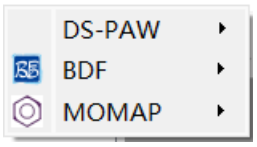


fig. 3.7: Simulator

- *BDF*: Quantum chemistry calculation software BDF.
- *DS-PAW*: First-principles plane wave calculation software DS-PAW.

3.1.6 Window

Click on *Window*, and the interface is shown in fig. 3.8.

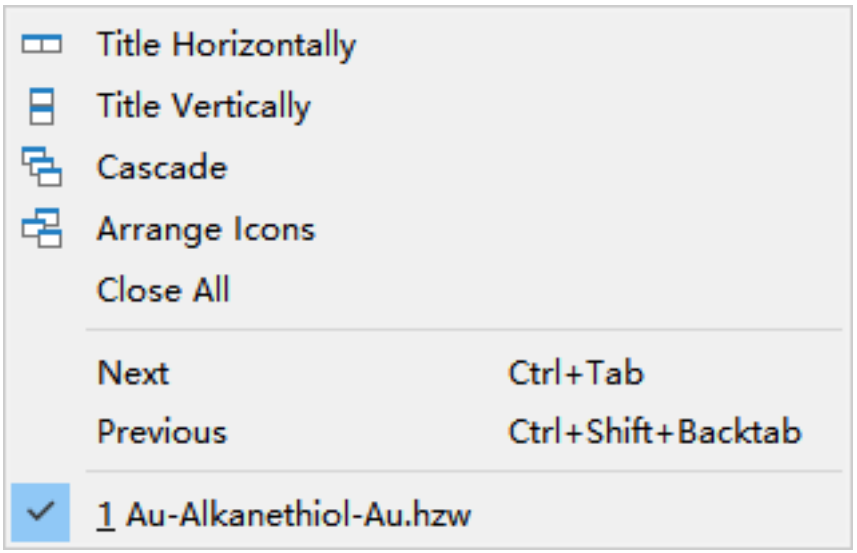


fig. 3.8: Window

- *Title Horizontally*: Horizontally arranges 3D Viewer windows of structure files.
- *Title Vertically*: Vertically arranges 3D Viewer windows of structure files.
- *Cascade*: Stacks 3D Viewer windows of structure files.
- *Arrange Icons*: Minimizes 3D Viewer windows of structure files.
- *Close All*: Closes 3D Viewer windows of structure files.

- *Next*: Selects the next 3D Viewer window of structure file.
- *Previous*: Selects the previous 3D Viewer window of structure file.

3.1.7 Help

Click on *Help*, and the interface is shown in fig. 3.9.

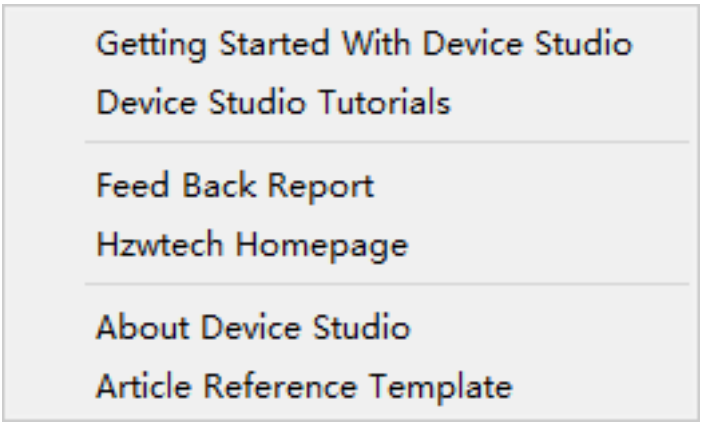


fig. 3.9: Help

- *Getting Started With Device Studio*: Connects Device Studio Quick Start Guide.
- *Device Studio Tutorials*: Connects Device Studio Usage Tutorial.
- *Feed Back Report*: Opens the Hongzhiwei Customer Information Feedback Collection Interface where users can provide product suggestions to Hongzhiwei.
- *Hzwtech Homepage*: Connects Hongzhiwei Technology (Shanghai) Co., Ltd. Homepage.
- *About Device Studio*: Opens the About Device Studio window to understand the Device Studio version number, issuing company, License usage period, etc.
- *Article Reference Template*: Opens the Device Studio Article Reference Template to facilitate correct citation of Device Studio in articles.

3.2 Toolbars

The Device Studio toolbars are shown in fig. 3.10. The numbers from left to right are numbered from 1 to 38. The English name of the icon can be viewed by placing the mouse arrow on the icon.

fig. 3.10: Toolbars

Number	Icon	Icon English Name	Function Description
1		Open Project	Opens Device Studio project file
2		Save Project	Saves current project and structure
3		New	Builds new structure, through which you can select to build device, crystal l or molecular structure
4		Import Local	Imports structure file from local
5		Undo	Undoes
6		Redo	Redoes
7		3D Viewer Selection Mode	Selects, clicks to enter selection mode, can select atoms by mouse click or drag to select
8		3D Viewer Rotation Mode	Rotates, clicks to enter rotation mode, can rotate 3D view of atom structure by dragging mouse
9		3D Viewer Zoom Mode	Zooms in or out, clicks to enter zoom mode, can zoom 3D view of atom structure by scrolling mouse middle key
10		3D Viewer Translation Mode	Translates, clicks to enter translation mode, can translate 3D view of atom structure by dragging mouse
11		3D Viewer zy View	Clicks to reset 3D view of structure (z-y plane), clicks down to select from different perspectives to view 3D view of structure
12		3D Viewer Fit to View	Clicks to move 3D view of structure to appropriate position according to screen
13		Display Style	Clicks to set display mode of atom structure

continues on next page

Table 3.1 – continued from previous page

Number	Icon	Icon English Name	Function Description
14		Structure Refinement Module	Clicks to enter atom structure refinement module, this module has fully upgraded 3D display effect of atom structure, displays atom structure in the form of equivalent atoms, and supports ball stick/polyhedron display mode, users can customize color, radius, and lighting parameters, create exclusive personal template
15		Add Atom	Adds atom, clicks to enter Device Studio periodic table, selects element, clicks in 3D view of structure to add atom
16		Add New Atom	Adds atom in the middle of selected multiple atoms. This icon needs to select multiple atoms to activate
17		Hydrogen passivation	Uses hydrogen atom to passivate crystal structure. Currently, only effective for Si and C elements
18		Delete Atom	Deletes selected atom
19		Replace Atom	Replaces selected atom
20		Edit Atom With Selected	Sets distance between 2 atoms or angle between 3 atoms. This icon needs to select 2 or more atoms to activate
21		Move Atom	Moves selected atom. This icon needs to select atom to activate
22		Rotate Atom	Rotates selected atom. This icon needs to select 2 or more atoms to activate
23		Mirror Atom	Mirrors selected atom. This icon needs to select atom to activate
24		Stretch Cell	Stretches or compresses primitive cell while keeping fractional coordinates unchanged
25		alternate axes	Rotates lattice basis vectors A, B, C of structure

continues on next page

Table 3.1 – continued from previous page

Number	Icon	Icon English Name	Function Description
26		alternate coordinate	Rotates X, Y, Z of structure
27		Wrap	Wraps atoms outside lattice along unit axis to lattice, clicks down to select Wrap Along a/b/c
28		Center	Centers all atoms or selected atoms as a whole in lattice cell, clicks down to select Center Along a/b/c
29		Fit Cell	Automatically matches minimum unit lattice basis vector, clicks down to select Fit Cell Along a/b/c
30		Minimize Structure	Performs structure optimization on molecular structure through molecular force field calculation, clicks down to select suitable force field. This icon can only activate when structure to be displayed is molecular structure
31		Convert to Molecule	Converts current structure to molecular
32		Convert to Crystal	Converts current structure to crystal
33		Convert to Device	Converts current structure to device
34		Distance	Measures distance between 2 atoms
35		Angle	Measures angle between 3 atoms
36		Dihedral angle	Measures dihedral angle between 4 atoms
37		Vector between two atoms	Measures vector between 2 atoms
38		Recalculate LinkerBond	Recalculates bond

> **Note**
>
> The Device Studio toolbars are important, so it is recommended that users read the function of each icon in *Toolbars* before using Device Studio. Also, for convenience of users'use, Device Studio has categorized the icons in the toolbars, and when the icon is **gray**, it cannot be activated unless the condition is met. If help is needed, consult the Hongzhiwei professional solution center team.

3.3 Project Management Area (Project Explorer)

Project Management Area is shown in fig. 3.11. If the project name is `DeviceStudio`, there are 3 structure files under this project, namely `Au-Alkanethiol-Au.hzw`, `NaCl.hzw`, and `azulene.hzw`. For structure files, such as `Au-Alkanethiol-Au.hzw`, as shown in the red frame of Figure 3.3-1, this area can manage input files for corresponding structure calculation, such as self-consistent calculation input file `scf.input`. Users can open and view the input file by right-clicking on the input file and selecting *Open with*, or find the file storage location in the computer by right-clicking on the input file and selecting *Open Containing Folder*. For structure files, if related calculation input files have been generated, they cannot be renamed; otherwise, if no related calculation input files have been generated, users can rename them by right-clicking on the structure file and selecting *Rename*, then renaming them.

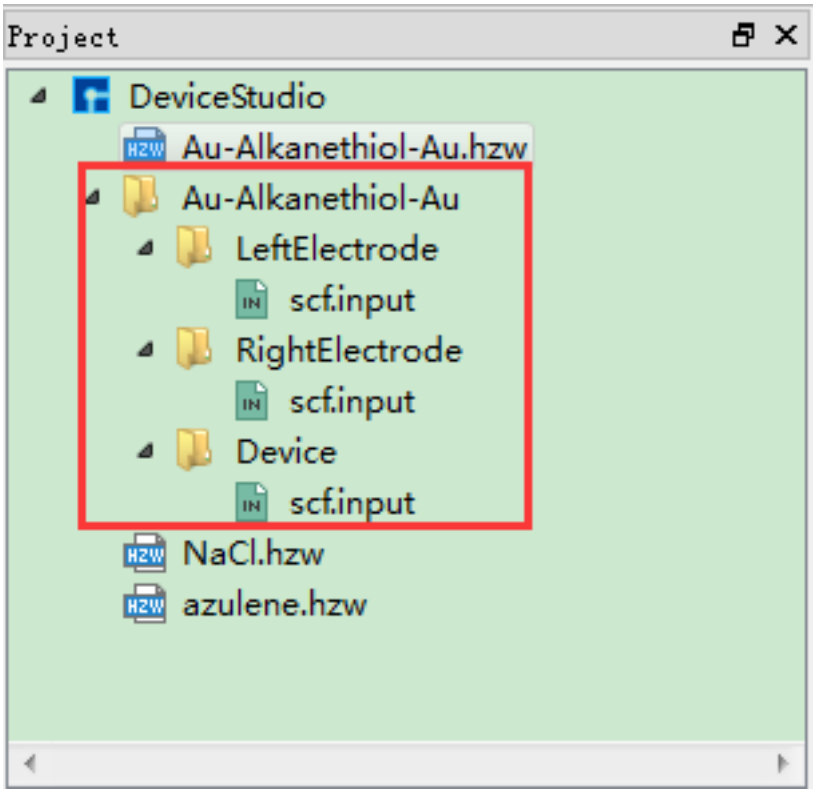


fig. 3.11: Project Management Area

To create or open an existing project, import or export structure files in the **Project Management Area**, please refer to the detailed description of *File*.

Note

Device Studio has optimized *Project Management Area (Project Explorer)*, so it is recommended that users name project files, structure files, etc. in English without spaces, Chinese characters, asterisks, etc. when submitting homework for calculation. After submitting homework, including **after submitting homework**, do not change file names. If you want to change them, it is recommended to change them before submitting homework for calculation.

3.4 Structure 3D Display Area (3D Viewer)

Structure 3D Display Area is shown in fig. 3.12. If the structure `Au-Alkanethiol-Au.hzw` is displayed in this area, users can open the structure file in the project management area by double-clicking on the structure file. In this area, users can zoom the 3D view of the structure by scrolling the mouse middle key; they can first select the *3D Viewer Translation Mode* shortcut icon in the toolbar or press the middle mouse button, and then drag the mouse to translate the 3D view of the

structure in this area; they can first select the *3D Viewer Rotation Mode* shortcut icon or press the right mouse button, and then drag the mouse to rotate the 3D view of the structure in this area.

Users can perform various operations such as adding, deleting, modifying, etc. on the structure in this area, and the 3D view of the structure can be displayed in real time in this area. Users can perform structure operations according to the function description of each shortcut icon in *Toolbars*.

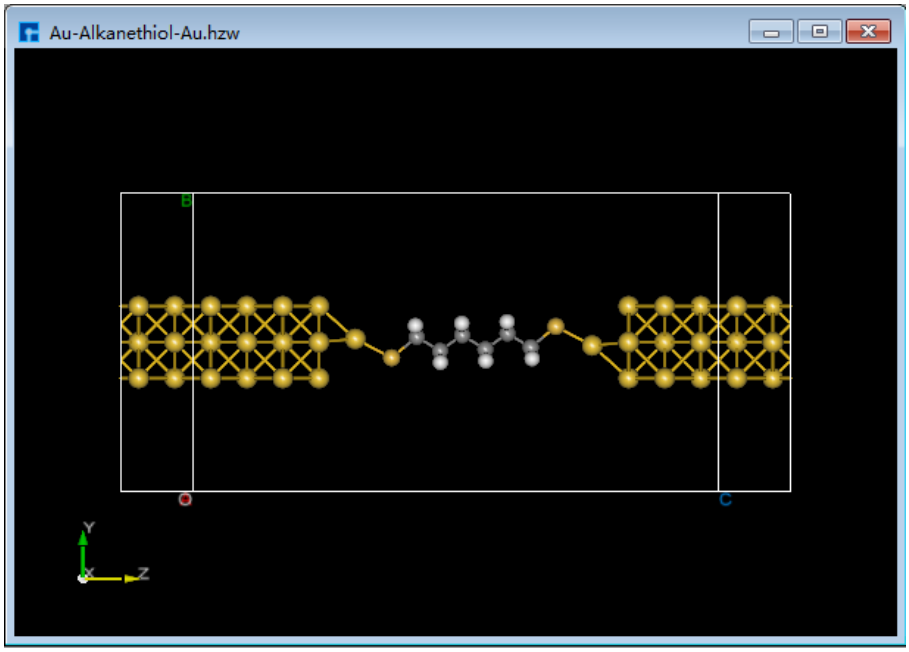
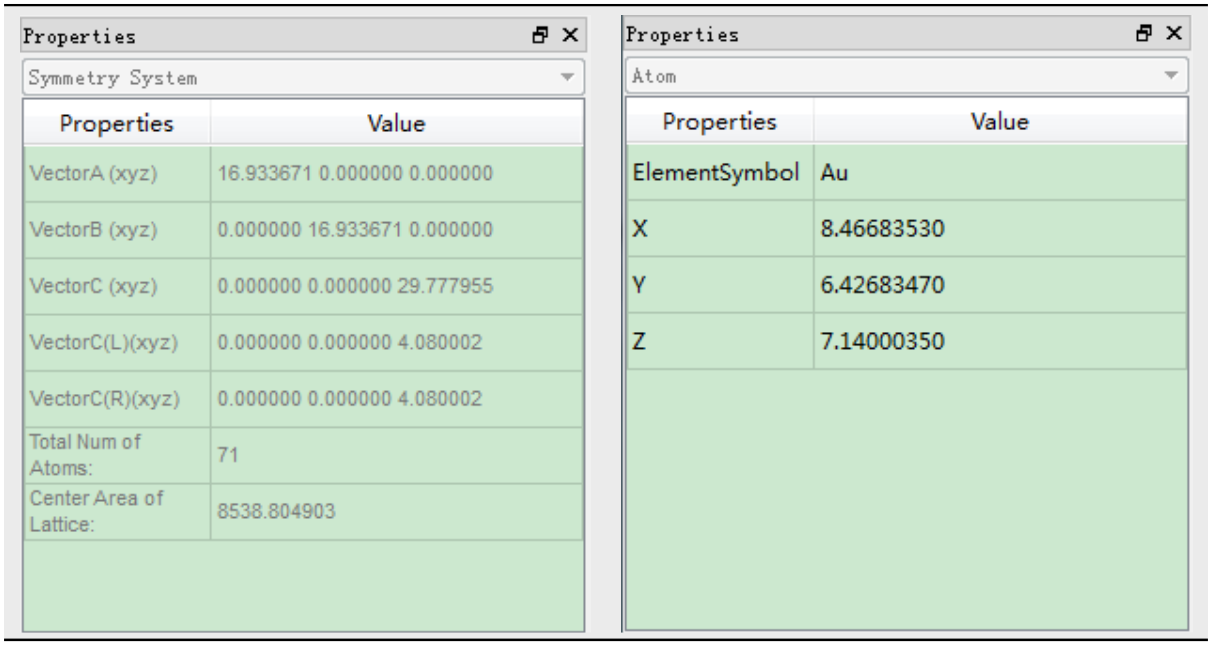


fig. 3.12: Au-Alkanethiol-Au's 3D Display

3.5 Structure Attribute Area (Properties Explorer)

If structure `Au-Alkanethiol-Au.hzw` is displayed in the 3D display area, **Structure Attribute Area** shows the system information of the structure as shown in `GraphicalInterface_13`; if a specific atom of `Au-Alkanethiol-Au.hzw` structure is selected, **Structure Attribute Area** shows the atom information of the structure as shown in `GraphicalInterface_14`, users can modify the coordinate position or replace the atom of the selected atom by double-clicking on the mouse.



3.6 Calculation Task Monitoring Management Area (Job Manager)

As shown in fig. 3.13, **Calculation Task Monitoring Management Area** contains 5 modules, with the function descriptions as follows. When the task is in queue, calculating, or completed, *Status* is Queued, Running, Completed respectively. After calculation is completed, part of calculation results will be automatically pulled back to local. If more calculation results are needed, click the download button to download and return.

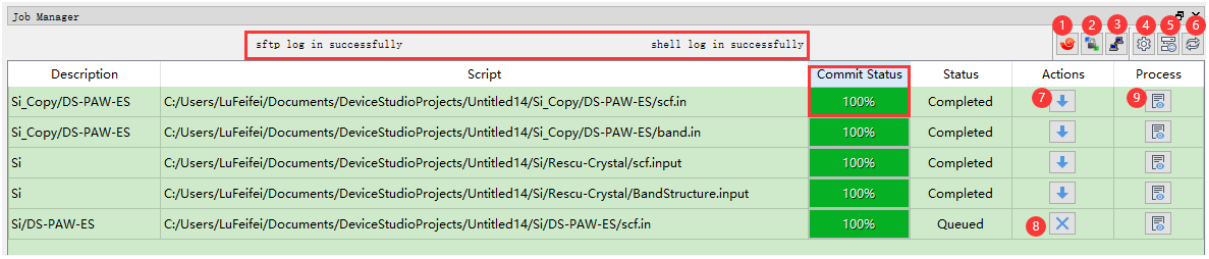


fig. 3.13: Calculation Task Monitoring Management Area

- *Description*: Structure name.
- *Script*: Location of task input file.
- *Commit Status*: Task file transmission progress.
- *Status*: Task calculation status.

- *Actions*: Task calculation operation.
- *Process*: Views task calculation log file to determine whether task calculation is completed through log file.

Calculation Task Monitoring Management Area (Job Manager) icon function is as follows table:

Number	Icon	Icon English Name	Function Description
1		/	Clicks to enter Xshell exe file directory setting
2		Open WinSCP	Clicks to connect current supercomputing server through WinSCP, as shown in fig. 7.19
3		Open PuTTY	Clicks to connect current supercomputing server through PuTTY, as shown in fig. 7.18
4		Reset IP	Clicks to enter MachineOptions interface, in which users can choose local or supercomputing server, or customize connection server. Connection server operation can refer to Nanodcal Connection Server section content
5		Reload to server	Reconnects server
6		refresh	Refreshes, clicks to refresh Calculation Task Monitoring Management Area status
7		Download	Downloads, clicks to enter Calculation Result Download Interface as shown in fig. 7.17
8		Cancel	Cancels, clicks to cancel calculation task
9		Inspect simulation data in real time	Clicks to view calculation result log file in real time

CHAPTER

FOUR

STRUCTURE MODELING

Device Studio supports importing structures from local or online databases, or building new structures based on imported ones. It supports creating various molecules, crystals, and typical device structures such as LCR/LR/FCB/FB/BCT/BT. Device Studio can automatically split crystal planes and build device structures according to user-specified matching accuracy requirements. It can automatically match and build multilayer device or crystal structures. It can generate special structures such as Nanoribbons, Nanotubes, clusters, grain boundaries, and random doping.

4.1 Supported File Types

Device Studio supports file types including `.hzw`, `.xyz`, `.cif`, `.dsxml`, `.pdb`, `.mol`, `.xsd`, `scf.input`, `.py`, `POSCAR`, `CONTCAR`, etc., where `.hzw` is Device Studio's proprietary file format. Device Studio can export structure files in `.hzw` and `.xyz` formats according to user needs, and can export 3D visualization results of structure files in `.png` image format. For crystal structures, it can identify their space group structure information and export structure files in `.cif` format.

4.2 Importing Structures

Before importing a structure, you need to create a new project or open an existing project, and import the structure based on an existing project. To create a project: double-click the Device Studio icon shortcut to log in and start the software. The graphical interface is shown in fig. 4.1. According to the interface prompts, select the button to create a new project (*Create a new Project*) or open an existing project (*Open an existing Project*), then click the *OK* button. If you choose to create a new project, you can name it according to your needs, such as naming this project `Device Studio`.

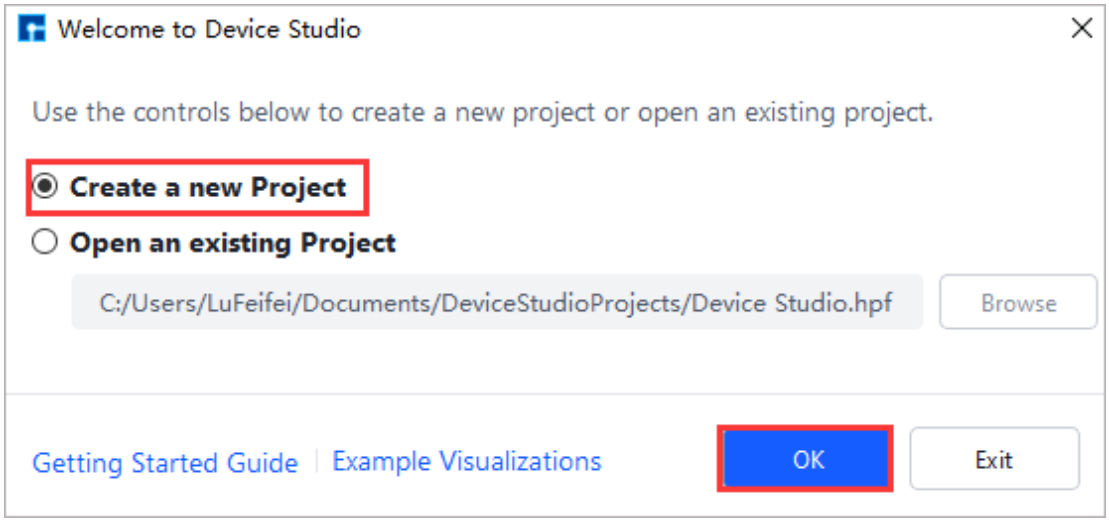


fig. 4.1: Graphical interface for selecting to create or open a project after starting the software

4.2.1 Importing Structures from Local Database

Device Studio comes with a local database containing over 500 commonly used or popular materials, which will be continuously updated and expanded. If users need a large-scale database, they can pay attention to Hongzhiwei's FIRST software, which includes three major databases: QuickMol, QuickCrystal, and ACED, with over **10 million** material entries. Users can import structures through the local database, such as importing the ZnO-MgO-Si device structure. The import operation is shown in the red part of fig. 4.2: *File* → *Import* → *Import Local*. Then a graphical interface pops up as shown in fig. 4.3. According to the interface prompts, find the folder containing ZnO-MgO-Si in the local database, select the ZnO-MgO-Si structure file, and click the open button in fig. 4.3 to import the ZnO-MgO-Si structure. The graphical interface after importing the ZnO-MgO-Si structure is shown in fig. 4.4, where the `ZnO-MgO-Si.hzw` structure file is in the Project Explorer area, and the 3D view of the structure is displayed in the 3D Viewer area.

Note

If you don't want to import the structure through the database, and you know the location of the structure file, such as the ZnO-MgO-Si structure, you can simply left-click to select the structure file and drag it to the Project Explorer area of Device Studio to import the structure. The 3D view of the structure will be displayed in the 3D Viewer area.

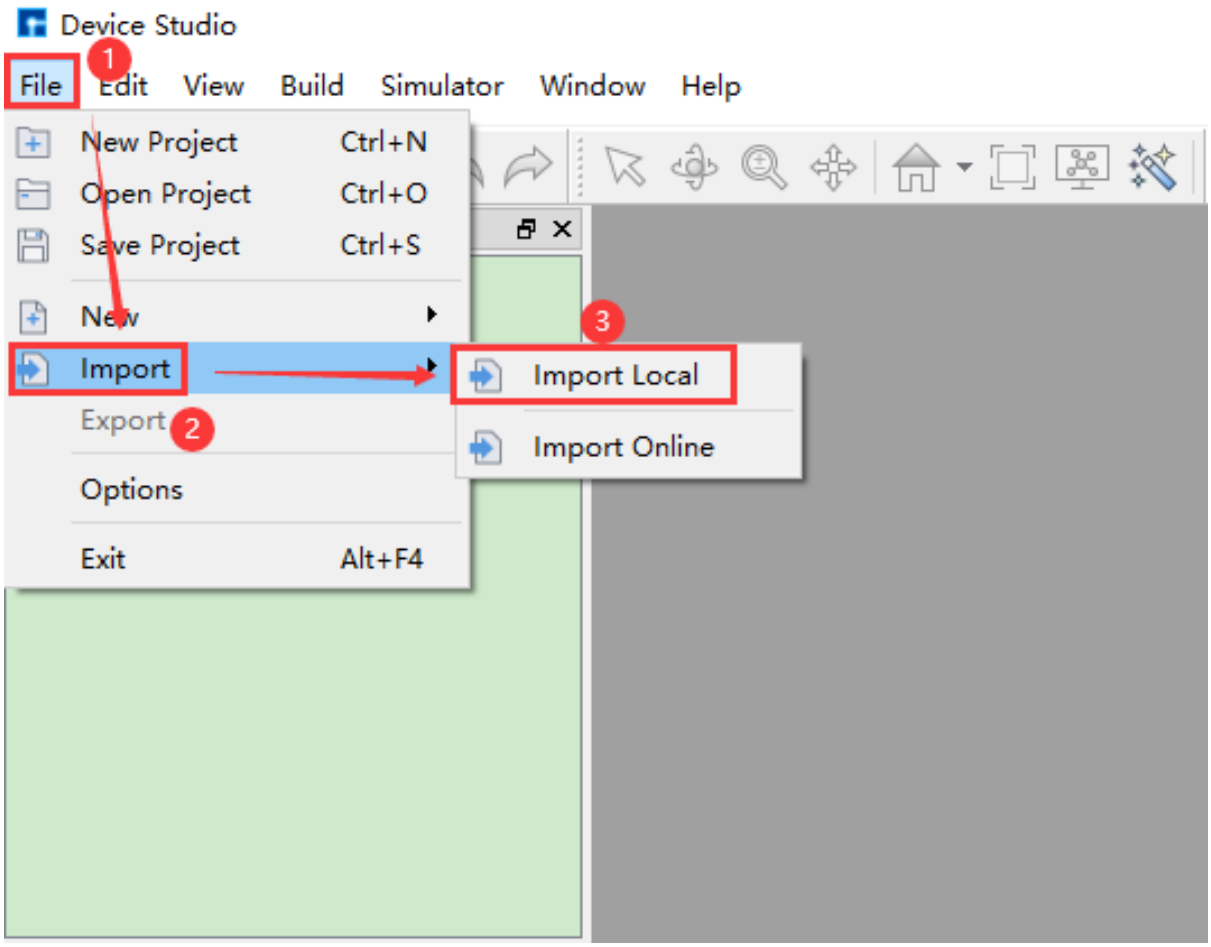


fig. 4.2: Pop-up interface for importing structure from local database

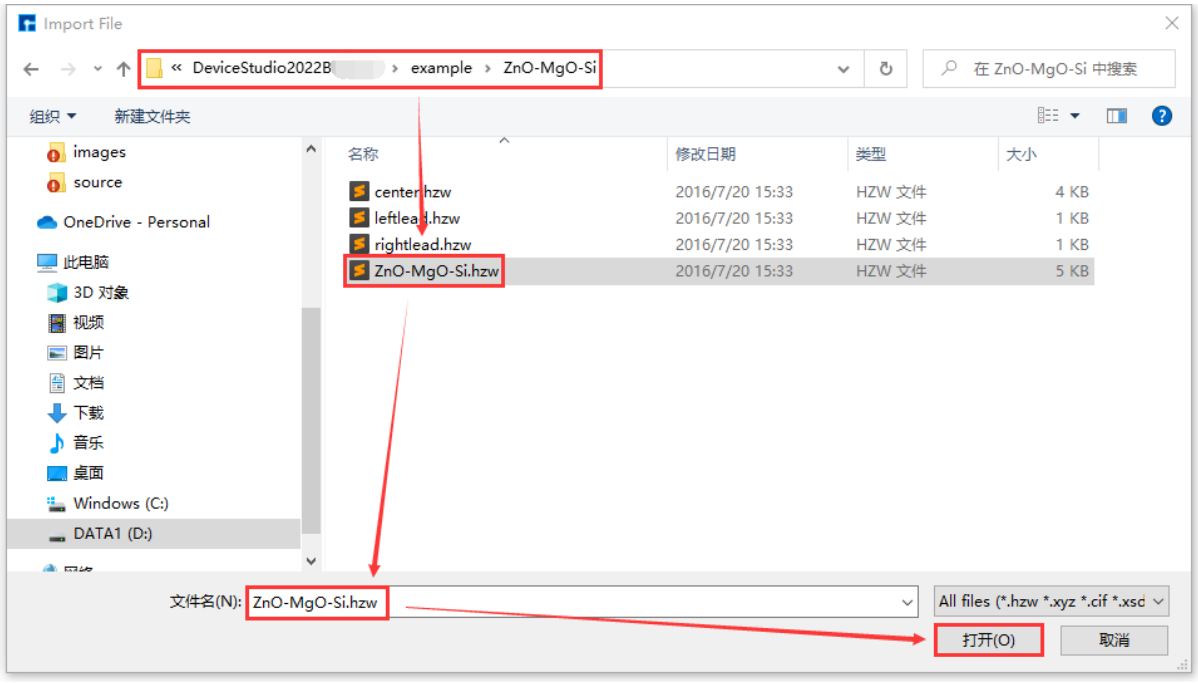


fig. 4.3: Interface for selecting ZnO-MgO-Si structure file

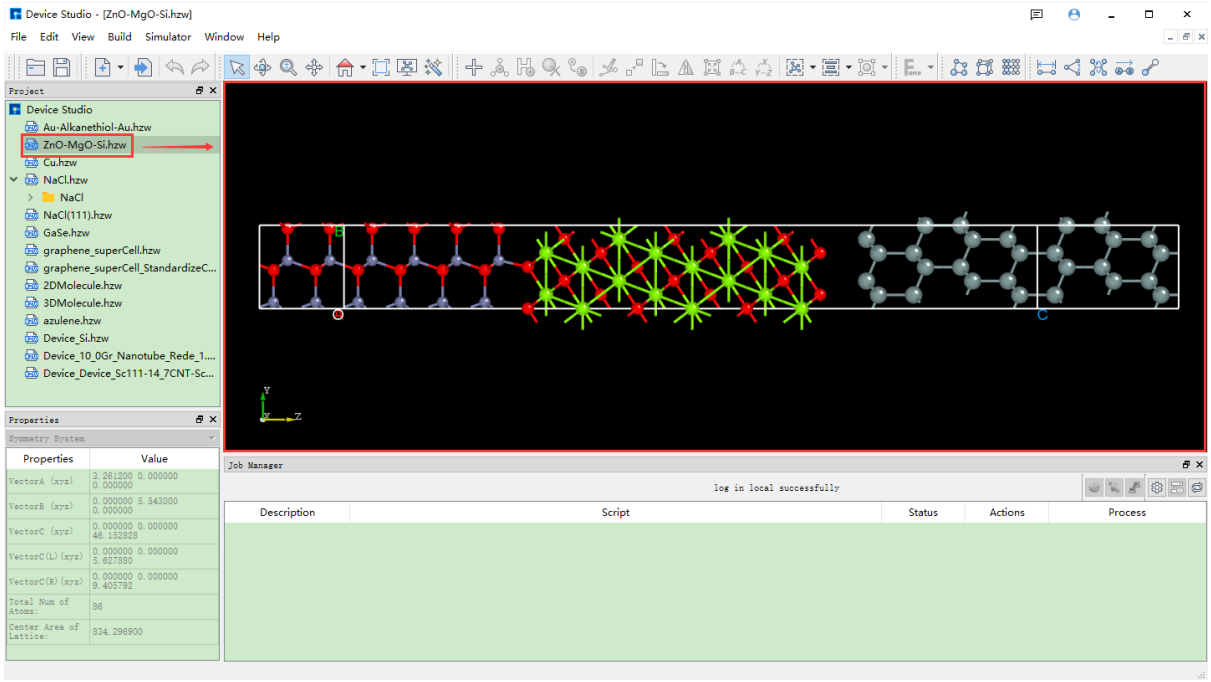


fig. 4.4: Device Studio interface after importing ZnO-MgO-Si structure

4.2.2 Importing Structures from Online Database

Device Studio supports connecting to the online Materials Project database. As shown in the red part of fig. 4.5: click *File* → *Import* → *Import Online* to pop up the interface for importing structures from the Materials Project database. In this interface, users can search for atomic structures by entering elements, chemical formulas, or mp numbers.

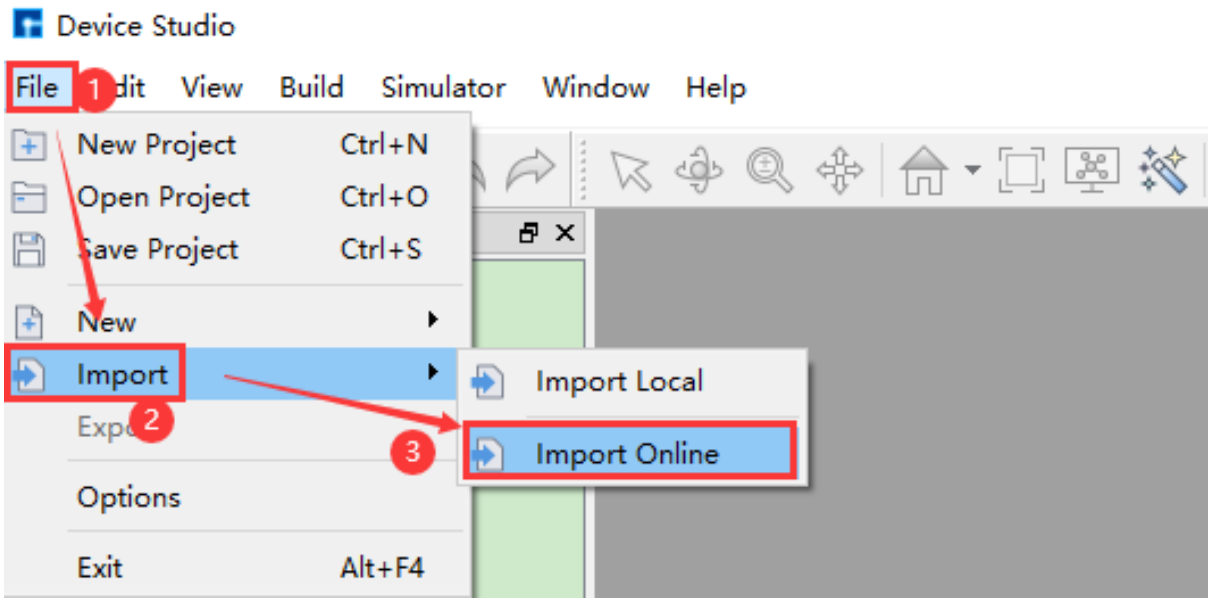


fig. 4.5: Pop-up interface for importing structure from online database

As shown in fig. 4.6, search for structures by entering elements. Enter the Si element and click the *Search* button or press the *Enter* key on the keyboard. Many atomic structures containing only Si elements will appear, such as the Si40 structure. The left side shows its detailed chemical formula, and the right side shows its corresponding space group structure. After selection, you can view the structure's chemical formula, space group symmetry information, and atomic coordinates in the red box area at the bottom left of the interface. You can view the 3D display of the structure in the red box area at the bottom right of the interface. For the 3D display of the structure, you can zoom in or out by scrolling the mouse wheel. You can right-click to select the structure and rotate the 3D view by dragging the mouse. After determining the atomic structure to search for, click the *Add* button in the interface to import the atomic structure. The structure file is saved in the software's project management area (Project Explorer), and you can view the 3D view of the atomic structure in the 3D display area. The Device Studio interface after importing the Si40 structure through the online Materials Project database is shown in fig. 4.7.

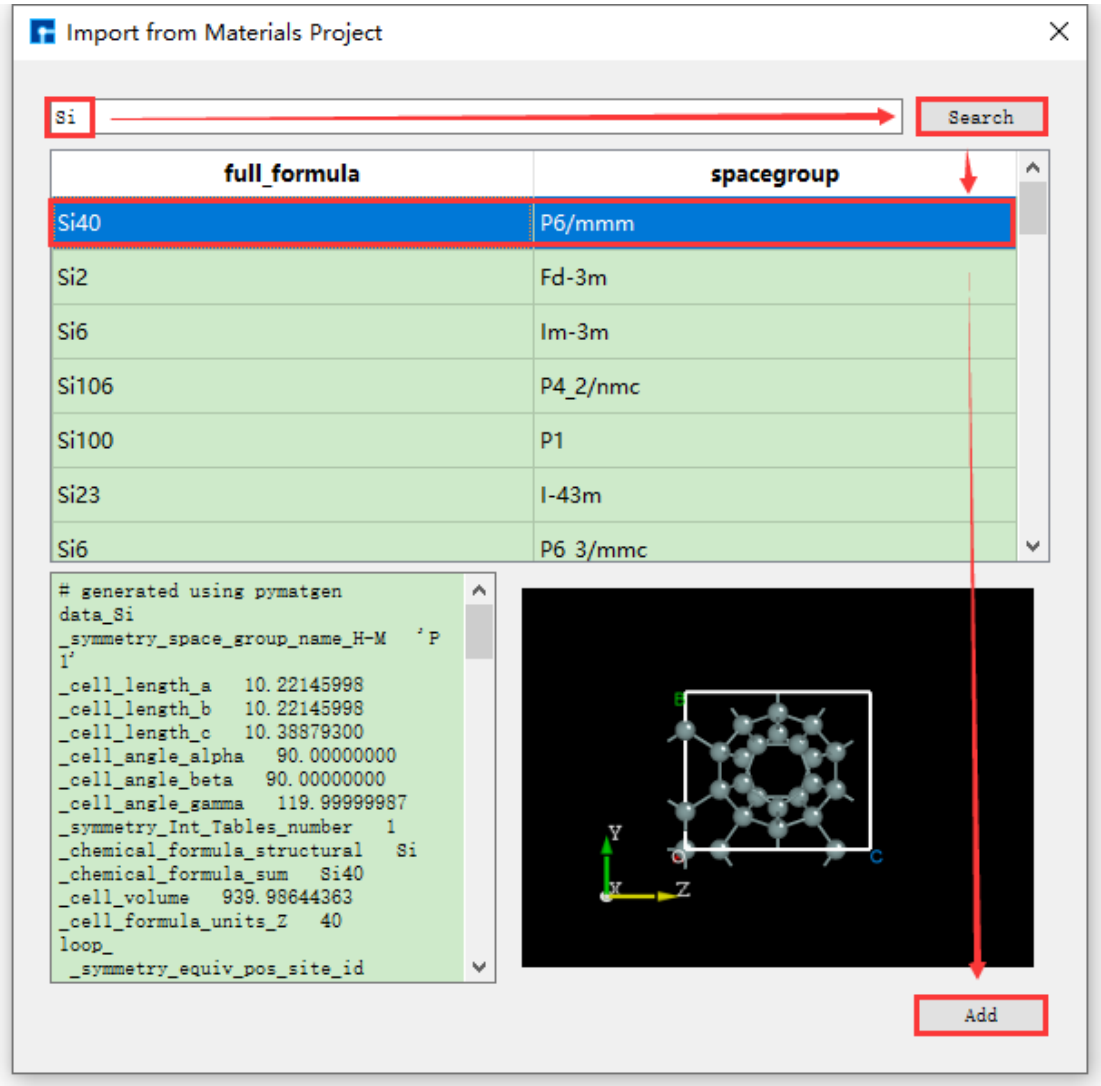


fig. 4.6: Materials Project element search and structure import operation interface

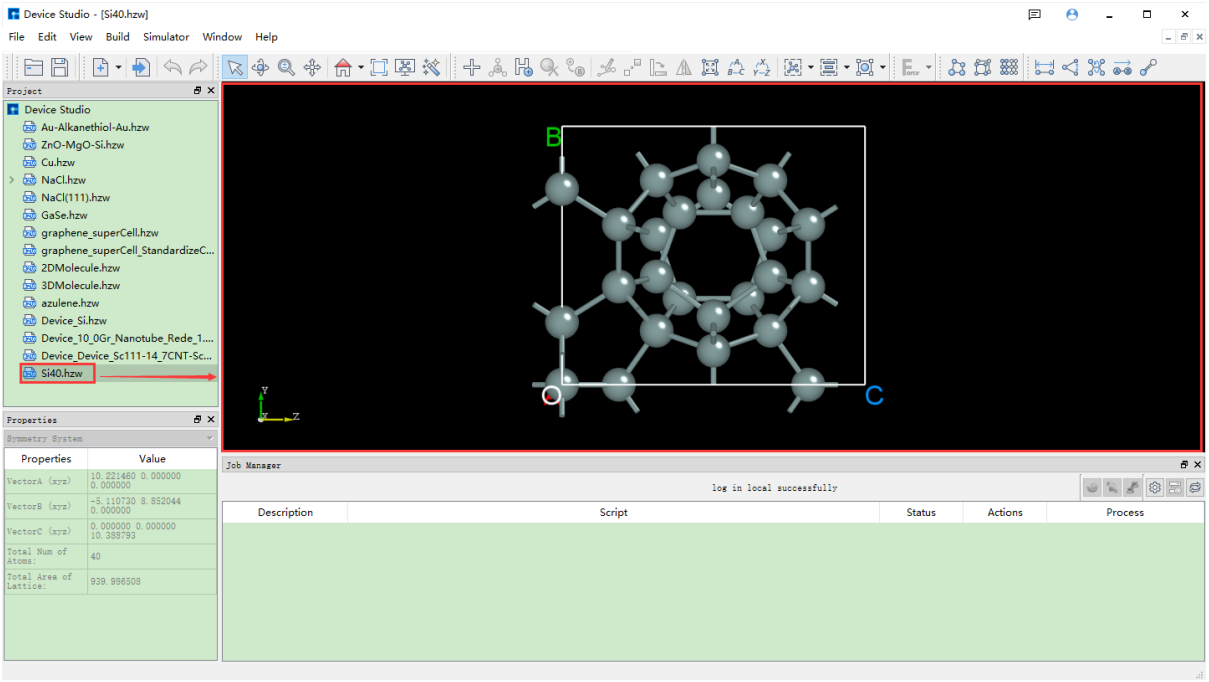


fig. 4.7: Device Studio interface after importing Si40 structure

The operations for searching and importing structures through chemical formulas and mp numbers are the same as those through element search and import. Their operation interfaces are shown in fig. 4.8 and fig. 4.9 respectively.

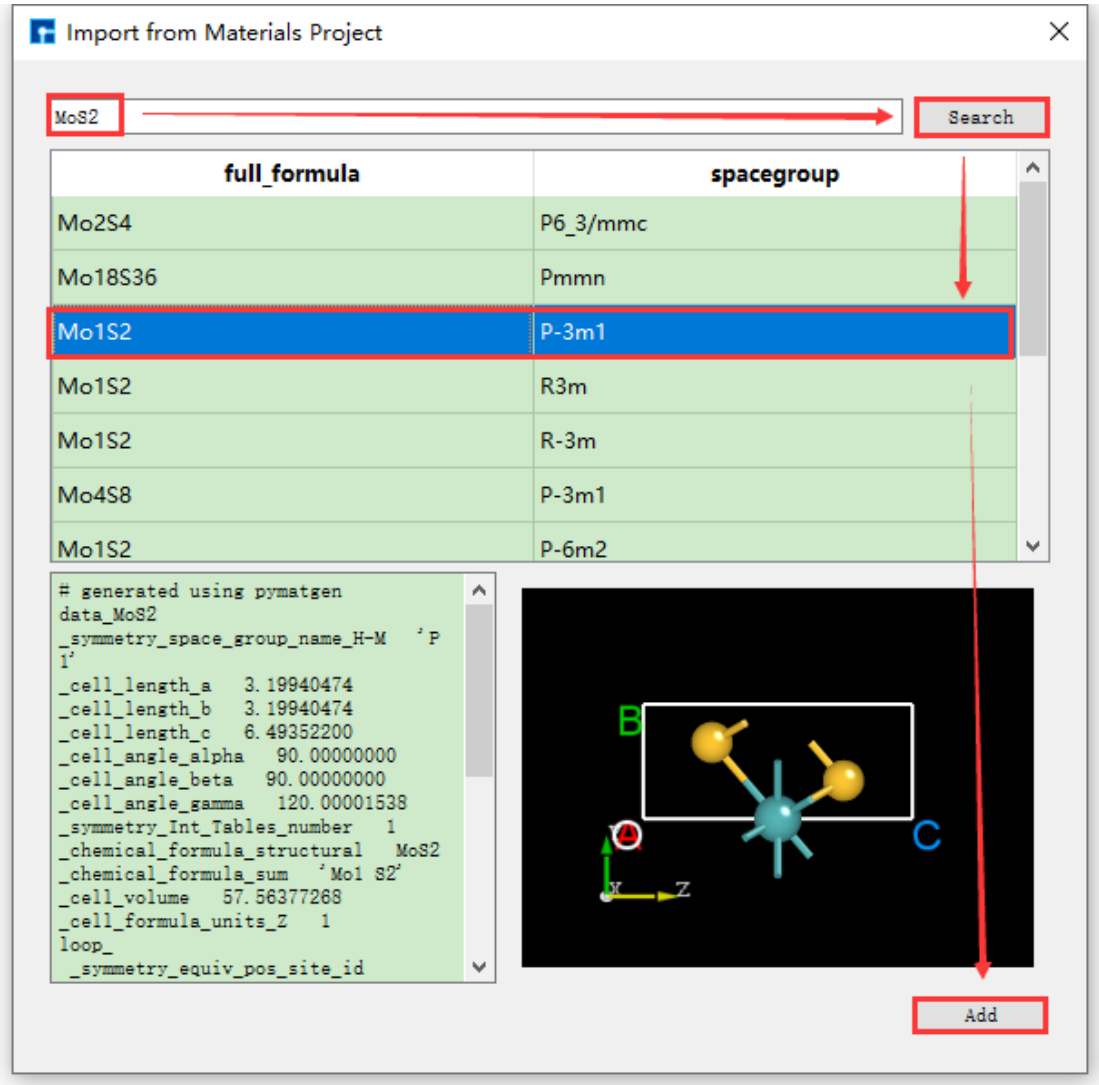


fig. 4.8: Materials Project chemical formula search and structure import operation interface

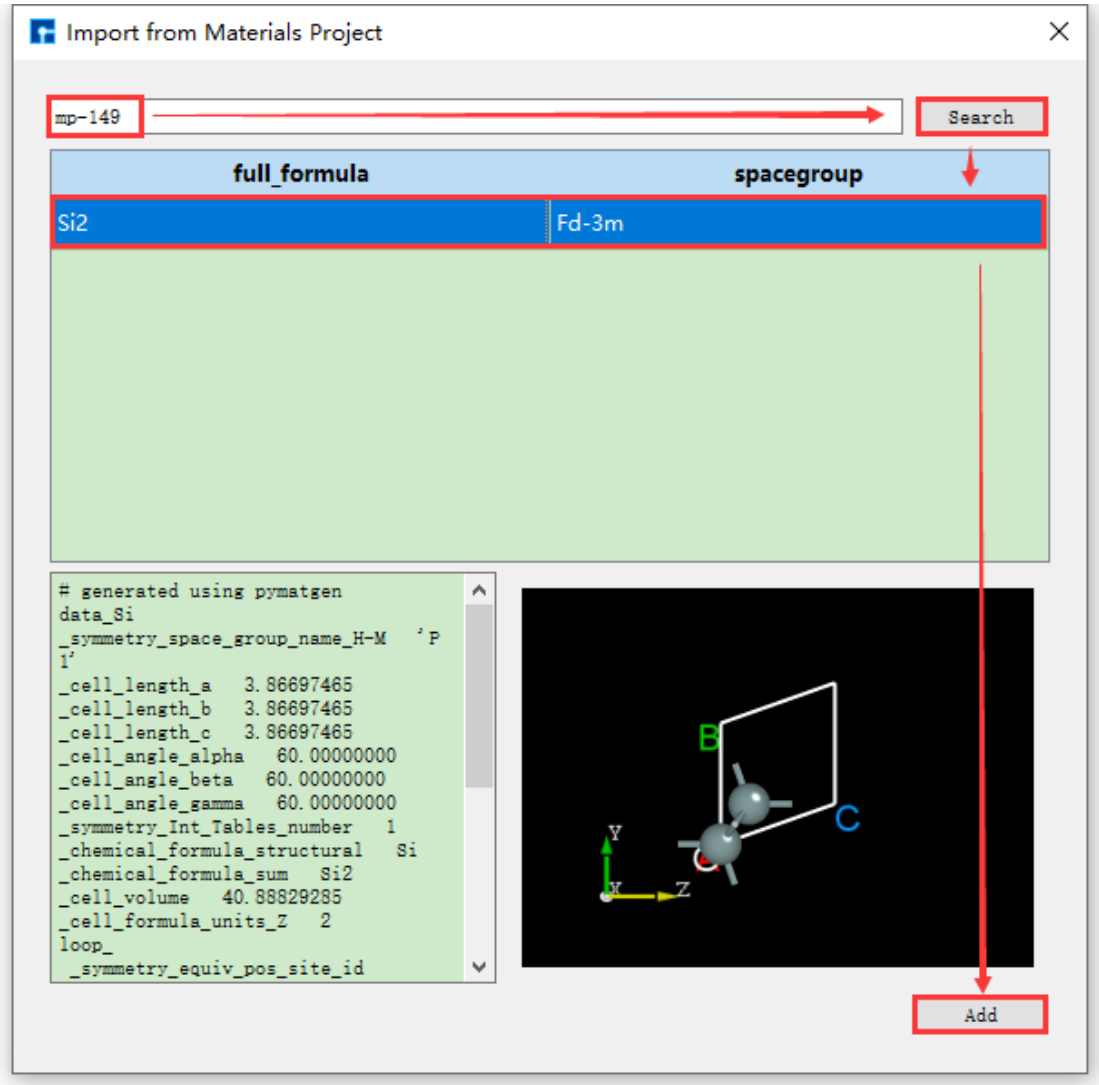


fig. 4.9: Materials Project mp number search and structure import operation interface

4.3 2D Molecular Modeling

Device Studio 2022A version adds the **2D Molecular Modeling** function. In the 2D molecular modeling interface, its toolbar contains various bonds and tools for drawing molecular structure formulas, including chemical bonds, ring templates, folded chains, boat structures, chair structures, arrows, borders, and text editing tools. Users can quickly and conveniently draw various 2D planar molecular structure formulas and write equations through this function, and it supports converting 2D molecular structures into 3D molecular structures.

Device Studio has the function of editing 2D molecular structures. Users can perform operations such as rotation, modifying bond width, bond length, bond position color, bond position type, bond position attribute conversion, adding hydrogen, removing hydrogen, adding charge, removing charge, etc. on the molecular structure.

Taking the construction of a 2D molecular structure with three connected benzene rings and its conversion to the corresponding 3D molecular structure as an example, the construction steps are shown in fig. 4.10, fig. 4.11, fig. 4.12, fig. 4.13, and fig. 4.14.

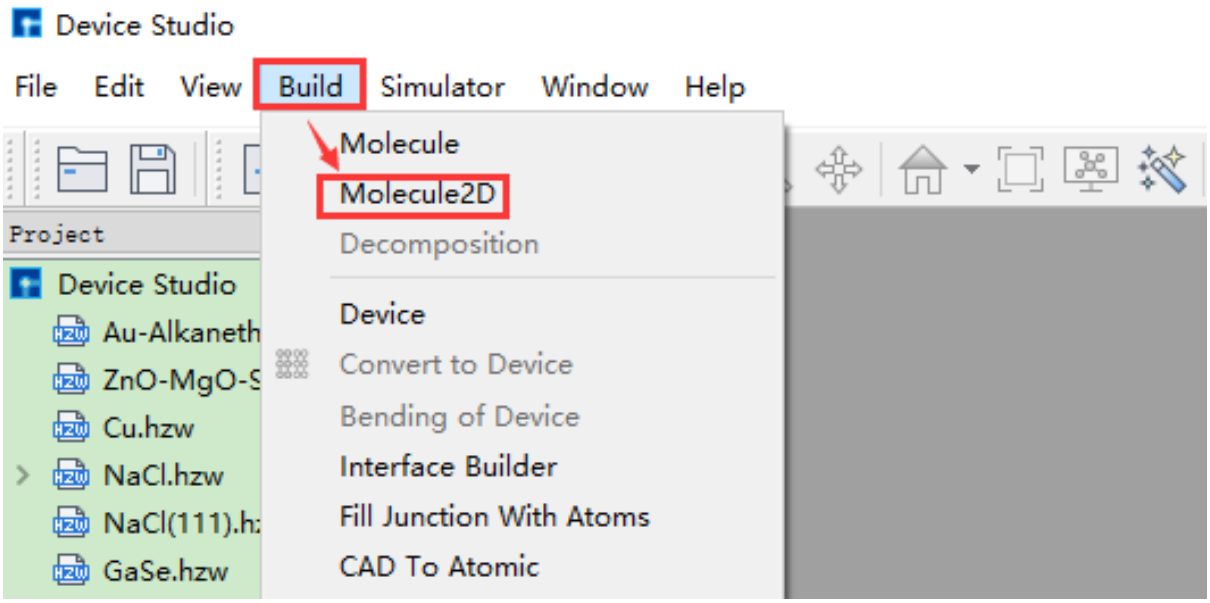


fig. 4.10: Pop-up 2D molecular modeling interface operation

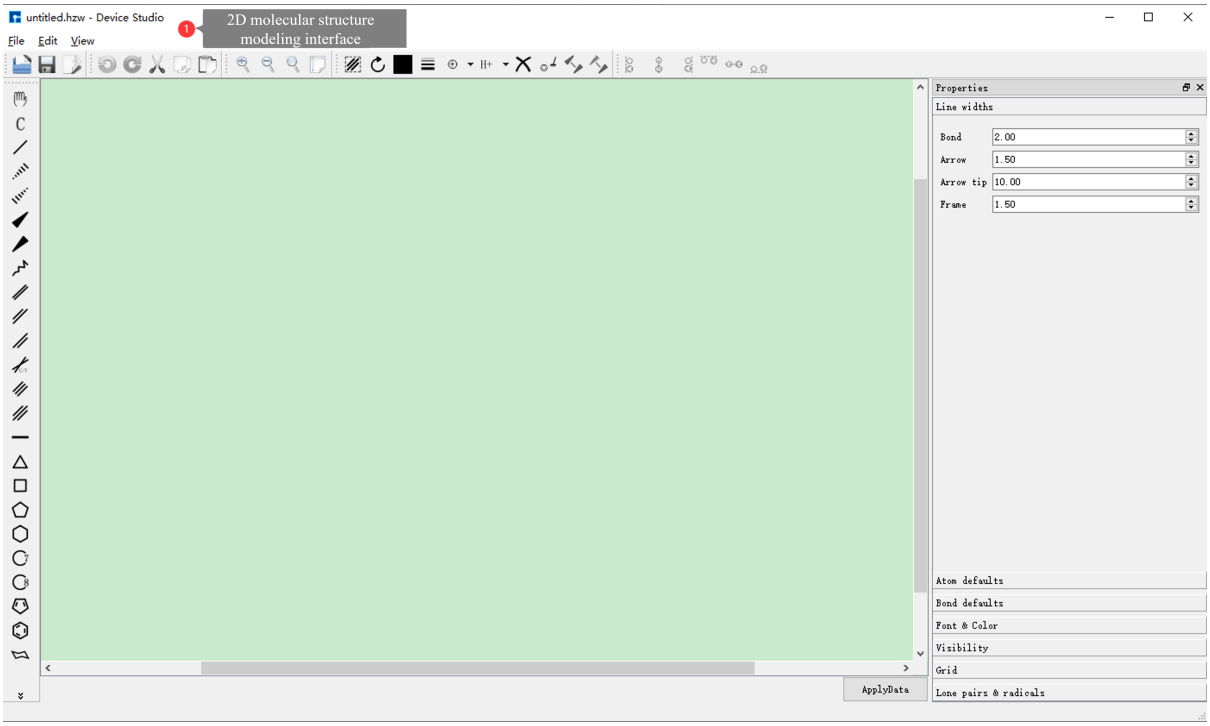


fig. 4.11: 2D molecular modeling interface

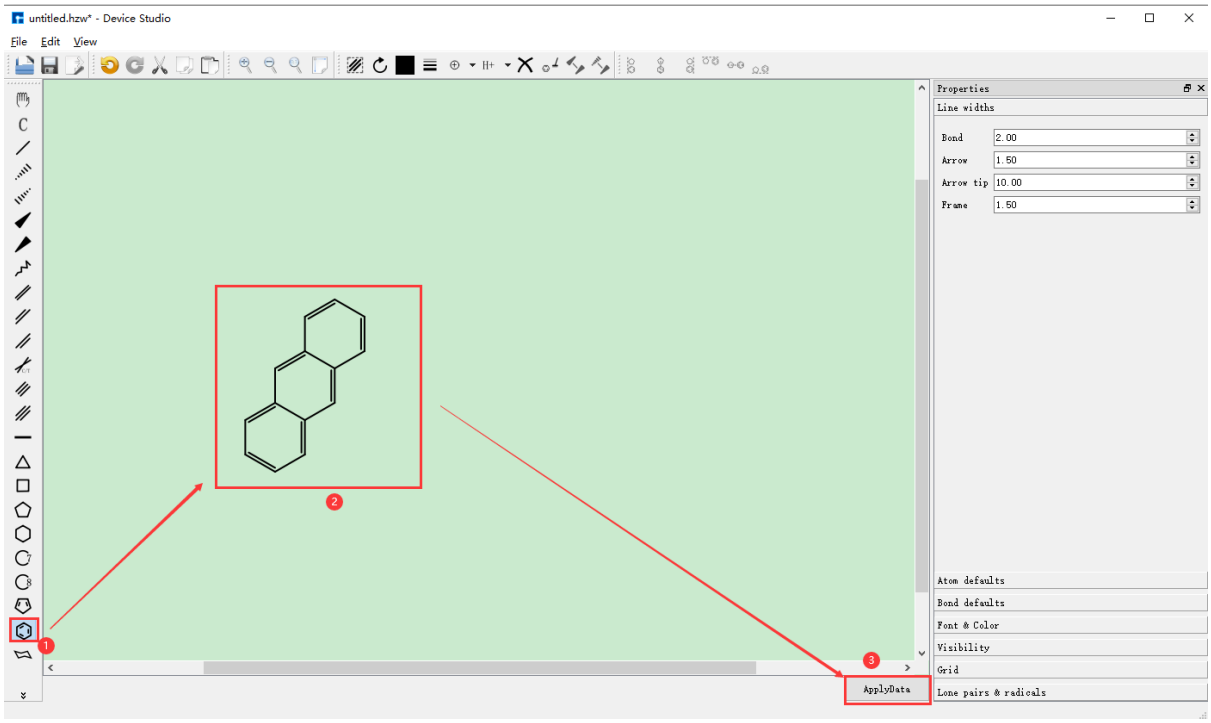


fig. 4.12: Building 2D molecular structure and converting to 3D molecular structure operation

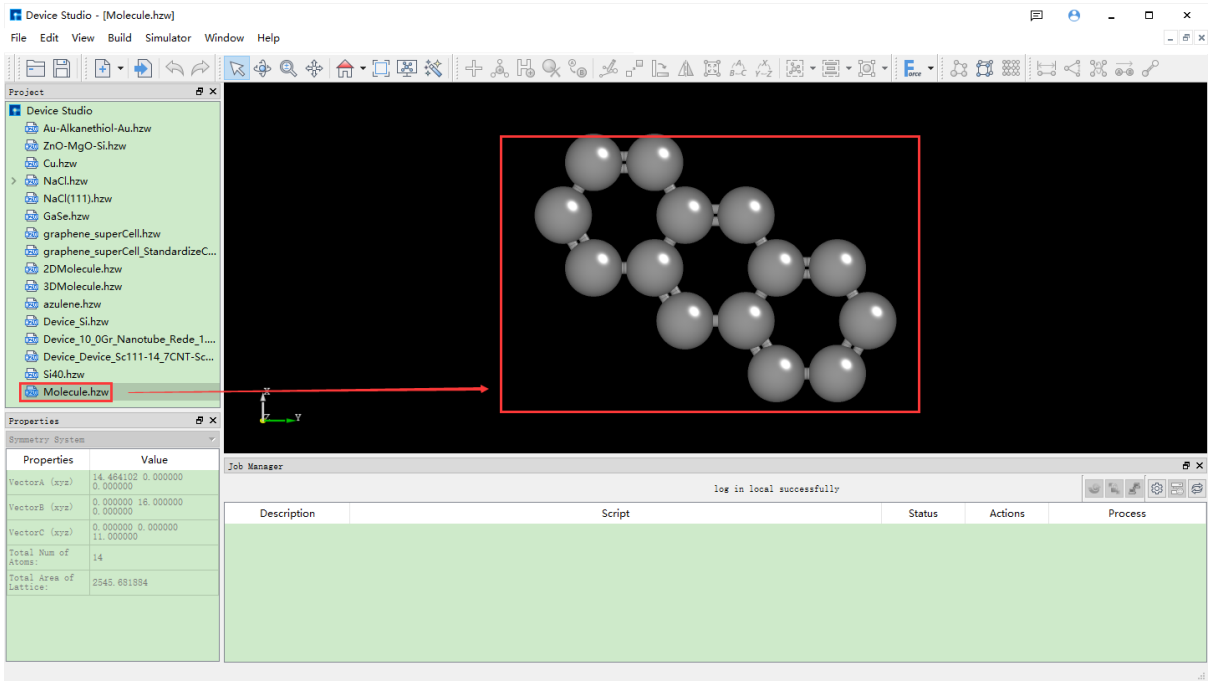


fig. 4.13: Device Studio interface after converting 2D molecular structure to 3D molecular structure

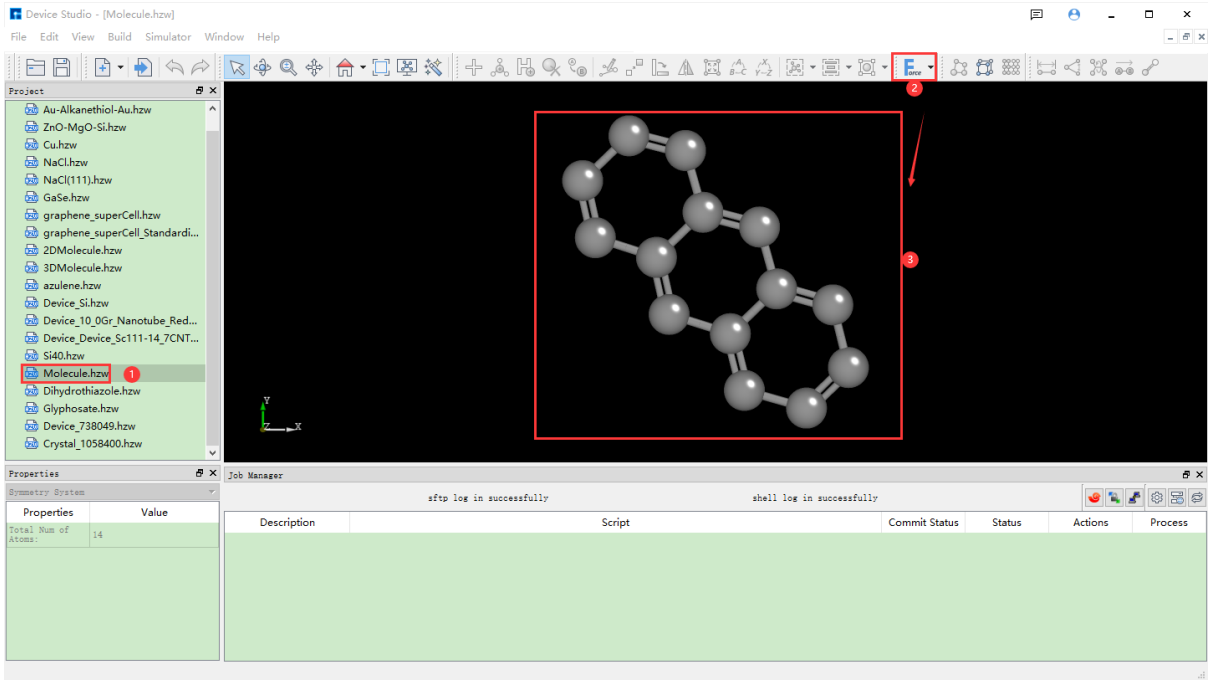


fig. 4.14: Optimizing converted 3D molecular structure operation

> **Note**
>
> The *Minimize Structure* labeled as ② in fig. 4.14 is for structural optimization of molecular structures through molecular force field calculations, defaulting to MMFF94. You can select an appropriate force field for structural optimization by clicking the dropdown button.

4.4 3D Molecular Modeling

Device Studio 2022A version adds the **3D Molecular Modeling** function. Users can quickly and conveniently build 3D molecular structures through this function. Device Studio supports editing 3D molecular structures and can view detailed information about atomic coordinates and bonds between atoms. It can perform a series of operations on molecular structures such as bond adjustment, atomic angle adjustment, dihedral angle adjustment, adding hydrogen, translation, rotation, renaming, copying fragments, adding, deleting, and modifying. The operation interface for building 3D molecular structures in Device Studio is shown in fig. 4.15, fig. 4.16, fig. 4.17, fig. 4.18, and fig. 4.19.

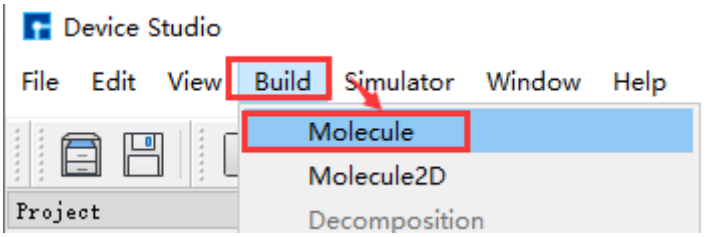


fig. 4.15: Pop-up 3D molecular modeling interface operation

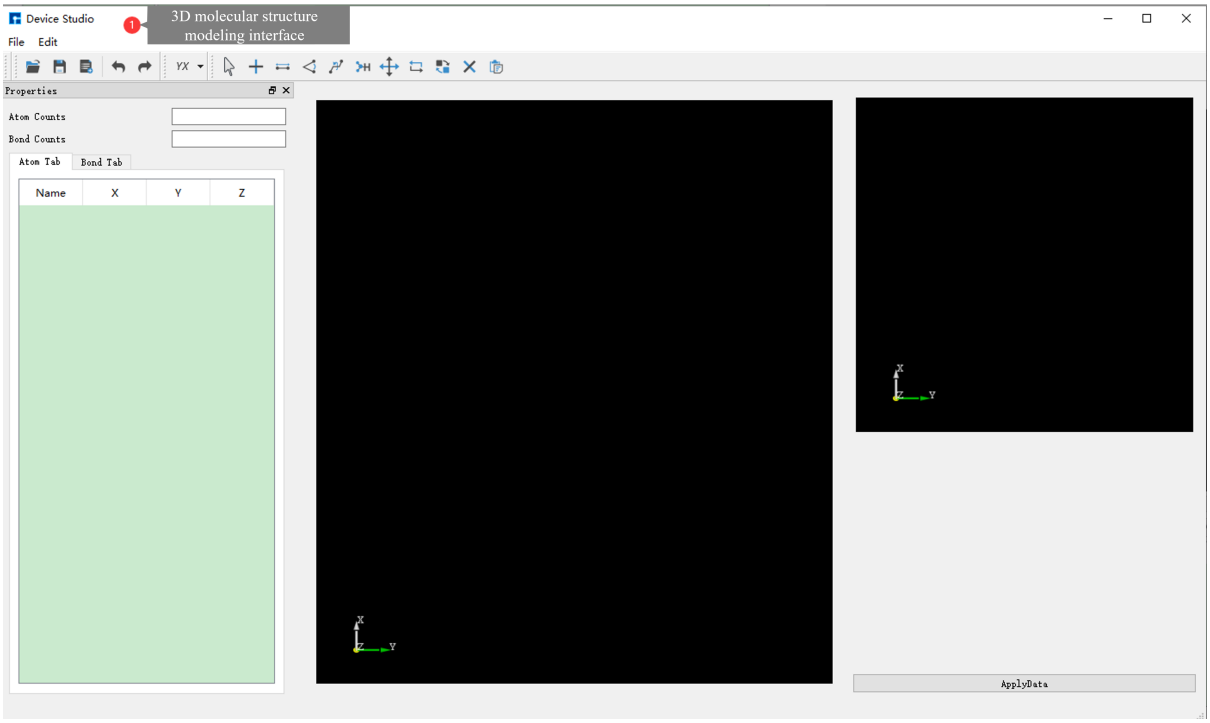


fig. 4.16: 3D molecular modeling interface

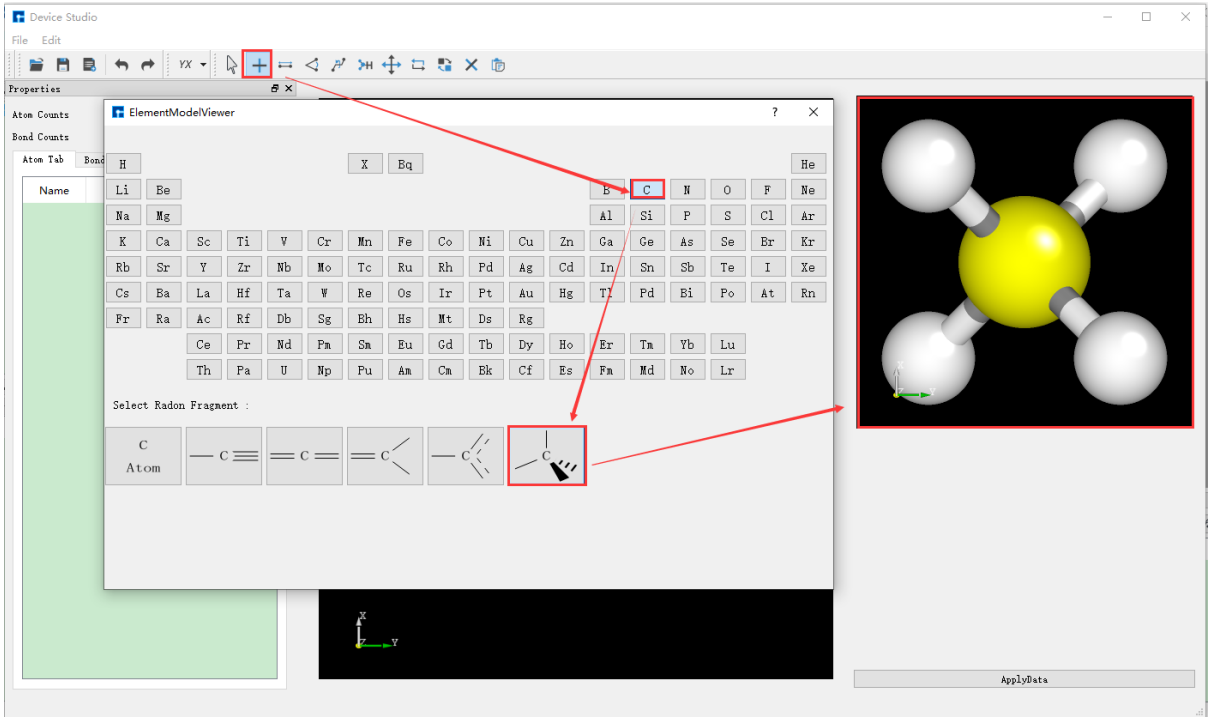


fig. 4.17: Building 3D molecular structure operation one

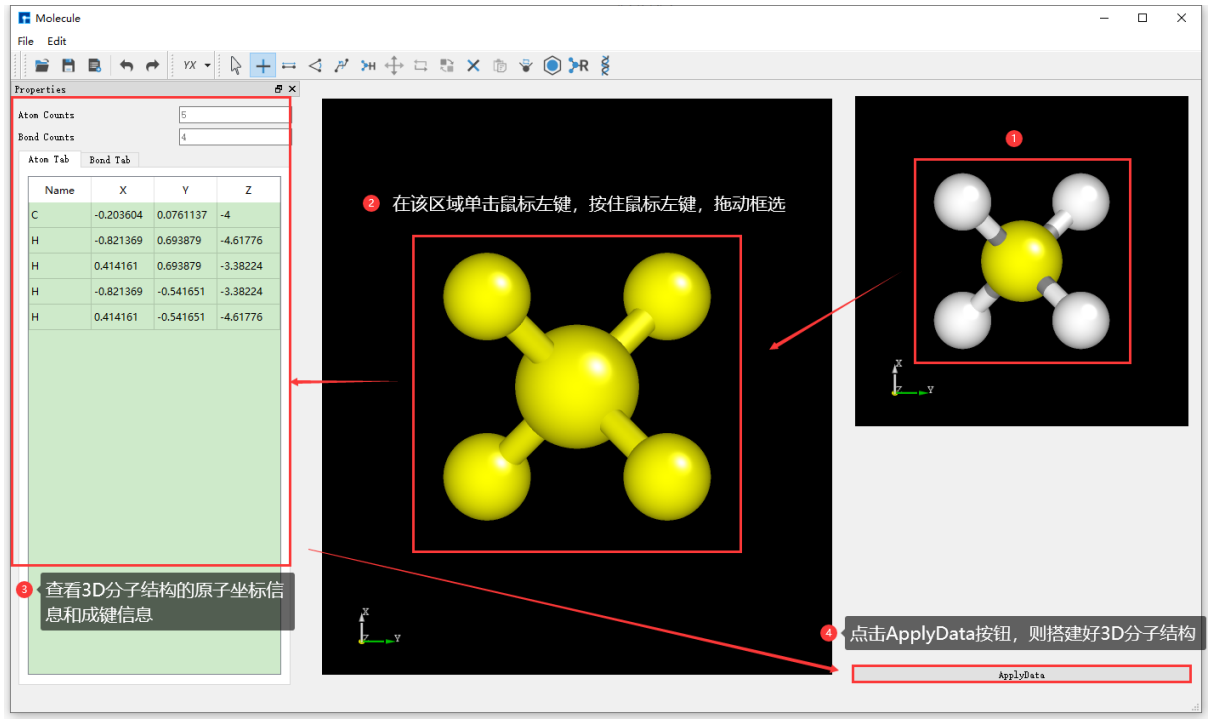


fig. 4.18: Building 3D molecular structure operation two

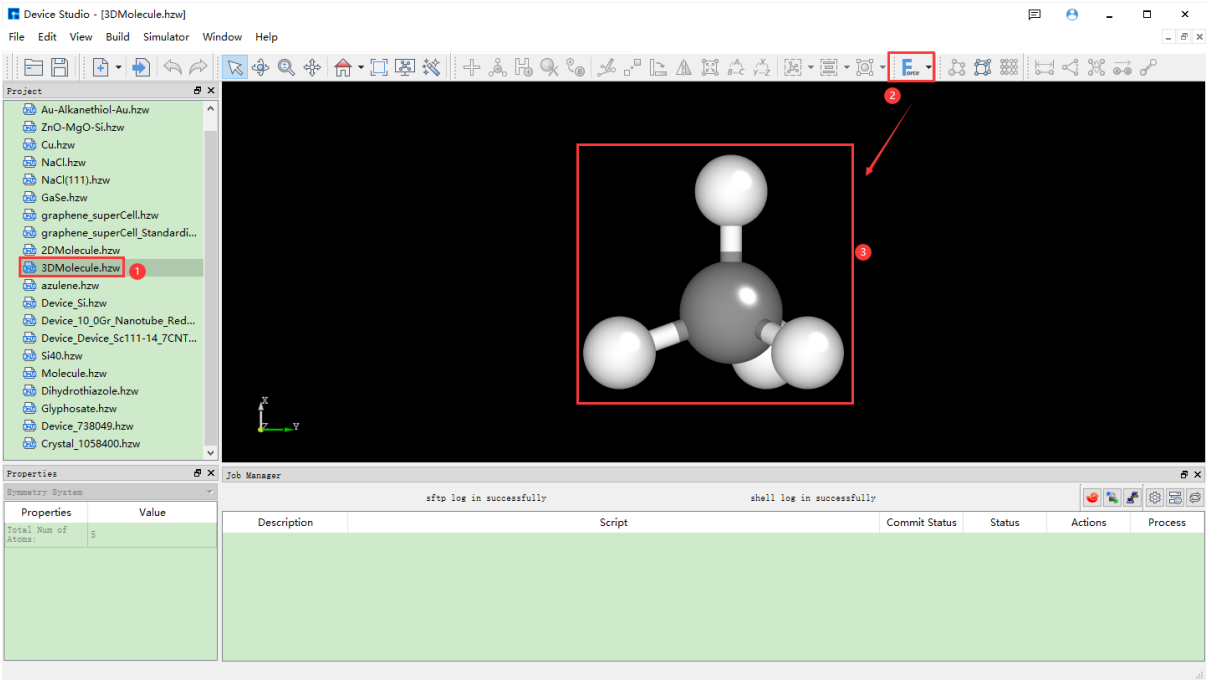


fig. 4.19: Optimizing built 3D molecular structure

4.5 Crystal Modeling

For crystal modeling, users can first search whether the structure exists in the local database or online database. If it exists, import it directly; if not, they can build it themselves or import a structure and build upon it. Users can choose how to build the crystal structure according to their needs.

Taking the construction of NaCl crystal structure as an example, click *Build* → *Crystal* in the Device Studio graphical interface, and the interface for building crystal structure pops up as shown in fig. 4.20.

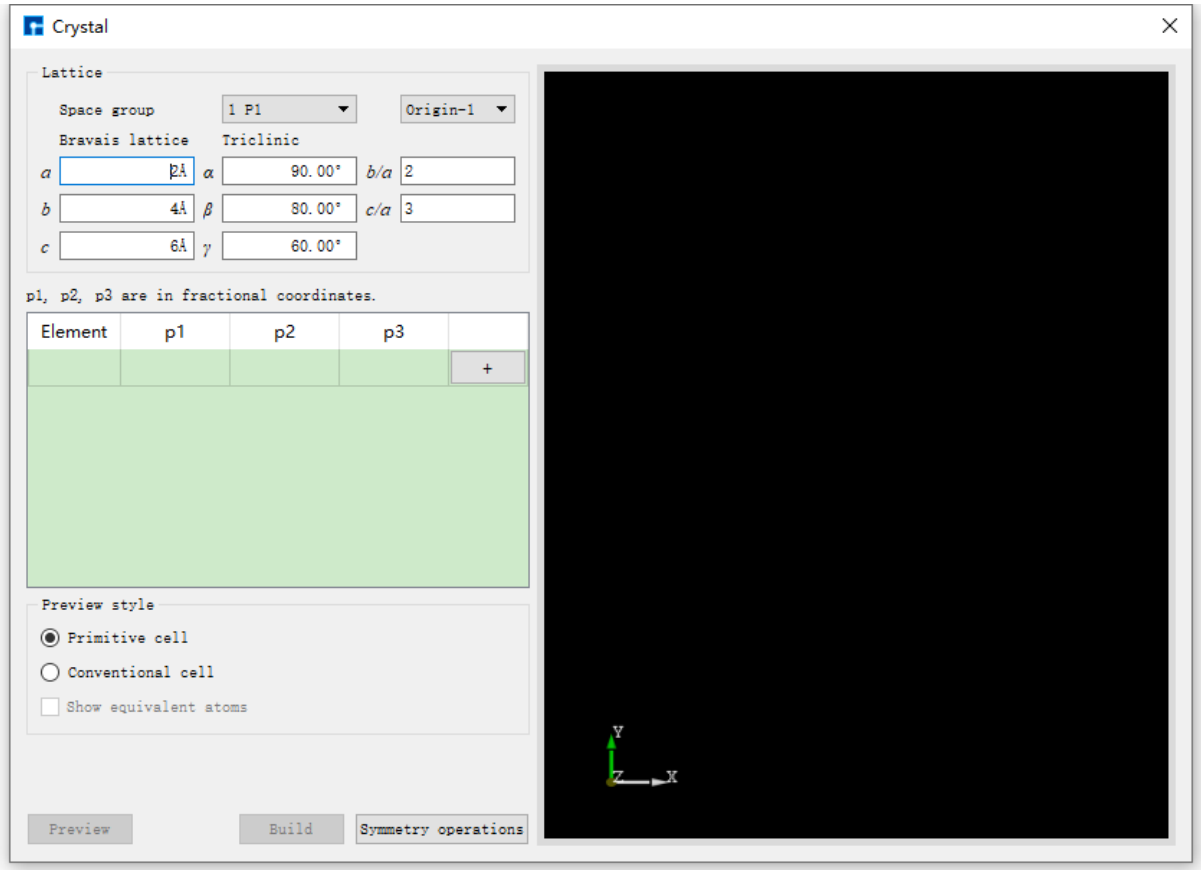


fig. 4.20: Crystal structure building interface

If you don't know the space group information of the NaCl crystal, when building the NaCl crystal structure in the interface shown in fig. 4.20, you can follow the red box selection and arrow direction shown in fig. 4.21, fill in or select the corresponding information step by step, click the *Preview* button to preview the built structure in the right area of the interface. This step is mainly used to check whether the built structure is correct and whether it is the desired structure. Then click *Build* to build the NaCl crystal structure. The structure file is saved in the software's project management area (Project Explorer), and you can view the 3D view of the structure in the 3D display area. Conversely, if you find that the built structure is incorrect during the preview process, you can rebuild it in the interface shown in fig. 4.20. During the structure building process, users can choose the *Preview style* in the interface according to their needs, that is, select *Primitive cell* or *Conventional cell*; choose whether to show equivalent position atoms, that is, whether to check *Show equivalent atoms*.

The p1, p2, p3 values of the NaCl crystal structure are shown in the following table:

Element	p1	p2	p3
Na	0	0	0
Na	0.5	0.5	0
Na	0.5	0	0.5
Na	0	0.5	0.5
Cl	0.5	0	0
Cl	0	0.5	0
Cl	0	0	0.5
Cl	0.5	0.5	0.5

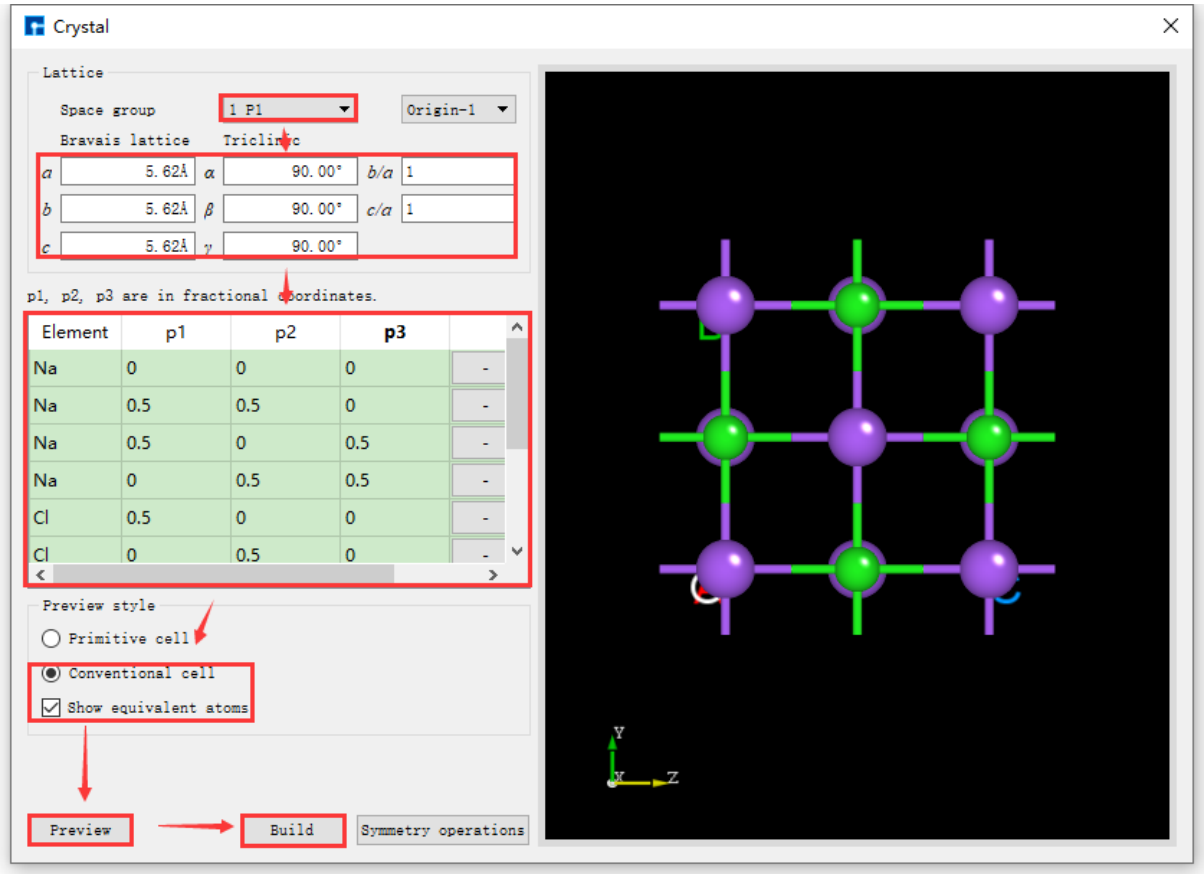


fig. 4.21: NaCl crystal structure building interface without space group information

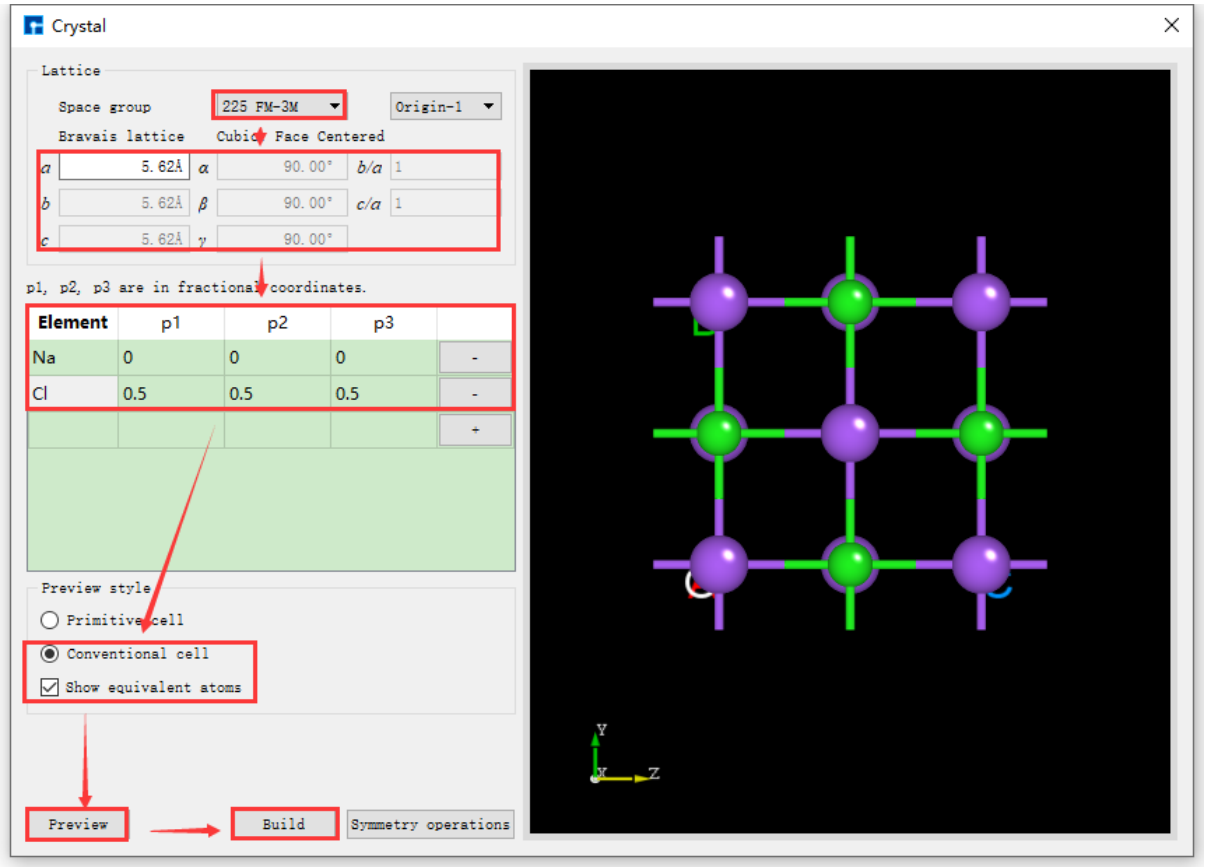


fig. 4.22: NaCl Crystal Structure Building Interface Based on Space Group Information

If the space group information of the structure is known, it can be built more conveniently and quickly. Device Studio supports the selection of 261 space groups (including 230 space groups and 31 extended subgroups). For example, the space group of NaCl crystal is `225 FM-3M`. Knowing this information, when building the NaCl crystal in the interface shown in fig. 4.20, you can fill in the corresponding information as indicated by the red box and arrow in fig. 4.22. Other operations are consistent with those without knowing the space group information and will not be described in detail here. Comparing fig. 4.21 and fig. 4.22, it is clear that knowing the space group information can simplify the construction of the crystal structure.

Figures fig. 4.21 and fig. 4.22 both show the result of displaying equivalent atoms when building the NaCl crystal structure, i.e., with the *Show equivalent atoms* option checked. If this option is unchecked, the interface will appear as shown in fig. 4.23. Clicking the *Build* button in the interface will build the NaCl crystal structure. The structure file is saved in the software's project management area, and a 3D view of the structure is displayed in the 3D display area. The interface after building the NaCl crystal structure is shown in fig. 4.24.

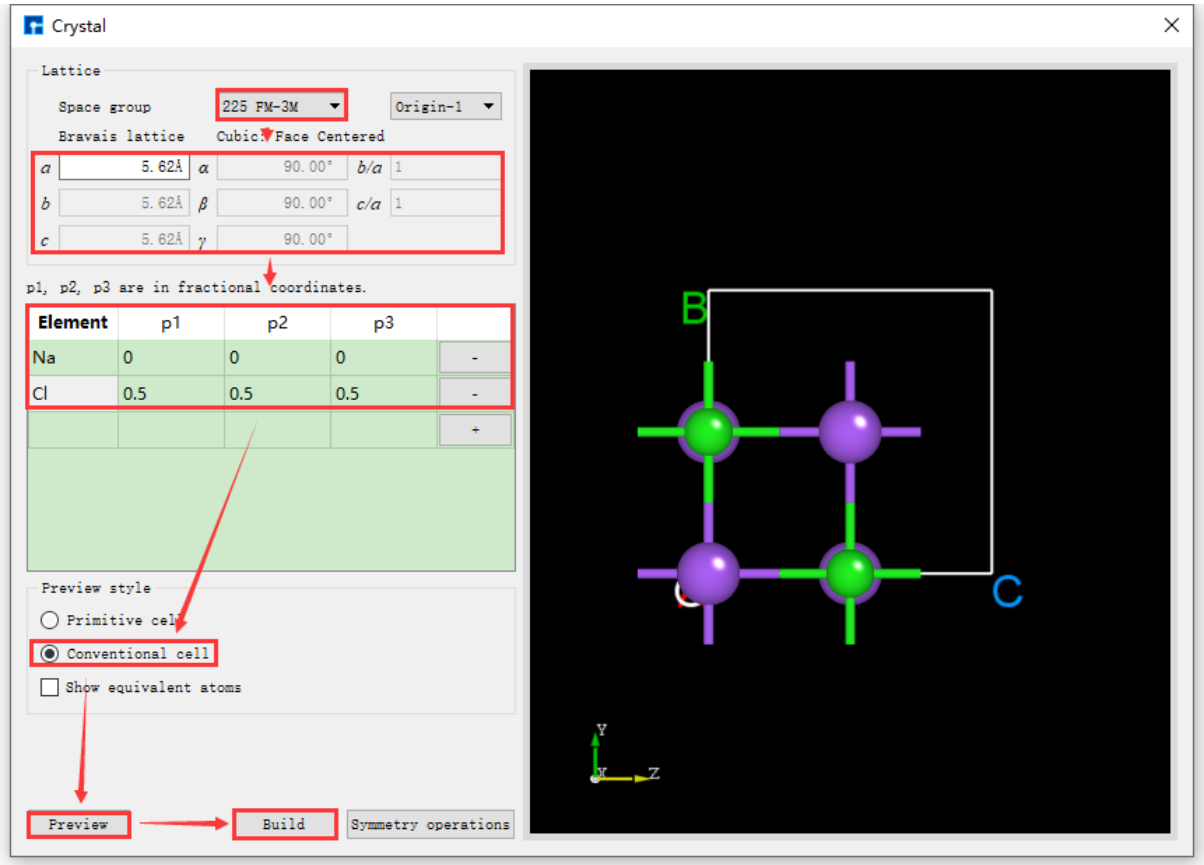


fig. 4.23: NaCl Crystal Structure Building Interface Without Equivalent Position Atoms Displayed

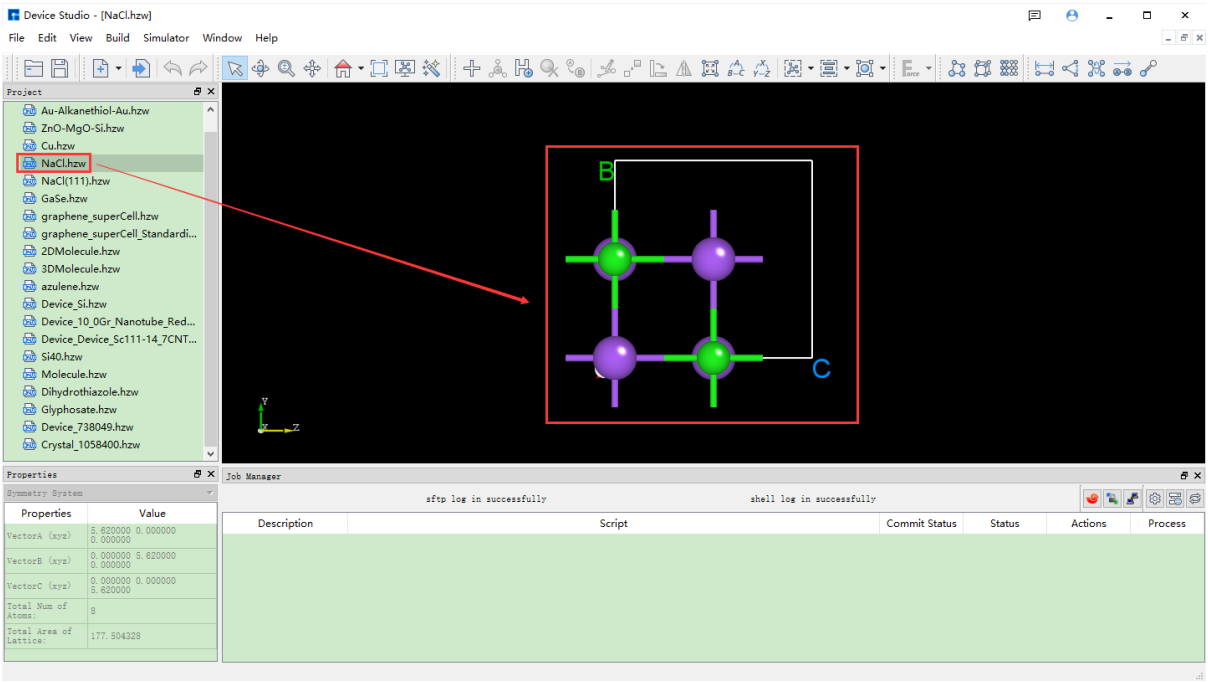


fig. 4.24: Device Studio Interface for Building NaCl Crystal Structure

4.6 Sections/Slices of Crystal Structure

Surface/Slab from Crystal Structure, this function is only available when a crystal structure exists. Taking the NaCl crystal structure built in the Crystal Modeling section as an example, to build a NaCl (1 1 1) crystal structure with a Thickness of 9.73 Å, click *Build* → *Surface/Slab* in the interface shown in fig. 4.24. The interface for building the surface/slab of the NaCl crystal structure will pop up as shown in fig. 4.25.

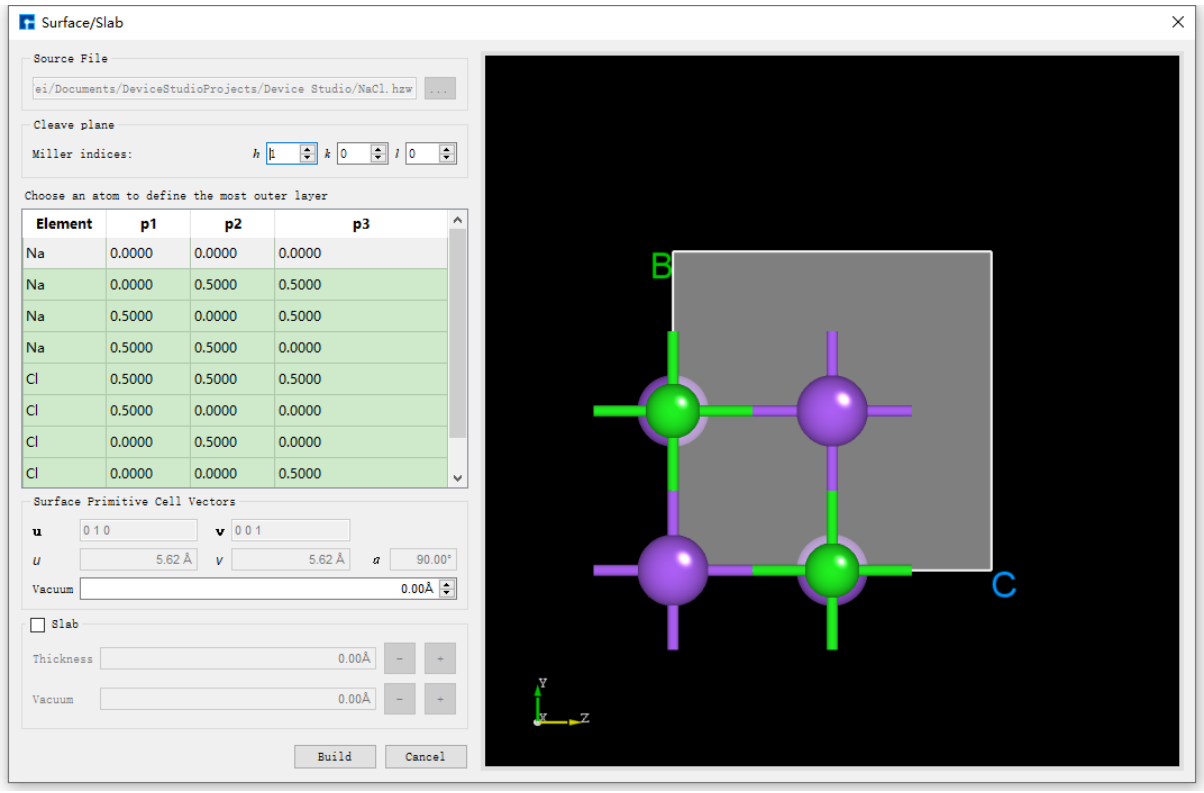


fig. 4.25: The interface for creating a slab/slice of the NaCl crystal structure

As shown in the red box and arrow in fig. 4.26, set the Miller index (1 1 1) in the interface shown in fig. 4.25. Select the Na (0.5000 0.5000 0.0000) atom as the starting atom for the slab in the dropdown table. Check the *Slab* box and click the + button after Thickness 5 times to set the Thickness to 9.73 Å. The structure can be previewed in the right panel. Click *Build* to build the 9.73 Å thick NaCl (1 1 1) crystal structure. The structure file is mounted in the Device Studio project management area, and the 3D view is displayed in the Device Studio 3D display area. The Device Studio interface after building the 9.73 Å thick NaCl (1 1 1) crystal structure is shown in fig. 4.27.

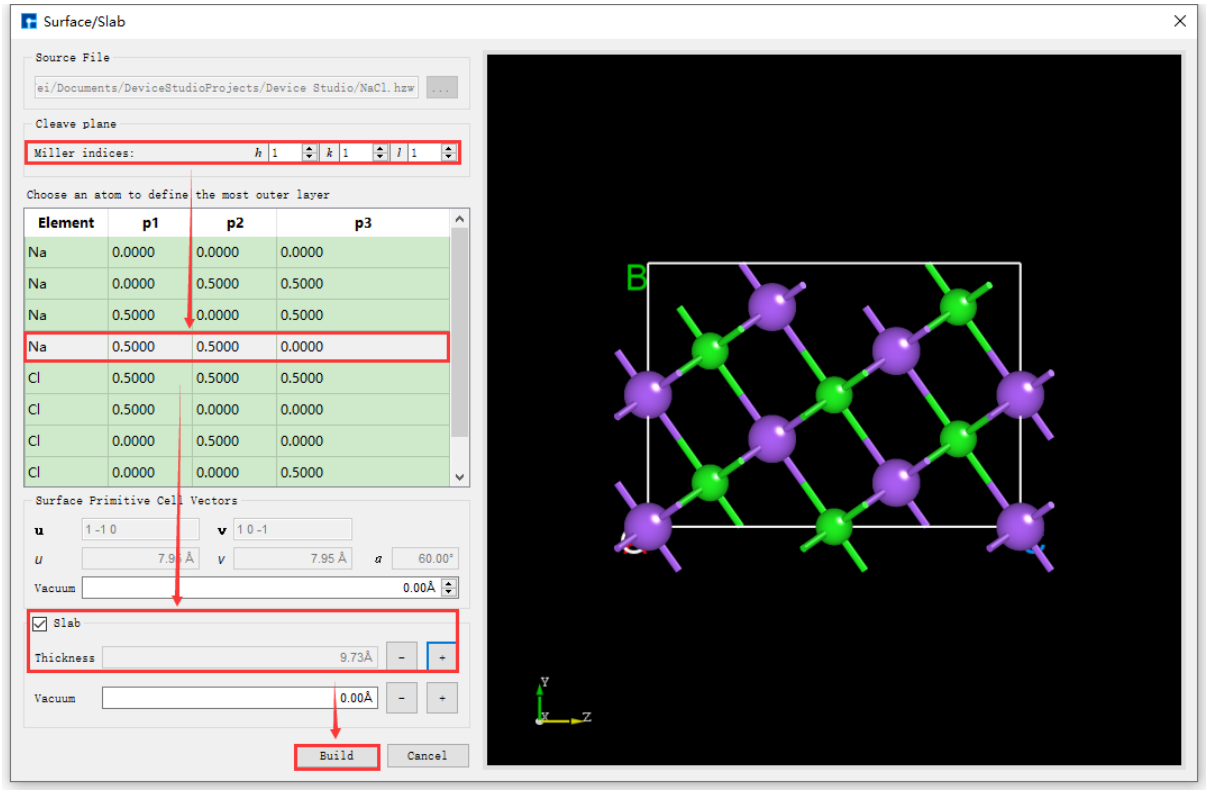


fig. 4.26: User interface for building a NaCl (1 1 1) crystal structure with a thickness of 9.73 Å.

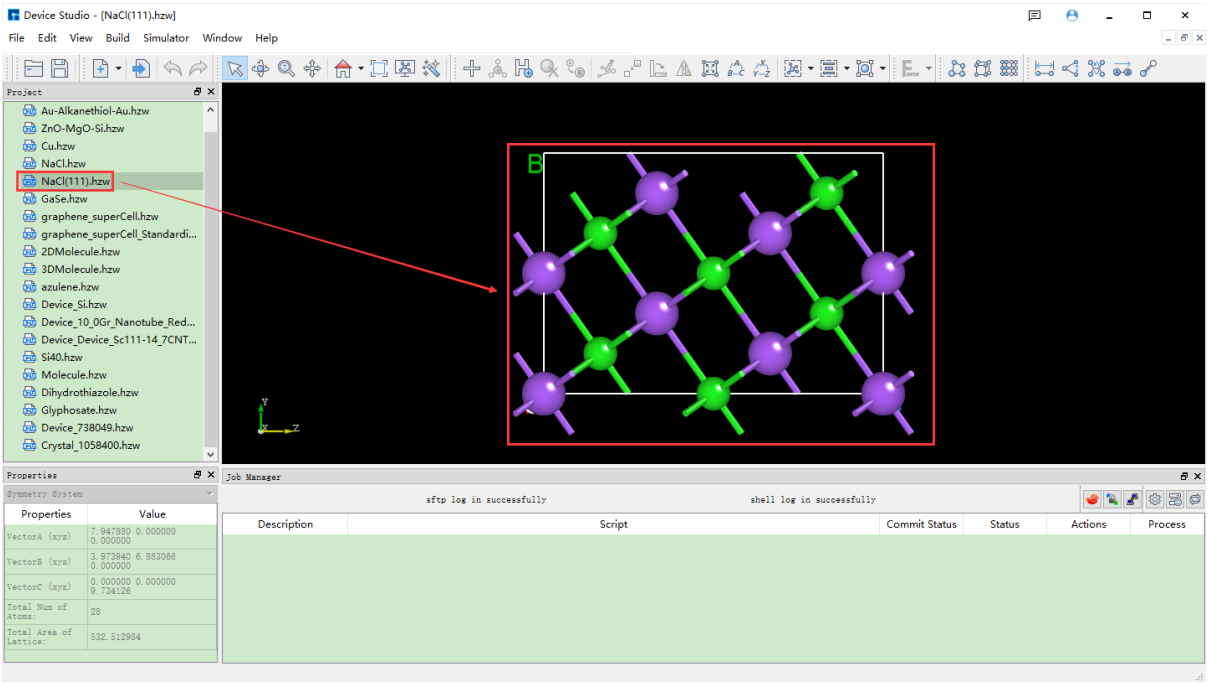


fig. 4.27: Set up the Device Studio interface for a NaCl (1 1 1) crystal structure with a Thickness of 9.73 Å.

4.7 Redefinition of the Unit Cell in Crystal Structures

After importing the Cu unit cell structure into Device Studio, the interface is shown as fig. 4.28. Click *Build* → *Redefine Crystal* in the interface to open the Cu unit cell structure crystal redefinition interface, as shown in fig. 4.29. Fill in the parameters according to the red boxed area in fig. 4.30. After filling in the parameters, click the *Preview* button to preview the supercell structure on the right side of the interface. Then, click the *Build* button to expand the Cu unit cell into a single cell. Simultaneously, the structure file `Cu_Rede.hzw` is mounted in the Device Studio project management area, and the 3D view of the structure is displayed in the Device Studio 3D display area, as shown in fig. 4.31.

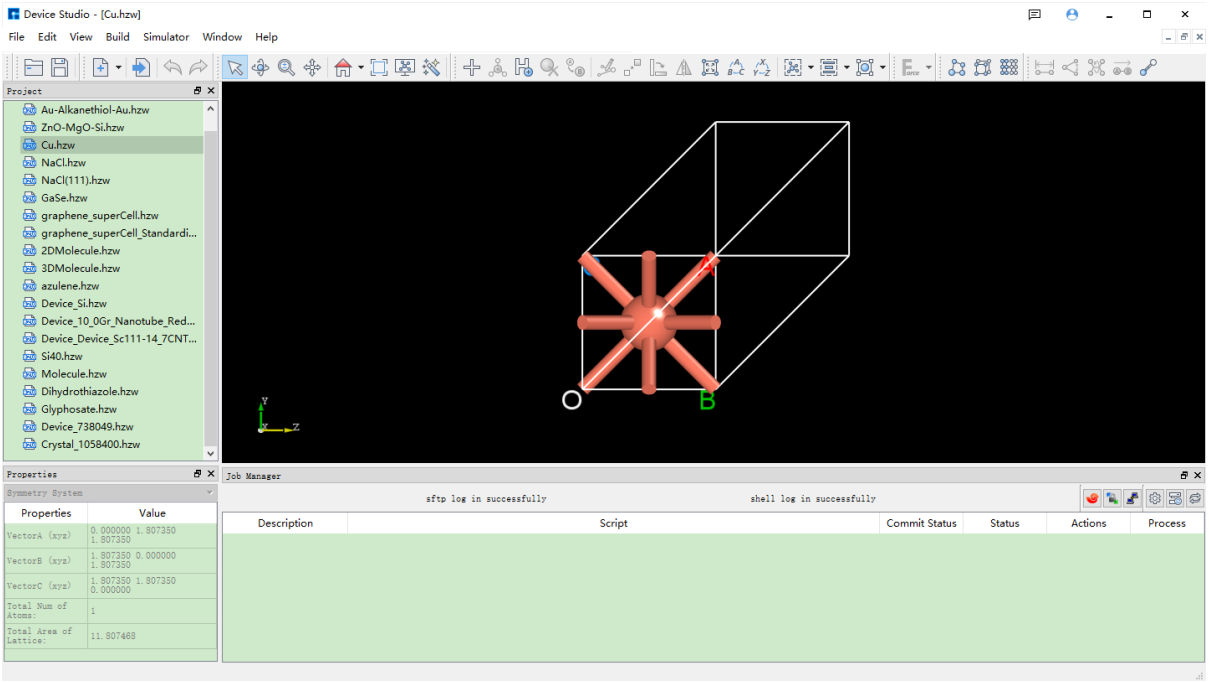


fig. 4.28: Device Studio interface after importing the Cu unit cell structure (`Cu.hzw`)

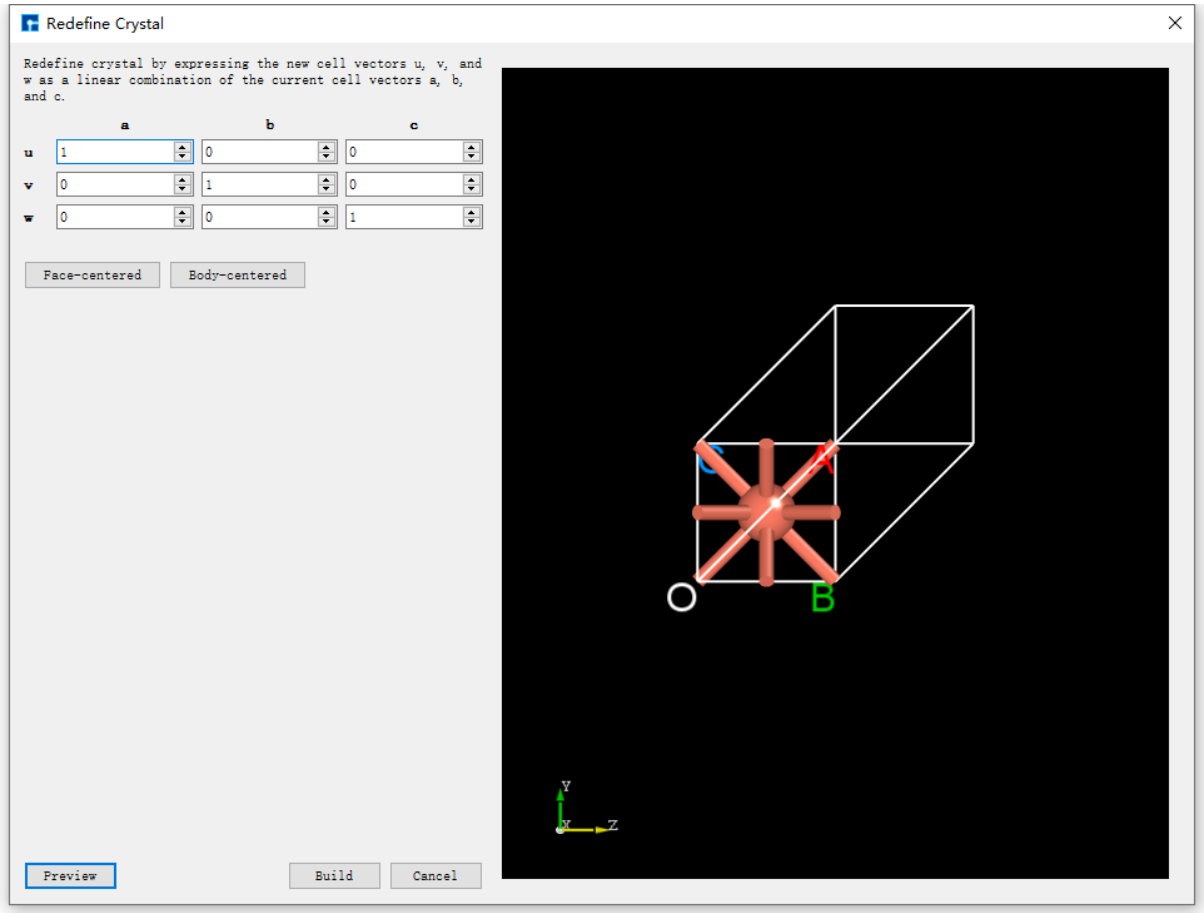


fig. 4.29: Cu Unit Cell Structure Redefinition Interface

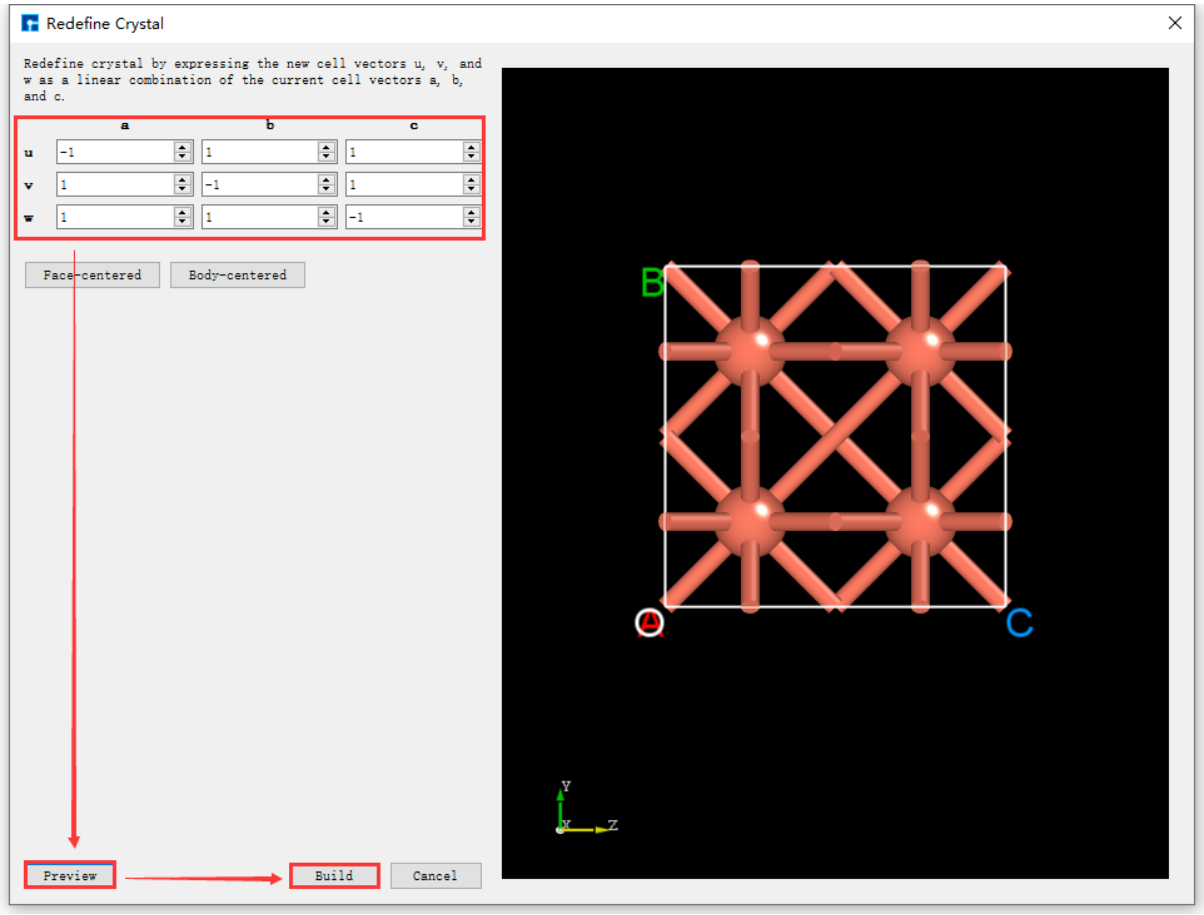


fig. 4.30: The interface for expanding the Cu unit cell structure into a supercell.

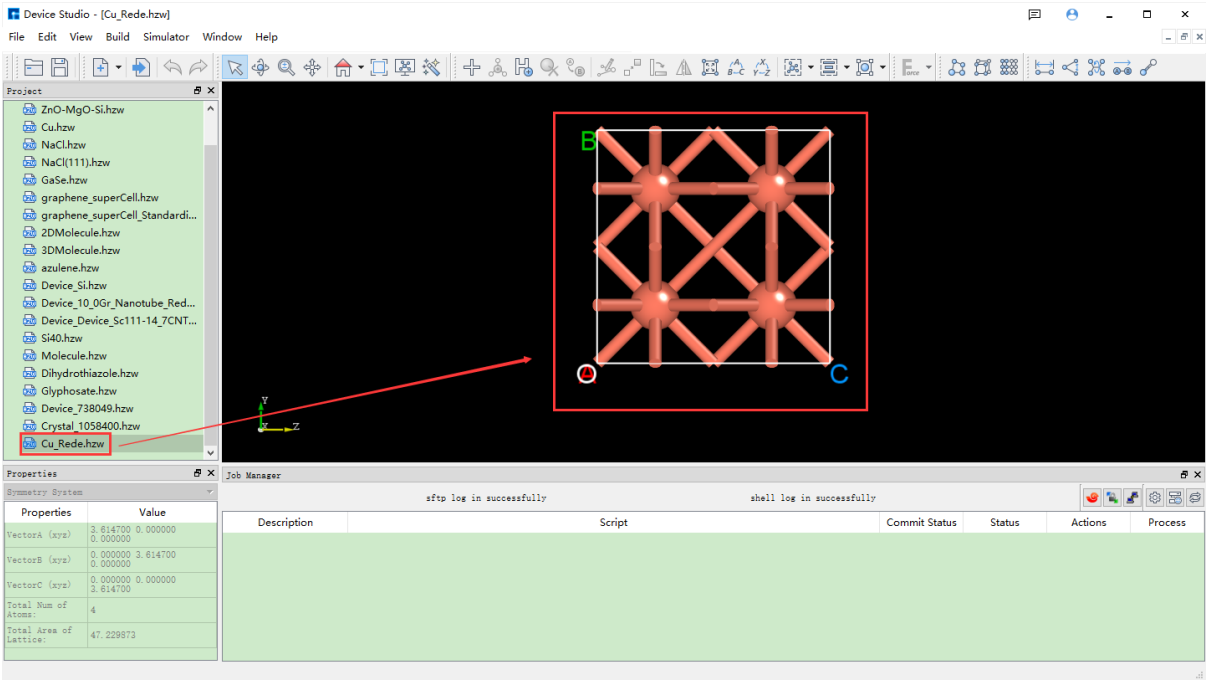


fig. 4.31: 3D view of the Cu unit cell (`Cu_Rede.hzw`) in Device Studio

The supercell can be built from the unit cell by using the "Redefine Crystal"function in Device Studio. The operation is the same as expanding the Cu primitive cell to a unit cell. For example, to expand the Cu unit cell to a 4x4x4 supercell, click fig. 4.31 *Build* → *Redefine Crystal*. The "Redefine Crystal"interface will pop up, as shown in fig. 4.32. Follow the steps indicated by the red boxes and arrows in fig. 4.32. After clicking the *Build* button, the Cu unit cell will be expanded to a 4x4x4 supercell. The structure file `Cu_Rede_Rede.hzw` will be mounted in the project management area of Device Studio, and the 3D view of the structure will be displayed in the 3D display area of Device Studio, as shown in fig. 4.33.

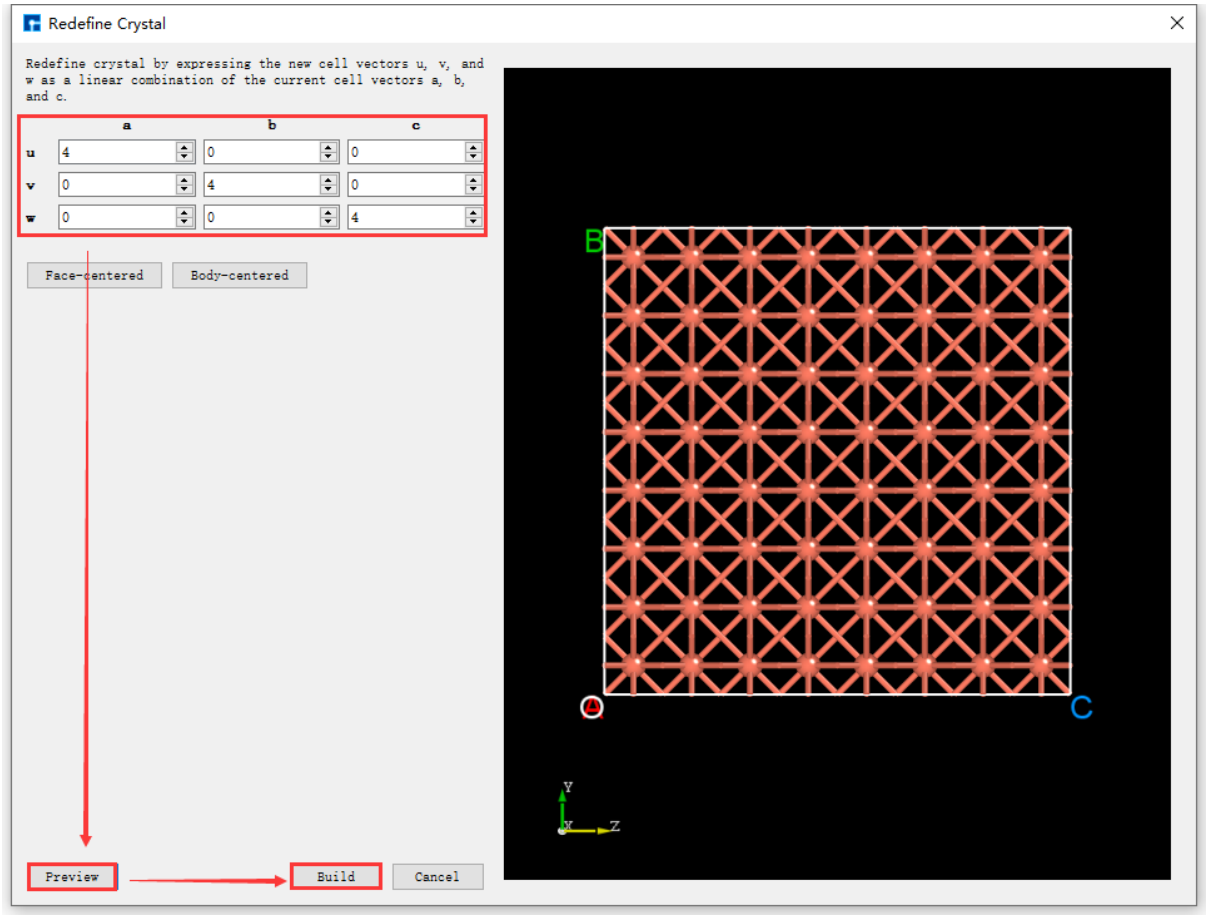


fig. 4.32: Interface for expanding the Cu unit cell to a 4x4x4 supercell

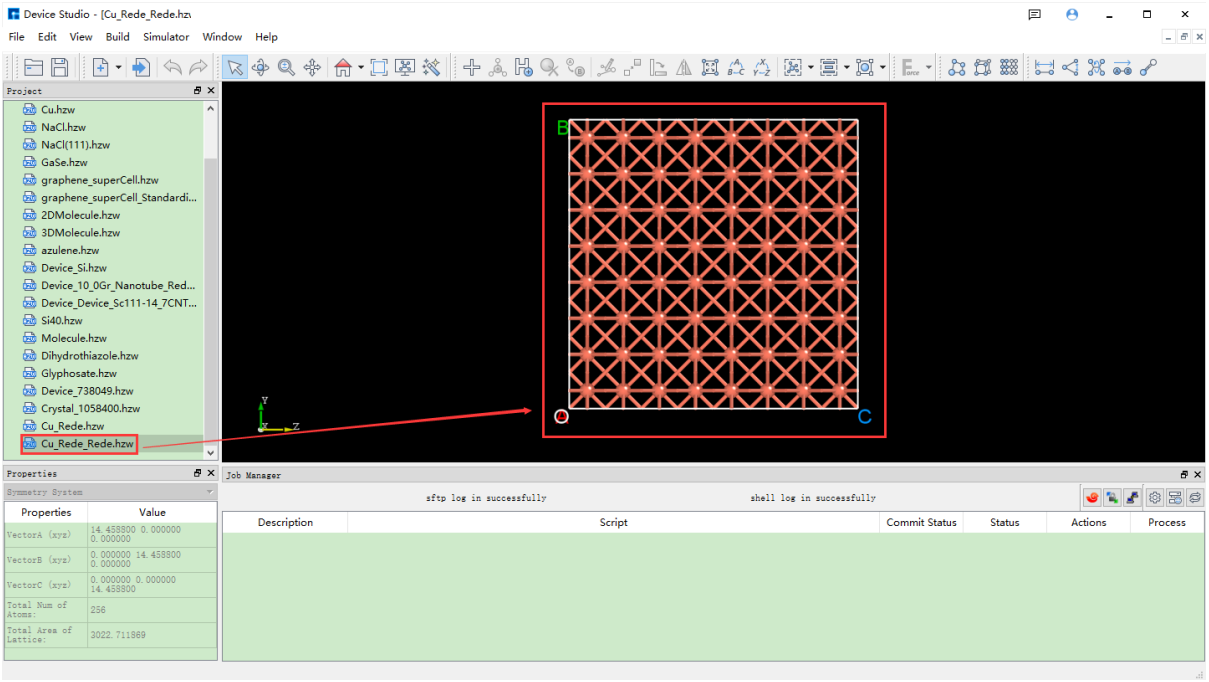


fig. 4.33: 3D view of the Cu supercell (`Cu_Rede_Rede.hzw`) structure in Device Studio

4.8 Device Modeling

Taking the construction of a gold-alkanethiol-gold (Au-Alkanethiol-Au) molecular device structure as an example, the following steps will detail the construction process.

4.8.1 Importing the Au Crystal Structure

***Import the Au crystal structure from the Device Studio local database**, i.e., import the Au primitive cell. The import process is not described in detail here; users can refer to local_database_import_structure. The interface after importing the Au crystal structure is shown in fig. 4.34.

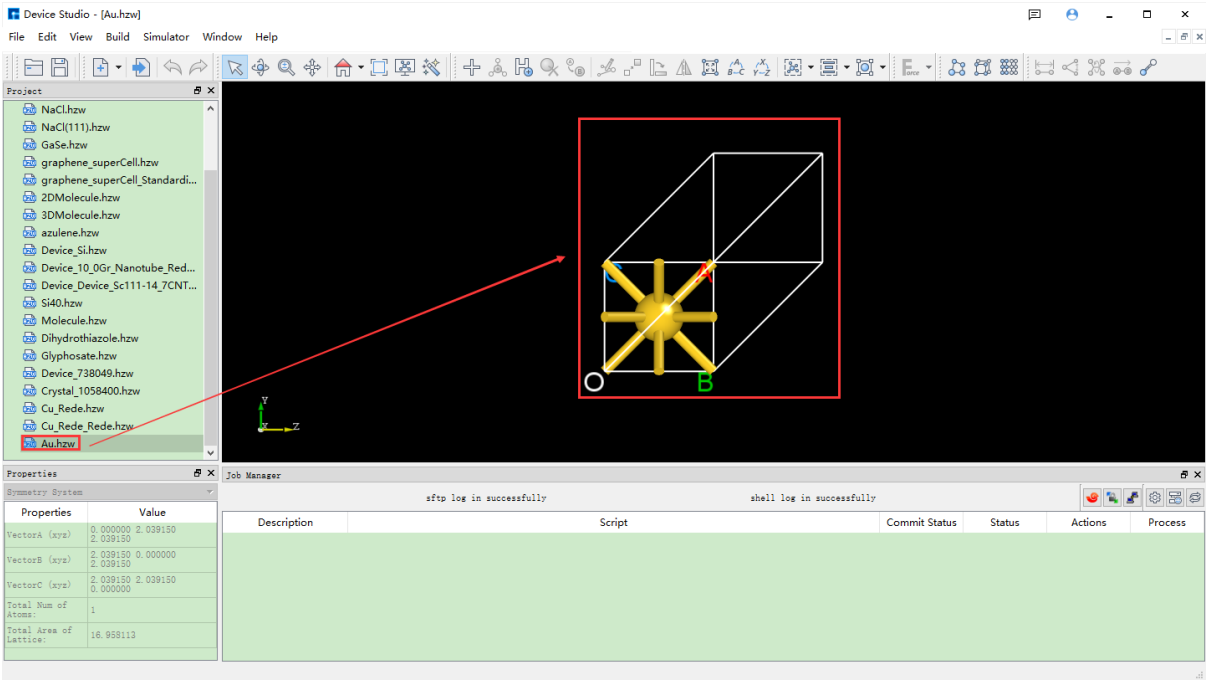


fig. 4.34: Interface after importing the Au crystal structure

4.8.2 Converting an Au primitive cell to an Au conventional cell

Click *Build* → *Redefine Crystal* in fig. 4.34, which will pop up the Redefine Crystal interface as shown in fig. 4.35. Click *Face-centered* → *Preview* in fig. 4.35, and the interface will change as shown in fig. 4.36. Users can preview the converted structure in the right area of fig. 4.36. After clicking *Build*, the Au primitive cell will be converted into an Au crystal cell. The structure file is saved in the software's project management area (Project Explorer), and a 3D view of the structure can be seen in the 3D display area, as shown in fig. 4.37. `Au.hzw` in fig. 4.37 corresponds to the Au primitive cell, and `Au_Rede.hzw` corresponds to the Au crystal cell. Users can select the structure file according to their computational needs, right-click and select *Rename* to rename the structure file.

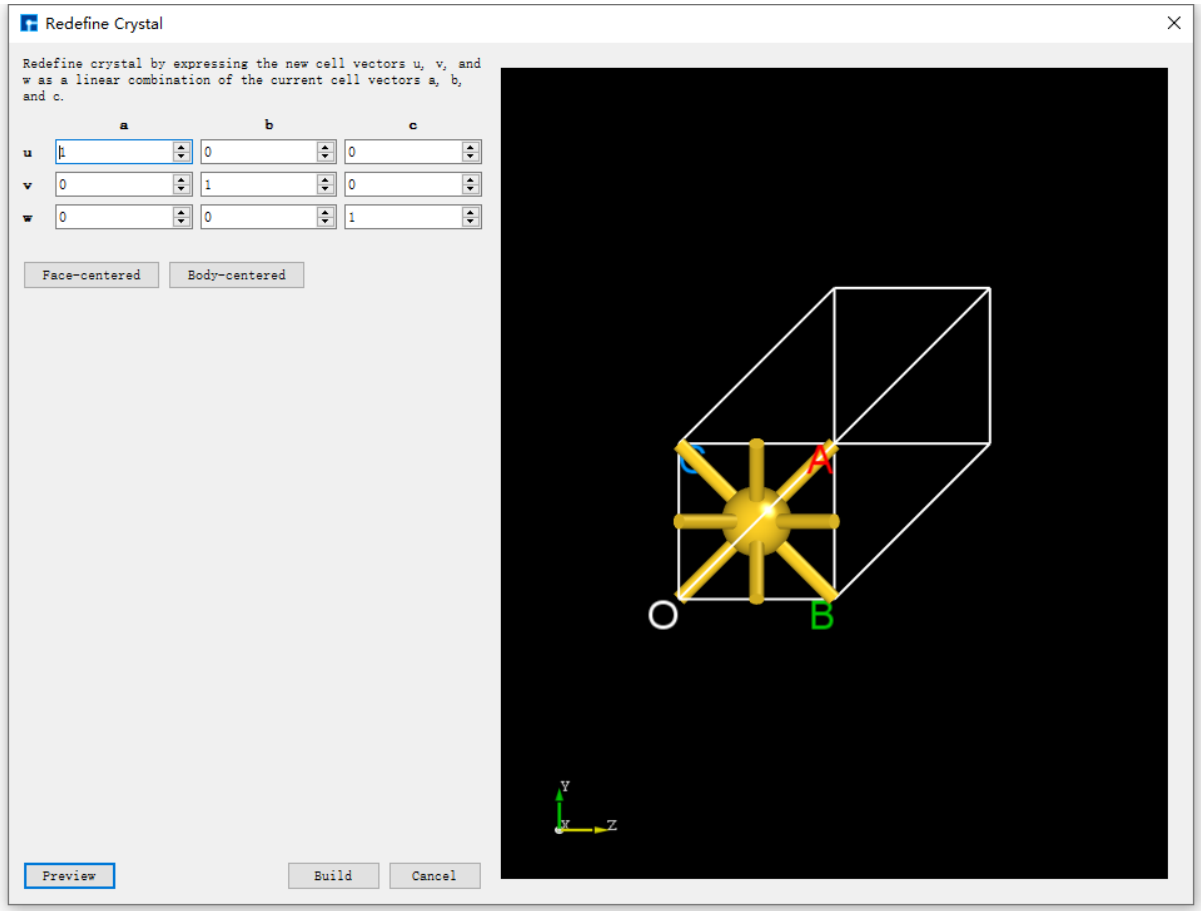


fig. 4.35: Redefine Crystal Interface for Au Unit Cell

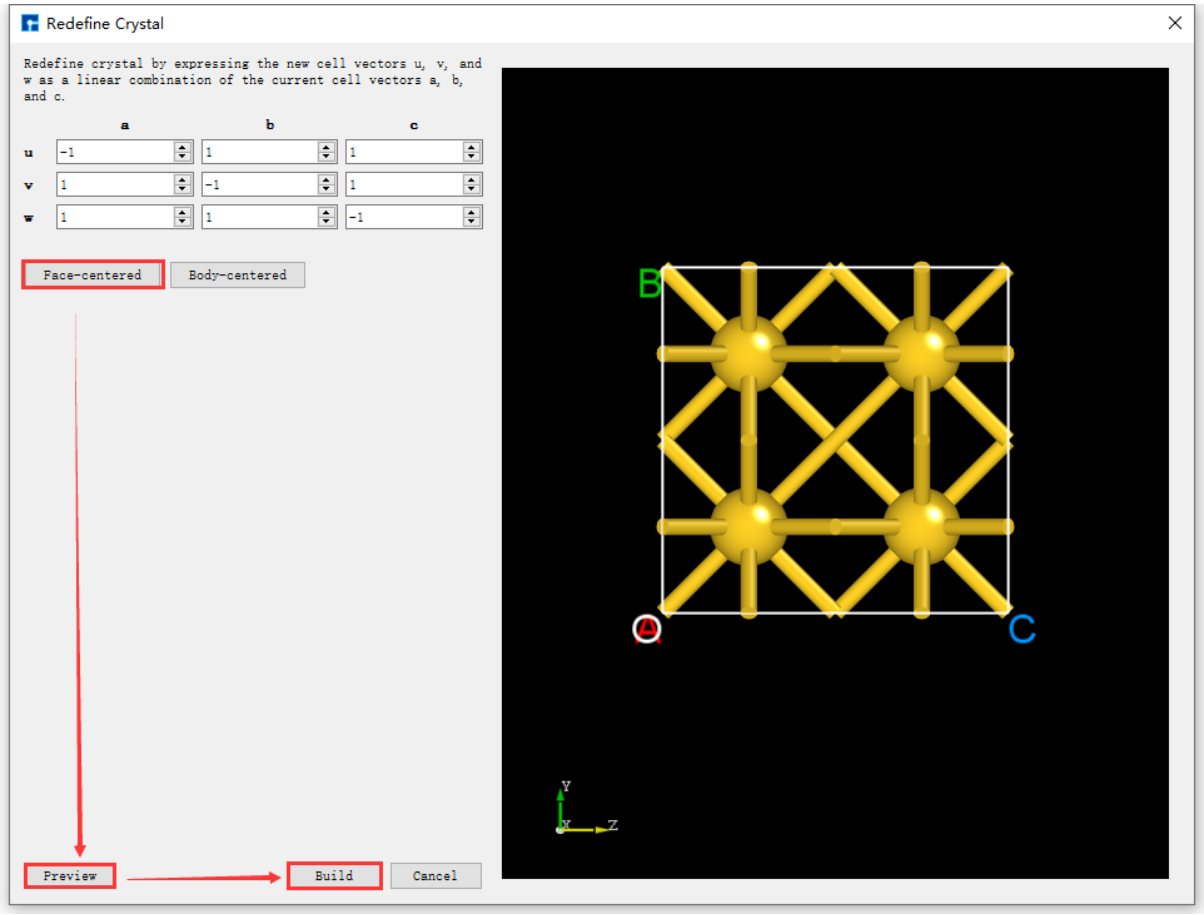


fig. 4.36: The operation interface for converting an Au unit cell to an Au crystal cell

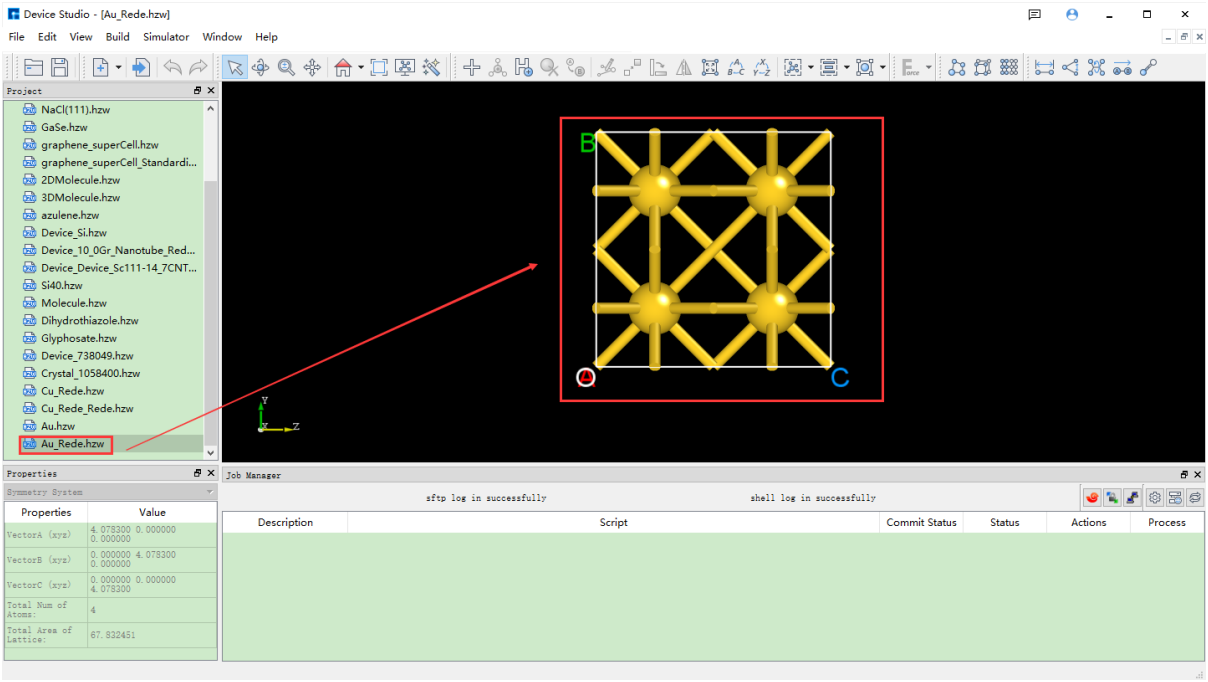


fig. 4.37: Interface after converting the Au primitive cell to the Au conventional cell

4.8.3 Converting an Au unit cell to an Au supercell

Convert the Au unit cell to a 2*2*4 supercell (referred to as: Au supercell). Click *Build* → *Redefine Crystal* in fig. 4.37 to open the Redefine Crystal interface. Modify the parameters as shown in the red box in fig. 4.38. Click *Preview* to preview the converted supercell structure. Clicking *Build* converts the Au unit cell into the Au supercell structure. The structure file is saved in the software's project management area (Project Explorer), and a 3D view of the structure can be seen in the 3D display area, as shown in fig. 4.39. `Au_Rede_Rede.hzw` in fig. 4.39 corresponds to the Au supercell; users can rename this structure file according to their computational needs.

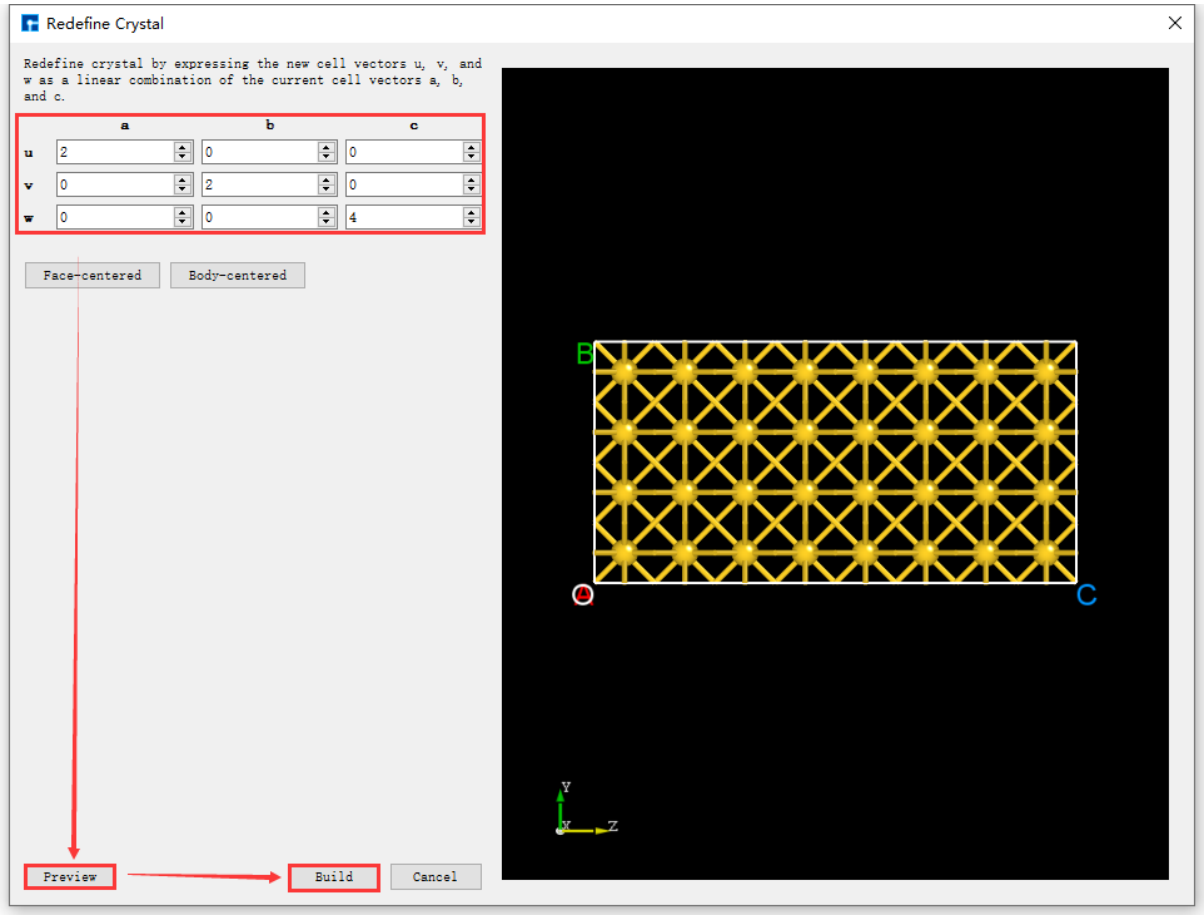


fig. 4.38: Operation interface for converting an Au unit cell to an Au supercell

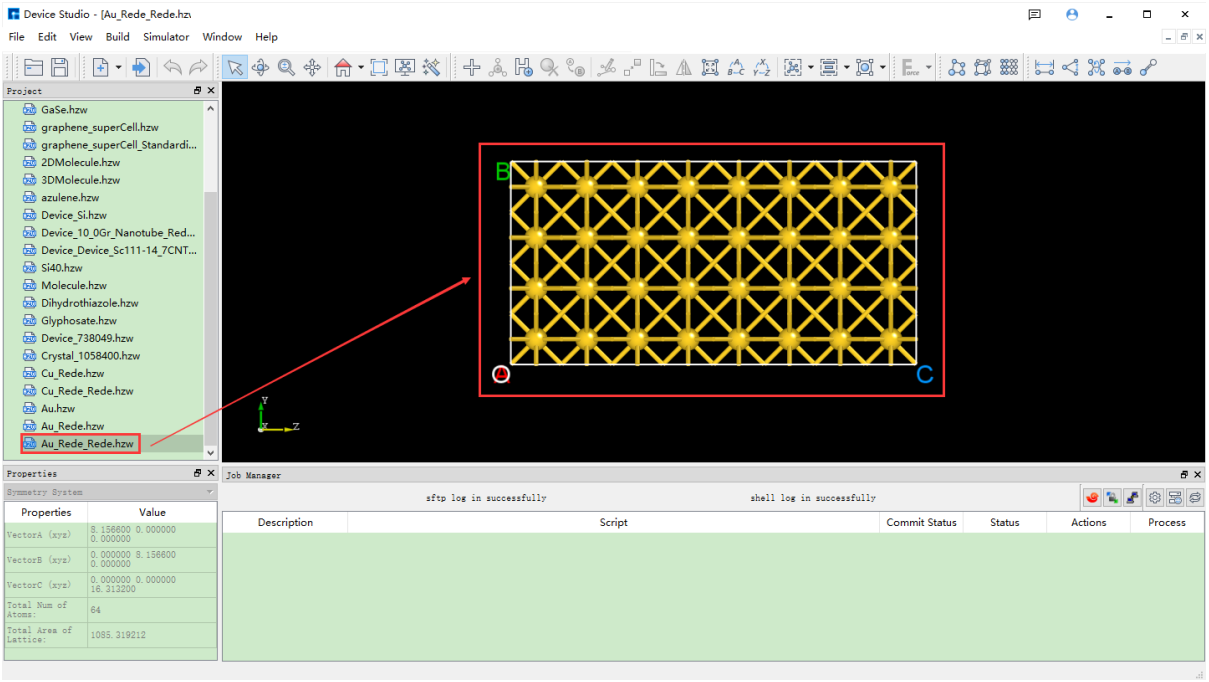


fig. 4.39: Interface after converting the Au unit cell to a Au supercell

4.8.4 Removing Redundant Atoms and Operations in the Au Supercell

***Remove redundant atoms from the Au supercell and center the structure within the unit cell.** To avoid accidentally deleting atoms and making them irretrievable, it is recommended to copy the Au supercell. Select the `Au_Rede_Rede.hzw` structure file → right-click → Copy. The CopyFile interface will appear, as shown in fig. 4.40. Users can rename the file according to their computational needs, such as Au_SuperCell, or directly use the default name. Then, click the *OK* button in the CopyFile interface. The `Au_SuperCell.hzw` structure file will be stored in the project management area. Double-click this structure file; its 3D view will be displayed as shown in fig. 4.41 (a).

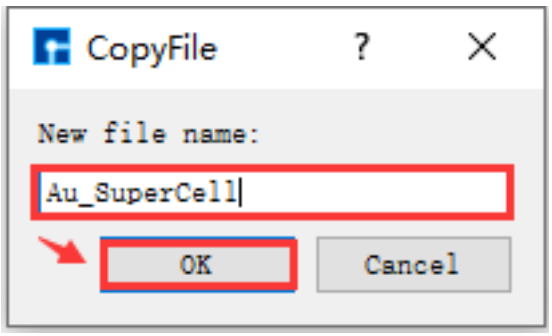


fig. 4.40: CopyFile Interface

(1) In the 3D display area, with the zy-plane view, mouse-select the area indicated by the red box in fig. 4.41 (a), then click the *Delete Atom* icon in the toolbar or press the *Delete* key on the keyboard to delete the selected atoms. The result is shown in fig. 4.42 (b).

(2) Click the dropdown button to the right of the *3D Viewer zy View* icon on the Toolbars and select *xy View* to switch from the zy-plane to the xy-plane, as shown in fig. 4.43 (c). Select the area within the red box in fig. 4.43 (c) using the mouse, and then click the *Delete Atom* icon on the Toolbars or press the *Delete* key to delete the selected atoms. After deletion, click the *3D Viewer zy View* icon on the Toolbars to switch back to the zy-plane, as shown in fig. 4.44 (d). First, select the area within the red box in fig. 4.44 (d) using the mouse; second, hold down the *Ctrl* key and click the area within the green box in fig. 4.44 (d) with the mouse; finally, click the *Delete Atom* icon on the Toolbars or press the *Delete* key to delete the selected atoms. The result is shown in fig. 4.45 (e).

(3) In the case of fig. 4.45 (e), clicking the *Center* icon on the Toolbars will center all atoms in the structure as a whole within the unit cell, as shown in fig. 4.46 (f). After completing the above series of operations, the structure file `Au_SuperCell.hzw` (Au_SuperCell supercell) is obtained, and its 3D view is shown in fig. 4.46 (f).

note

Selected atoms are highlighted in yellow, allowing users to easily identify them.

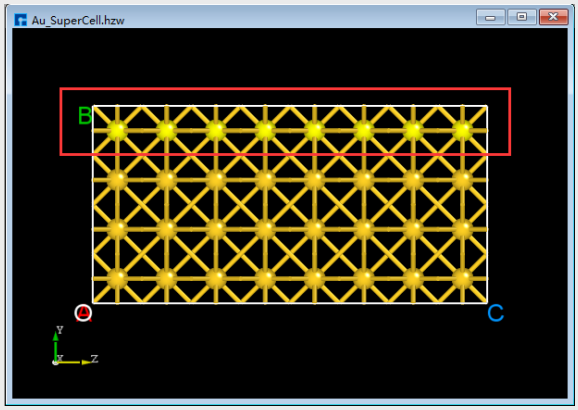


fig. 4.41: （a）

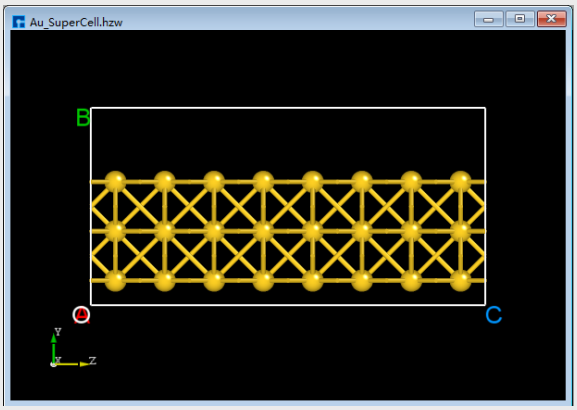


fig. 4.42: （b）

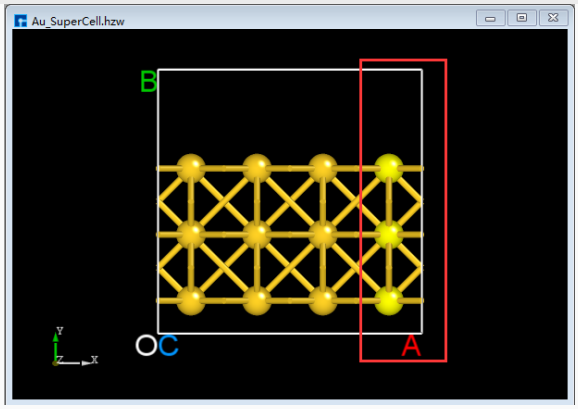


fig. 4.43: （c）

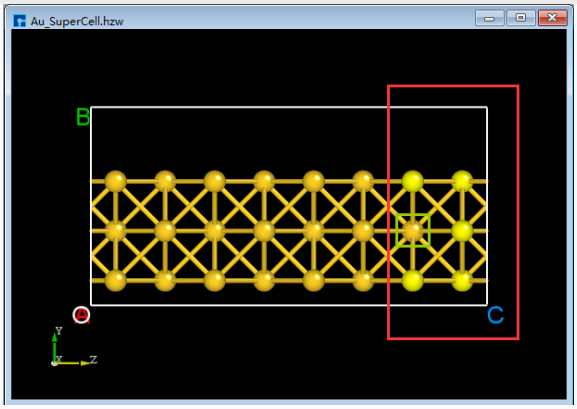


fig. 4.44: （d）

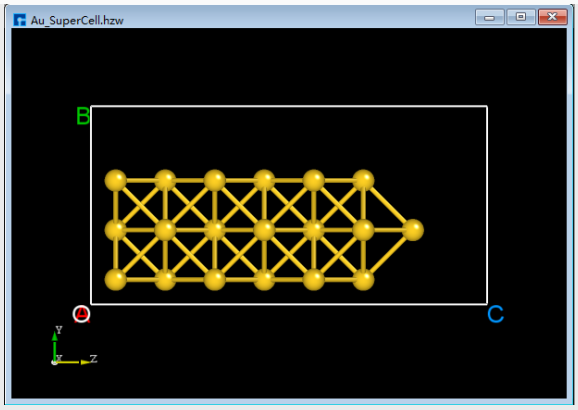


fig. 4.45: （e）

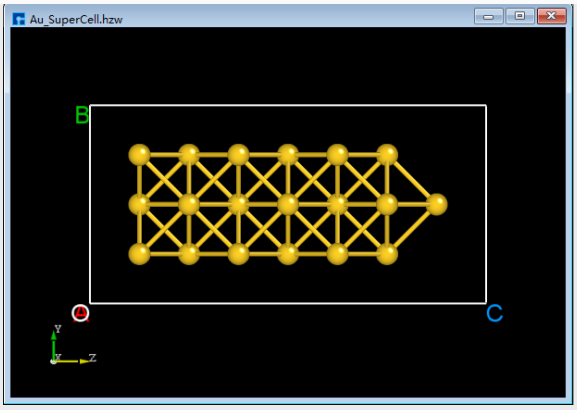


fig. 4.46: （f）

4.8.5 Set X and Y axis directions to vacuum

Set the X and Y axes of the Au_SuperCell supercell to vacuum. Duplicate the Au_SuperCell supercell and rename it Au_SuperCell_1. Double-click its structure file `Au_SuperCell_1.hzw` to display it in the 3D display area. Click the *Convert to Crystal* shortcut icon on the Toolbars to open the Convert to Crystal interface. Set the parameters as shown in the red box in fig. 4.47 → preview on the right side of the interface → *Build*. This will set the X and Y axes of the

Au_SuperCell_1 supercell to vacuum, as shown in fig. 4.48 (a). Click the *Center* shortcut icon on the Toolbars to center all atoms in the unit cell. After centering, the structure will appear as shown in fig. 4.49 (b). After completing these steps, the structure file `Au_SuperCell_1.hzw`, representing the Au_SuperCell_1 supercell, will have a 3D view as shown in fig. 4.49 (b).

note

Copying and renaming the structural files is for the convenience of this tutorial and to prevent irreversible errors after a series of operations. Users can decide whether to copy and rename them based on their modeling needs. Generally, for accidental deletions or misoperations, you can click the *Undo* shortcut icon on the Toolbars or press the *Ctrl+Z* shortcut to undo.

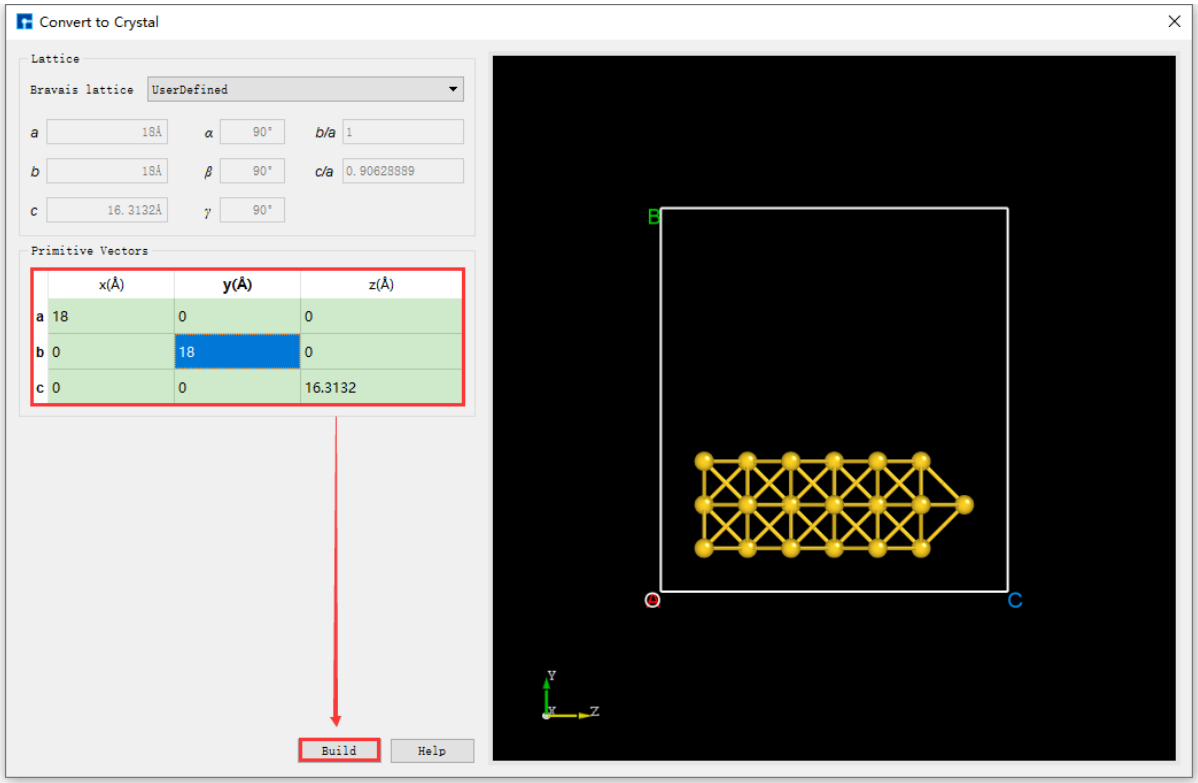


fig. 4.47: Convert to Crystal interface

note

After clicking the *Build* button in the fig. 4.47 interface, if the 3D view of the `Au_SuperCell_1.hzw` structure does not appear in the appropriate location in the 3D display area, the user can reset the 3D view to the appropriate location by clicking the *3D Viewer zy View* shortcut icon on the Toolbars or by pressing the shortcut key *Ctrl+R*. The reset 3D

view of the structure is shown in fig. 4.49 (b). **Users can use this method to reset the 3D view whenever it is not in the appropriate location in the 3D display area during the modeling process.**

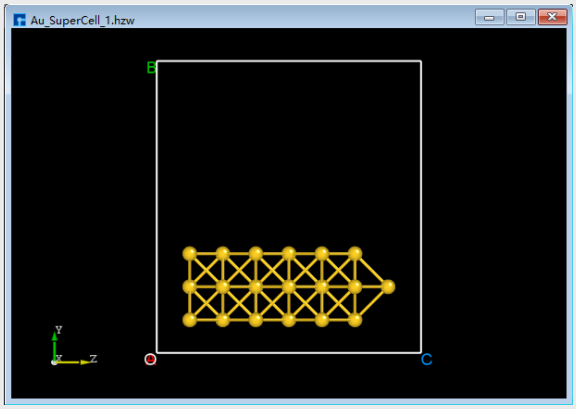


fig. 4.48: （a）

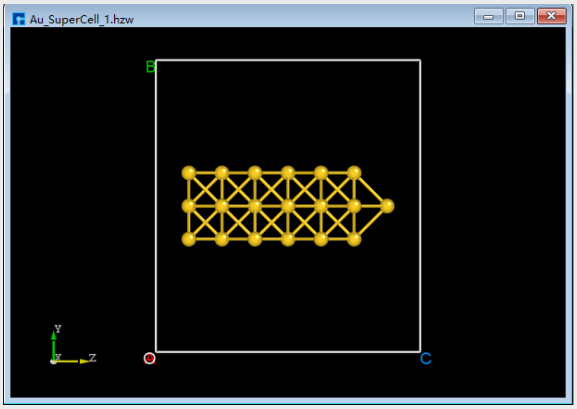


fig. 4.49: （b）

4.8.6 Mirror the structure and reset the lattice constants

Mirror the selected atoms, reset the lattice constant, and center the structure. As shown in fig. 4.50, select all atoms → click the *Mirror Atom* shortcut icon → the Mirror interface pops up → set parameters → check Copy → click *Apply*. The structure will then be as shown in fig. 4.52 (a). Based on fig. 4.52 (a), click the *Convert to Crystal* shortcut icon. The Convert to Crystal interface will pop up, as shown in fig. 4.51. Set the parameters as shown in the red box in the figure. Preview the structure with the reset lattice constant on the right side of the interface. Click *Build*, then click the *Center* shortcut icon to center all atoms of the structure with the reset lattice constant in the unit cell. The centered structure is shown in fig. 4.53 (b).

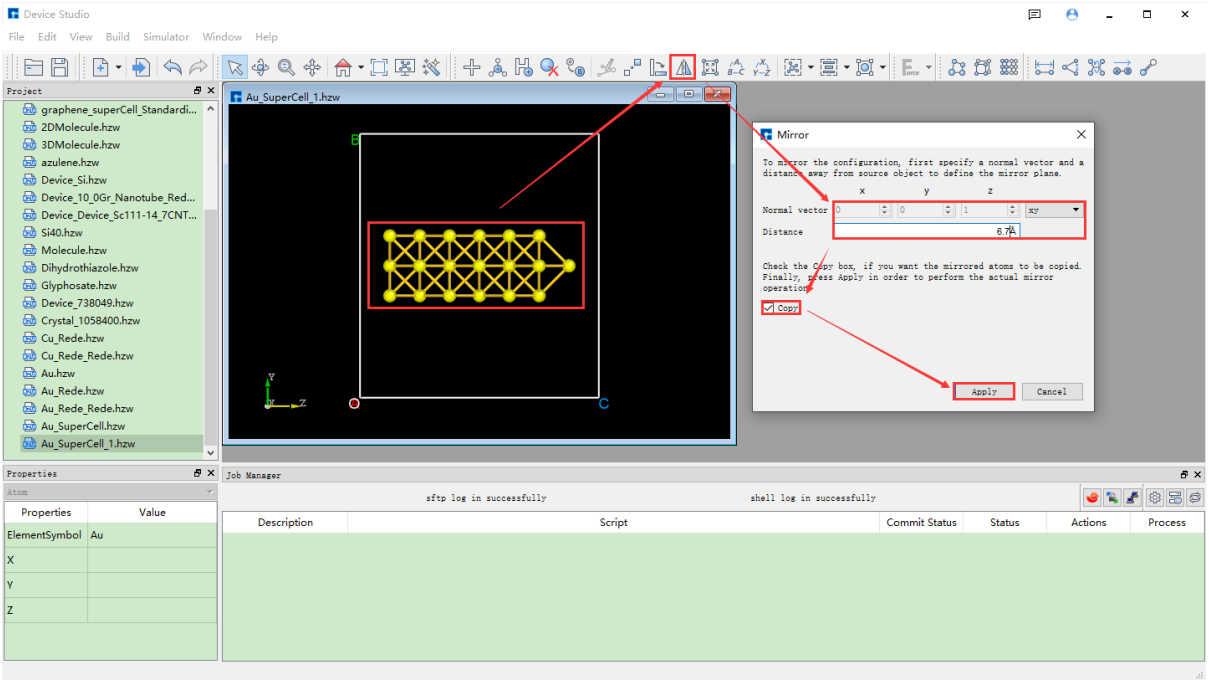


fig. 4.50: Au_SuperCell_1 Supercell Mirroring Operation Interface

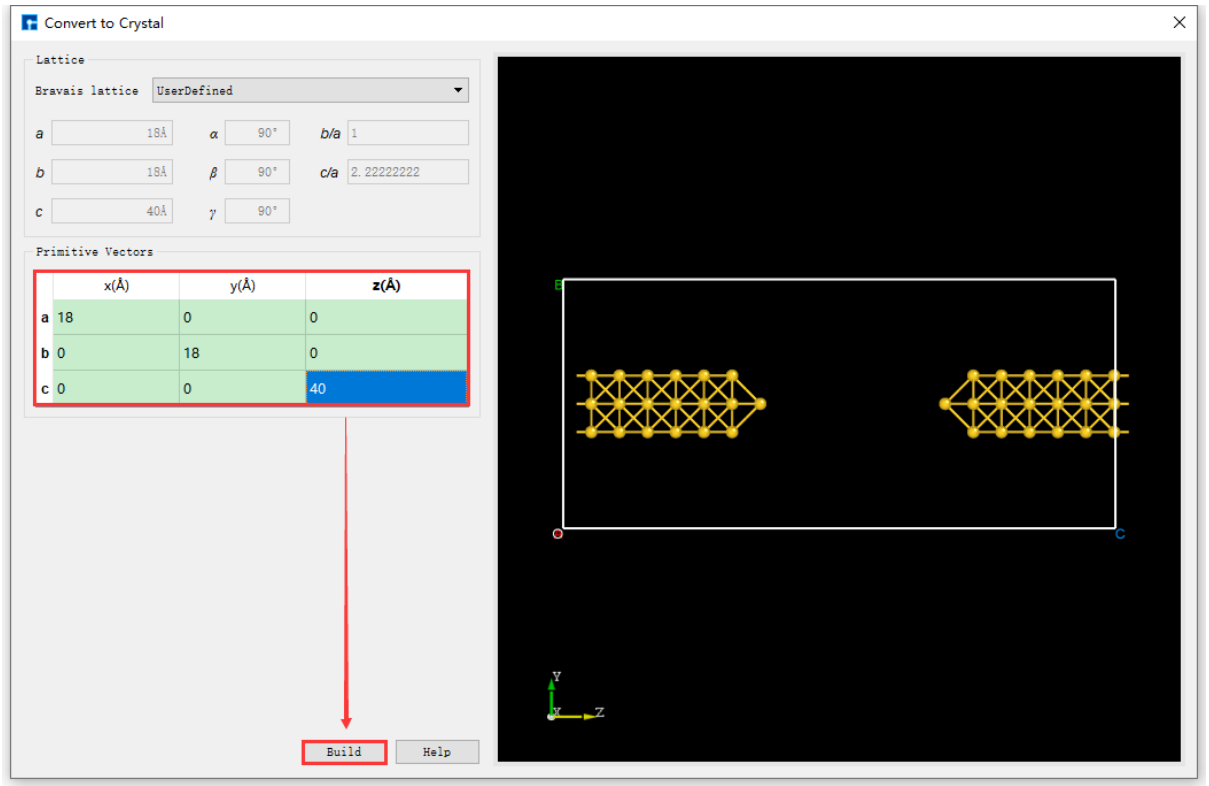


fig. 4.51: Au_SuperCell_1 Supercell Lattice Constant Resetting Operation Interface

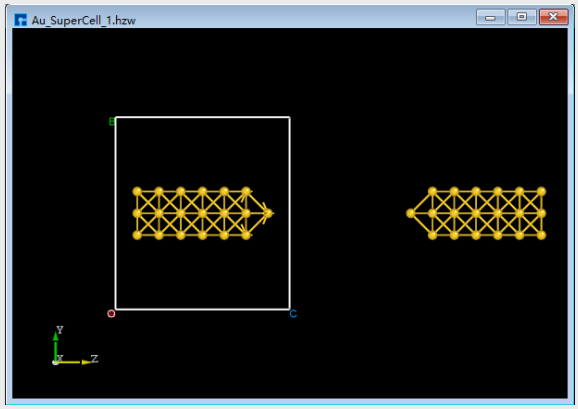


fig. 4.52: （a）

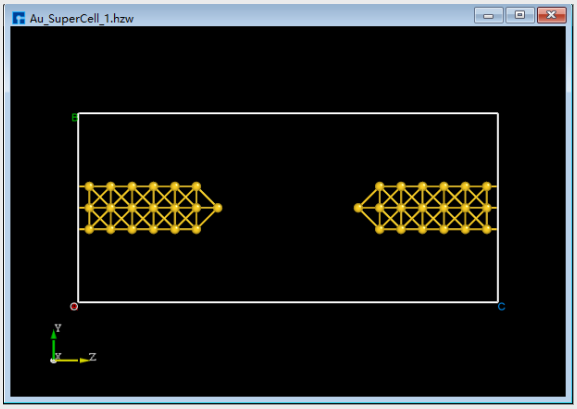


fig. 4.53: （b）

4.8.7 Setting up a Two-Port Device Structure

Import the alkanethiol molecule structure and copy it to the center of the Au_SuperCell_1 supercell structure. Then, build the two-port device structure.

(1) Import the alkanethiol molecular structure as shown in fig. 4.54.

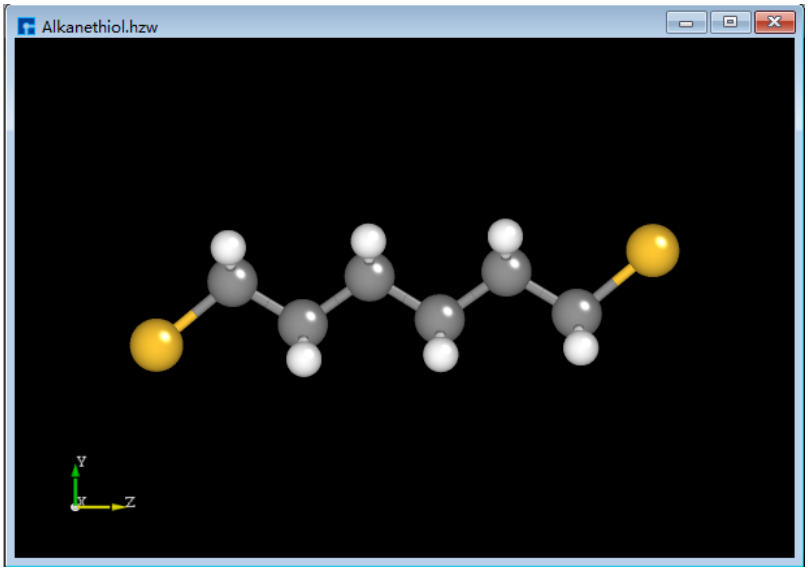


fig. 4.54: Alkanethiol molecule

(2) Double-click *Au_SuperCell_1.hzw* to open the Au_SuperCell_1 supercell structure. Box-select the alkanethiol molecule structure and press the shortcut key *Ctrl+C* to copy it. Click the left side of the interface in fig. 4.53 (b) and press the shortcut key *Ctrl+V* to paste the alkanethiol molecule structure into the Au_SuperCell_1 supercell structure, as shown in fig. 4.55 (a). To easily move the pasted alkanethiol molecule structure to the center of the Au_SuperCell_1 supercell structure, click the drop-down button to the right of the

3D Viewer zy View shortcut icon and select *ZX zx View* to switch from the zy plane to the zx plane, as shown in fig. 4.56 (b). Select the alkanethiol molecule structure and click the *Center* shortcut icon to move the alkanethiol molecule structure to the center of the Au_SuperCell_1 supercell structure, as shown in fig. 4.57 (c). Click the *3D Viewer zy View* shortcut icon to switch back to the zy plane, as shown in fig. 4.58 (d).

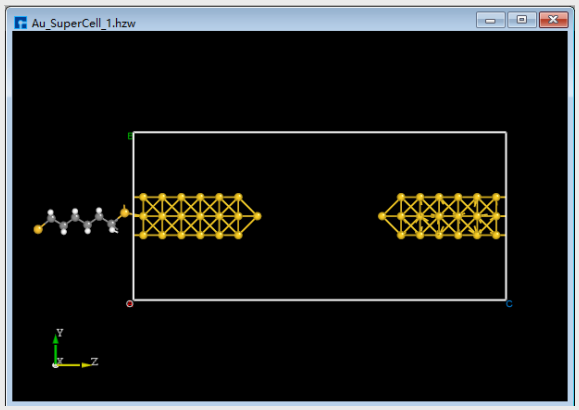


fig. 4.55: （a）

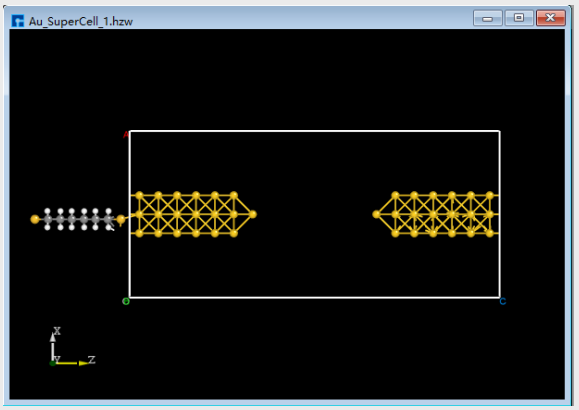


fig. 4.56: （b）

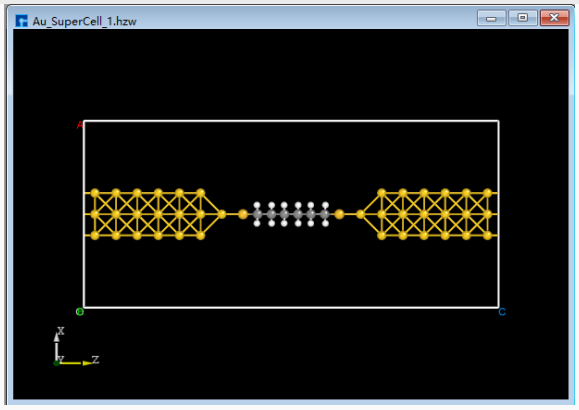


fig. 4.57: （c）

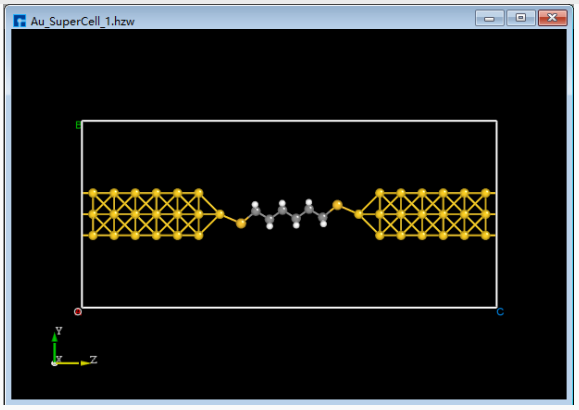


fig. 4.58: （d）

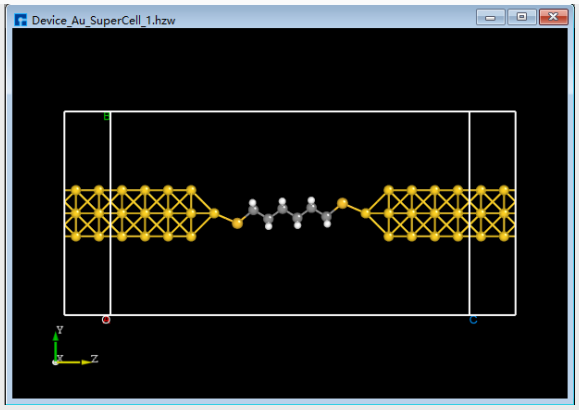


fig. 4.59: （e）

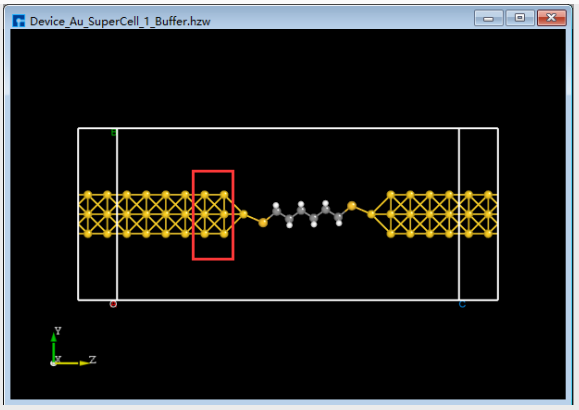


fig. 4.60: （f）

(3) Click the *Convert to Device* shortcut icon. The Convert to Device interface will pop up, as shown in fig. 4.61. Select the parts in the red boxes, then click *Preview* to preview the

two-port device structure on the right side of the interface. Clicking *Build* will generate the two-port device structure `Device_Au_SuperCell_1.hzw`, as shown in fig. 4.59 (e).

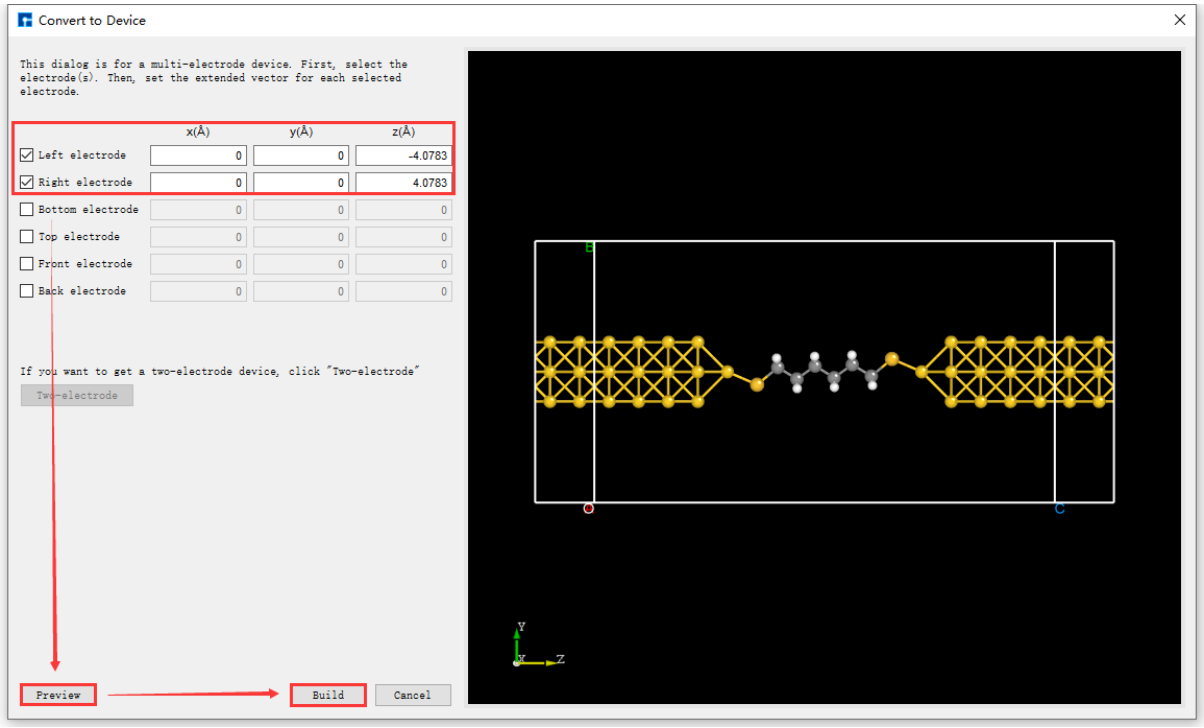


fig. 4.61: Convert to Device Interface

4.8.8 Adding a Buffer Layer to the Device Structure

Users can choose whether to add a buffer layer to the built two-port device structure based on computational needs; there is no mandatory requirement. For example, to add a buffer layer to the *Device_Au_SuperCell_1.hzw* device structure near the electrode along the transport direction (Z-axis), using an atom-layer incremental method, double-click to open the device structure → click *Simulator* → *Nanodcal* → *Add Buffer* in the software menu bar. The Add Buffer interface, as shown in fig. 4.62, will appear. Click the + button twice after Left. A preview of the buffer layer added to the left side of the device along the transport direction will be shown on the right side of the interface. Clicking *Build* will generate the two-port device structure with the added buffer layer, *Device_Au_SuperCell_1_Buffer.hzw*, as shown in fig. 4.60 (f).

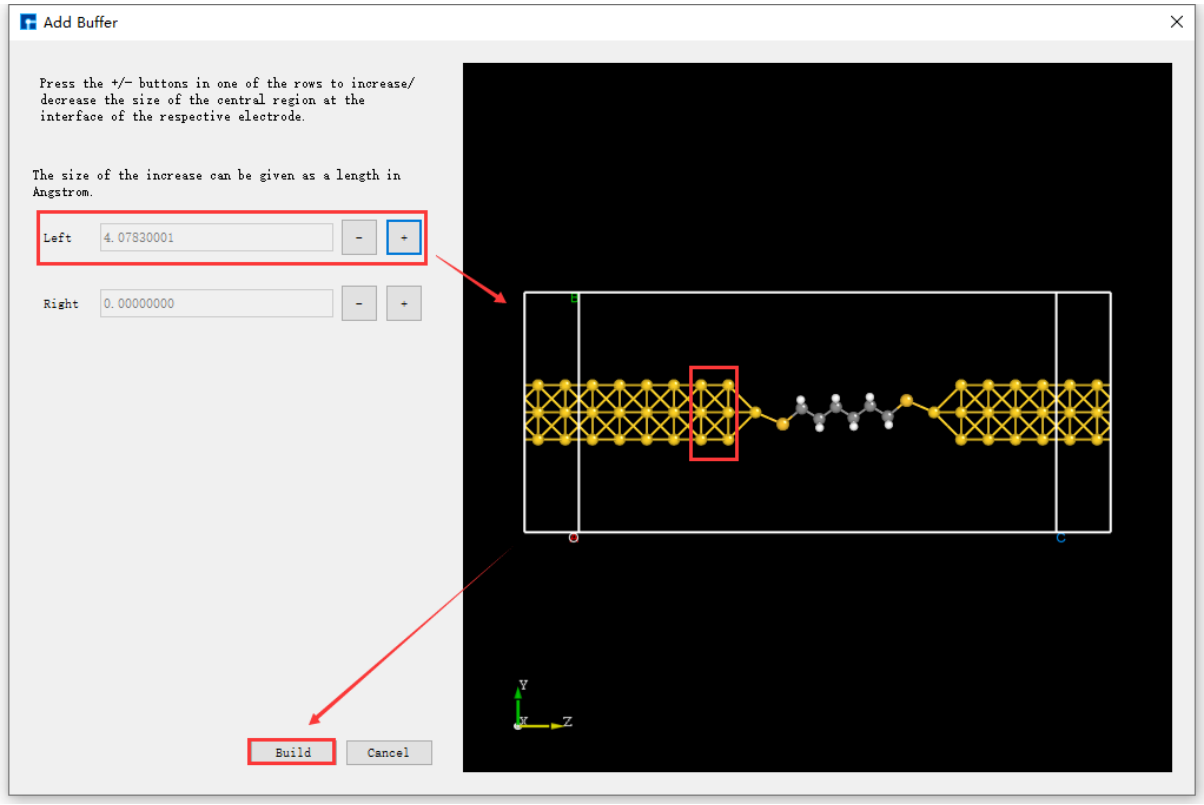


fig. 4.62: Add Buffer Interface

note

The addition of buffer layers to the device structure described above is merely an example; users can decide whether to add buffer layers near both ends of the electrodes and how many layers to add, based on their computational needs.

4.9 Export Structure

For a built structure, such as the two-port device structure `Device_Au_SuperCell_1_Buffer.hzw`, to export this structure file, double-click to open the structure file → click *File* → *Export* in the software to bring up the export interface. Users can select the storage location, name the structure file (or use the default name), and choose the storage format as needed.

CHAPTER

FIVE

STRUCTURE EDITING AND INFORMATION MEASUREMENT

For structure manipulation, users should first carefully read the descriptions of each shortcut icon in *Toolbars*, then perform the corresponding operations as needed. The structure view after the operation can be viewed in the 3D display area.

5.1 Basic Operations for 3D Structure Display

Device Studio supports viewing the 3D structure from ZY, XY, XZ, YZ, YX, and ZX planes, as shown in the NaCl (111) crystal structure in the 3D display area (`NaCl(111).hzw`). Users can reset the structure to the ZY plane by clicking the *3D Viewer zy View* shortcut icon in the toolbar. Clicking the dropdown button of this shortcut icon allows selection of XY, XZ, YZ, YX, or ZX planes to view the 3D structure of the NaCl (111) crystal. The 3D views of the NaCl (111) crystal structure from the ZY, XY, XZ, YZ, YX, and ZX planes in the 3D display area are shown in fig. 5.1, fig. 5.2, fig. 5.3, fig. 5.4, fig. 5.5, and fig. 5.6, respectively.

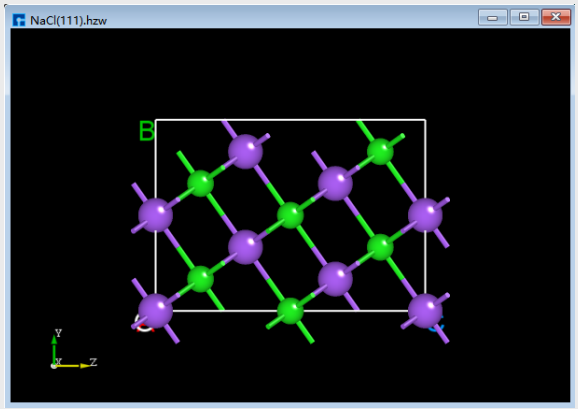


fig. 5.1: 3D View of NaCl (1 1 1) ZY Plane

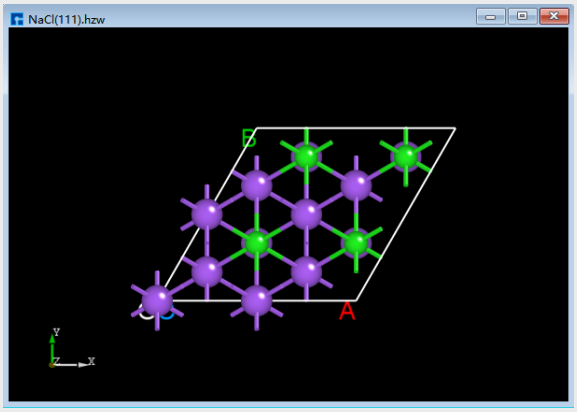


fig. 5.2: 3D View of NaCl (1 1 1) XY Plane

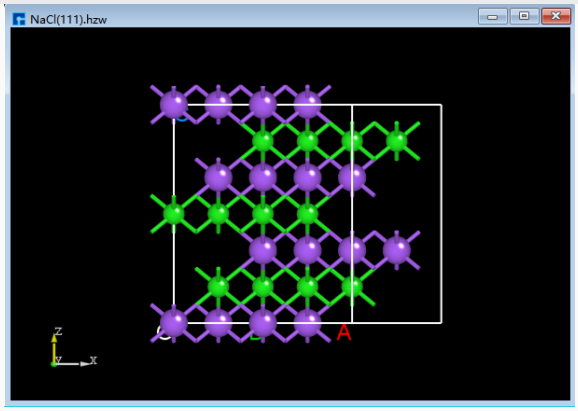


fig. 5.3: 3D view of NaCl (1 1 1) XZ plane

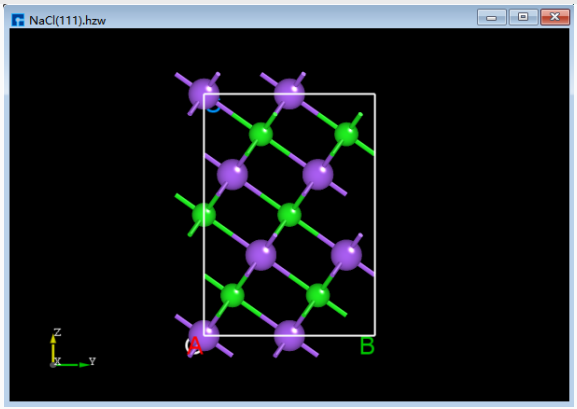


fig. 5.4: 3D view of NaCl (111) YZ plane

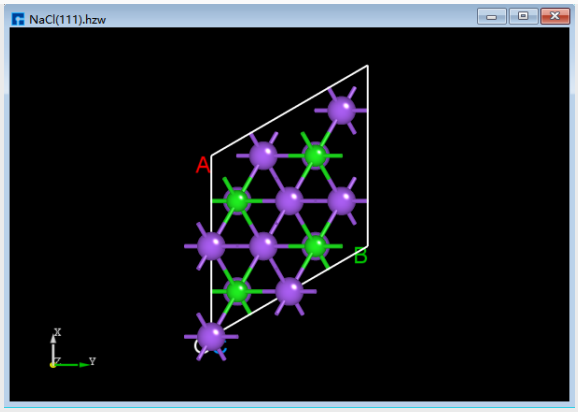


fig. 5.5: 3D view of NaCl (1 1 1) YX plane

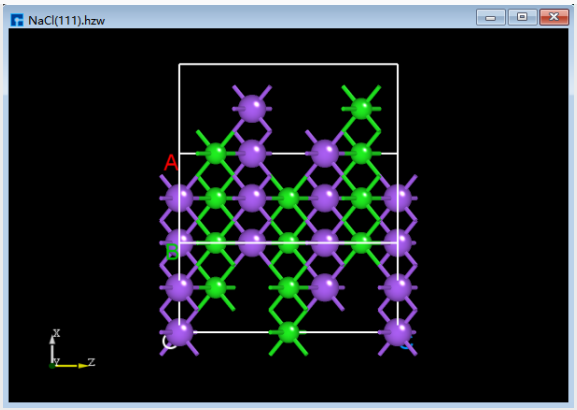


fig. 5.6: 3D view of NaCl (1 1 1) ZX plane

In the 3D structure display area, users can zoom in or out of the 3D view of the structure by scrolling the middle mouse button; they can pan the 3D view of the structure in this area by first selecting the *3D Viewer Translation Mode* shortcut icon in the toolbar or holding down the middle mouse button and dragging the mouse; they can rotate the 3D view of the structure in this area by first selecting the *3D Viewer Rotation Mode* shortcut icon in the toolbar or holding down the right mouse button and dragging the mouse.

5.2 Structure Modification Operations

Taking crystalline MoS₂ as an example to illustrate a series of structural modification operations, prepare the structure file (`MoS2.hzw`). Drag and drop this file into the Project Explorer area of the software to import the structure. The 3D view of the structure in the zy plane is shown in fig. 5.12 (a).

5.2.1 Adding Atoms

To add a Cr atom to crystalline MoS₂, as shown in red in fig. 5.7, click the *Add Atom* shortcut icon in the Toolbars. The periodic table will pop up. Select Cr in the periodic table and click *OK*. Click the left mouse button at position ④ in the interface shown in fig. 5.7. Then click the *Recalculate LinkerBond* shortcut icon to recalculate bond lengths. This completes the operation of adding a Cr atom to MoS₂. The completed 3D view is shown in fig. 5.13 (b).

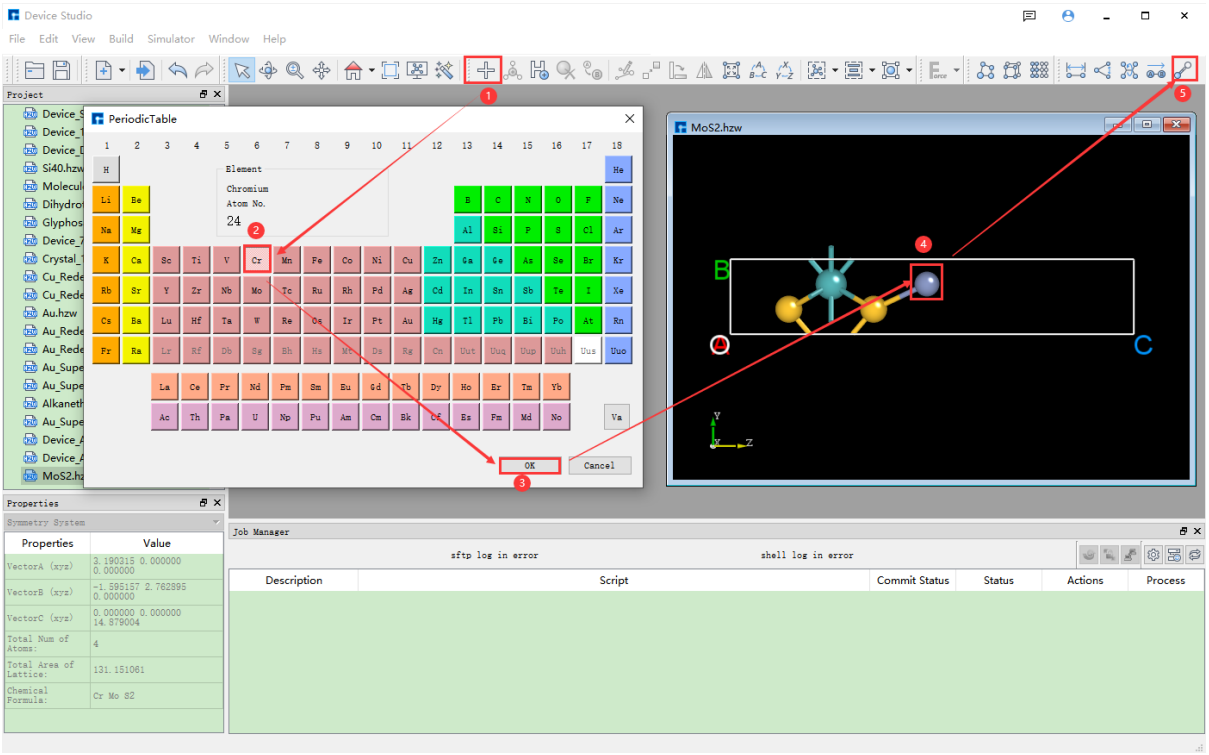


fig. 5.7: Add atomic operation interface

5.2.2 Delete Atom

To delete an S atom, as shown in the structure in fig. 5.13 (b), follow the steps illustrated in the red portion of fig. 5.8. Select the S atom to be deleted, click the *Delete Atom* shortcut icon on the toolbar, or press the *Delete* key. Then, click the *Recalculate LinkerBond* shortcut icon to recalculate bond lengths. The 3D view after deleting the S atom is shown in fig. 5.14 (c).

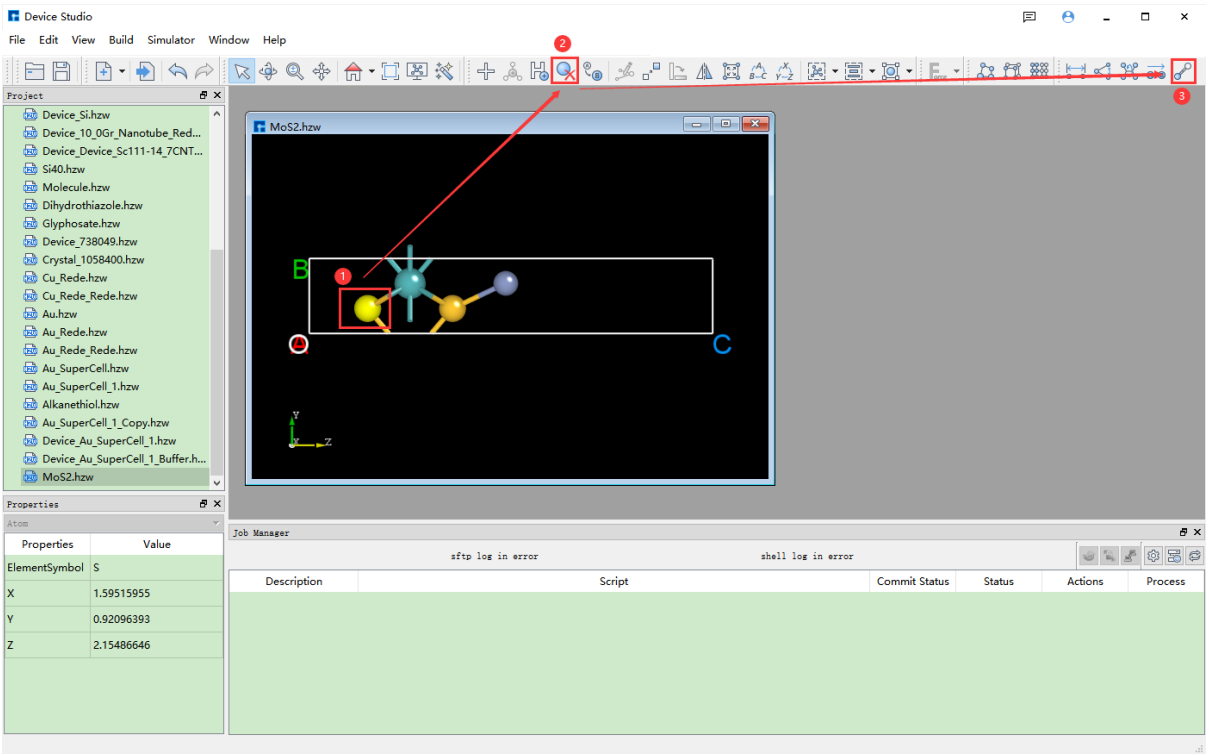


fig. 5.8: Remove Atom Operation Interface

5.2.3 Replacement Atom

To replace a Cr atom with a W atom in the structure shown in fig. 5.14 (c), follow the steps shown in red in fig. 5.9. Select the Cr atom to be replaced, click the *Replace Atom* shortcut icon in the Toolbars, select W from the periodic table that appears, click *OK*, and then click the *Recalculate LinkerBond* shortcut icon to complete the replacement. The 3D view of the resulting structure is shown in fig. 5.15 (d).

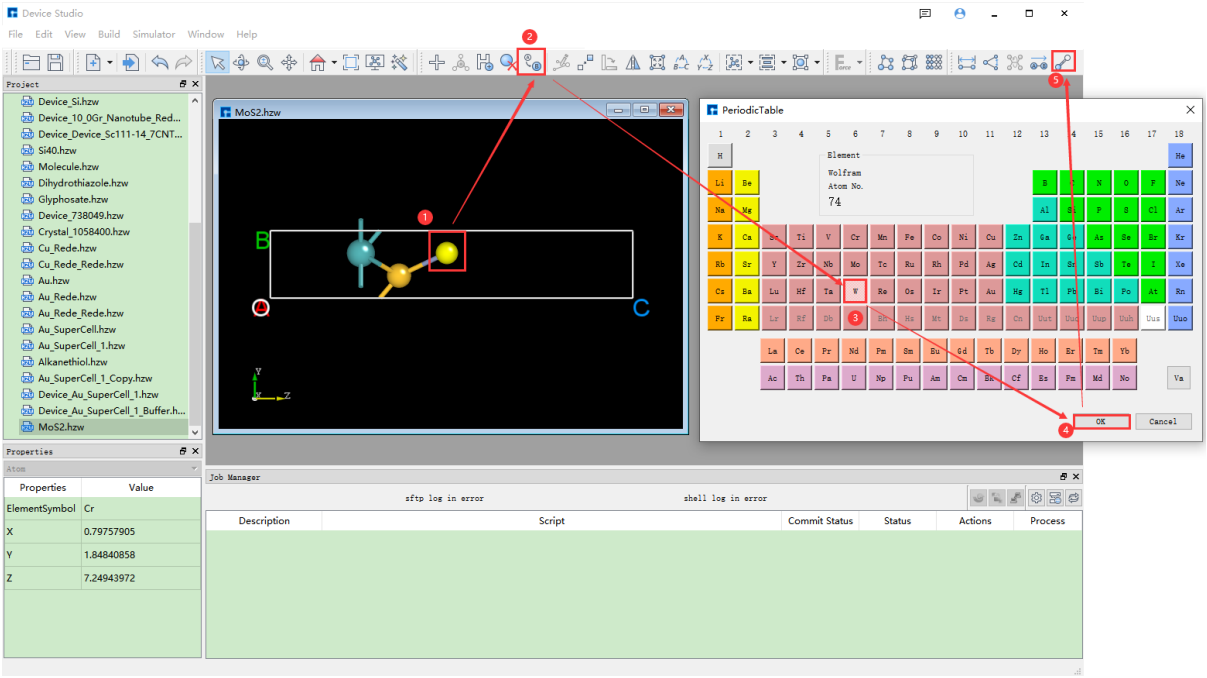


fig. 5.9: Replace Atomic Operation Interface

5.2.4 Modifying Atomic Coordinates

To modify the coordinates of the W atom from (0.79757905, 1.84840857, 7.24943971) in fig. 5.15 (d) to (1.0, 1.5, 12.0), follow the steps shown in red in fig. 5.10. First, select the W atom with the mouse. The coordinates of the selected W atom, (0.5951619, 1.47565329, 7.18570423), will be displayed in the Properties Explorer. Then, double-click the appropriate fields and enter 1.0, 1.5, and 12.0 respectively to modify the W atom's coordinates. Finally, click the *Recalculate LinkerBond* shortcut icon to recalculate bond lengths. The 3D view of the structure after modifying the atomic coordinates is shown in fig. 5.16 (e).

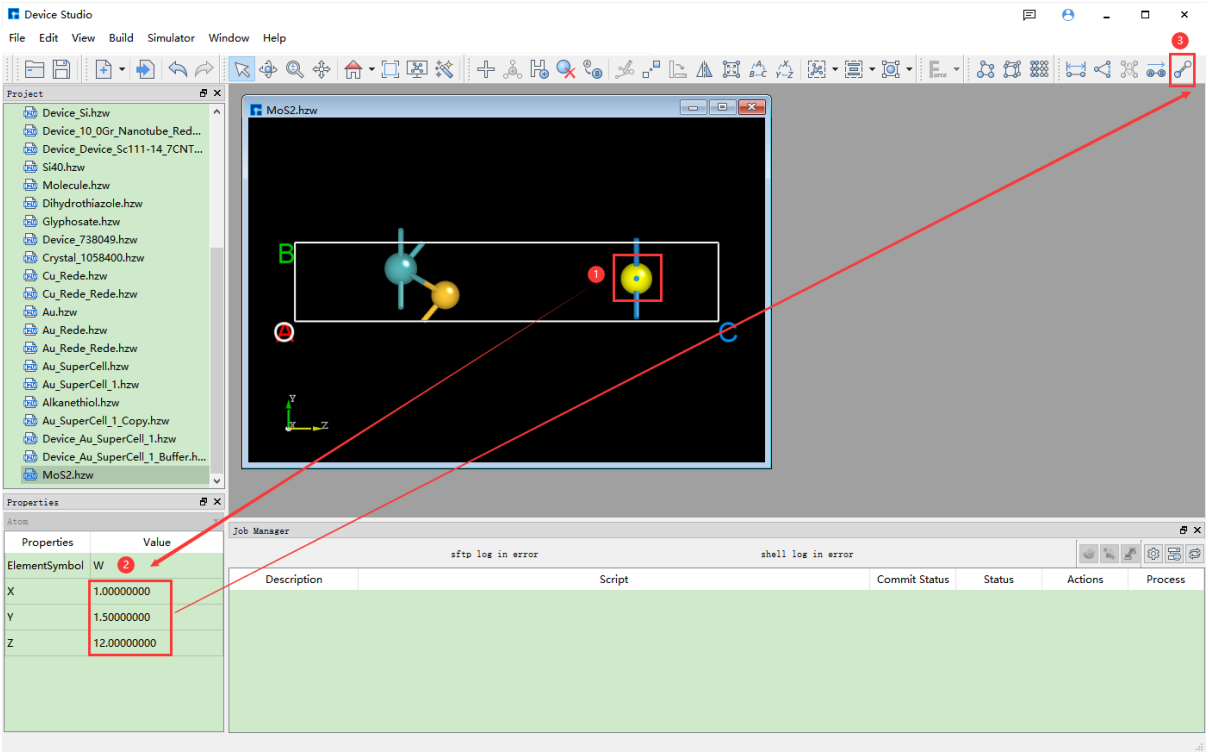


fig. 5.10: Modify Atomic Coordinates Operation Interface

5.2.5 Move the selected atom

For the structure shown in fig. 5.16 (e), move the two leftmost atoms as shown in the red portion of fig. 5.11. First, select the two leftmost atoms with the mouse. Click the *Move Atom* shortcut icon to open the Move Atom dialog. Enter the distance to move in the dialog and click to move along the positive Z direction (+z). After moving, click the *Recalculate LinkerBond* shortcut icon to recalculate the bond lengths. The 3D view of the structure after moving is shown in fig. 5.17 (f).

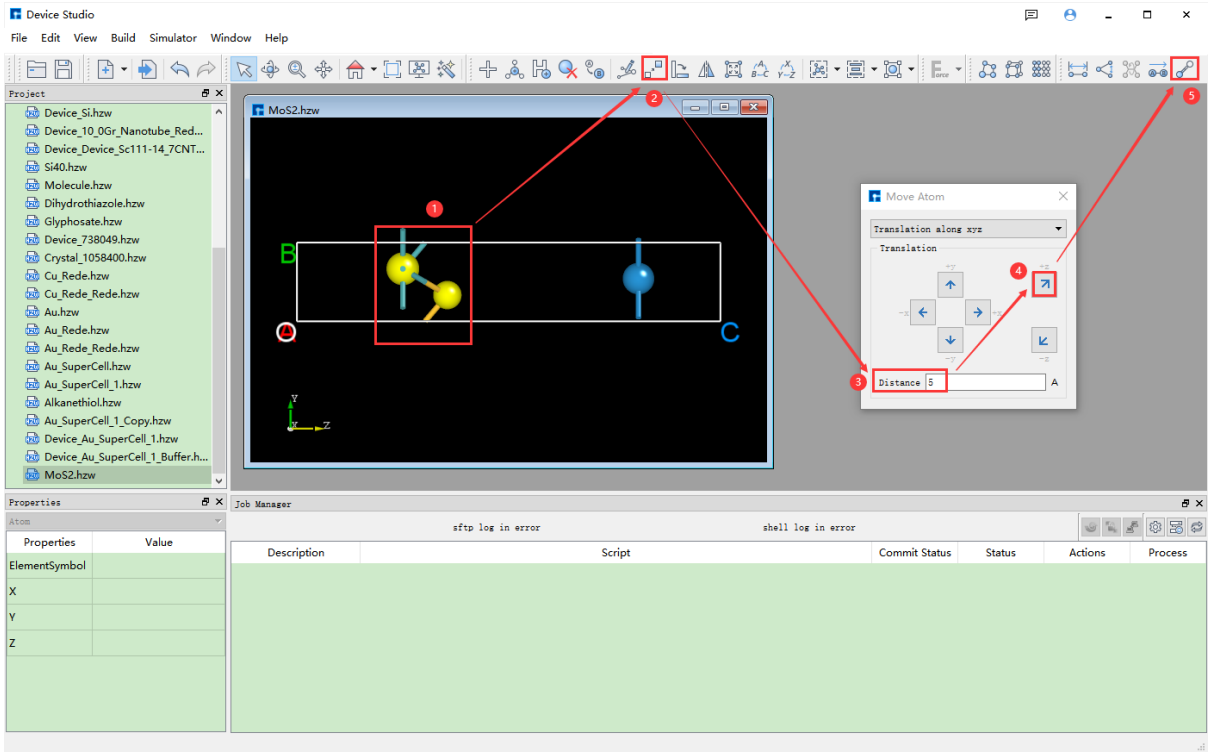


fig. 5.11: Move the selected atomic operation interface

note

This only describes a portion of the structural modification operations. Users can refer to the descriptions of each shortcut icon in *Toolbars* for details and perform corresponding structural operations as needed.

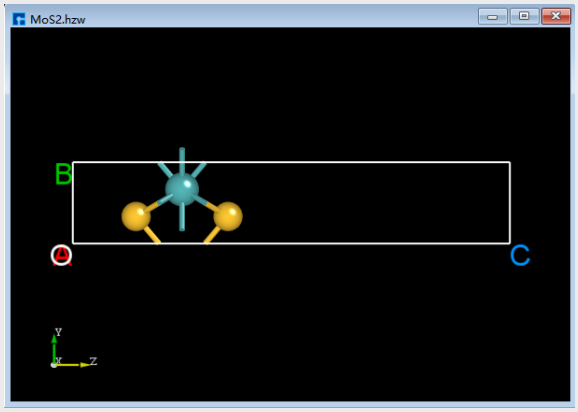


fig. 5.12: （a）

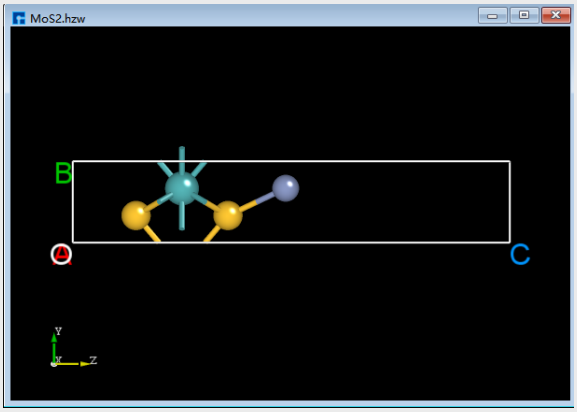


fig. 5.13: （b）

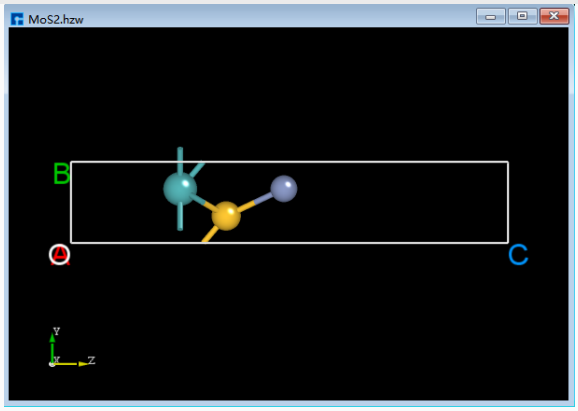


fig. 5.14: （c）

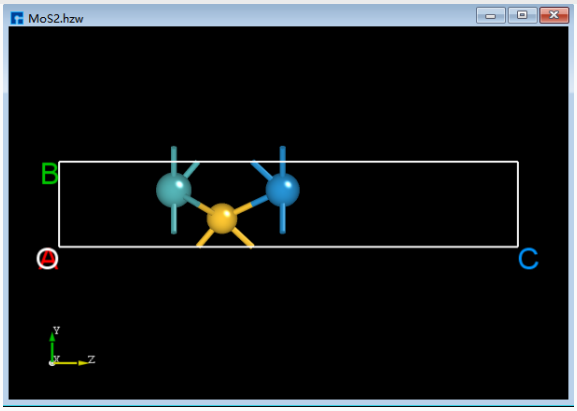


fig. 5.15: （d）

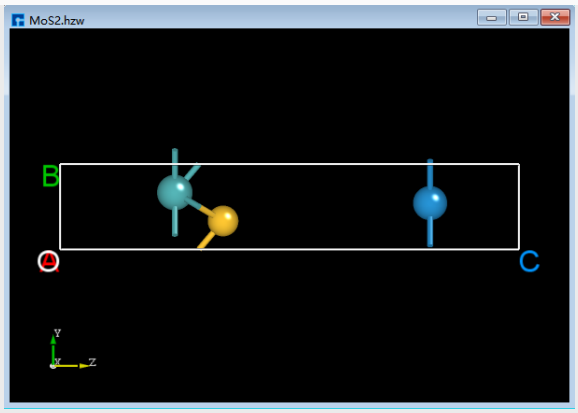


fig. 5.16: （e）

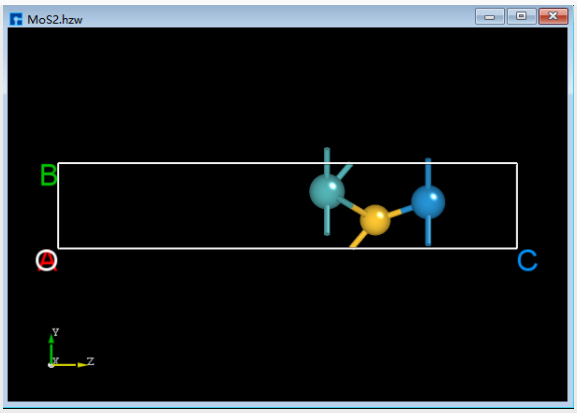


fig. 5.17: （f）

5.3 Information Measurement of Structure

A series of operations for measuring structural information is described using the Si8 crystal structure as an example. Prepare the structure file (`Si8.hzw`), and drag and drop it into the Project Explorer of the software to import the structure. The 3D view of the structure's zy plane is shown in fig. 5.18.

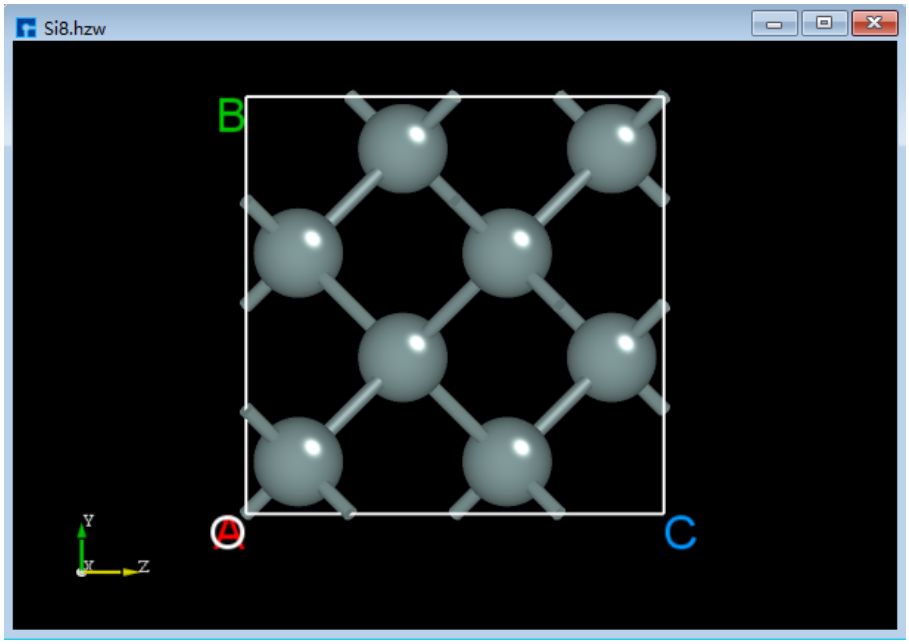


fig. 5.18: Si8 Crystal Structure

注意事项

To measure structural information, multiple atoms often need to be selected. It is recommended that users first select the corresponding shortcut icon on the *Toolbars* and then hold down the *Ctrl* key while individually selecting atoms in the structure. Without holding down the *Ctrl* key, multiple atom selection via mouse clicks is not possible, and therefore structural information measurement cannot be performed.

5.3.1 Measuring the distance between two atoms

For the crystal structure shown in fig. 5.18, click the *Distance* shortcut icon on the Toolbars, hold down the *Ctrl* key on the keyboard, and then select two atoms in the structure with the mouse to measure the distance between the selected two atoms, as shown in fig. 5.19 (a). If you do not want to keep the measurement numbers, right-click and select "Clear Annotation".

5.3.2 Measuring the vector between two atoms

For a crystal structure as shown in fig. 5.18, click the *Vector between two atoms* shortcut icon on the Toolbars, hold down the *Ctrl* key on the keyboard, and then select two atoms in the structure with the mouse to measure the vector between the selected two atoms, as shown in fig. 5.20 (b).

5.3.3 Measuring the Angle Between Three Atoms

For a crystal structure as shown in fig. 5.18, click the *Angle* shortcut icon on the Toolbars, hold down the *Ctrl* key on the keyboard, and then select three atoms in the structure with the mouse to measure the angle between the selected three atoms, as shown in fig. 5.21 (c).

5.3.4 Measuring the dihedral angle between four atoms

For a crystal structure as shown in fig. 5.18, click the *Dihedral angle* shortcut icon on the Toolbars, hold down the *Ctrl* key on the keyboard, and then select four atoms in the structure with the mouse to measure the dihedral angle between the selected four atoms, as shown in fig. 5.22 (d).

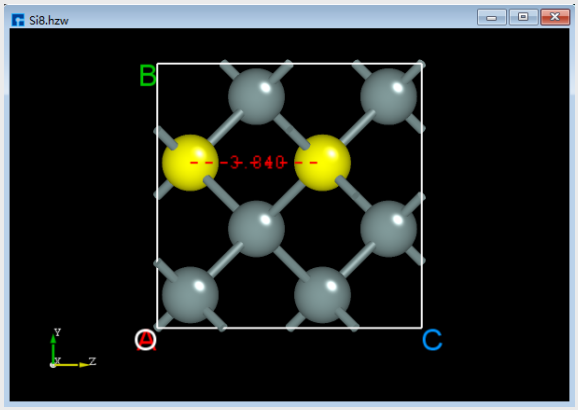


fig. 5.19: （a）

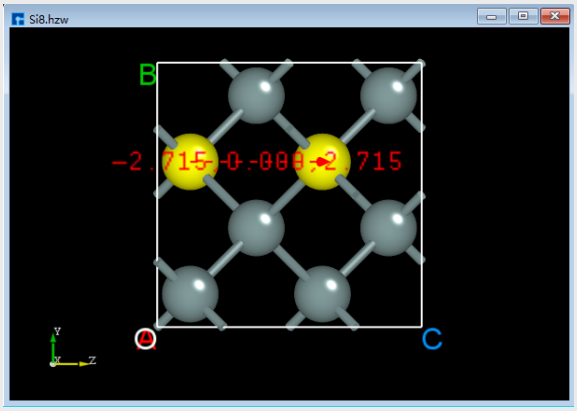


fig. 5.20: （b）

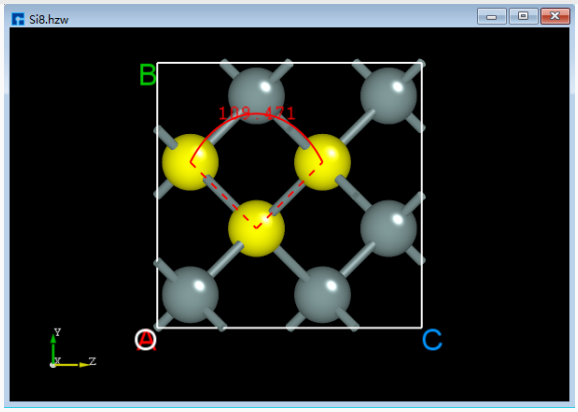


fig. 5.21: （c）

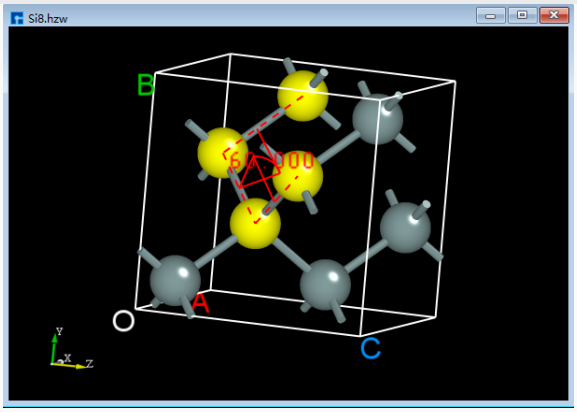


fig. 5.22: （d）

CHAPTER

SIX

ATOMIC STRUCTURE REFINEMENT MODULE

The Device Studio's new Structure Refinement Module (SRM) significantly enhances the rendering and anti-aliasing of 3D atomic structure displays. It displays atomic structures using equivalent atoms, supporting both ball-and-stick and polyhedral modes. In polyhedral mode, polyhedron transparency can be adjusted. Users can modify the color, radius, and lighting of individual atoms, multiple atoms of the same element, or groups of atoms. The SRM includes Device Studio initial templates, allowing users to create custom templates with defined color, radius, and lighting parameters, which can then be applied to imported atomic structures.

This chapter will use the **Si16O32 crystal structure** (`Si16O32.hzw`) as an example to detail the functions of the Structure Refinement Module.

***Key Features of the Atomic Structure Refinement Module** are as follows:

- – Added an atomic structure refinement module, comprehensively upgrading the rendering and anti-aliasing effects of the 3D atomic structure display;
  - – * Smoother and more three-dimensional atomic structure display for improved visualization.
- – Added support for displaying atomic structures as **equivalent atoms**, with options for ball-and-stick or polyhedron modes;
  - – * Users can select the display mode for atomic structures: ball-and-stick or polyhedron;
  - – * In polyhedron mode, users can adjust the polyhedron's color and transparency.
- – Added support for 3D structure view editing;
  - – * Supports modifying the color, radius, and lighting of a single atom, multiple atoms of the same element, or multiple atoms within an atomic structure.
- – Added Device Studio template functionality;

  - * Two Device Studio initial templates are currently available, allowing users to select and apply a template to the atomic structure;
  - * Templates are configured based on the periodic table of elements, including parameters such as color, radius, lighting, and background color.

- – Added support for creating user-specific templates;
  - * Users can set parameters such as template color, radius, lighting, and background color to generate and apply custom templates.
- – Added support for controlling the display or hiding of Axes, Cell, and OABC in the SRM structure display area;
- – Added support for setting the background color of the 3D structure view (SRM structure display area);
  - * Supports setting the background color of the SRM structure display area, including gradient effects.
- – Added structure import, save, and export functionalities.
  - * Supports importing and displaying *.dsxml*, *.hzw*, *.xyz*, *.cif*, *.pdb*, and *.mol* structure files;
  - * Supports exporting *.hzw*, *.xyz*, and *.cif* structure files;
  - * Supports exporting 3D views of atomic structures in *.png*, *.jpg*, *.bmp*, *.pdf*, *.tif*, and *.eps* image formats.

note

- – The *.dsxml* format is exclusive to the Device Studio atomic structure refinement module. To continue editing a structure file in a subsequent session, it is recommended to save it as a *.dsxml* file via the **Atomic Structure Refinement Module** interface, such as in fig. 6.1, by clicking *File* → *Save As*.
- – Since the Structure Refinement module displays the structure file in a **3D view**, and `.mol` structure files are available in both 2D and 3D formats, users who need to import this type of structure file into the Structure Refinement module are advised to import the 3D `.mol` structure file.

6.1 Introduction to the Graphical User Interface of the Atomic Structure Refinement Module

The graphical user interface (GUI) of the Structure Refinement Module (SRM) is shown in fig. 6.1.

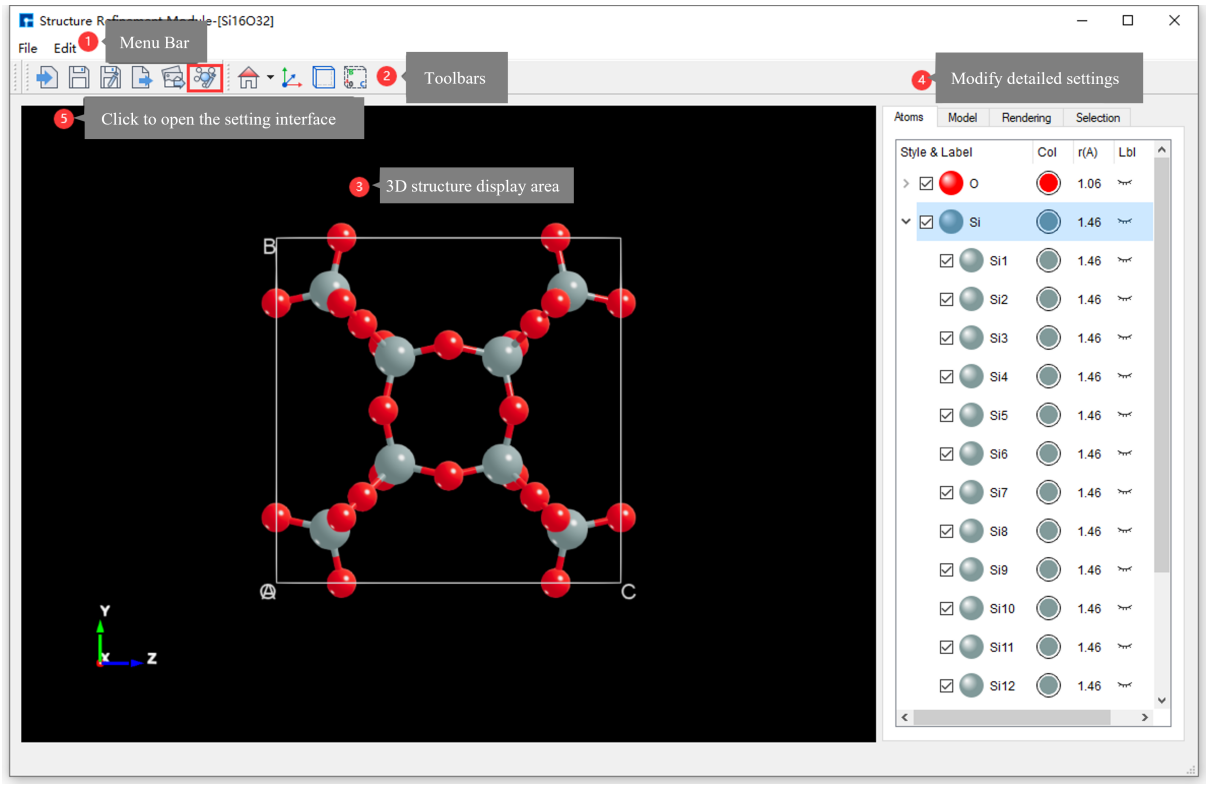


fig. 6.1: Atomic Structure Refinement Module Graphical User Interface

6.1.1 SRM Menu Bar

The Structure Refinement Module (SRM) menu bar is shown in fig. 6.2.

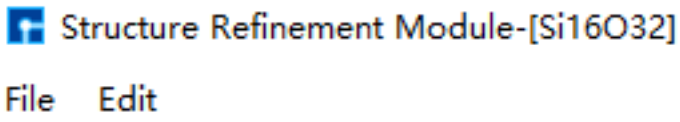


fig. 6.2: Atomic Structure Refinement Module Menu Bar

6.1.1.1 SRM Menu Bar - File

Clicking *File* on the Structure Refinement Module (SRM) menu bar displays the interface shown in fig. 6.3.

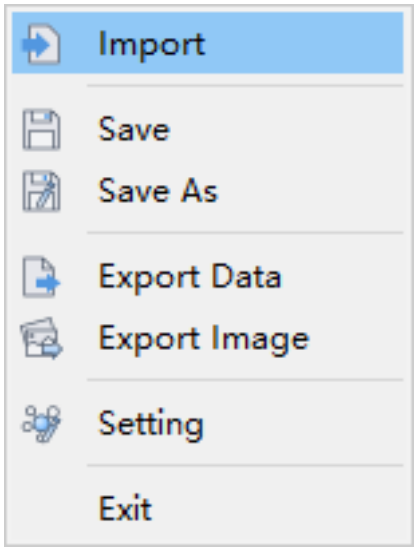


fig. 6.3: SRM - Menu Bar - File

- – *Import* : Clicking this opens a dialog box (as shown in fig. 6.27) for importing structure files (`.dsxml`, `.hzw`, `.xyz`, `.cif`, `.pdb`, `.mol`), allowing users to import atomic structures as needed.
- – *Save*: Initially grayed out and disabled. It becomes highlighted and enabled after the user edits the atomic structure. Clicking it saves the user's edits to the atomic structure parameters. This action subsequently invokes the *Save As* dialog (as shown in fig. 6.4) to save the structure file (`.dsxml`).
- – *Save As* : Clicking this button opens a dialog box for saving the structure file (`.dsxml`), allowing the user to name the file and choose a save location, as shown in fig. 6.4.
- – *Export Data* : Clicking this button opens a dialog for exporting structure files (`.hzw`, `.xyz`, `.cif`). Users can select the file format, name the file as needed, and choose a storage location, as shown in fig. 6.5.
- – *Export Image*: Clicking this button opens a dialog for exporting image files (`.png`, `.jpg`, `.bmp`, `.pdf`, `.tif`, `.eps`). Users can name the image file as needed and select a storage location, as shown in fig. 6.6.
- – *Setting* : Clicking this opens the Setting interface, which contains Device Studio templates. Parameters such as element radius, color, and lighting can be set within the

templates.

- – *Exit* : Click to close the atomic structure refinement module interface.

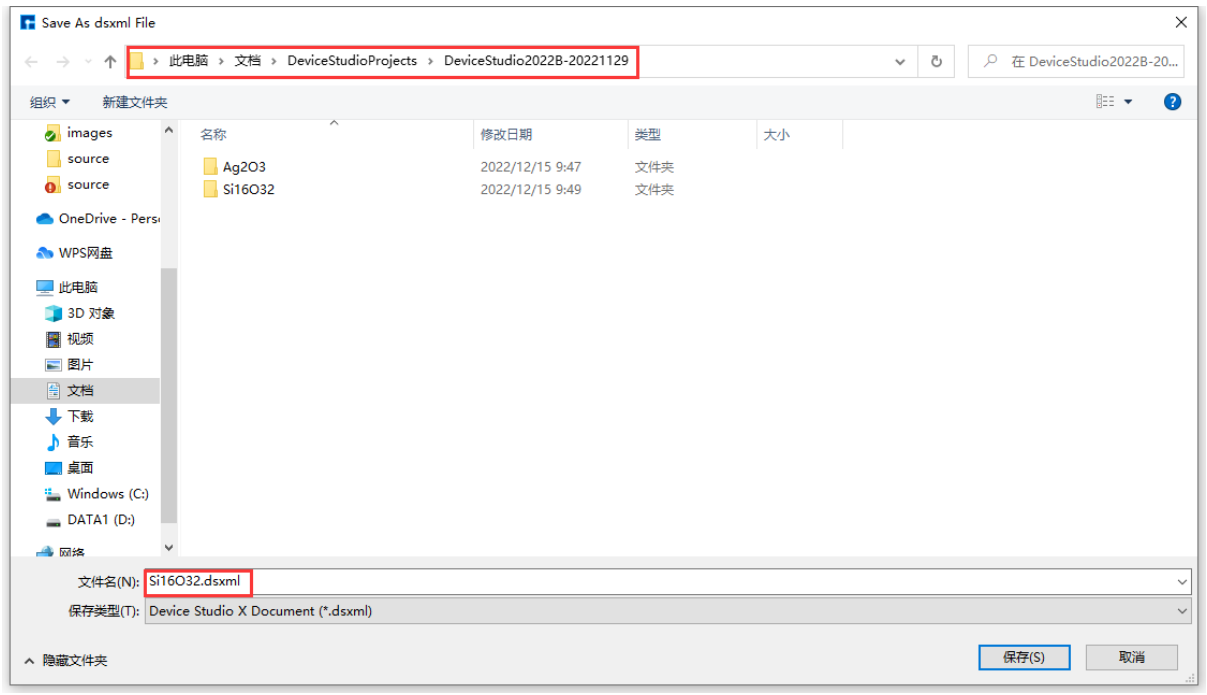


fig. 6.4: Save Structure File (`.dsxml`) Interface

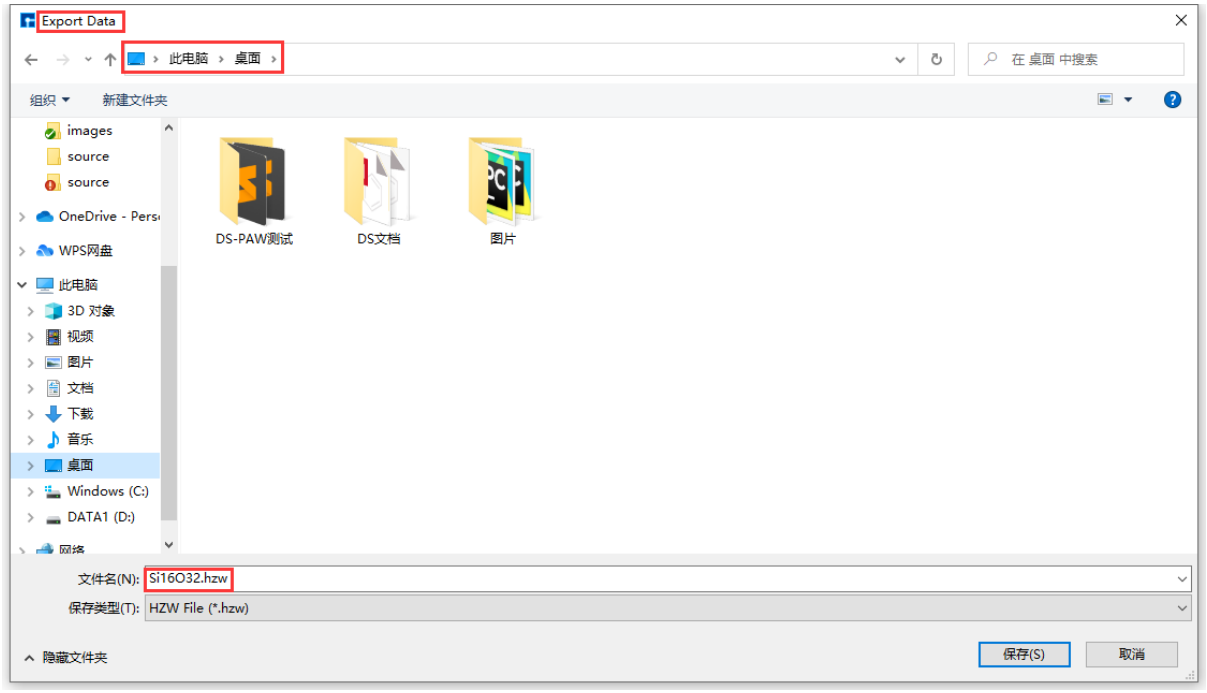


fig. 6.5: Export Structure Files (`.hzw`, `.xyz`, `.cif`) Interface

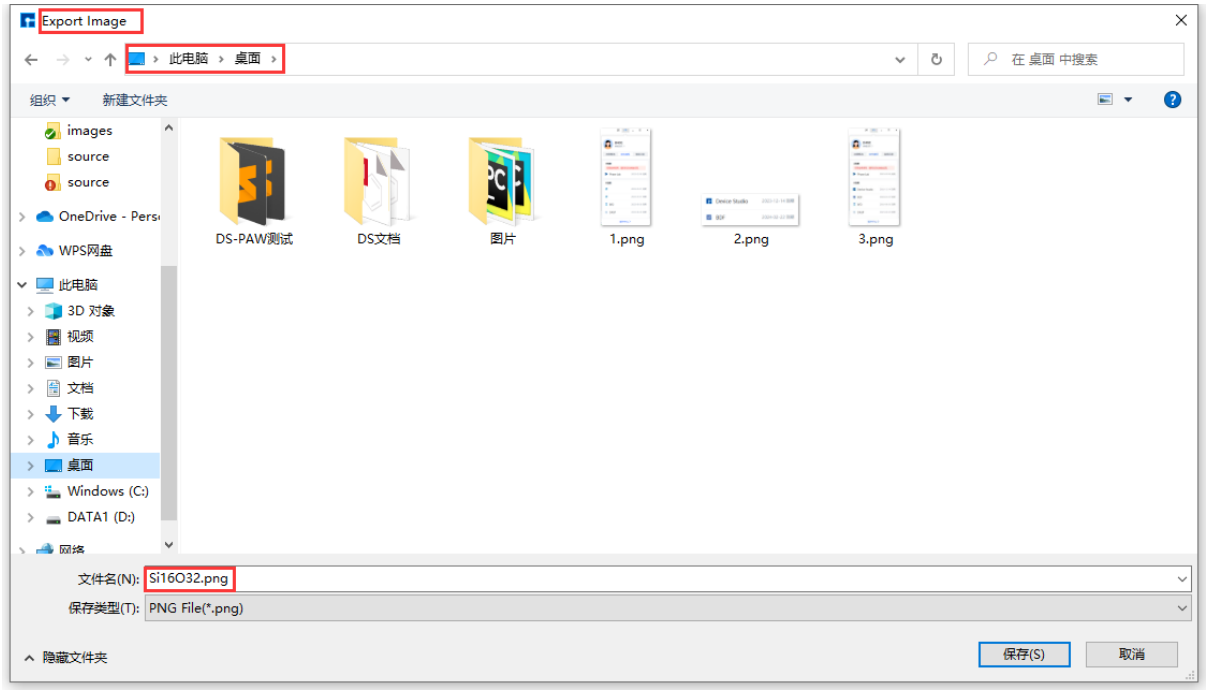


fig. 6.6: Export Image Files (.png, .jpg, .bmp, .pdf, .tif, .eps) Interface

6.1.1.2 SRM Menu Bar - Edit

Click *Edit* on the Structure Refinement Module (SRM) menu bar; the interface is shown in fig. 6.7.

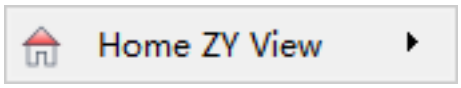


fig. 6.7: SRM - Menu Bar - Edit

- – *Home ZY View*: Clicking this restores the atomic structure to its initial state in the structure display area. The dropdown allows selection of different 3D views of the structure.

note

The *Home ZY View* primarily targets atomic structures that have been rotated, translated, zoomed, or scaled. Users can restore the initial state with a single click as needed.

6.1.2 SRM Toolbar

The Structure Refinement Module (SRM) menu bar is shown in fig. 6.8.

fig. 6.8: Structure Refinement Module Toolbar

The functions of each icon in the SRM toolbar are shown in the table below:

Number	Icon	Icon Name	Function Description
1		Import	After clicking, a dialog box for importing structural files pops up, allowing users to import atomic structures as needed.
2		Save	After clicking, save the user's edited parameters for the atomic structure.
3		Save As	After clicking, a dialog box pops up for saving the structure file (`.dsxml`), allowing you to save the structure file.
4		Export Data	After clicking, a dialog box pops up for exporting structural files (`.hzw`, `.xyz`, `.cif`), allowing users to select the desired file format.
5		Export Image	After clicking, a dialog box will pop up allowing you to export the image file (`.png`, `.jpg`, `.bmp`, `.pdf`, `.tif`, `.eps`). Users can name the structure file and select a storage location as needed.
6		Setting	After clicking, the Setting interface pops up. This interface contains Device Studio templates, allowing you to set parameters such as the radius, color, and lighting of elements in the template.
7		Home ZY View	After clicking, restores the initial state of the atomic structure in the structure display area. Clicking the dropdown allows you to view the 3D structure from different perspectives.
8		Show Axes	Show Axes
9		Hide Axes	Hide Axes
10		Show Cell	Show Cell when the structure is a crystal or a device.
11		Hide Cell	Hide the Cell when the structure is a crystal or device.
12		Show OABC	Show OABC when the structure is a crystal or device.
13		Hide OABC	Hide OABC when the structure is a crystal or device.

note

The first seven icons in the SRM toolbar correspond to those in the SRM menu bar; detailed functions can be found in the SRM menu bar. The *Show Cell*, *Hide Cell*, *Show OABC*, and *Hide OABC* functions are only activated when the imported structure is a crystal or device.

6.1.3 SRM - Structure Display Area

The Structure Refinement Module (SRM) structure display area, as shown in fig. 6.9, has the following functions:

- – Displays a 3D view of the atomic structure;
- – Supports zooming the 3D view of the atomic structure in and out by scrolling the **mouse wheel**.
- – Supports rotating the 3D view of the atomic structure by holding down the **right mouse button** and dragging the mouse.
- – Supports panning the 3D view of the atomic structure by holding down the **middle mouse button** and dragging the mouse;
- – Real-time display of atomic structure edits is supported.

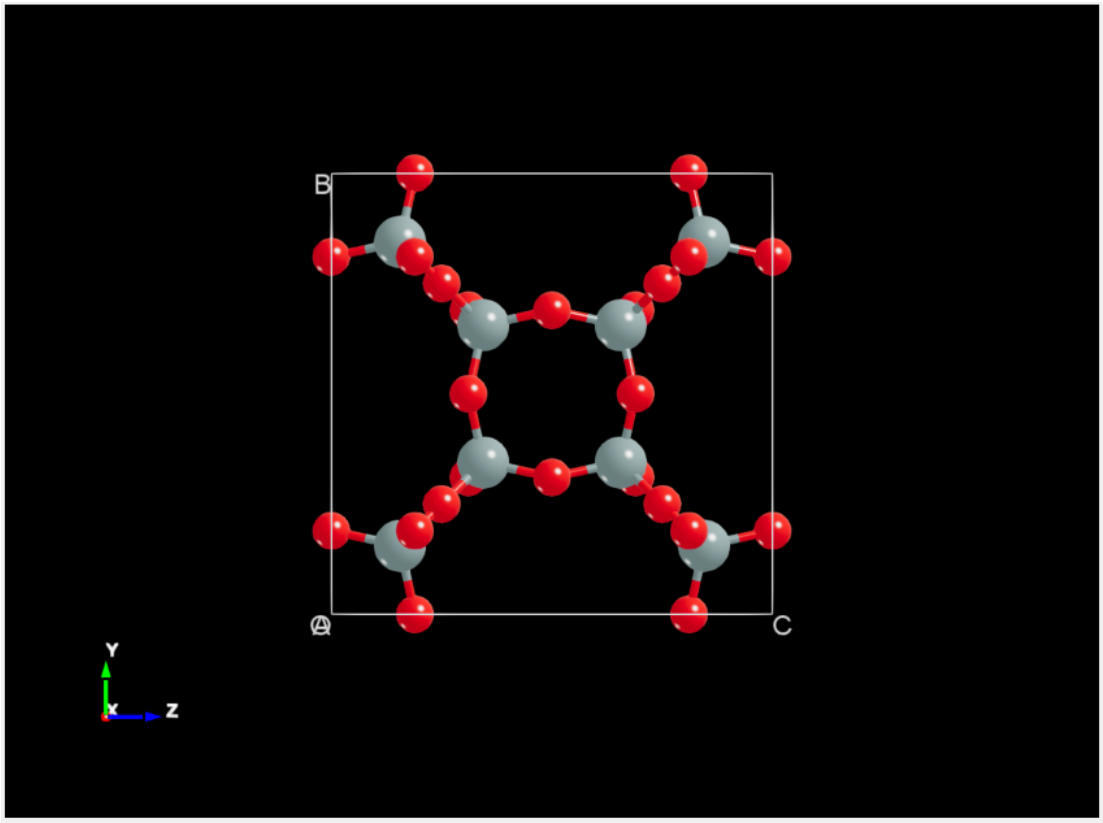


fig. 6.9: Atomic Structure Refinement Module Structure Display Area

6.1.4 SRM Parameter Adjustment Area

The Structure Refinement Module (SRM) parameter area, as shown in fig. 6.10, is divided into four sections: Atoms, Model, Rendering, and Selection. Each section will be explained below.

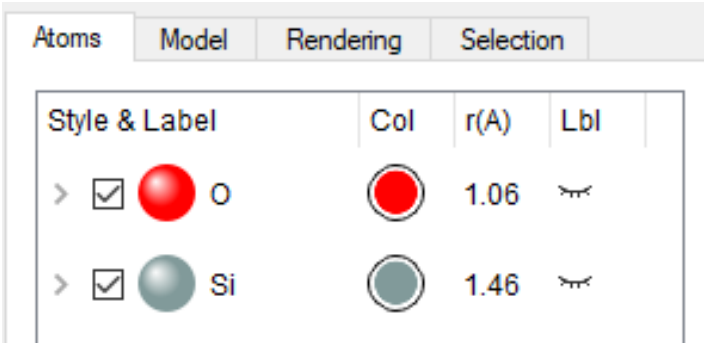


fig. 6.10: Atomic Structure Refinement Module Parameter Adjustment Area

note

The atomic structure refinement module parameter adjustment area is activated only after a structure has been imported; otherwise, it is grayed out and unusable. Descriptions of this area's functionality are provided only when it is activated and usable.

6.1.4.1 SRM - Parameter Adjustment Area - Atoms Area

The Atoms area in the parameter adjustment region of the Structure Refinement Module (SRM), as shown in fig. 6.11, provides the following functionality:

- – Supports collapsing atoms in the atomic structure by element pattern or expanding them by label pattern; the default is collapsing by element pattern.
- – Supports modifying the color and radius of atoms of the same element within the atomic structure;
- – Supports modifying the color and radius of a single atom in the atomic structure;
- – Supports showing or hiding all atoms of the same element in the atomic structure.
- – Show or hide individual atoms in the atomic structure;
- – Supports showing or hiding the labels of all atoms of the same element in the atomic structure;
- – Supports showing or hiding the label of a specific atom in the atomic structure.

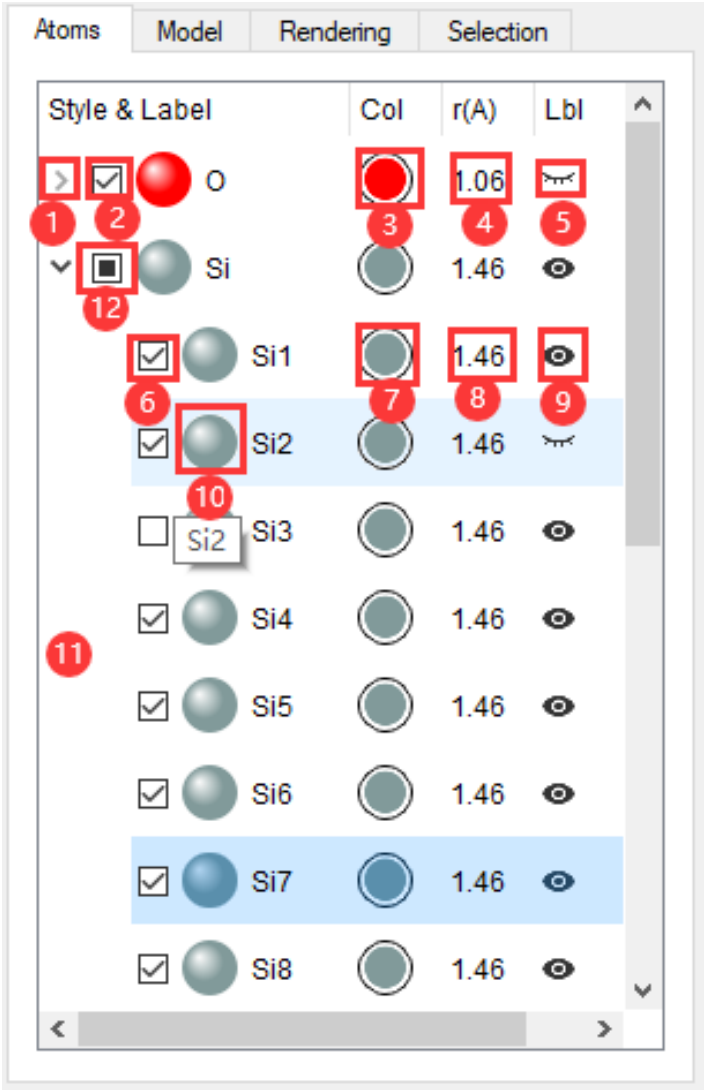


fig. 6.11: Atoms Area in the Structure Refinement Module Parameter Adjustment Region

The following describes the functions of each labeled item in the Atoms area of the Structure Refinement Module (SRM) parameter adjustment region, as shown in fig. 6.11:

- – Label ① in fig. 6.11: Collapse atoms in the structure by element type or expand them by label.
  - – * When the button arrow points down, clicking it will collapse all expanded ○ atoms according to the ○ element pattern;
  - – * When the button arrow points right, clicking will expand all ○ atoms according to the label mode.
- – Number ② in fig. 6.11: Show or hide all atoms of the same element in the structure in the SRM structure display area;

  - ∗ Checked, all ○ atoms are shown in the SRM structure display area;
  - ∗ Unchecked, all ○ atoms are hidden in the SRM structure display area.

- – Number ③ in fig. 6.11: Modify the color of the same element in the structure;
  - ∗ Click ③ in fig. 6.11 → The Select Color interface pops up as shown in fig. 6.12 → Select a color or enter RGB values → Click the *OK* button to modify the color of the ○ element (i.e., the color of all ○ atoms).

note

When the atomic structure is displayed in polyhedral mode, modifying the color of atoms or elements in the structure will change the color of the polyhedra. Users can use this method to modify the color of the polyhedra.

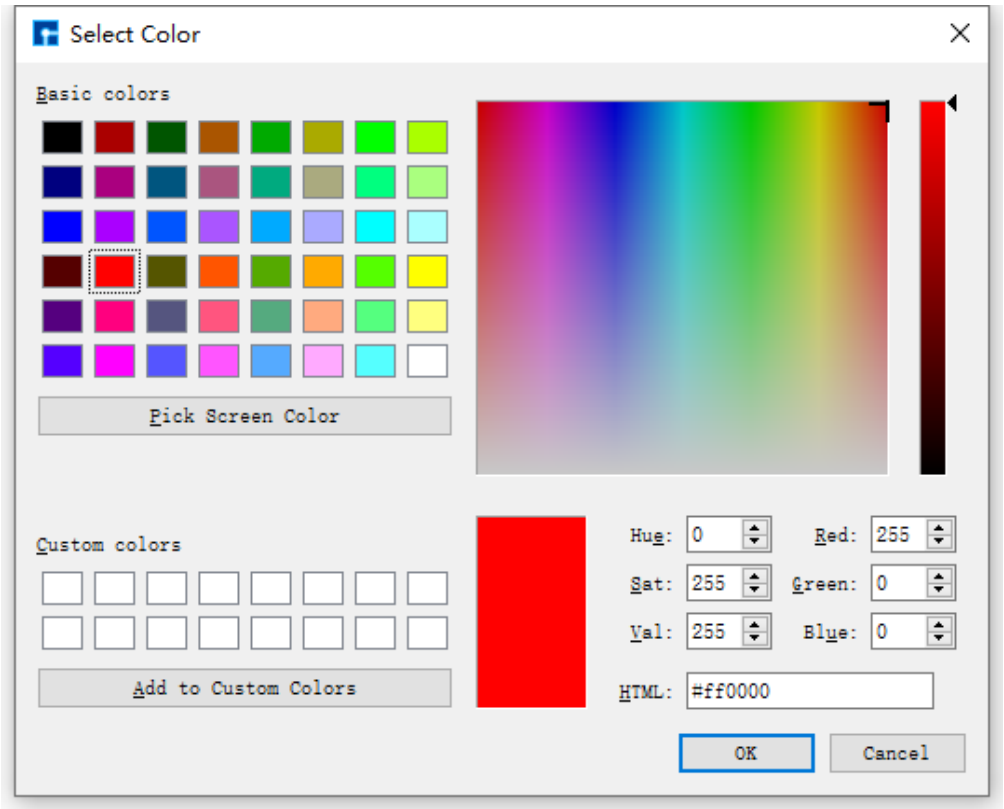


fig. 6.12: Select Color Interface

- – Label ④ in fig. 6.11: Modify the radius of the same element in the structure;
  - ∗ Double-click label ④ in fig. 6.11 → modify the radius value to change the radius of the ○ element (i.e., the radius of all ○ atoms).

note

This radius value is of Double type and is rounded to two decimal places.

- – Item ⑤ in fig. 6.11: Shows or hides the labels of all atoms of the same element in the SRM structure display area;
  - – * When the eye button is closed, the labels of all O atoms are hidden in the SRM structure display area;
  - – * When the eye button is open, the SRM structure display area shows the labels of all O atoms.
- – Item ⑥ in fig. 6.11: Shows or hides a specific atom in the SRM structure display area;
  - – * Checking this box displays the Si1 atom in the SRM structure display area;
  - – * Unchecking this will hide the Si1 atom in the SRM structure display area.
- – No. ⑦ in fig. 6.11: Modify the color of an atom in the structure;
  - – * Click label ⑦ in fig. 6.11 → The Select Color interface, as shown in fig. 6.12, will pop up → Select a color or enter RGB values → Click the *OK* button to modify the color of the Si1 atom.
- – Label ⑧ in fig. 6.11: Modify the radius of an atom in the structure;
  - – * Double-click label ⑧ in fig. 6.11 → modify the radius value to change the radius of the Si1 atom.
- – Number ⑨ in fig. 6.11: Show or hide the label of a specific atom in the SRM structure display area;
  - – * When the eye button is closed, the label of the Si1 atom is hidden in the SRM structure display area;
  - – * When the eye button is open, the label of the Si1 atom is displayed in the SRM structure display area.
- – fig. 6.11, label ⑩: Hovering the mouse over this location will display the atom label;
  - – * If the atom label is too long to be fully displayed, place the mouse cursor over it to show the complete label. For example, placing the cursor over label ⑩ in fig. 6.11 will display the complete label Si2.

- – Number □ in fig. 6.11: This can be any location in the Atoms area. You can modify the color or radius of all elements in the structure by right-clicking.
  - – * Change the color of all elements in the structure: Right-click → Color → Device Studio template 1 or Device Studio template 2;
  - – * Modify the radius of all elements in the structure: Right-click → Radius → Device Studio template 1 or Device Studio template 2.

note

Device Studio templates 1 and 2 are initial templates for Device Studio. These templates are configured based on the periodic table and include parameters such as color, radius, lighting, and background color. Selecting a template applies all of its parameters to the structure.

6.1.4.2 SRM - Parameter Adjustment Area - Model Area

The Model area in the parameter adjustment region of the Structure Refinement Module (SRM), as shown in fig. 6.13, provides the following functionalities:

- – Supports selecting the display mode of the atomic structure: ball-and-stick mode or polyhedral mode;
- – In polyhedron mode, the polyhedron transparency can be adjusted;
- – Supports controlling the visibility of Axes, Cell, and OABC within the SRM structure display area.
- – Supports setting the background color of the SRM structure display area, including gradient effects.

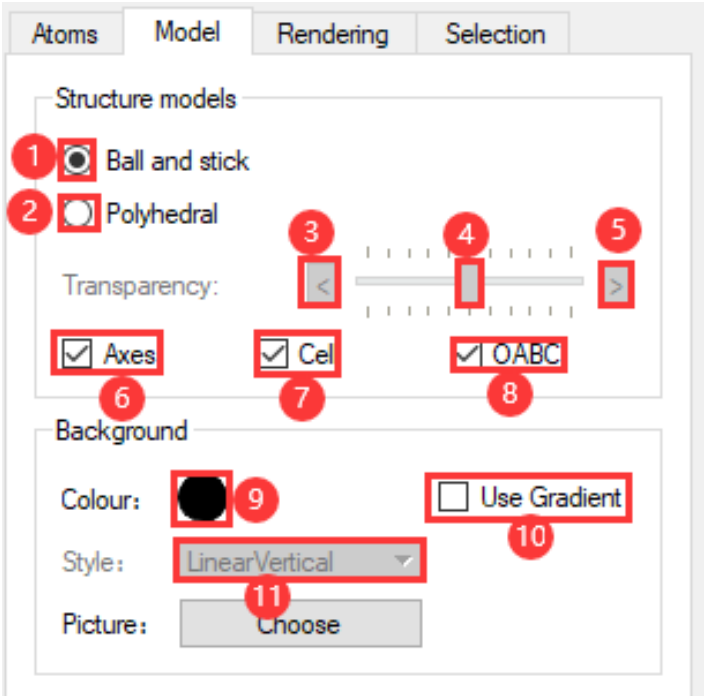


fig. 6.13: Structure Refinement Module Parameter Adjustment Area - Model Area

The following describes the functions of each labeled item in the Model area of the Structure Refinement Module (SRM) parameter adjustment region, as shown in fig. 6.13:

- – In fig. 6.13, label ①: Clicking ① selects the ball-and-stick model for displaying the atomic structure;
- – In fig. 6.13, label ②: Clicking ② selects the polyhedral model for displaying the atomic structure;
- – In fig. 6.13, label ③: In polyhedral mode, clicking area ③ increases the transparency of the polyhedra, making them increasingly transparent;
- – In fig. 6.13, label ④: In polyhedral mode, dragging label ④ adjusts the transparency of the atomic structure polyhedra;
  - – * Left-click and drag the button in area ④ to the left to increase the polyhedron's transparency, making it more transparent.
  - – * Click and hold the button in area ④ with the left mouse button and drag to the right to decrease the polyhedron's transparency, making it increasingly opaque.
- – In fig. 6.13, clicking area ⑤ in polyhedron mode reduces the polyhedron's transparency, making it increasingly opaque;

note

Items ③, ④, and ⑤ in fig. 6.13 (i.e., polyhedron transparency adjustment) are only active when item ② (Polyhedral) is selected, meaning the atomic structure display mode is set to polyhedral. Otherwise, they are grayed out and unavailable. Only one of the ball-and-stick and polyhedral modes can be selected at a time.

- – Number ⑥ in fig. 6.13: Shows or hides coordinate axes in the SRM structure display area;
  - – * Checked, the coordinate axes of the atomic structure will be displayed in the SRM structure display area;
  - – * Unchecked, the atomic structure coordinate axes are hidden in the SRM structure display area.
- – Item ⑦ in fig. 6.13: When the structure is a crystal or device, show or hide its cell in the SRM structure display area;
  - – * When checked, the atomic structure's cell is displayed in the SRM structure display area;
  - – * Unchecked, the atomic structure Cell is hidden in the SRM structure display area.
- – Item ⑧ in fig. 6.13: When the structure is a crystal or device, show or hide its OABC in the SRM structure display area;
  - – * When checked, the OABC of the atomic structure is displayed in the SRM structure display area;
  - – * Unchecked, hides the OABC atomic structure in the SRM structure display area.

note

Labels ⑦ and ⑧ in fig. 6.13 are only activated when the imported structure is a crystal or device; if the imported structure is a molecule, both functions are grayed out and unavailable.

- – Number ⑨ in fig. 6.13: Modifies the background color of the SRM structure display area;
  - – * Click label ⑨ in fig. 6.13 → A Select Color dialog box will pop up as shown in fig. 6.12 → Select a color or enter RGB values → Click the *OK* button to modify the background color of the SRM structure display area.

- – Number ⑩ in fig. 6.13 sets the background color of the SRM structure display area to a gradient effect;
  - – * Checked: Sets the background color to a gradient effect;
  - – * Unchecking this option disables the background gradient effect.
- – In fig. 6.13, item ⑪: When item ⑩ (i.e., Use Gradient) in fig. 6.13 is checked, click the dropdown button to select the gradient type for the background color.

note

In fig. 6.13, item ⑪ is activated only when item ⑩ (i.e., Use Gradient) is checked; otherwise, it is grayed out and unavailable.

6.1.4.3 SRM - Parameter Adjustment Area - Rendering Area

The Rendering area in the Structure Refinement Module (SRM) parameter adjustment region, as shown in fig. 6.14, is divided into three parts: **Atom**, **Bonds**, and **Lighting**. These allow for lighting adjustments to atoms, bonds, and the entire atomic structure, respectively. Atom and bond lighting is controlled by three parameters: Multiplier, Diffuse, and Shininess. The **Lighting** section adjusts the lighting of the entire atomic structure. This module provides the following functionality:

- – Supports individual lighting adjustments for atoms and bonds within the atomic structure;
- – Global illumination adjustment for the entire atomic structure is supported.
  - – * Supports illuminating the atomic structure with multiple light beams, up to a maximum of four.
  - – * Supports adjusting the position of the light beams on the atom.
  - – * Supports adjusting the beam intensity;
  - – * Supports adjusting the ambient light parameters.

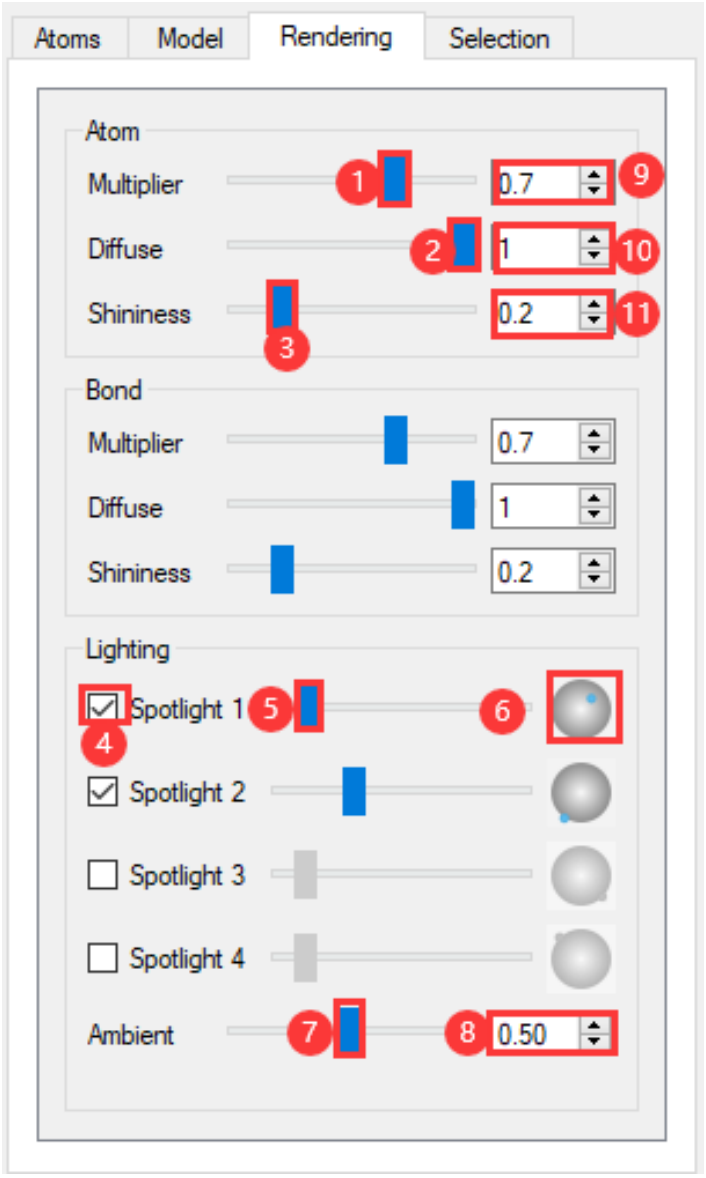


fig. 6.14: Structure Refinement Module Parameter Adjustment Area - Rendering Area

The following describes the functionality of each labeled feature in the Rendering area of the Structure Refinement Module (SRM) parameter adjustment region, i.e., fig. 6.14:

- – **Atom** section: Adjusts the lighting of atoms in the atomic structure;
  - ∗ Labels ①, ②, ③ and ⑨, ⑩, ⓫ in fig. 6.14: Adjust the lighting of atoms in the structure by dragging the **slider** at positions ①, ②, ③ or setting the **numerical value** at positions ⑨, ⑩, ⓫. This is achieved by adjusting the Multiplier (highlight coefficient), Diffuse (diffuse reflection coefficient), and Shininess (shininess) parameters, and the effect can be seen in real time in the SRM structure display area.
- – **Bond** section: Adjusts the lighting of bonds in the atomic structure;

  - The lighting parameters in this section are adjusted in the same way as in the **Atom** section and will not be described here.

- **Lighting** section: Adjusts the overall lighting of the atomic structure. Spotlight 1 to Spotlight 4 represent four light sources, initially positioned at four fixed locations (two frontal, two rear). A maximum of four spotlights can illuminate the atomic structure.

  - Item ④ in fig. 6.14: Controls whether a light beam (e.g., Spotlight 1) illuminates the atom, with real-time effects visible in the SRM structure display area.

    - Checked, the beam (e.g., Spotlight 1) illuminates the atoms;

    - Unchecked, the beam (e.g., Spotlight 1) will not illuminate the atom.

  - Item ⑤ in fig. 6.14: Adjusts the brightness of the beam (e.g., Spotlight 1), with real-time effects visible in the SRM structure display area.

    - Click the button in area ⑤ with the left mouse button, hold and drag to the left to decrease the beam brightness, making it dimmer.

    - Click and hold the button in area ⑤ with the left mouse button and drag to the right to increase the beam brightness.

  - Number ⑥ in fig. 6.14: Adjusts the position of the beam illuminating the atom, with the adjustment effect visible in real time in the SRM structure display area;

    - Clicking label ⑥ in fig. 6.14 adjusts the beam's position on the atom, as shown in fig. 6.15.

  - Click labels ⑦ and ⑧ in fig. 6.14, drag label ⑦ to **slide the button** or set the value at label ⑧ to adjust the atom structure lighting via the Ambient parameter. The adjustment effect can be seen in real-time in the SRM structure display area.

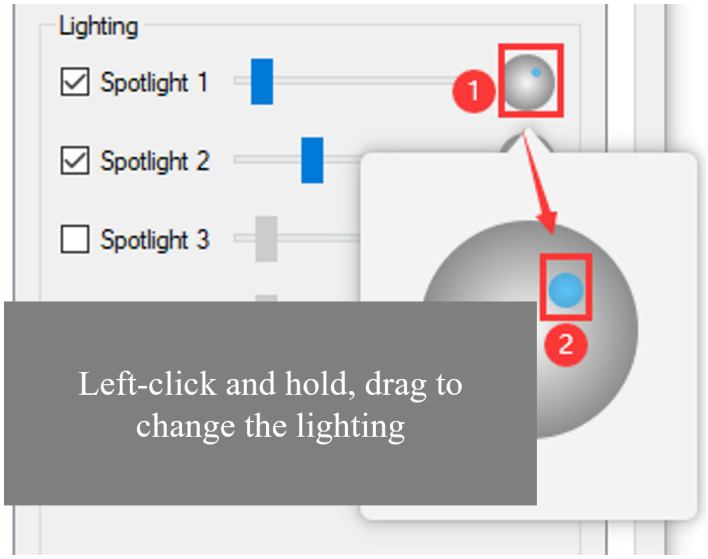


fig. 6.15: User interface for adjusting the beam's position on the atoms.

note

- – Multiplier (specular coefficient) ranges from [0, 1], with a default value of 0.7 for both **Atom** and **Bond** sections;
- – Diffuse (Diffuse Reflection Coefficient) ranges from [0, 1], with a default value of 1 for both **Atom** and **Bond** sections;
- – Shininess (glossiness) ranges from [0.001, 1], with a default value of 1 for both **Atom** and **Bond** sections;
- – Ambient (ambient light) ranges from [0, 1], with a default value of 0.5.

6.1.4.4 SRM Parameter Adjustment Area - Selection Area

The Selection area in the Structure Refinement Module (SRM) parameter adjustment region is initially grayed out and unavailable. It is activated by selecting an atom in the SRM structure display area. For example, selecting atom `O43` in the Si16O32 crystal structure in the SRM structure display area will display the properties of atom `O43` in the Selection area, as shown in fig. 6.16. The module's functions are as follows:

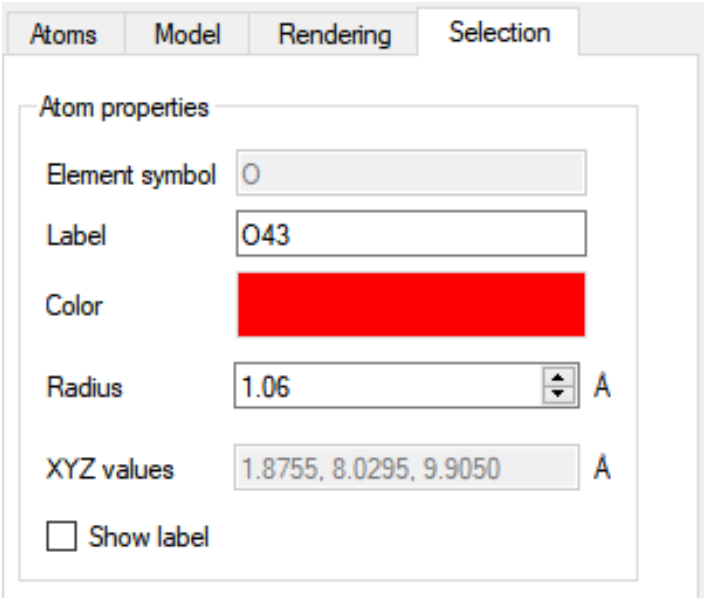


fig. 6.16: Atom Structure Refinement Module Parameter Adjustment Area - Selection Area

- – *Element symbol* : Displays the element symbol of the selected atom (e.g., `O43` atom), not editable;
- – *Label* : Displays the label of the selected atom (e.g., atom `O43`). It is editable.
- – *Color* : Displays the color of the selected atom (e.g., `O43` atom). Clicking the color button after *Color* → opens the Select Color interface as shown in fig. 6.12 → select a color or enter RGB values → click the *OK* button to modify the color of the `O43` atom;
- – *Radius* : Displays the radius of the selected atom (e.g., `O43` atom), and allows editing.
- – *XYZ values* : Displays the coordinates of the selected atom (e.g., atom `O43`), which are not editable;
- – *Show label* : When checked, shows the label of the selected atom (e.g., `O43` atom) in the SRM structure display area; otherwise, hides it.

6.1.5 SRM Setting Interface

Click the *Setting* icon in the Structure Refinement Module (SRM) graphical user interface SRM toolbar as shown in fig. 6.17, to open the SRM Setting interface as shown in fig. 6.18. This module provides the following functionalities:

- – Supports user selection of Device Studio initial templates and their application to the structure;

  - * Initial templates Device Studio template 1 and Device Studio template 2 are shown in fig. 6.18 and fig. 6.19 respectively.

- – Users can customize parameters such as color, radius, lighting, and background color to generate and apply a personalized template.

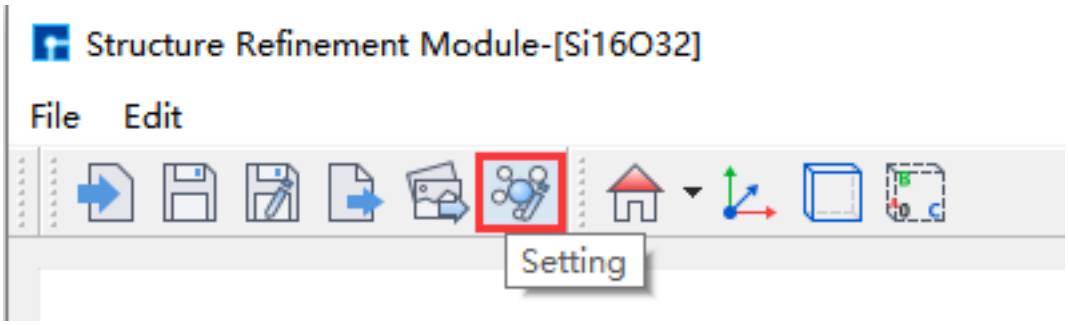


fig. 6.17: Steps to Open the Setting Interface

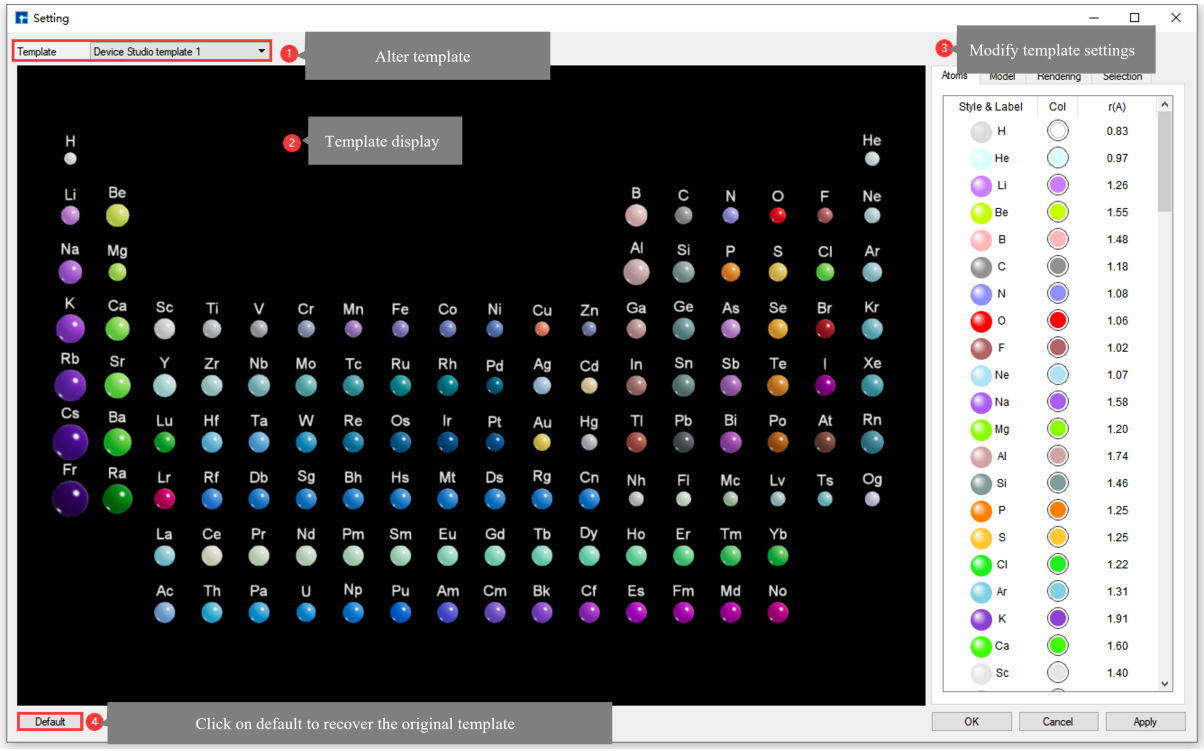


fig. 6.18: Settings Interface (Device Studio template 1)

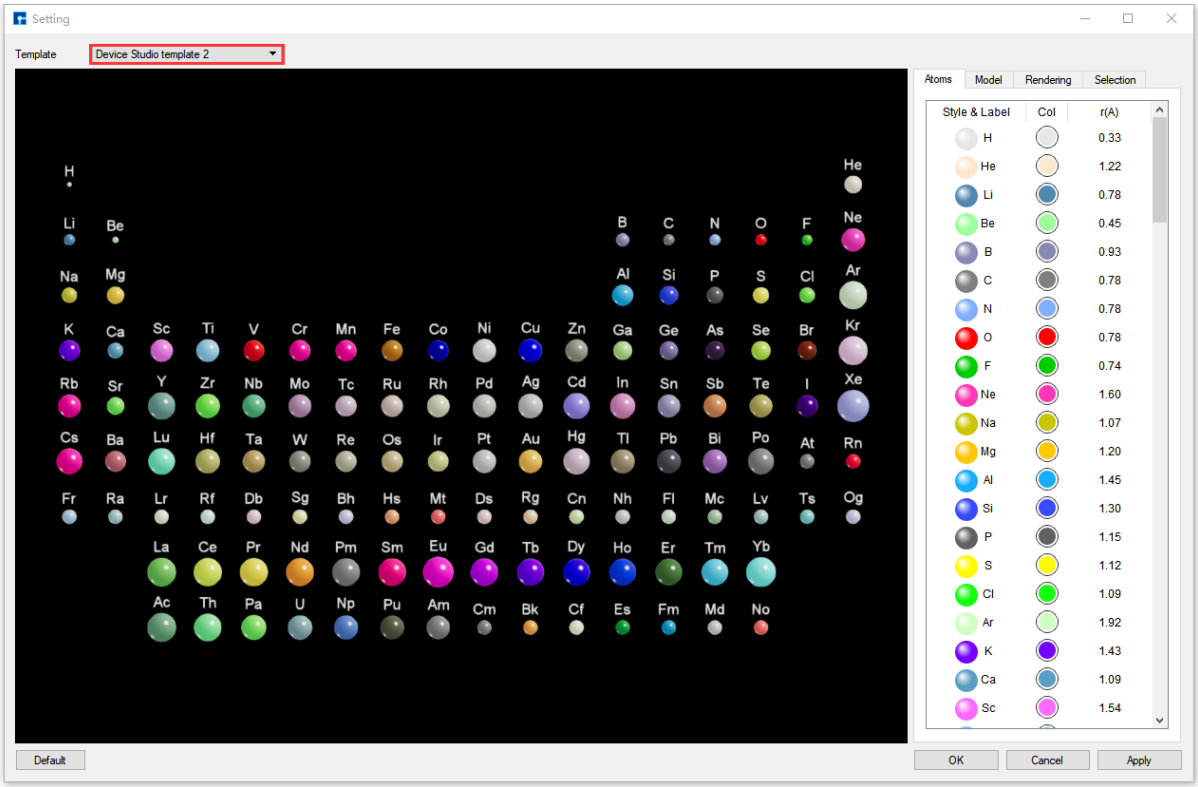


fig. 6.19: Settings Interface (Device Studio template 2)

Functional description of parameters in the Setting interface of the atomic structure refinement module fig. 6.18:

- – Template Selection Area:
  - * The Structure Refinement module currently includes two Device Studio initial templates, Device Studio template 1 and Device Studio template 2, as shown in fig. 6.18 and fig. 6.19 respectively. A dropdown button allows selection; Device Studio template 1 is used by default. The templates contain:
    - * · The template is arranged according to the periodic table, and by default displays all atoms in the periodic table structure;
    - * · Labels for all atoms in the default periodic table structure;
    - * · Default element color parameter;
    - * · Default element radius parameter;
    - * · Default lighting parameters;
    - * · The default background color for displaying the periodic table structure is black.

- – Template Display Area:
  - * Displays the template element periodic table structure file, and also displays real-time adjustments to template parameters in this area;
- – Template Parameter Adjustment Area:
  - * This area has the same functionality as the SRM parameter adjustment area in the atomic structure refinement module, except that the **polyhedral mode** for selecting the periodic table structure of template elements is unavailable. Further details are omitted here.
- – *Default* : Clicking this button restores the Device Studio initial template;
- – *OK* : Clicking this button closes the Setting interface, saves the template parameters, and applies the parameters to the structure in the atomic structure refinement template interface;
- – *Cancel* : Clicking this button closes the Setting window without saving the template parameters;
- – *Apply* : Click this button to save the template parameters without closing the Setting interface, and apply the parameters to the structure in the atomic structure refinement template interface.

note

To generate a user-specific template, you can modify the initial Device Studio templates, Device Studio template 1 and Device Studio template 2, based on fig. 6.18 and fig. 6.19 respectively. Adjust parameters such as color, radius, lighting, and background color, then click *OK* or *Apply* in the Setting interface. Refer to *SRM Parameter Adjustment Area* for detailed parameter adjustment instructions.

6.2 Importing Structures into the Atomic Structure Refinement Module

Before using the Structure Refinement Module (SRM), you need to log in and start and create a project. To import the Si16O32 crystal structure, drag and drop the Si16O32 structure file into the Device Studio *Project Management Area (Project Explorer)* area (import structure). There are two ways to import the structure into the SRM via the Device Studio main interface.

1. Method 1: If the structure (e.g., Si16O32 crystal structure) is already displayed on the Device Studio main interface, as shown in fig. 6.20, the Si16O32 crystal structure can be imported into the Structure Refinement Module as shown in fig. 6.21;

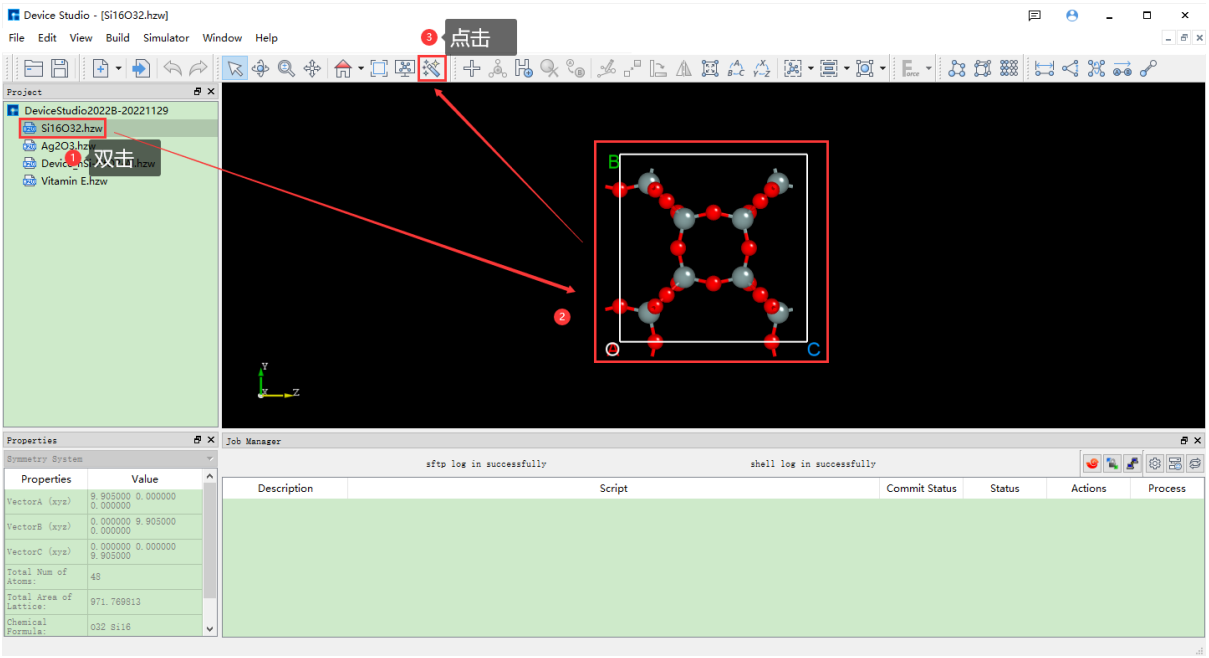


fig. 6.20: Device Studio main interface showing the Si16O32 crystal structure (**without equivalent atoms shown**).

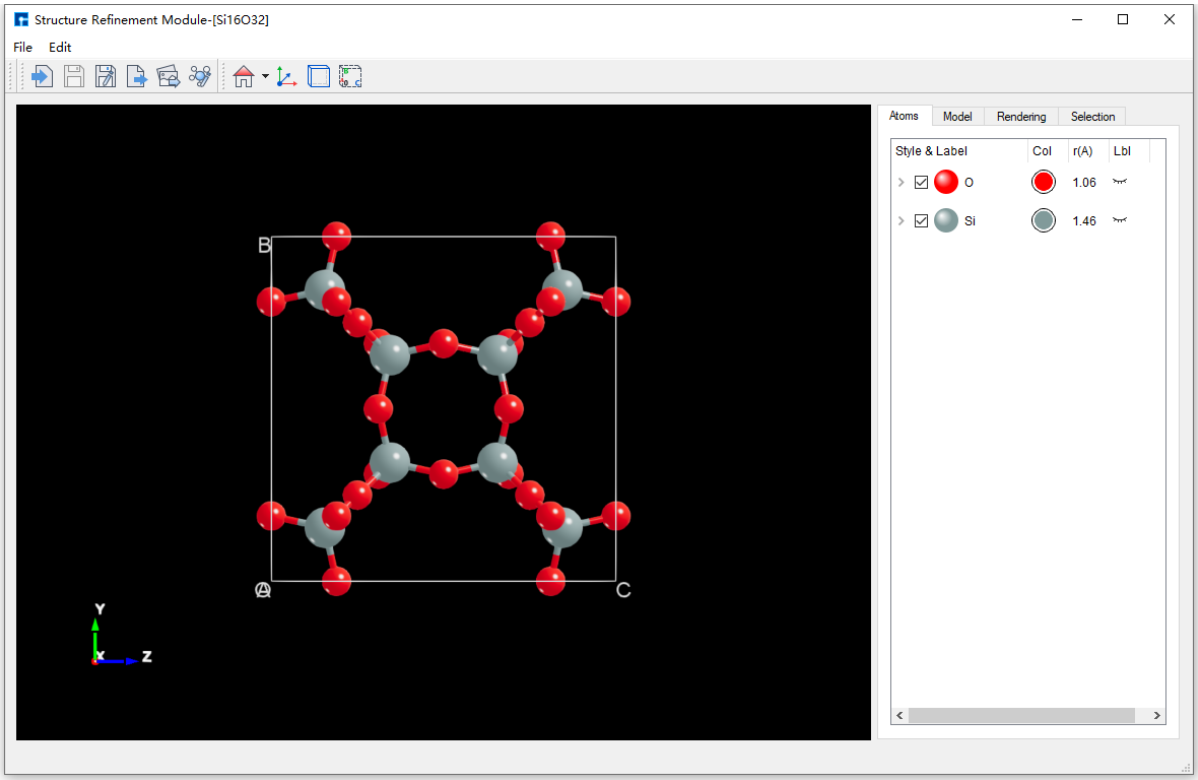


fig. 6.21: Import the atomic structure refinement module interface for the Si16O32 crystal structure (**show equivalent atoms**).

The Si16O32 crystal structure is displayed in the Device Studio main interface and the atomic structure refinement module interface with **equivalent atoms not shown** and **equivalent atoms shown**, respectively, as shown in fig. 6.22 and fig. 6.23.

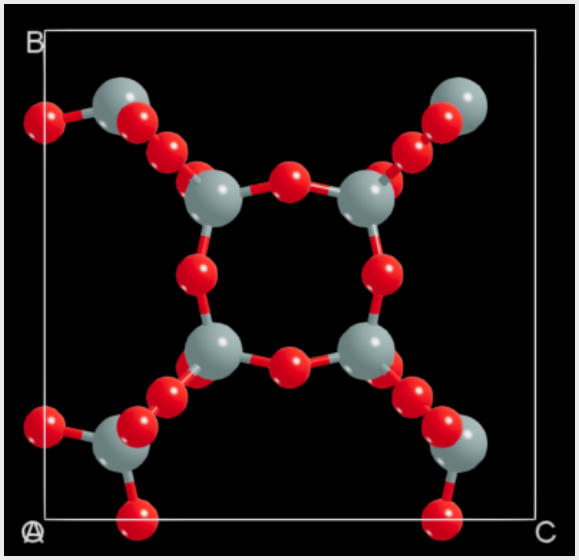


fig. 6.22: The Si16O32 crystal structure does not show equivalent atoms

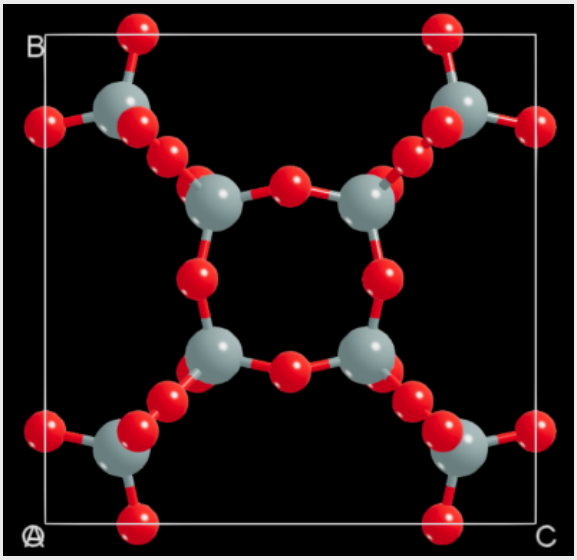


fig. 6.23: The Si16O32 crystal structure shows equivalent atoms

2. Method 2: If the structure is not displayed in the Device Studio main interface, as shown in fig. 6.24, you can enter the atomic structure refinement module as shown in fig. 6.25. As shown in fig. 6.26 and fig. 6.27, you can import the Si16O32 crystal structure into the atomic structure refinement module. The atomic structure refinement module interface after importing the Si16O32 crystal structure is shown in fig. 6.21.

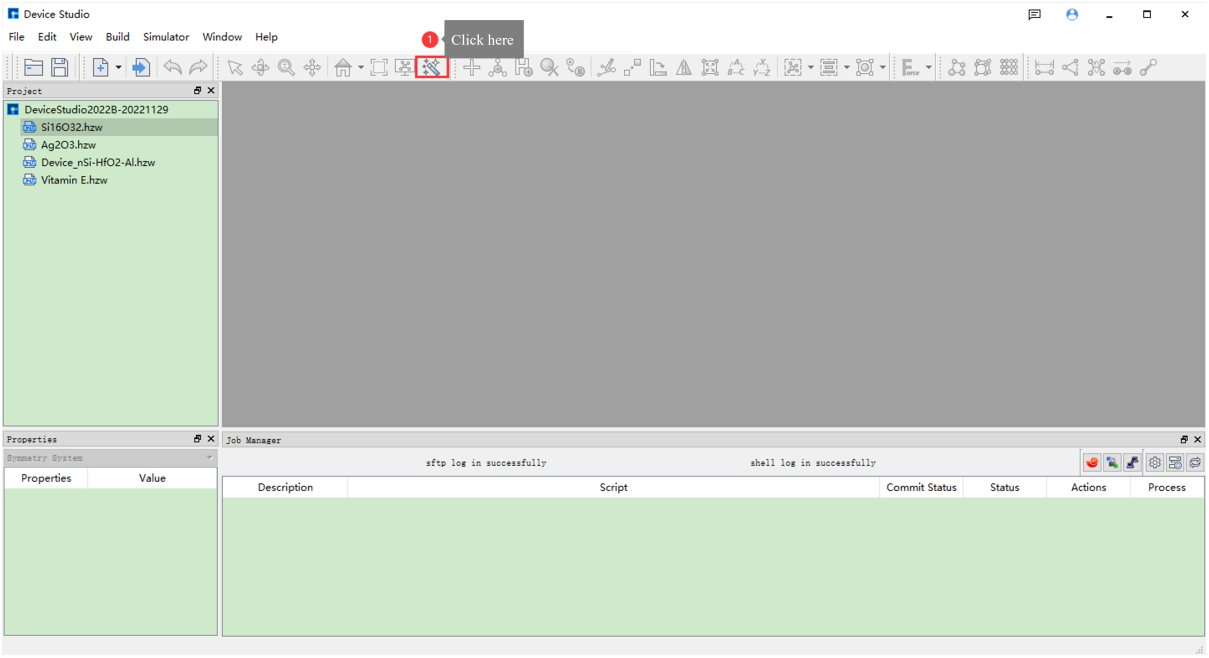


fig. 6.24: Device Studio main interface without structure displayed

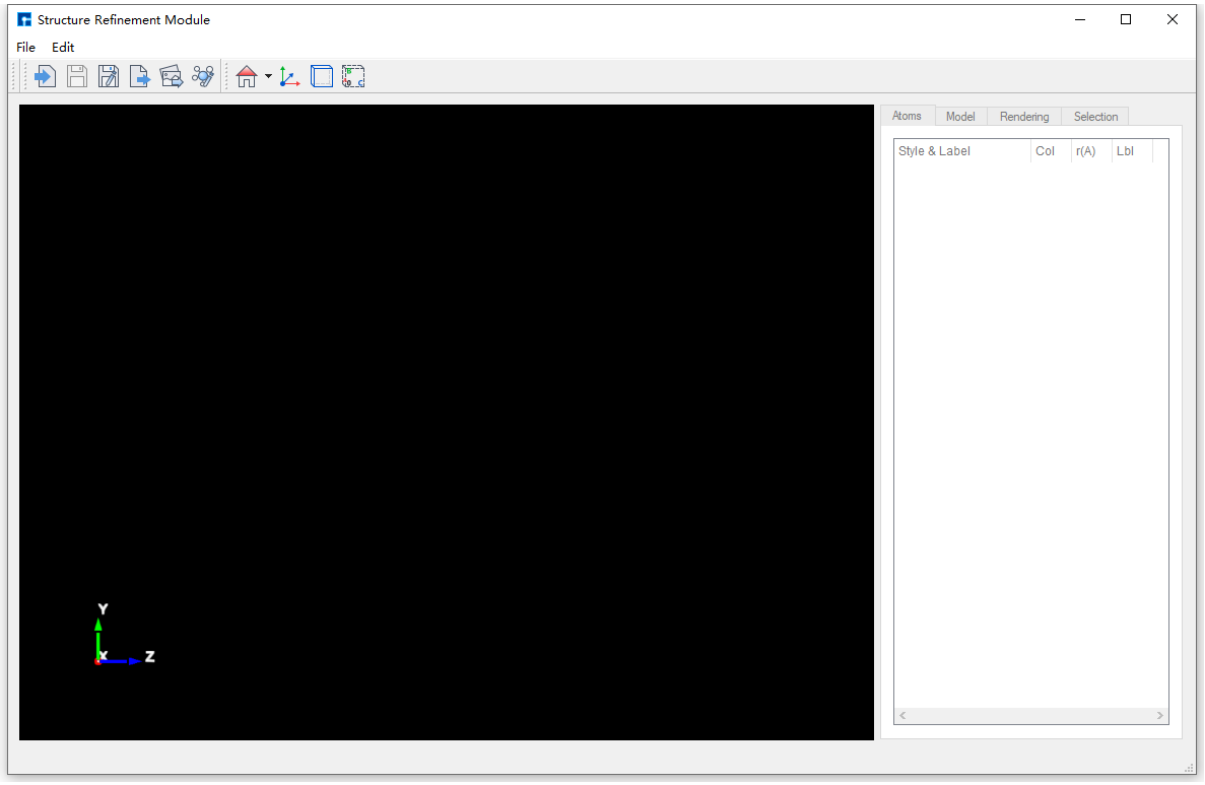


fig. 6.25: The atomic structure refinement module interface is not displayed.

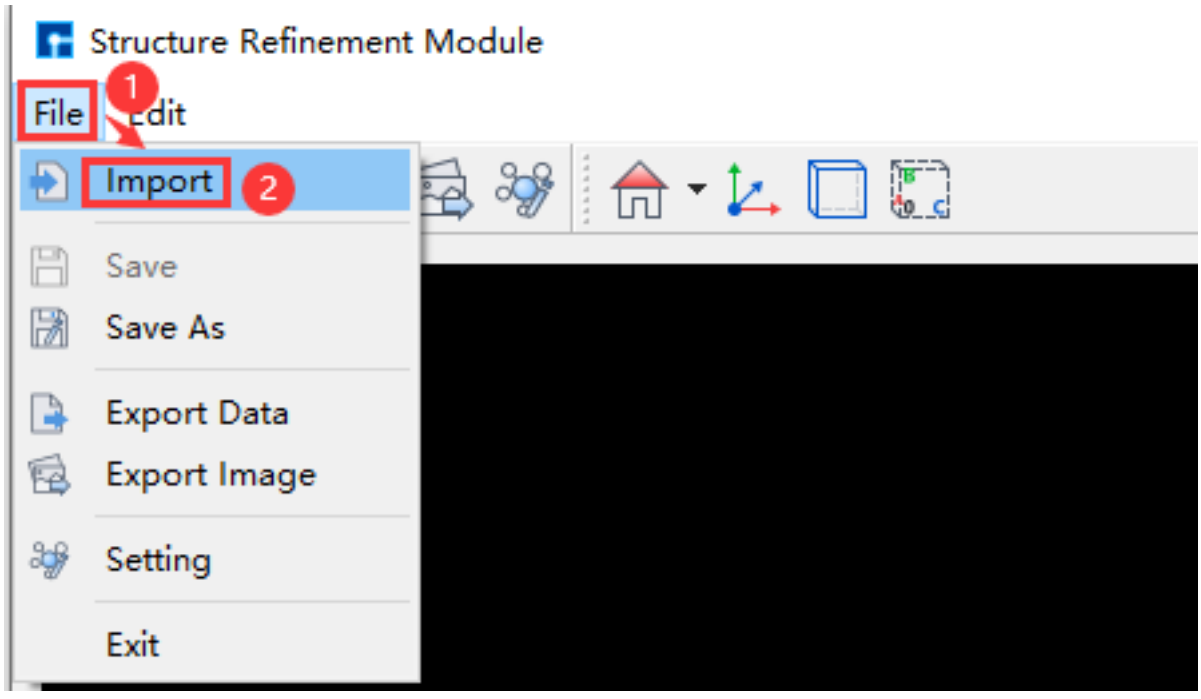


fig. 6.26: The Atomic Structure Refinement Module pops up; import structure operation interface.

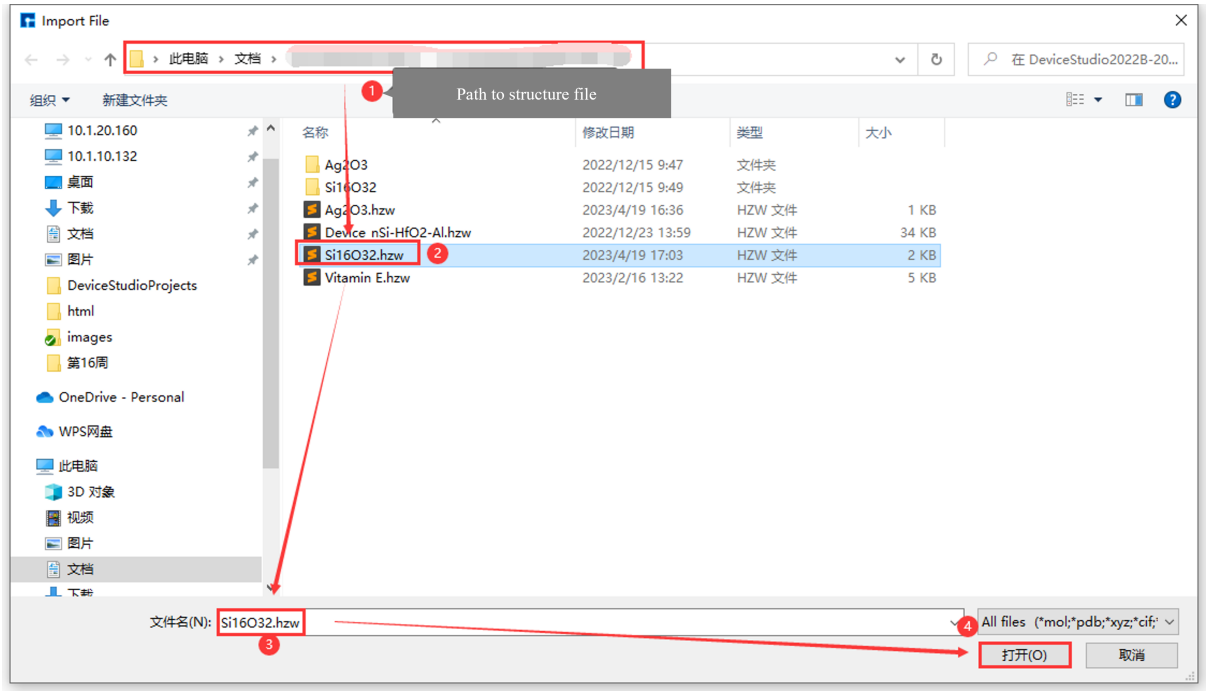
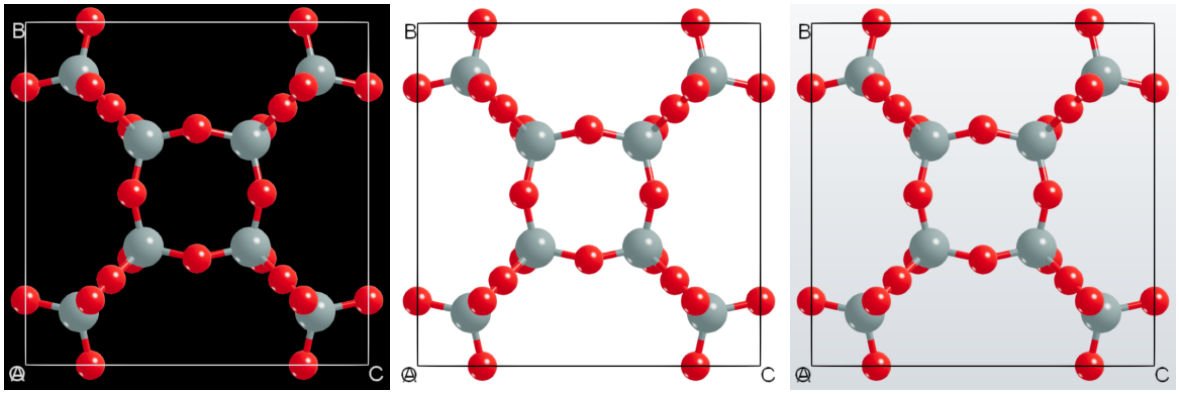


fig. 6.27: Select the Si16O32 crystal structure file to import into the atomic structure refinement module interface.

6.3 Modify the background color of the atomic structure refinement module

Modifying the background color of the Atomic Structure Refinement module requires a loaded structure. For example, if you have already loaded the **Si16O32 crystal structure** as shown in fig. 6.21, refer to Importing a structure into the Atomic Structure Refinement module for instructions on importing a structure. Detailed instructions for importing are omitted here.

To illustrate, this section details how to modify the background color of the Si16O32 crystal structure display within the Atomic Structure Refinement module, specifically changing the background color of the SRM structure display area, using the **Si16O32 crystal structure** as an example.



1. As shown in fig. 6.28, the interface for modifying the **background color** of the displayed Si16O32 crystal structure from **pure black** to **pure white** is shown.

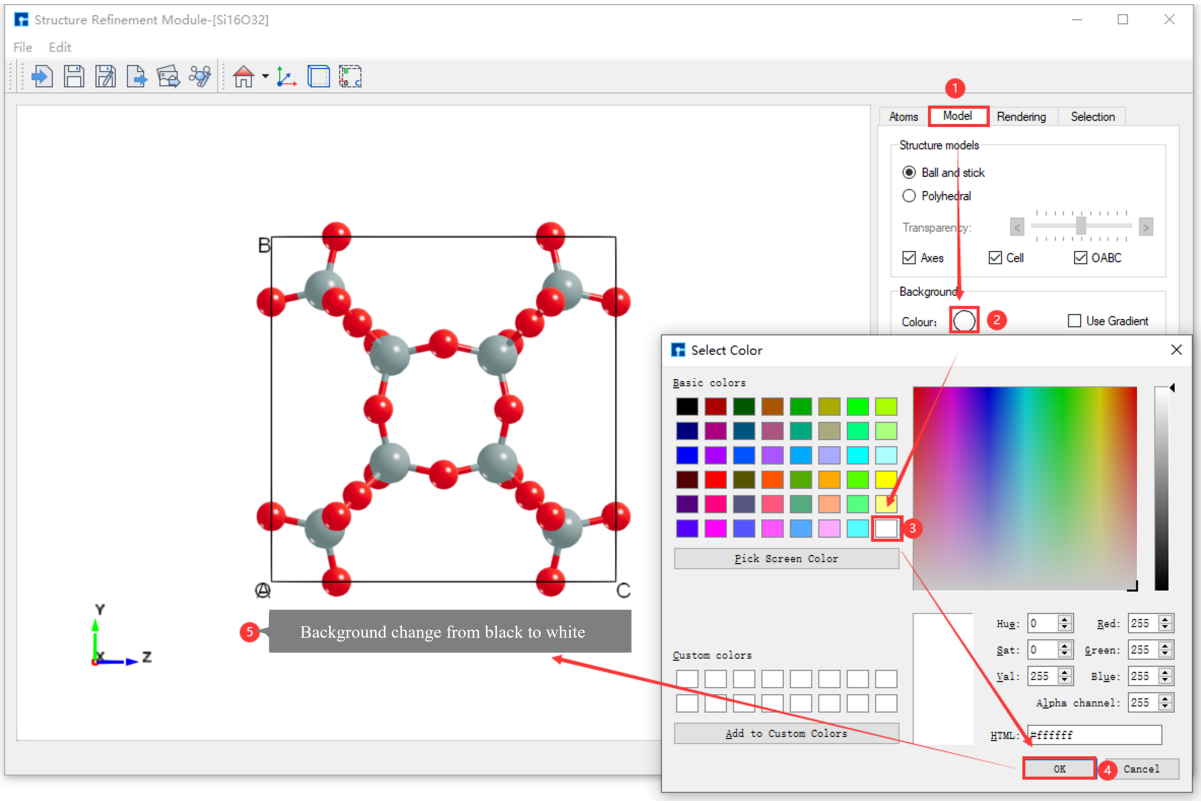


fig. 6.28: The operation interface for changing the background color of the displayed Si16O32 crystal structure from **pure black** to **pure white**.

2. As shown in fig. 6.29, this is the interface for changing the background color of the displayed Si16O32 crystal structure from **pure white** to a **gradient effect**.

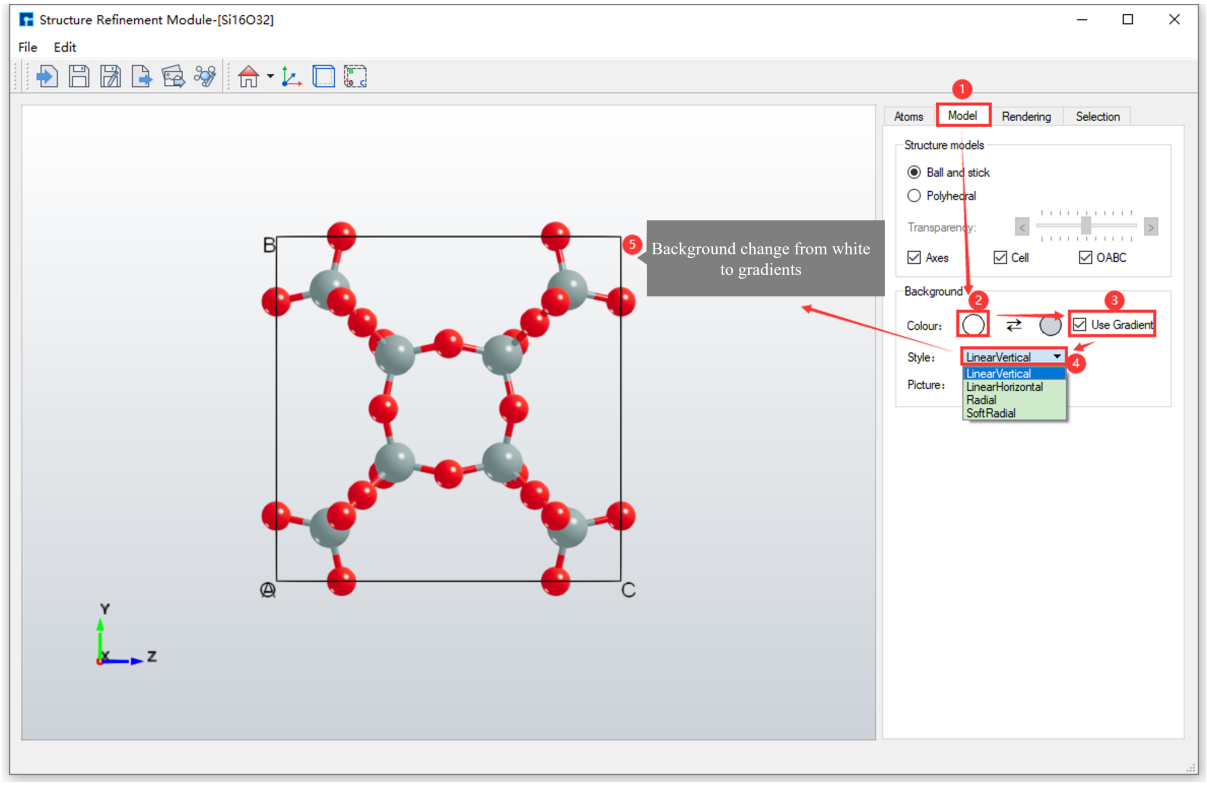


fig. 6.29: The interface displays the modification of the **background color** of the Si16O32 crystal structure from **pure white** to a **gradient effect**.

3. Based on fig. 6.29, click the dropdown button in area ④ of fig. 6.29 to select the gradient type for the background color.

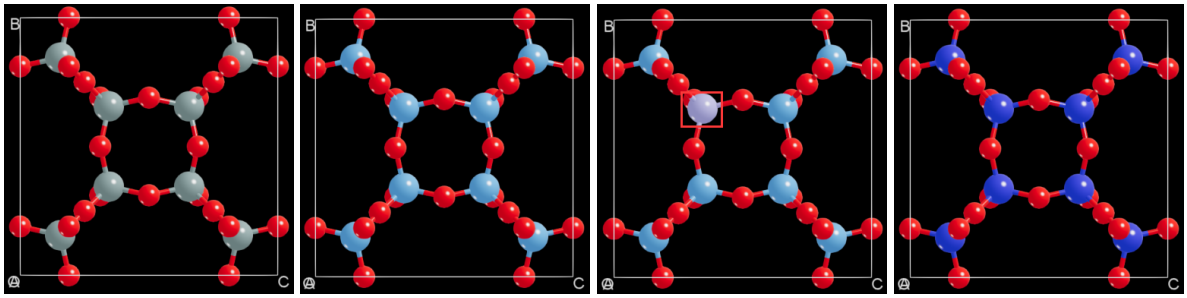
note

The background color of the atomic structure refinement module is primarily modified through *SRM - Parameter Adjustment Area - Model Area*. Users can read this section for details.

6.4 Modifying the color of atoms in the structure

To modify the color of atoms in the structure, you need to import the structure first. For example, if you have already imported the **Si16O32 crystal structure** into the Atomic Structure Refinement module as shown in fig. 6.21, you can refer to the section Importing structures into the Atomic Structure Refinement module for details on importing structures. The specific steps will not be detailed here.

Taking the **Si16O32 crystal structure** as an example, this section details how to modify the color of atoms within the **Si16O32 crystal structure** in the Atomic Structure Refinement module.



6.4.1 Modifying the Color of the Same Element within a Structure

As shown in fig. 6.30, this interface allows modification of the color of the Si element (i.e., all Si atoms) in the Si16O32 crystal structure to **blue** (RGB value: `[85 170 255]`).

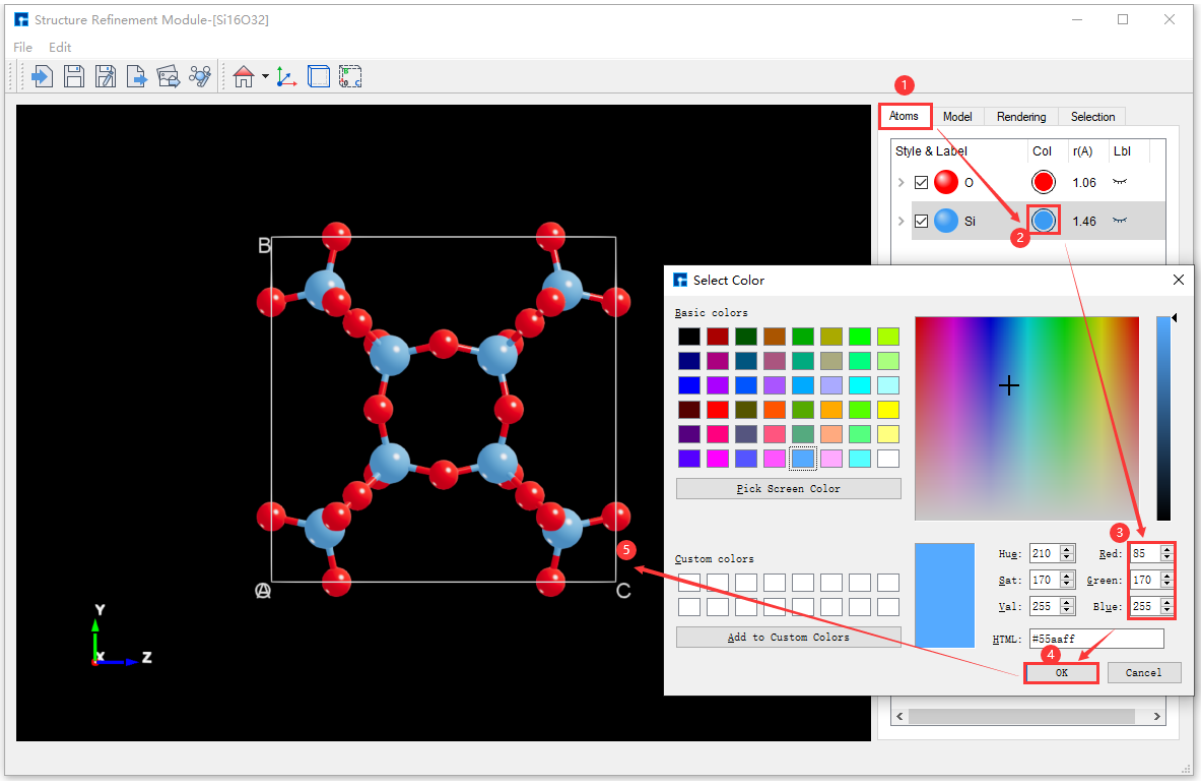


fig. 6.30: The interface for modifying the color of the `Si` element in the Si16O32 crystal structure to **blue** (RGB value `[85 170 255]`)

6.4.2 Change the color of an atom in the structure

There are two ways to change the color of atom `Si11` in the Si16O32 crystal structure to RGB value `[170 170 255]`, based on fig. 6.30.

1. Method 1: Without selecting the `Si11` atom, as shown in fig. 6.31, the interface for modifying the color of the `Si11` atom in the Si16O32 crystal structure to RGB value `[170 170 255]` is displayed;

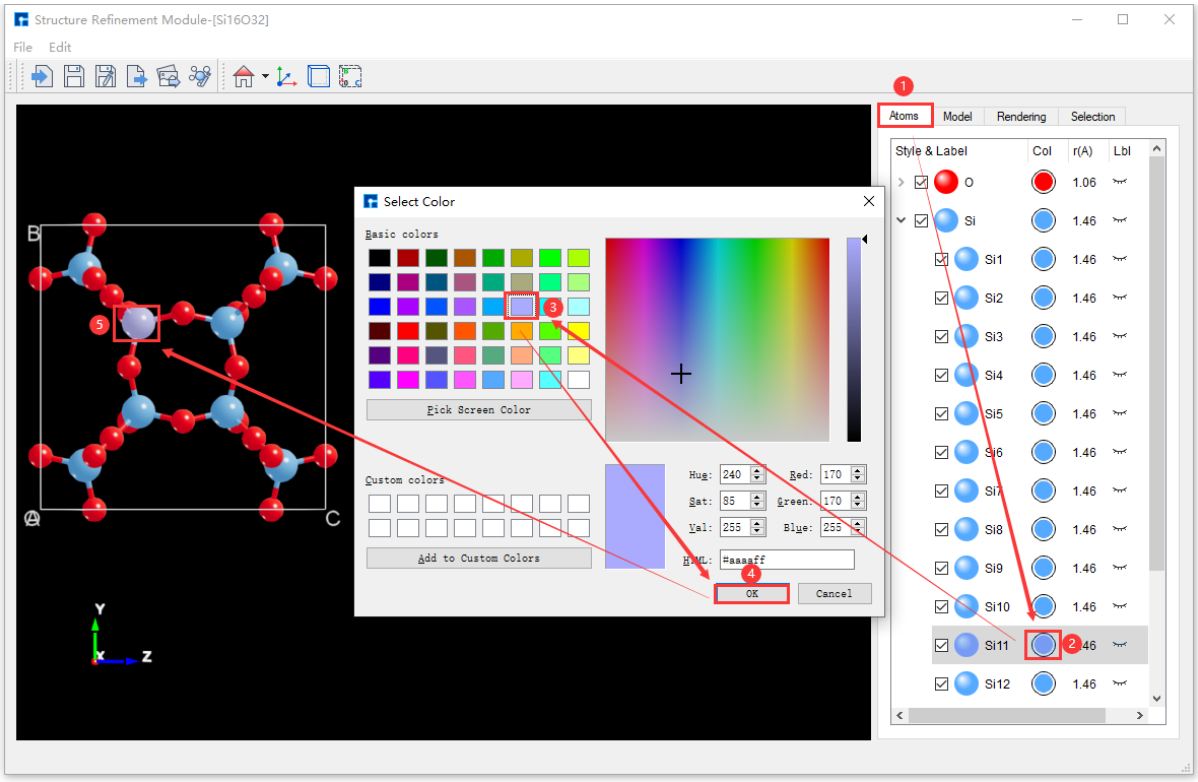


fig. 6.31: Unselected atoms: Modify the color of the `Si11` atom in the `Si16O32` crystal structure to RGB value `[170 170 255]` in the operation interface.

2. Method 2: Click on the `Si11` atom with the mouse, as shown in fig. 6.32, to modify the color of the `Si11` atom in the Si16O32 crystal structure to RGB value `[170 170 255]`.

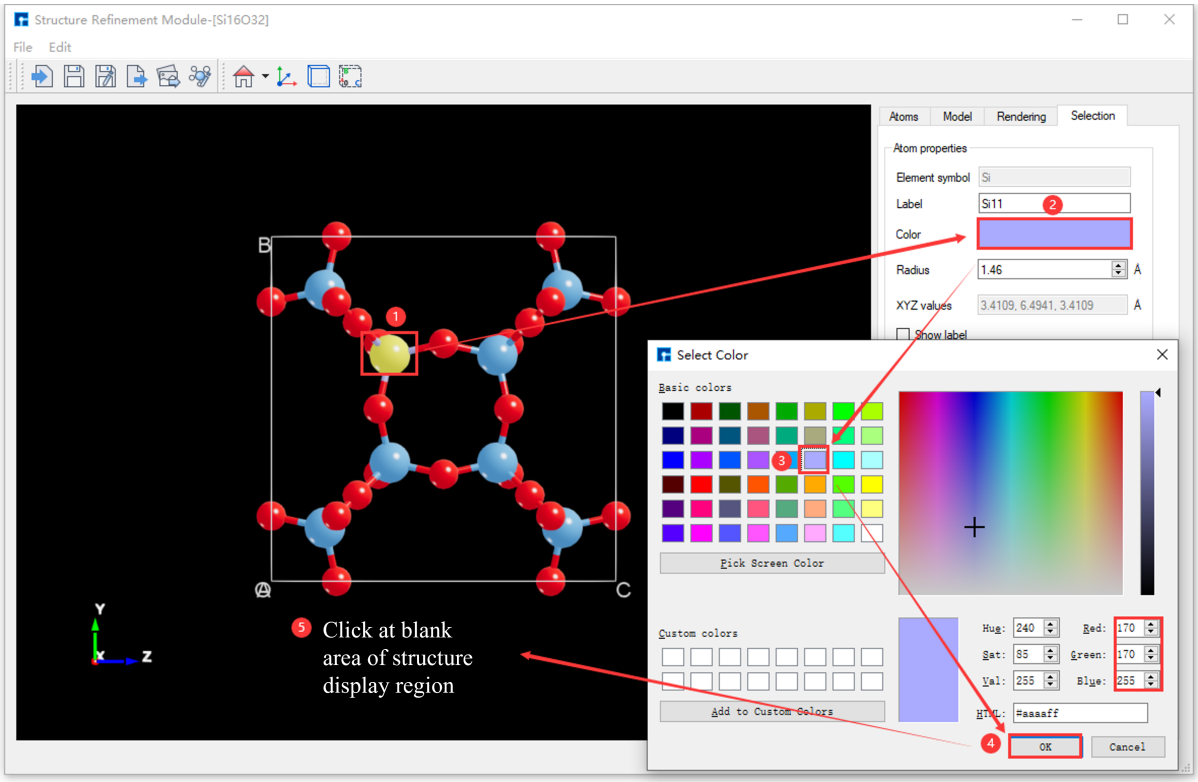


fig. 6.32: Select Atom: Modify the color of atom `Si11` in the `Si16O32` crystal structure to RGB value `[170 170 255]` in the operation interface.

6.4.3 Change the color of all elements in the structure

The initial Device Studio templates, Device Studio template 1 and Device Studio template 2, are shown in fig. 6.18 and fig. 6.19, respectively.

The Si16O32 crystal structure contains two elements, Si and O. Figure fig. 6.33 shows the interface for modifying the color of all elements in the Si16O32 crystal structure (essentially switching to the colors of Device Studio template 2) based on fig. 6.32. The modified interface is shown in fig. 6.34.

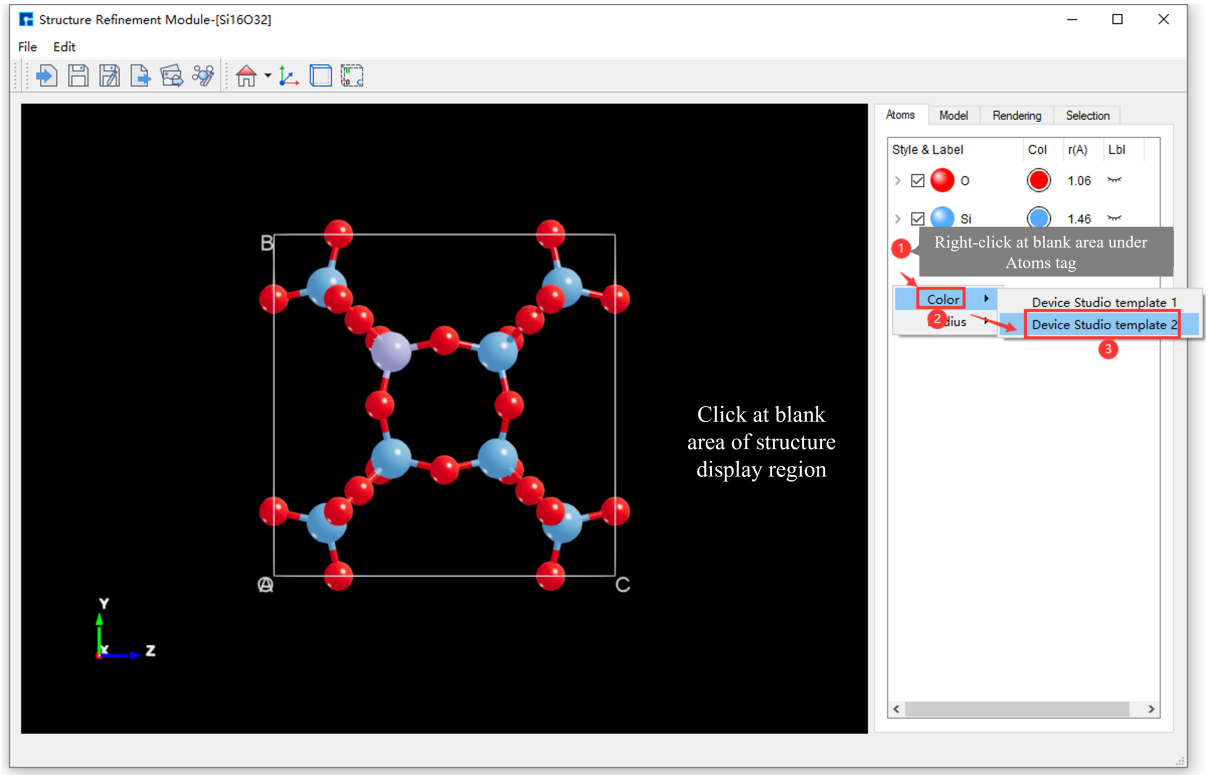


fig. 6.33: User interface for modifying the color of all elements in the Si16O32 crystal structure.

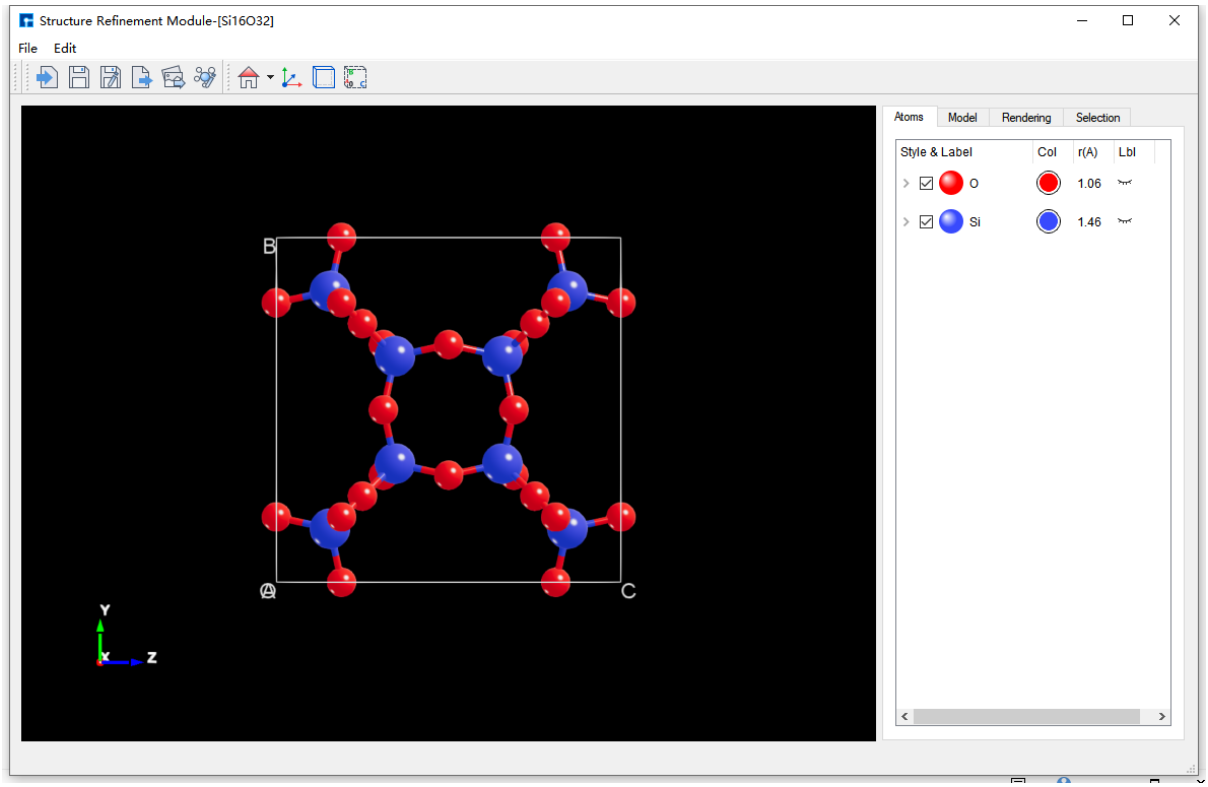


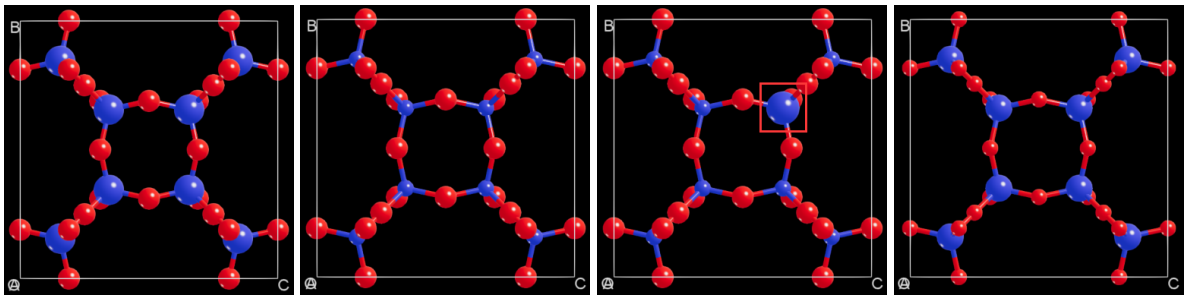
fig. 6.34: The interface after modifying the color of all elements in the Si16O32 crystal structure.

note

Modify the color of all elements in the structure by right-clicking in the blank area of *SRM - Parameter Adjustment Area - Atoms Area* → Color → Device Studio template 1 or Device Studio template 2. This only applies the color parameters from the template to the structure; radius parameters are not applied.

6.5 Modify the radius of atoms in the structure

Modify the atomic radii in the structure. This modification requires that the structure be imported. Based on fig. 6.34, this section details how to modify the atomic radii in the Si16O32 crystal structure as an example within the atomic structure refinement module.



6.5.1 Modify the radius of the same element in the structure

As shown in fig. 6.35, this is the interface for modifying the radius of the Si element (i.e., all Si atoms) in the Si16O32 crystal structure from 1.46 to 0.80.

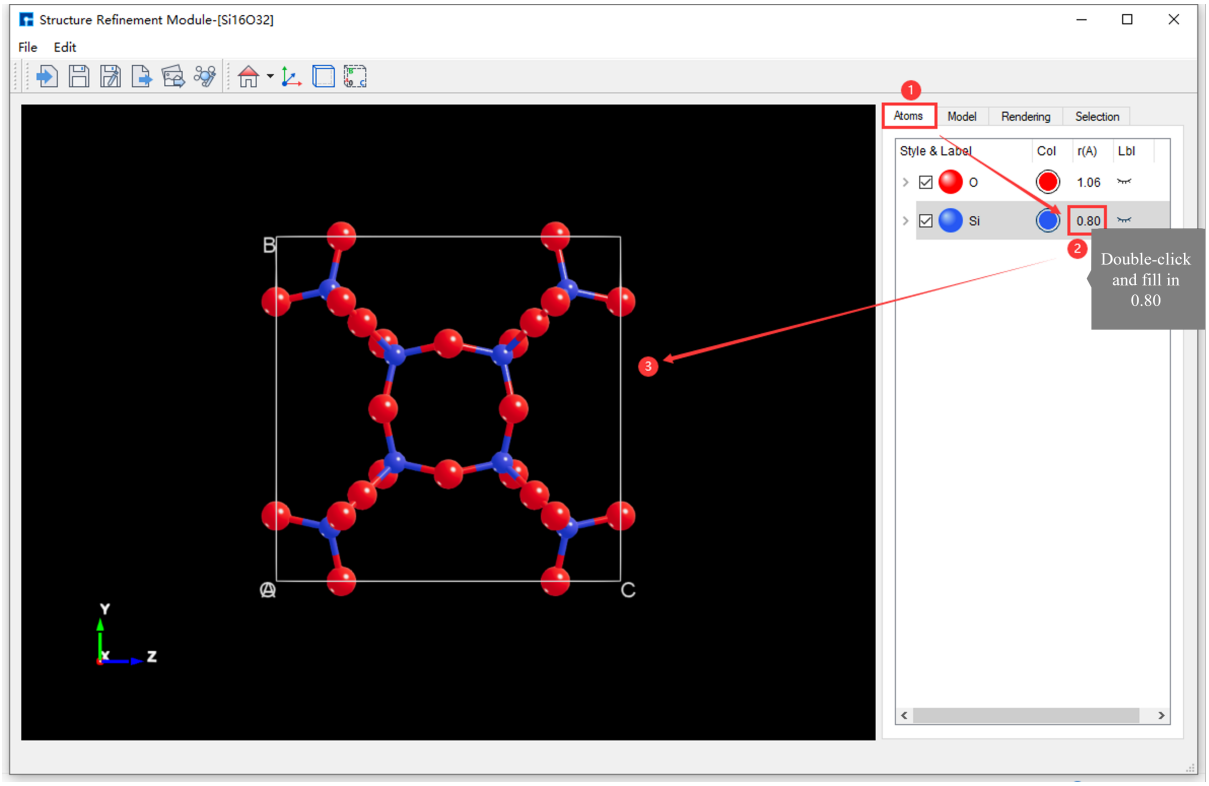


fig. 6.35: The interface for modifying the radius of the `Si` element in the Si16O32 crystal structure from `1.46` to `0.80`

6.5.2 Modify the radius of an atom in the structure

Based on fig. 6.35, there are two ways to modify the radius of the `Si16` atom in the Si16O32 crystal structure from `0.80` to `1.60`.

1. Method 1: Without selecting the `Si16` atom, as shown in fig. 6.36, the interface for modifying the radius of the `Si16` atom in the Si16O32 crystal structure from `0.80` to `1.60` is displayed;

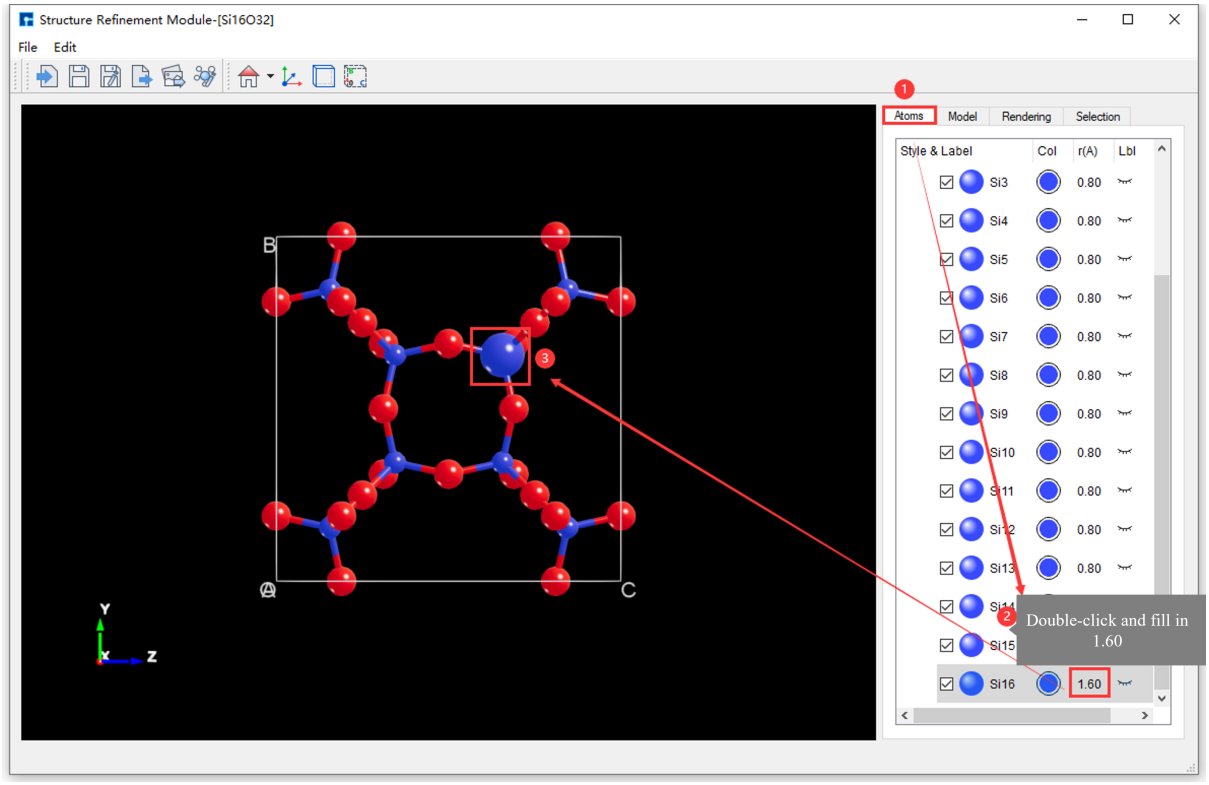


fig. 6.36: Unselected Atoms: Interface for modifying the radius of the `Si16` atom in the `Si16O32` crystal structure from `0.80` to `1.60`.

2. Method 2: Click on the `Si16` atom with the mouse, as shown in fig. 6.37, to modify the radius of the `Si16` atom in the Si16O32 crystal structure from `0.80` to `1.60`.

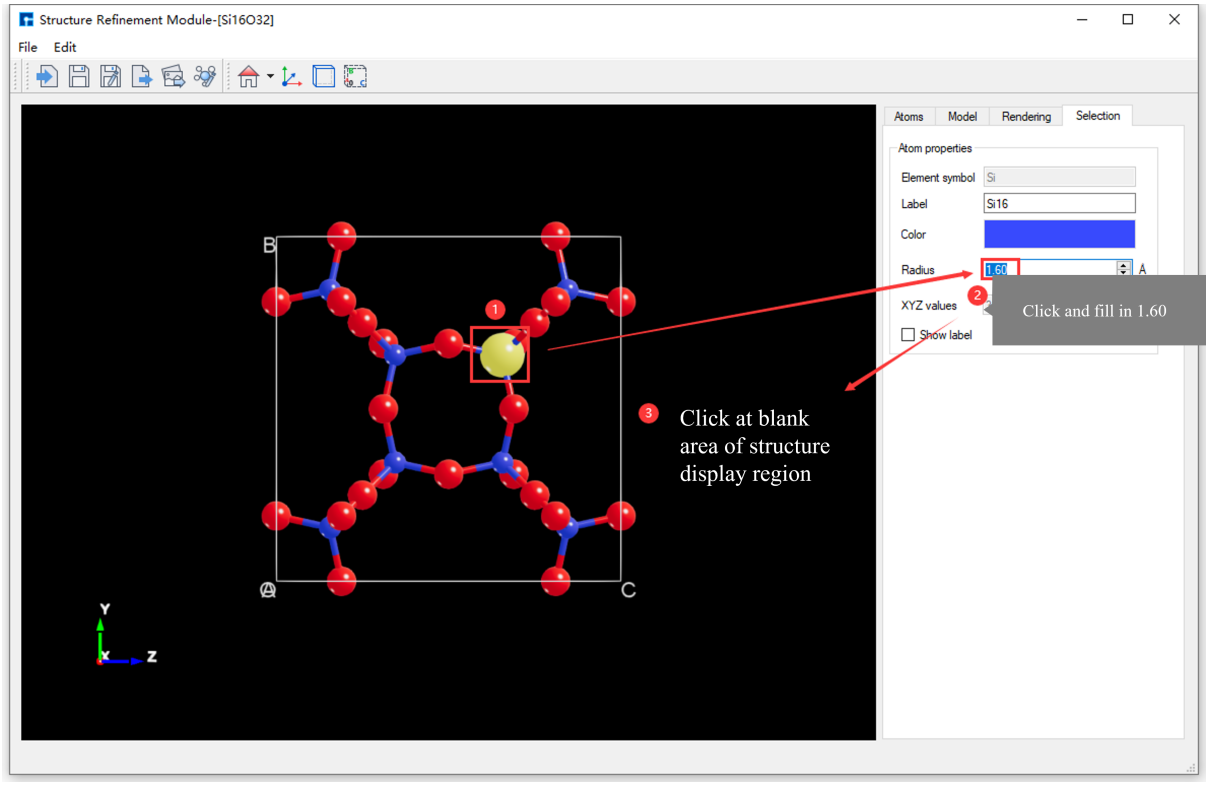


fig. 6.37: Select Atoms: Interface for modifying the radius of the Si16 atom in the Si16O32 crystal structure from 0.80 to 1.60.

6.5.3 Modify the radius of all elements in the structure

The initial Device Studio templates, Device Studio template 1 and Device Studio template 2, are shown in fig. 6.18 and fig. 6.19, respectively.

The Si16O32 crystal structure contains two elements, Si and O. The interface for modifying the radii of all elements in the Si16O32 crystal structure based on fig. 6.37 (effectively switching to the radii of Device Studio template 2) is shown in fig. 6.38. The interface after modification is shown in fig. 6.39.

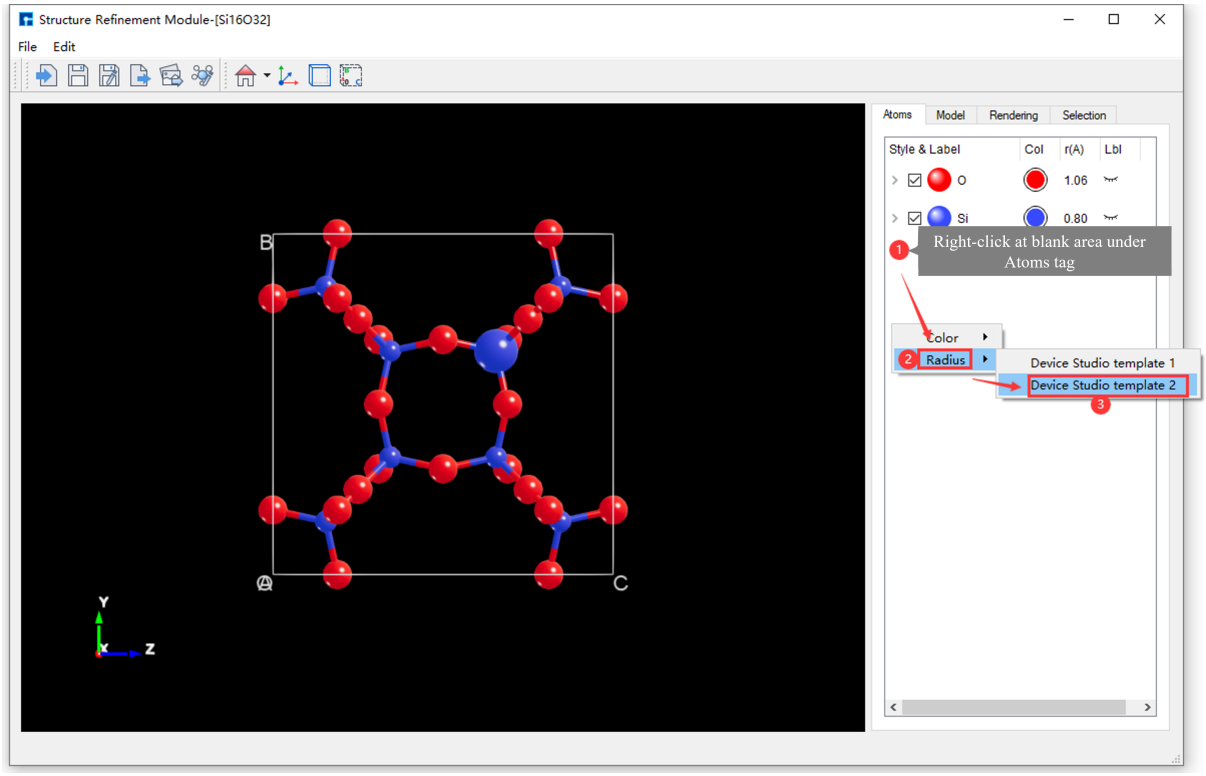


fig. 6.38: User interface for modifying the radii of all elements in the Si16O32 crystal structure.

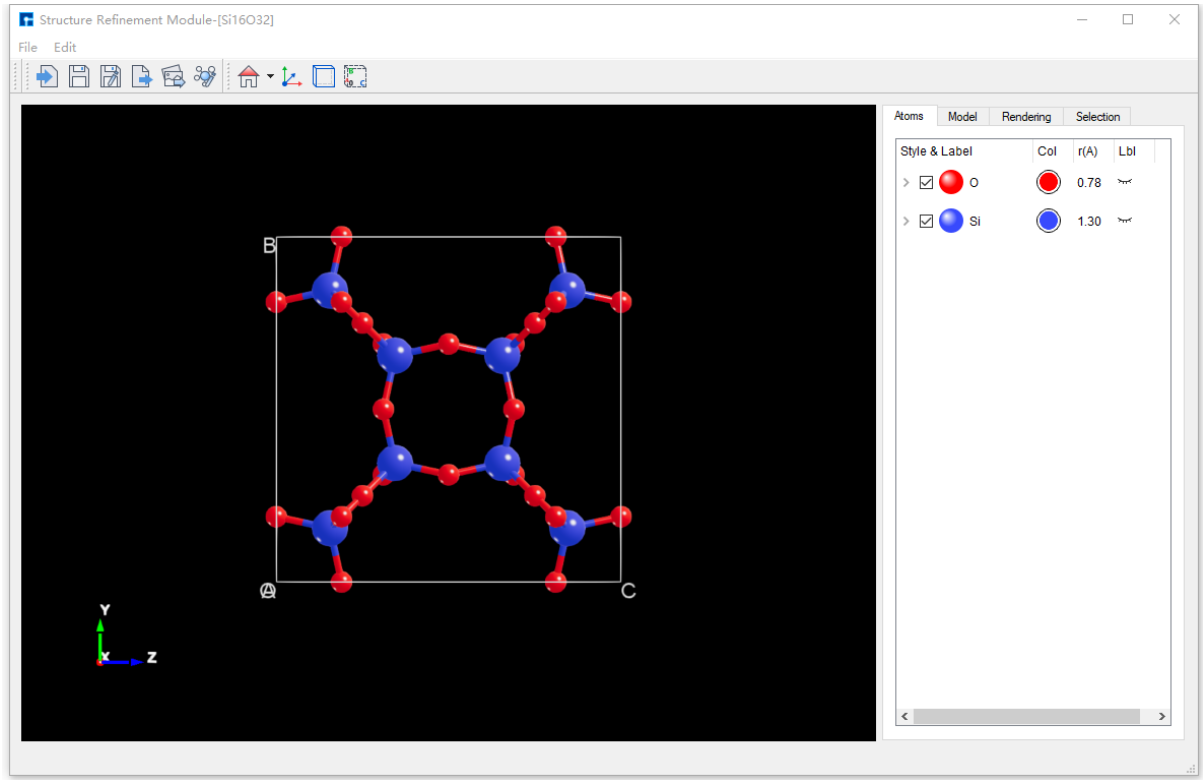


fig. 6.39: Interface after modifying the atomic radii of all elements in the Si16O32 crystal structure

note

Modify the radius of all elements in the structure by right-clicking in the blank area of *SRM - Parameter Adjustment Area - Atoms Area* → Radius → Device Studio template 1 or Device Studio template 2. This only applies the radius parameter from the template to the structure; color parameters are not applied.

6.6 Ball-and-stick/polyhedral model of the structure

The structure imported by default from the atomic structure refinement module is displayed in **ball-and-stick mode**, as shown in fig. 6.40 for the Si16O32 crystal structure displayed in **ball-and-stick mode**.

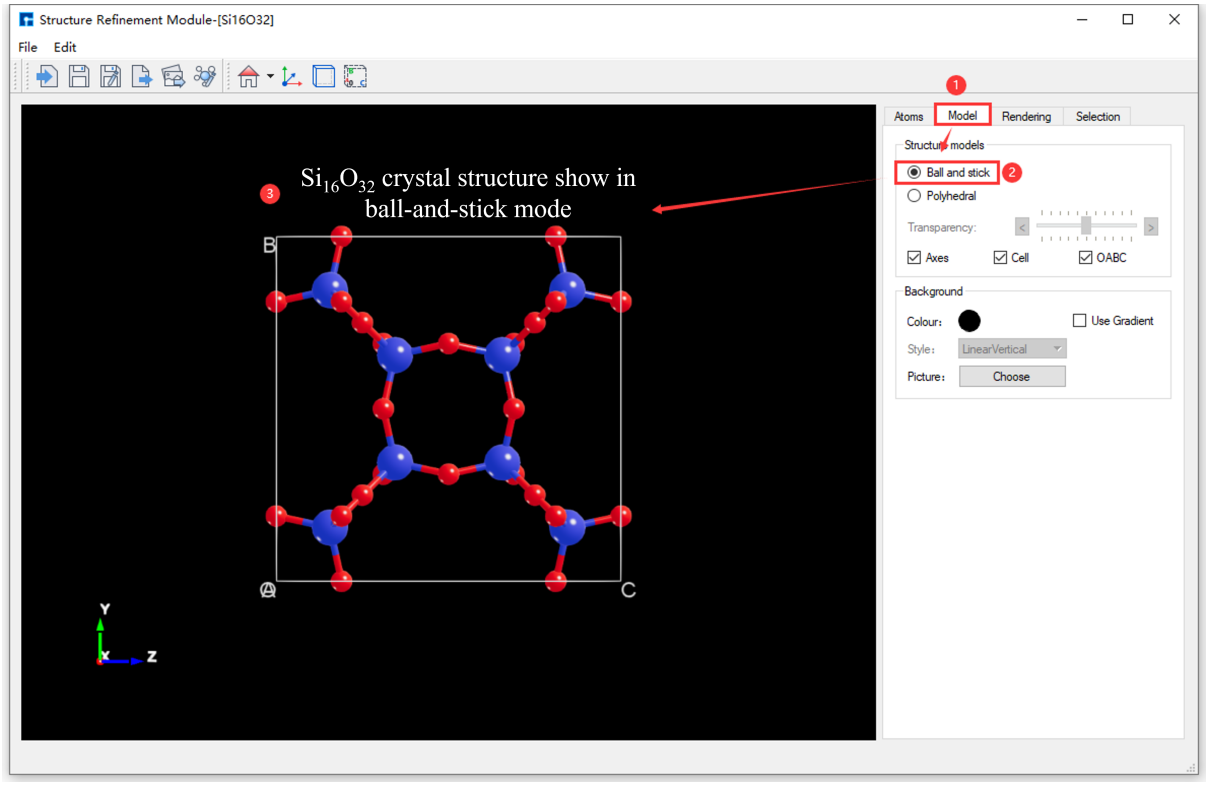


fig. 6.40: Si16O32 crystal structure shown in **ball-and-stick model**

note

To hide bonds in the atomic structure, for example, in the Si16O32 crystal structure, select the Si16O32 crystal structure with your mouse and press the *Delete* key.

As shown in fig. 6.41, this is the interface for switching the Si16O32 crystal structure from **ball-and-stick model** to **polyhedral model**.

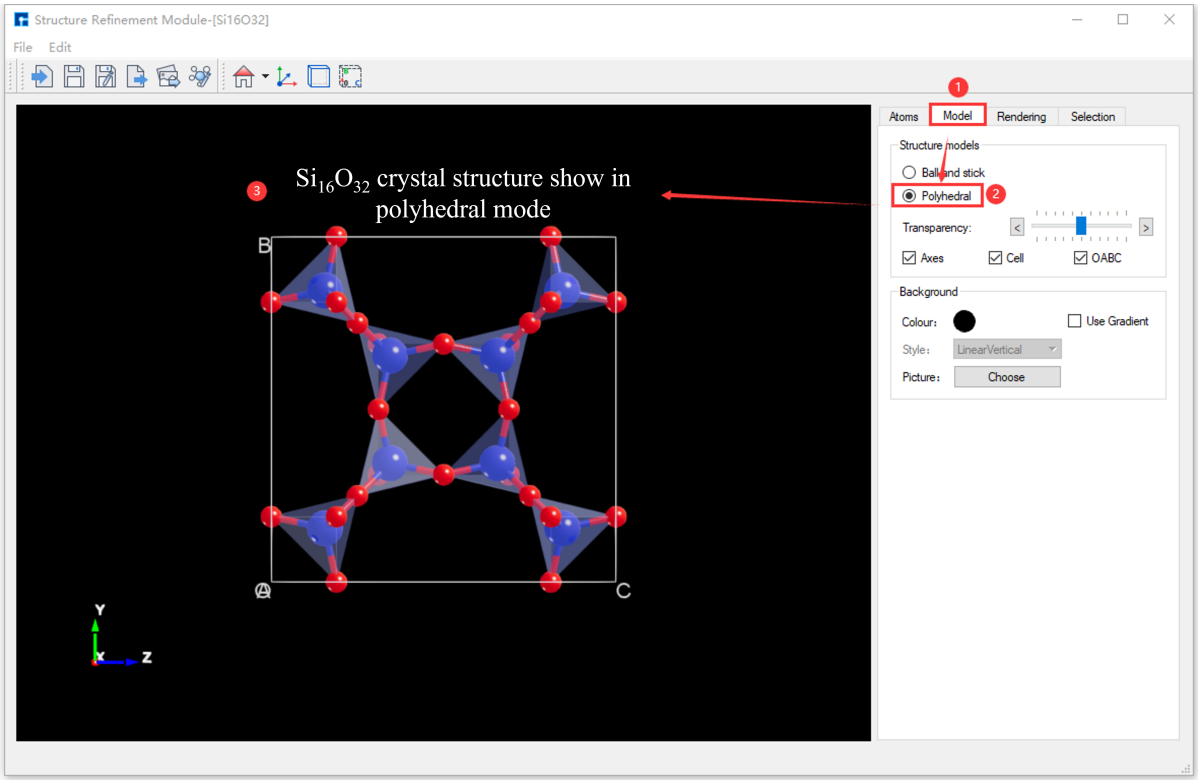


fig. 6.41: Si16O32 crystal structure displayed in **polyhedral mode**

To adjust the polyhedron transparency, please refer to the *SRM - Parameter Adjustment Area - Model Area* section, which details how to do so.

6.7 Adjusting Lighting Parameters of Structures

The atomic structure refinement module supports adjusting lighting parameters for the structure; detailed instructions are omitted here, and users may refer to section *SRM - Parameter Adjustment Area - Rendering Area*.

- – Supports individual lighting adjustment for atoms and bonds within the atomic structure;
- – Supports global illumination adjustment for the entire atomic structure.
  - – * Supports illuminating the atomic structure with multiple light beams, up to four.
  - – * Supports adjusting the position of the light beams on the atom.
  - – * Supports adjusting the beam intensity;

- * Supports adjusting the ambient light parameters.

CHAPTER

SEVEN

KEY FEATURES

7.1 Supercell Identification of Primitive Cell

Device Studio features a **supercell-to-primitive-cell recognition** function, which is very easy to operate. For example, as shown in fig. 7.1 (3D view of the graphene supercell structure in the XY plane), importing a graphene supercell structure in Device Studio, and clicking *Build* → *StandardizeCell* will recognize the graphene supercell structure as a primitive cell structure, as shown in fig. 7.2.

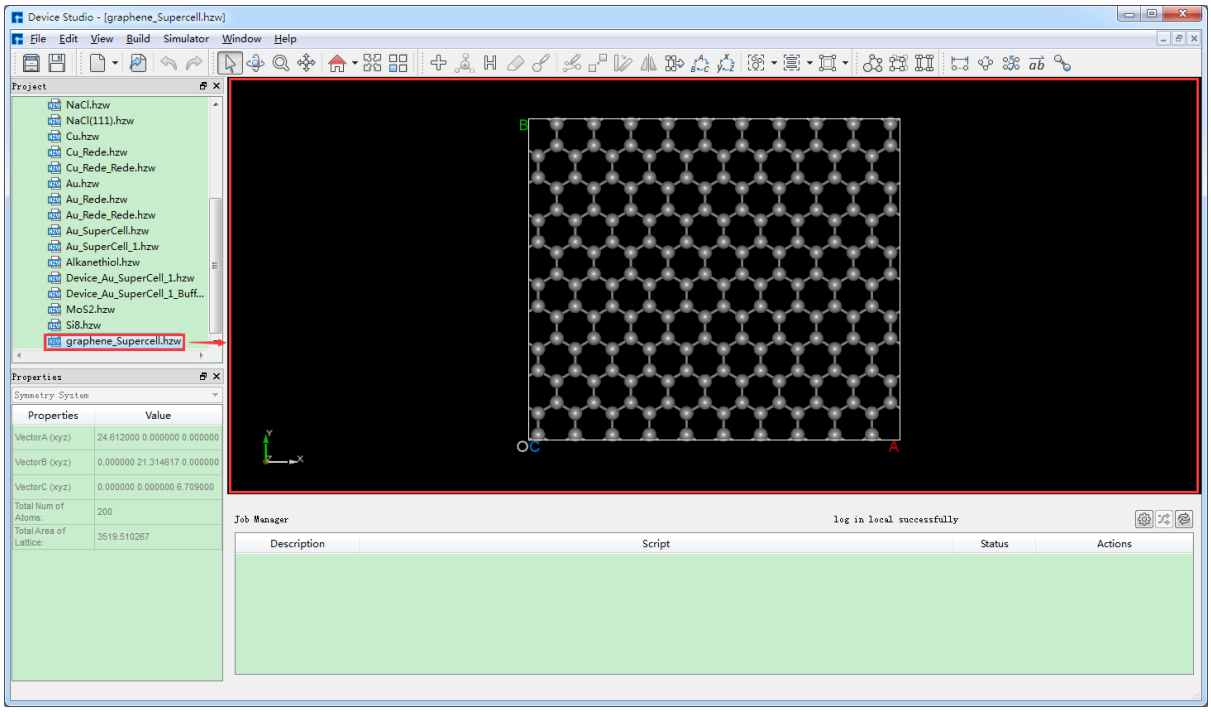


fig. 7.1: Import the graphene supercell structure into the Device Studio interface

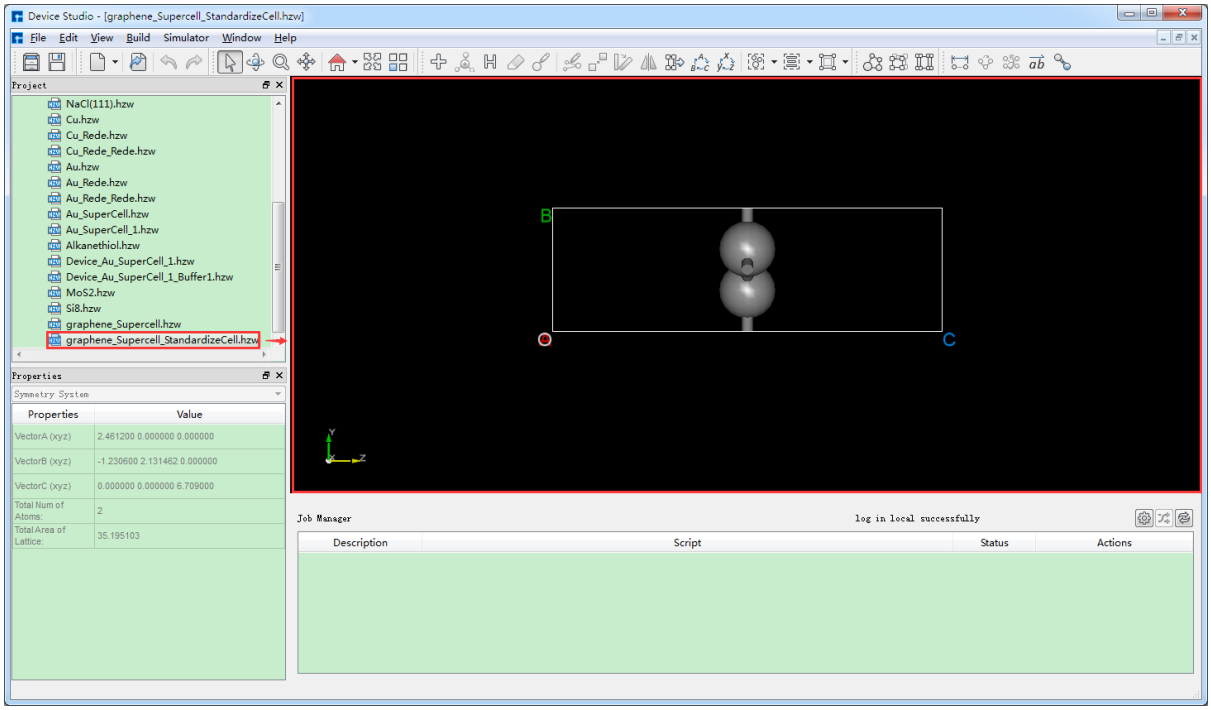


fig. 7.2: Graphene unit cell structure

7.2 Flexible Device Structure Modeling

Device Studio allows for the construction of flexible device structures. Taking the gold-alkanethiol-gold (Au-Alkanethiol-Au) flexible device structure as an example, first import the Au-Alkanethiol-Au molecular device structure into Device Studio as shown in fig. 7.3. In the fig. 7.3 interface, click *Build* → *Bending of Device*. The Bent interface for constructing the flexible device structure will pop up. In the Bent interface, select *Both Side* and set the relevant parameters as shown in fig. 7.4. Click *Preview* to preview the constructed flexible device structure, and click *Build* to complete the construction of the Au-Alkanethiol-Au flexible device structure. The structure file `Au-Alkanethiol-Au_bent.hzw` will be mounted in the Device Studio Project Explorer area. The Device Studio interface after constructing the Au-Alkanethiol-Au flexible device structure is shown in fig. 7.5.

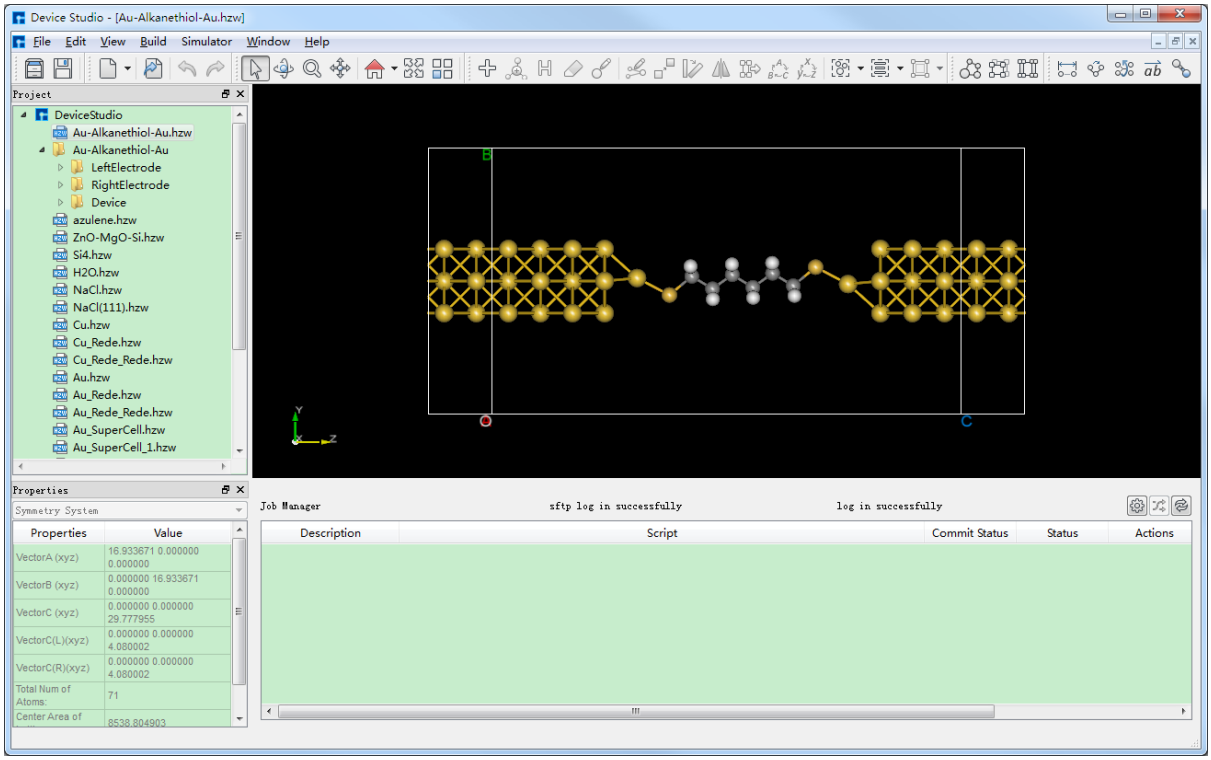


fig. 7.3: Device Studio interface after importing the Gold-Alkanethiol-Gold (Au-Alkanethiol-Au) molecular device structure

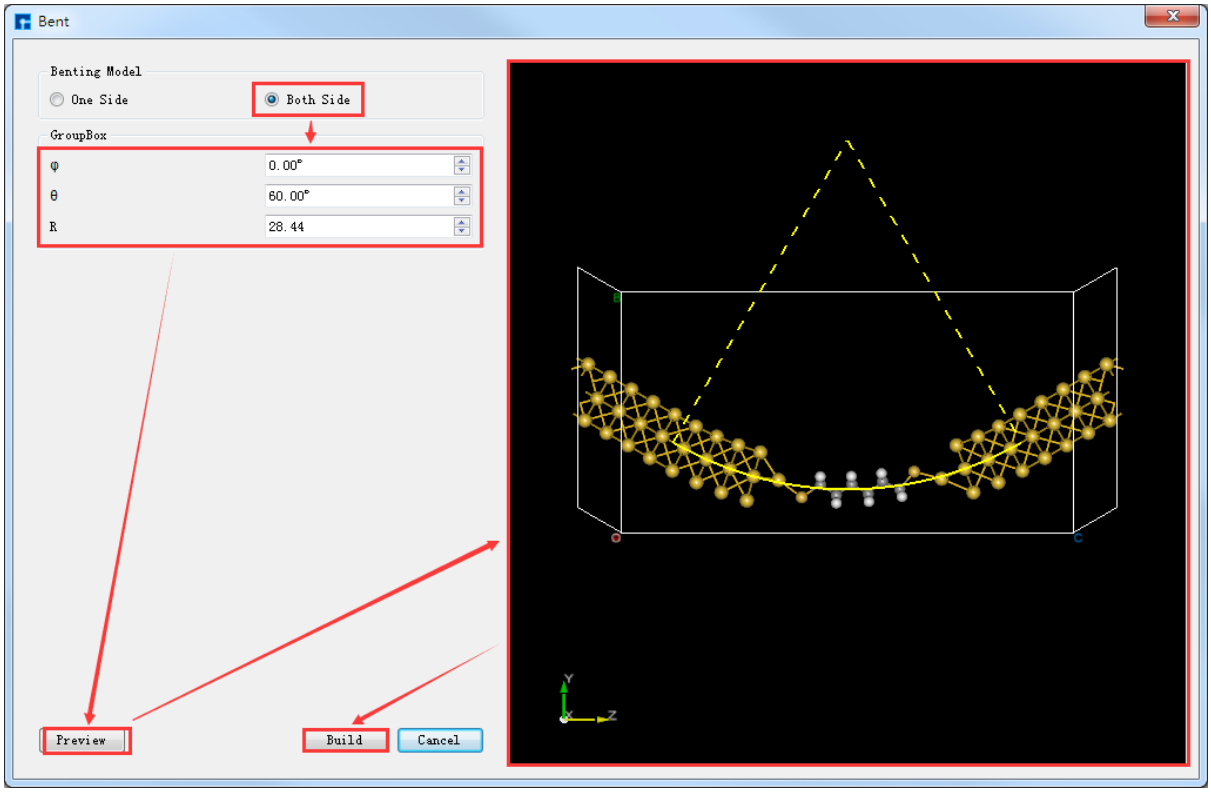


fig. 7.4: Constructing the Bent Interface of a **Flexible Device Structure**

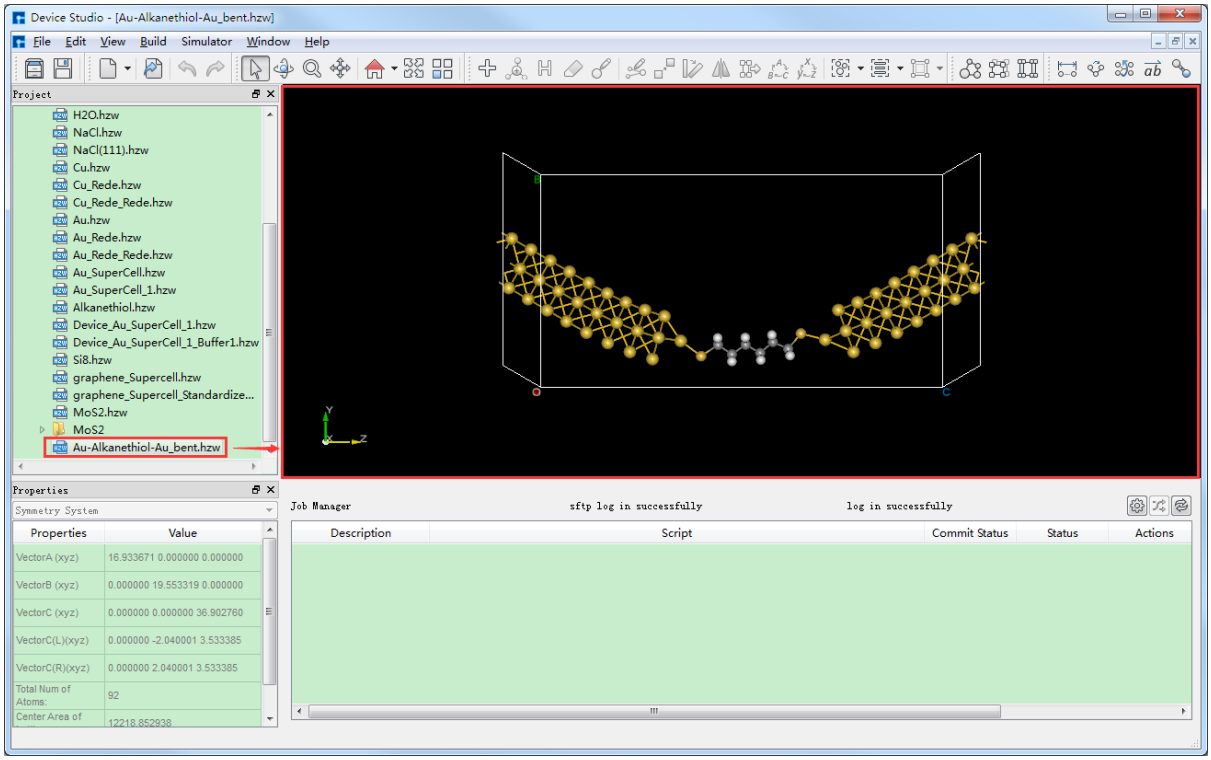


fig. 7.5: Device Studio interface for setting up a flexible **device structure** of Gold-Alkanethiol-Gold (Au-Alkanethiol-Au)

7.3 Identifying the Space Group Information of Crystal Structures

Device Studio can identify the space group and symmetry information of crystal structures. For example, in the Device Studio graphical user interface shown in fig. 7.6, for the GaSe crystal structure, clicking on Clicking *Build* → *Symmetry* will open the Symmetry interface as shown in fig. 7.7. The space group information for the GaSe crystal structure can be found in fig. 7.7 (a), and clicking Clicking the *Operators* button in the Symmetry interface displays the symmetry information of the GaSe crystal structure, as shown in fig. 7.8.

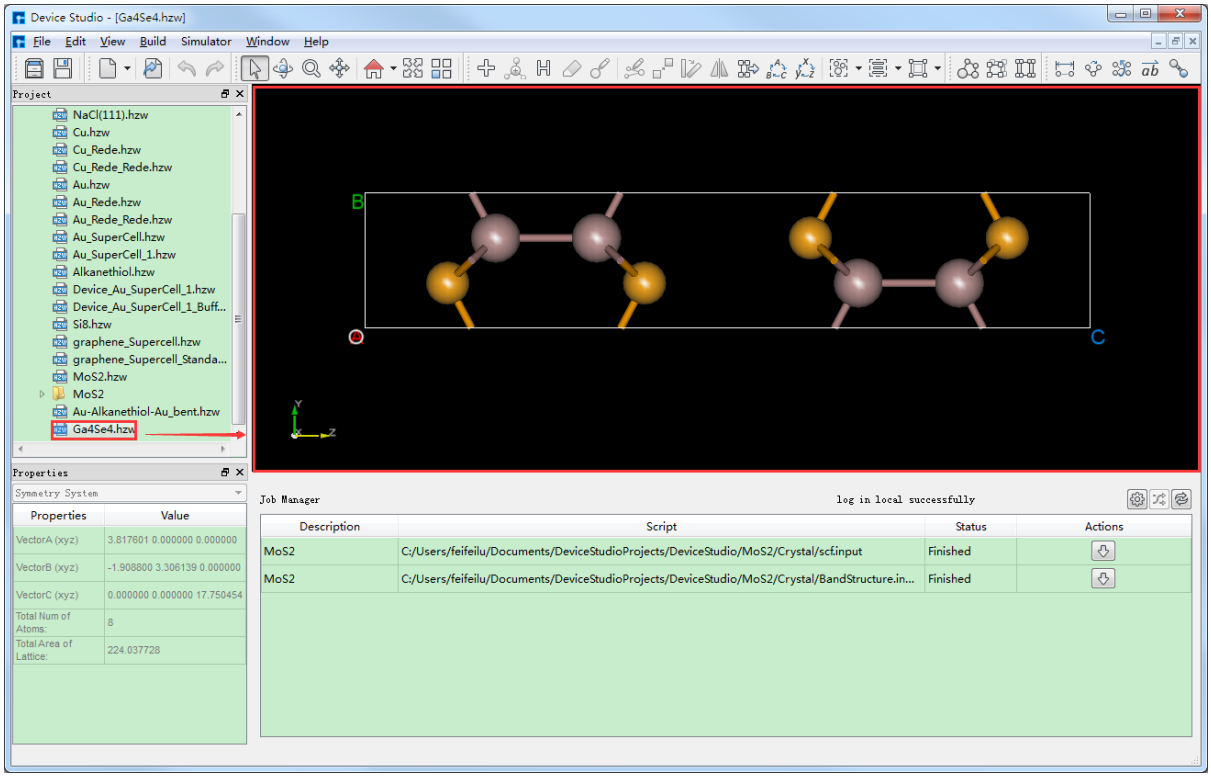


fig. 7.6: Device Studio interface displaying the GaSe crystal structure

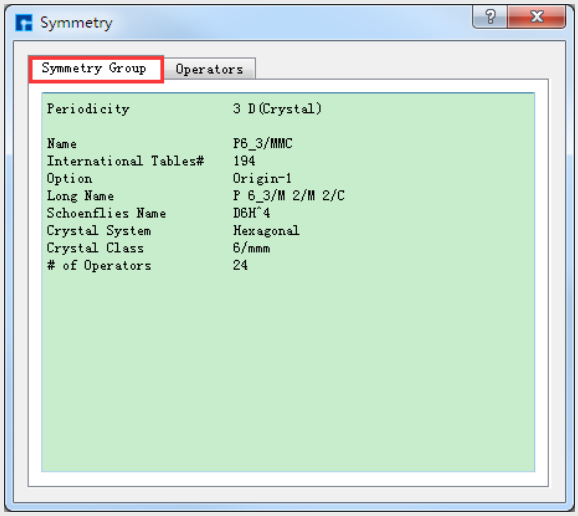


fig. 7.7: Space group information of the GaSe crystal structure

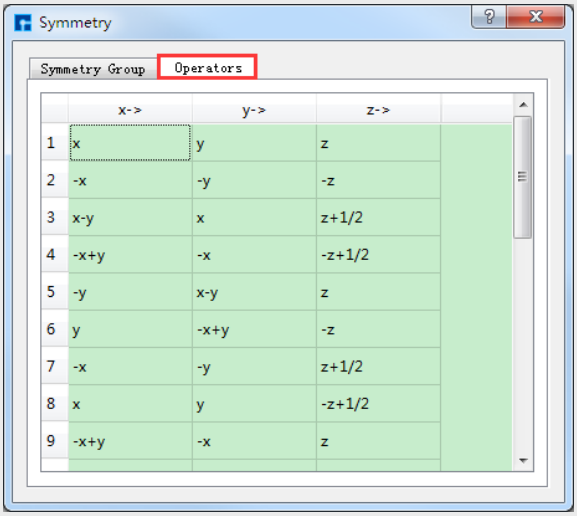


fig. 7.8: Symmetry information of the GaSe crystal structure

7.4 Splitting Molecular Structures

Device Studio features a molecular structure decomposition function, which splits a crystal structure into individual molecular structures. For example, in the Device Studio graphical interface shown in fig. 7.9, for the C5H17AlN2O8P2 crystal structure, Clicking *Build* → *Decomposition* in the interface will decompose the C5H17AlN2O8P2 crystal structure into 6 molecular structures, as shown in fig. 7.10, fig. 7.11, and fig. 7.12. as shown in fig. 7.13, fig. 7.14, and fig. 7.15.

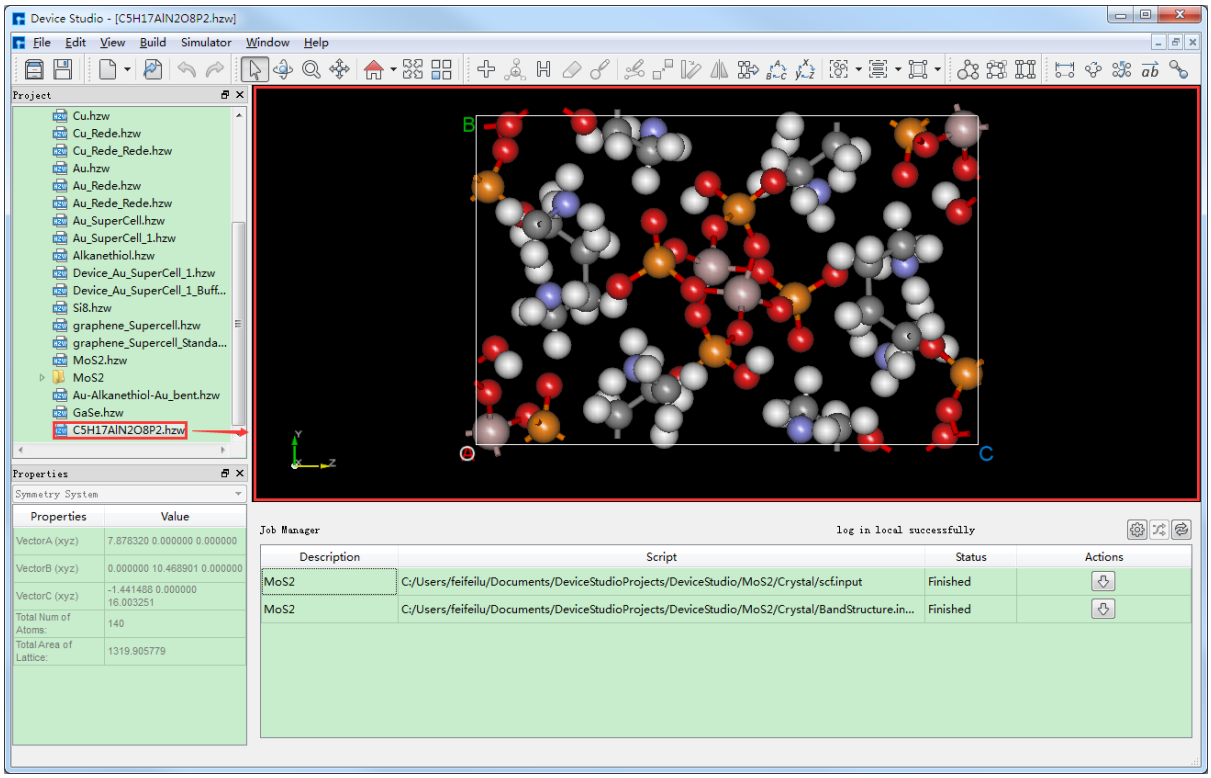


fig. 7.9: Device Studio interface displaying the crystal structure of C5H17AlN2O8P2

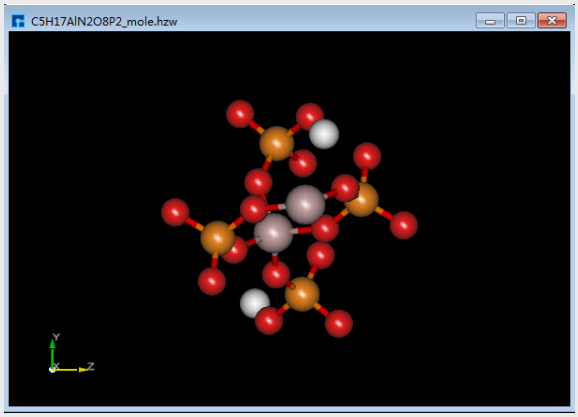


fig. 7.10: C5H17AlN2O8P2_mole

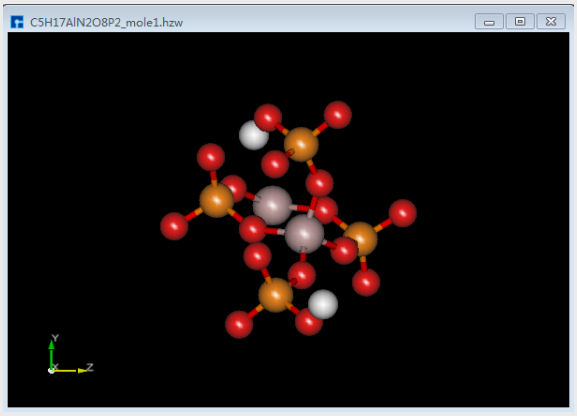


fig. 7.11: C5H17AlN2O8P2_mole1

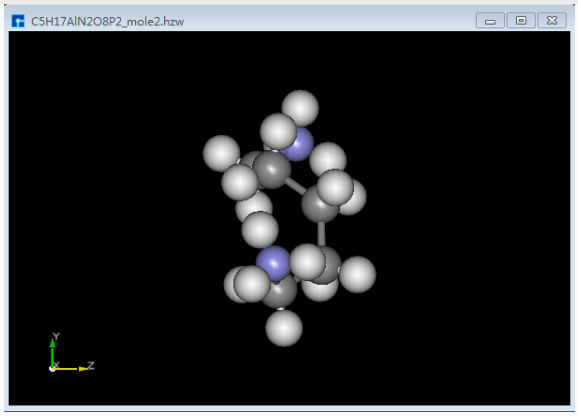


fig. 7.12: C5H17AlN2O8P2_mole2

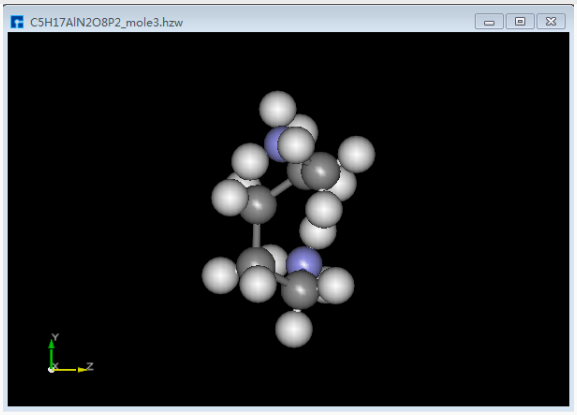


fig. 7.13: C5H17AlN2O8P2_mole3

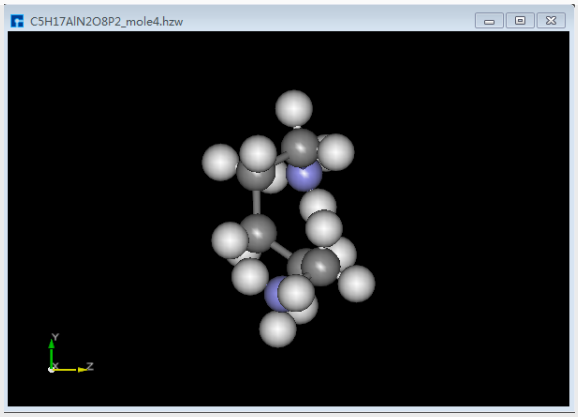


fig. 7.14: C5H17AlN2O8P2_mole4

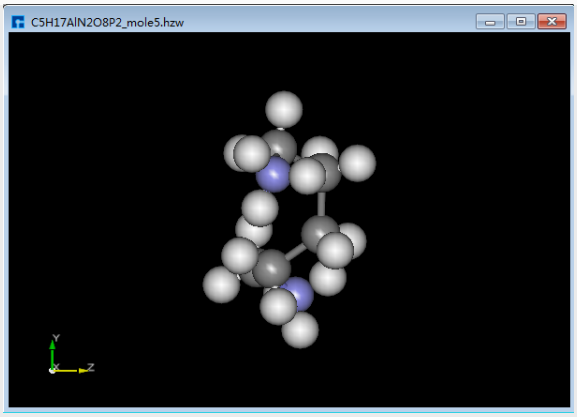


fig. 7.15: C5H17AlN2O8P2_mole5

7.5 Task Monitoring and Management

Device Studio's *Calculation Task Monitoring Management Area (Job Manager)*, as shown in fig. 7.16, integrates **PuTTY** and **WinSCP** modules, supporting the free configuration of server parameters, directories, and scripts. Commands are supported, along with automatic task status refresh and disconnection alerts. For information on configuring server connections in the Job

Manager's task monitoring and management area, please refer to the section Nanodcal 连接服务器.

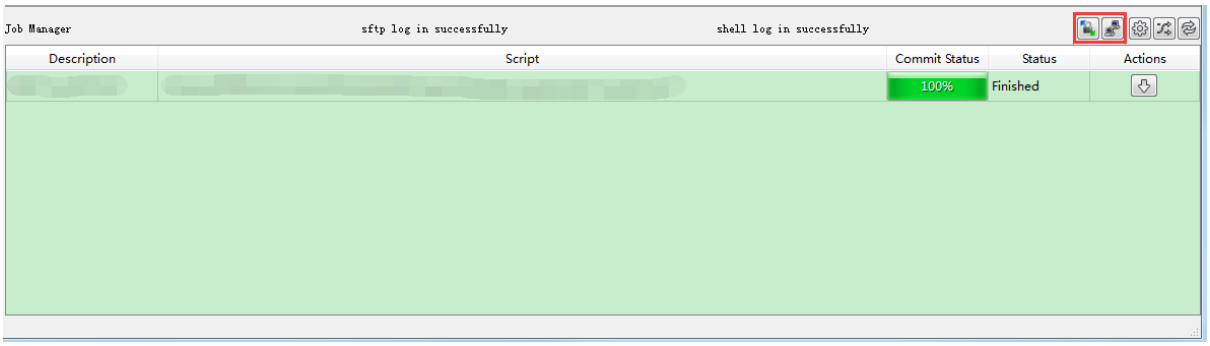


fig. 7.16: Device Studio's *Calculation Task Monitoring Management Area (Job Manager)*

If the job calculation is complete, click the *Download* button under *Action* in the Job Manager to open the download interface for the calculation results, as shown in fig. 7.17, then click *Download* on the interface. The results can then be downloaded and viewed in the Project Explorer area of the software. Alternatively, users can connect to the server already connected to Device Studio by clicking the **Open PuTTY** and **Open WinSCP** icons in fig. 7.16, as shown in fig. 7.18 and fig. 7.19, respectively.

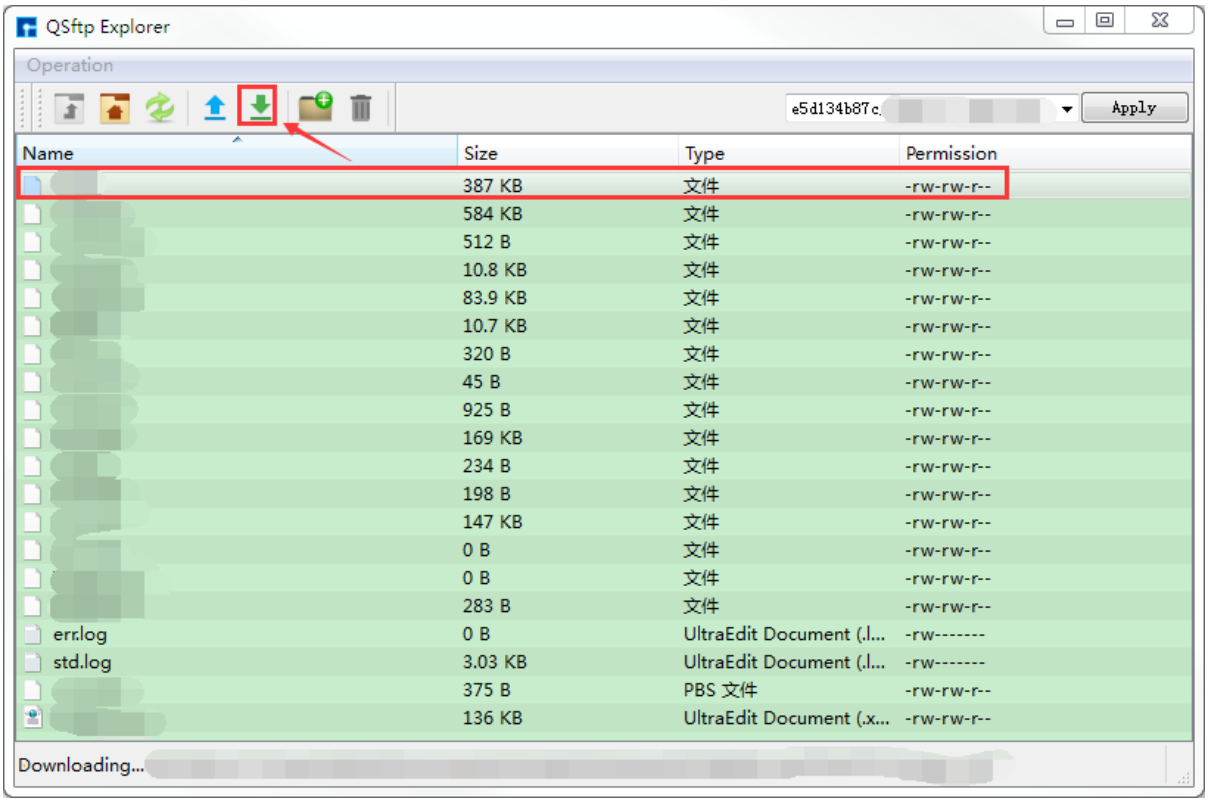


fig. 7.17: Device Studio's *Calculation Task Monitoring Management Area (Job Manager)* interface for downloading computation results

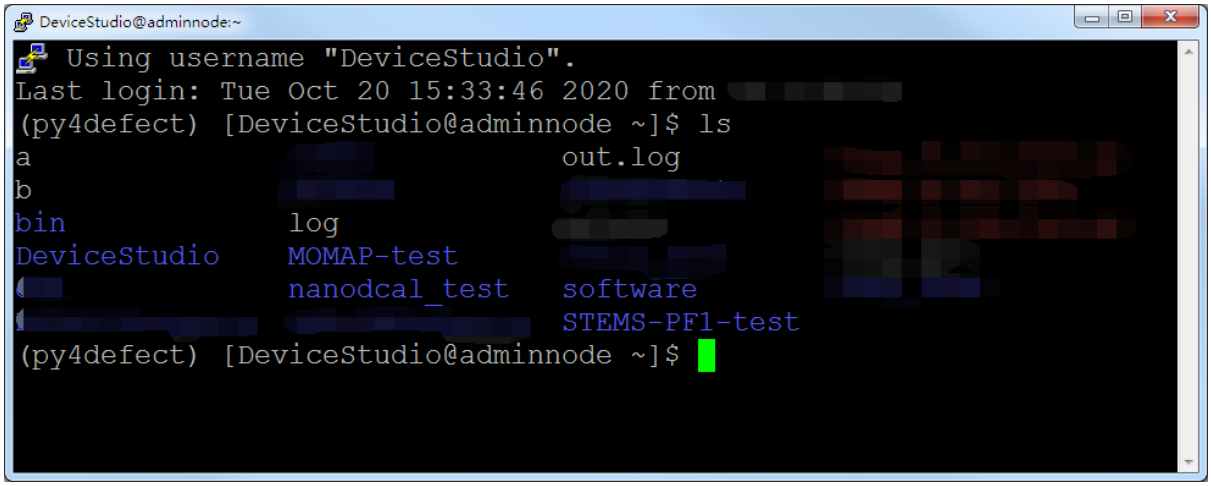


fig. 7.18: ***PuTTY** Server Connection Interface

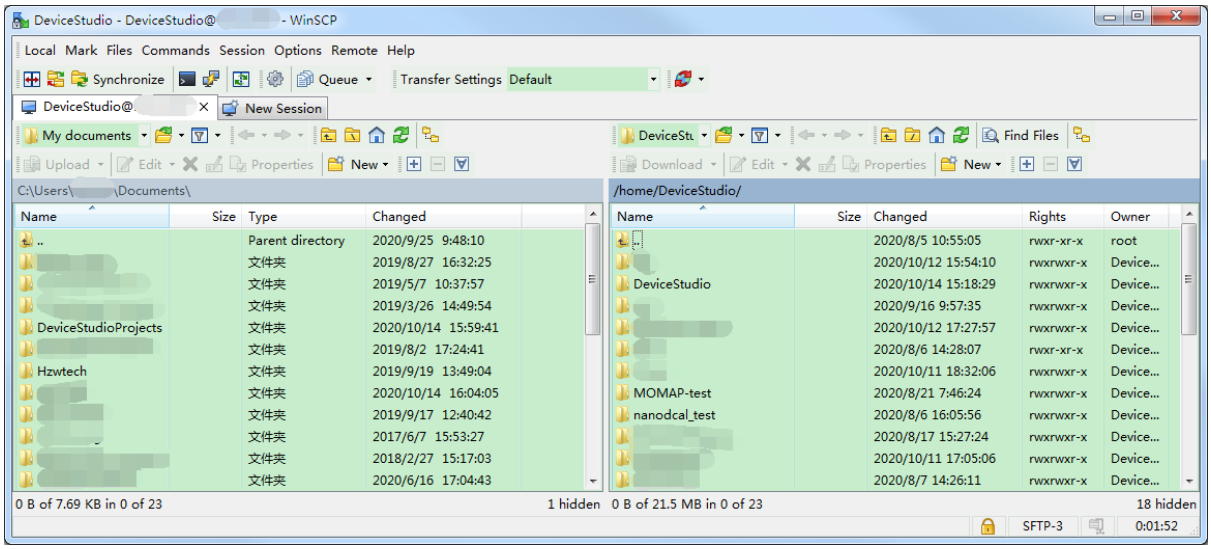


fig. 7.19: ***WinSCP** Server Connection Interface

CHAPTER

EIGHT

COMMON FUNCTIONS

8.1 Modify Device Studio Main Interface Background Color

Modify the background color of the atomic structure display in the Device Studio main interface, i.e., modify the *Structure 3D Display Area (3D Viewer)* background color in Device Studio. There are two ways to modify it, using the **Si16O32 crystal structure** as an example for detailed explanation.

1. Method One: When a structure (e.g., Si16O32 crystal structure) is already displayed in the Device Studio main interface, as shown in fig. 8.1, this is the operation interface for changing the **background color** of the Si16O32 crystal structure display from **pure black** to **pure white**.

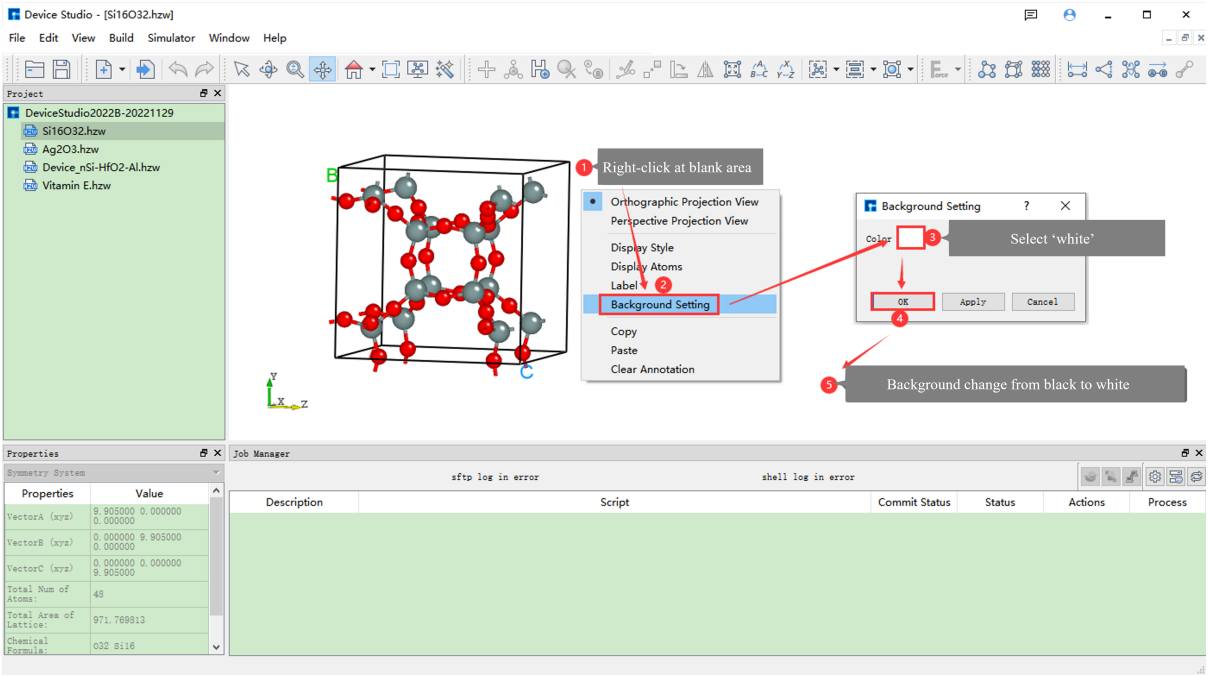


fig. 8.1: Operation Interface for Changing the **Background Color** of Si16O32 Crystal Structure Display from **Pure Black** to **Pure White**

> **Note**
>
> Method One can only be used when a structure is already displayed in the Device Studio main interface.

2. Method Two: When no structure is displayed in the Device Studio main interface, as shown in fig. 8.2, fig. 8.3, and fig. 8.4, these are the operation steps for changing the **background color** of the Si16O32 crystal structure display from **pure black** to **pure white**.

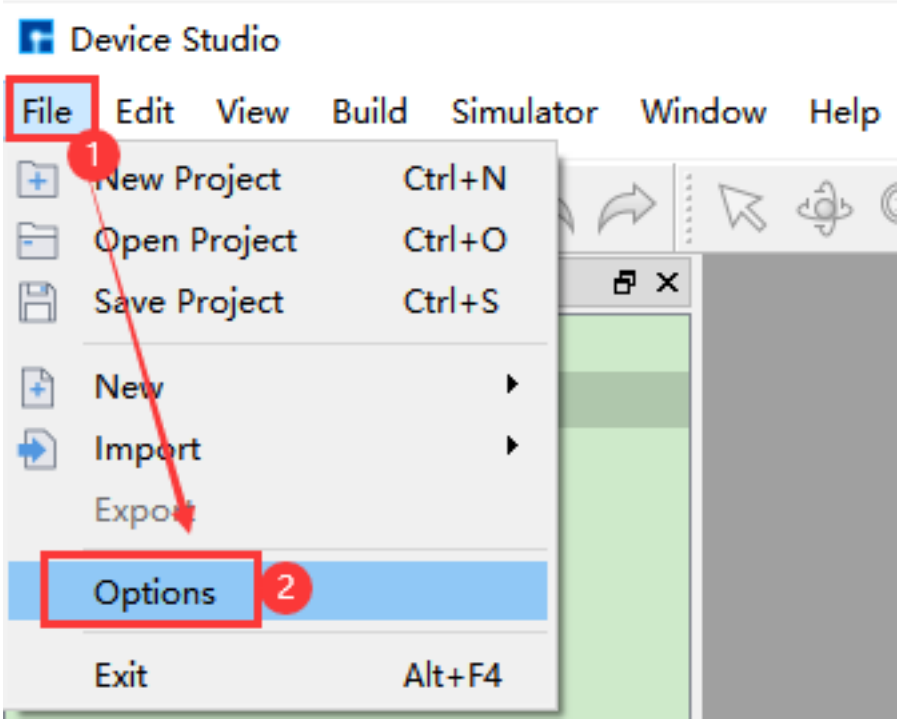


fig. 8.2: Step One: Change the **Background Color** of Structure Display in Device Studio Main Interface from **Pure Black** to **Pure White**

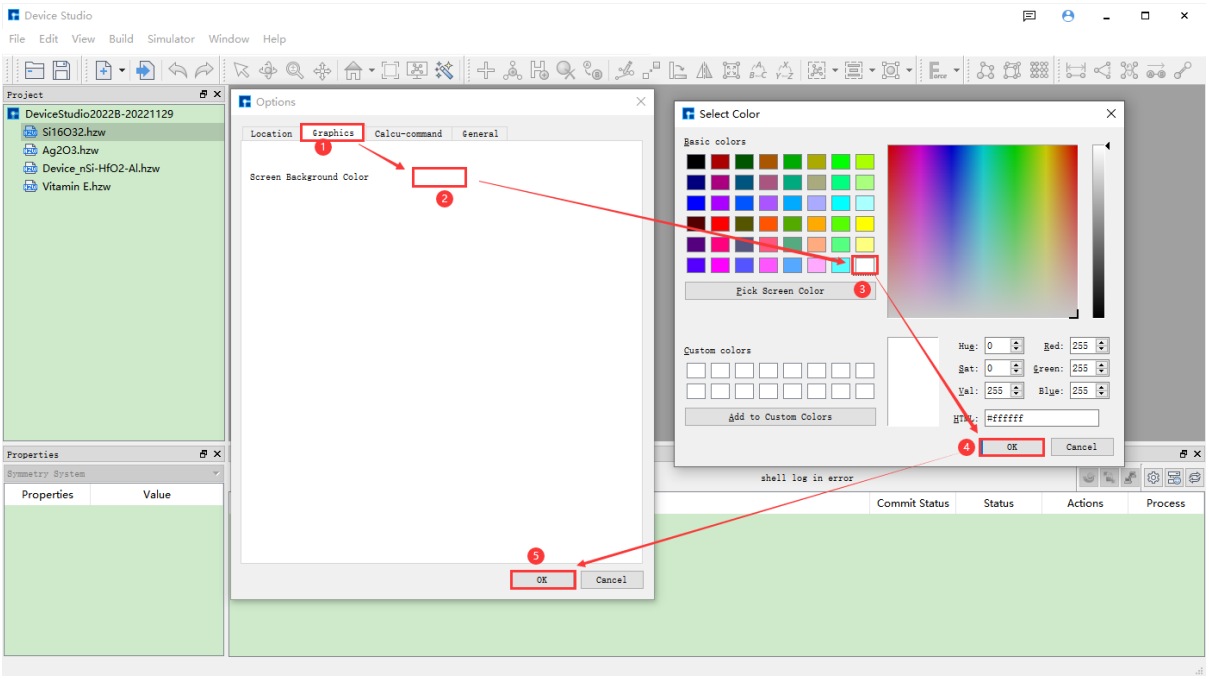


fig. 8.3: Step Two: Change the **Background Color** of Structure Display in Device Studio Main Interface from **Pure Black** to **Pure White**

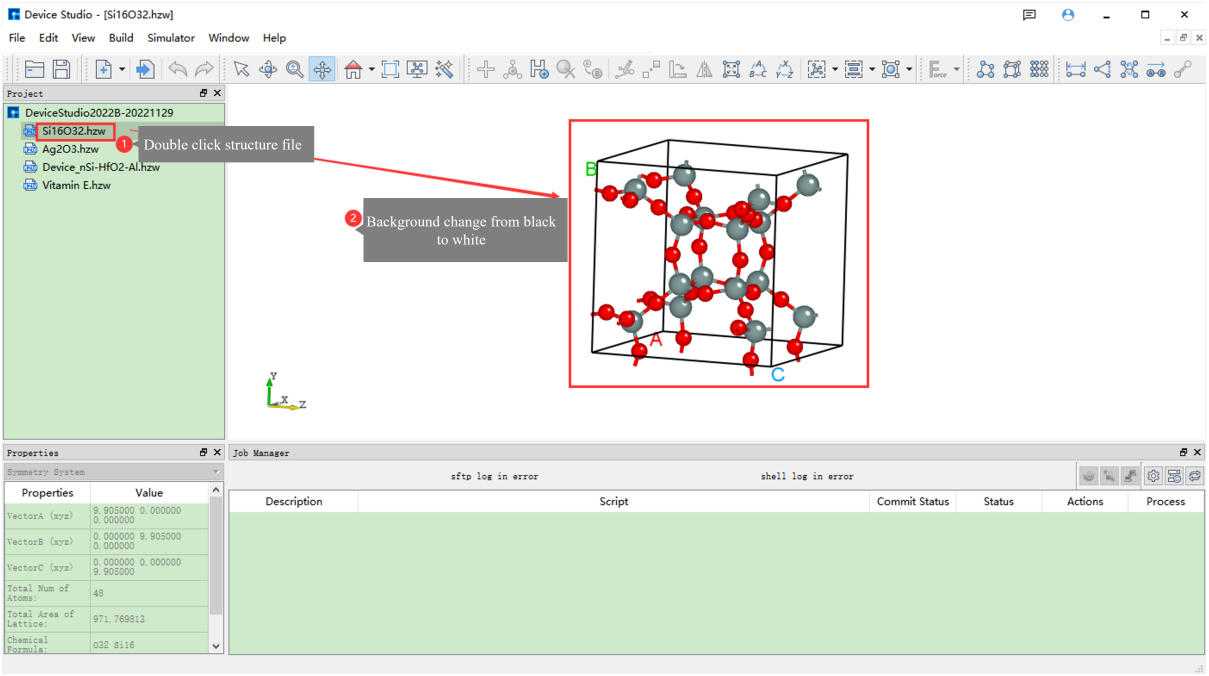


fig. 8.4: Step Three: Change the **Background Color** of Structure Display in Device Studio Main Interface from **Pure Black** to **Pure White**

Important Note

This section mainly describes **how to modify the background color of atomic structure display in the Device Studio main interface**, i.e., modify the *Structure 3D Display Area (3D Viewer)* background color in Device Studio. This does not affect the background color of the Atomic Structure Refinement Module. If you want to modify the background color of the atomic structure refinement module, please refer to the Modify Atomic Structure Refinement Module Background Color section.

8.2 Device Studio Citation Instructions

When using any module of Device Studio for **Atomic-level Material Modeling (Million-scale)**, **High-performance Scientific Simulation Computing**, **Computation Task Monitoring and Management**, or **Data Visualization**, please cite Device Studio in your article using the following citation template:

Device Studio[1] program provides a number of functions for performing visualization, modeling and simulation. And XXX simulation using XXX software integrated in Device Studio program.

Reference：

[1] Hongzhiwei Technology, Device Studio, Version 2023A, China, 2023. Available online:https://cloud.hzwtech.com/web/product-service?id=6 (accessed on XXX, XXX).

CHAPTER

NINE

SCIENTIFIC COMPUTING SOFTWARE APPLICATION EXAMPLES

9.1 BDF Example

BDF (Beijing Density Functional) is an independent and complete **quantum chemistry calculation software package** with complete independent intellectual property rights. It is also the first **program based on modern density functional theory that can accurately calculate the total ground state energy of molecular systems with complete relativistic density functional** (early similar programs could not accurately calculate total energy due to poor numerical integration accuracy).

BDF **Official User Manual Website**: https://bdf-manual.readthedocs.io/zh_CN/latest/index.html

BDF Development Team Information:

- **International Quantum Molecular Science Academy Academician Wenjian Liu's Research Team**.
- **Hongzhiwei Development Team, Service Team**.

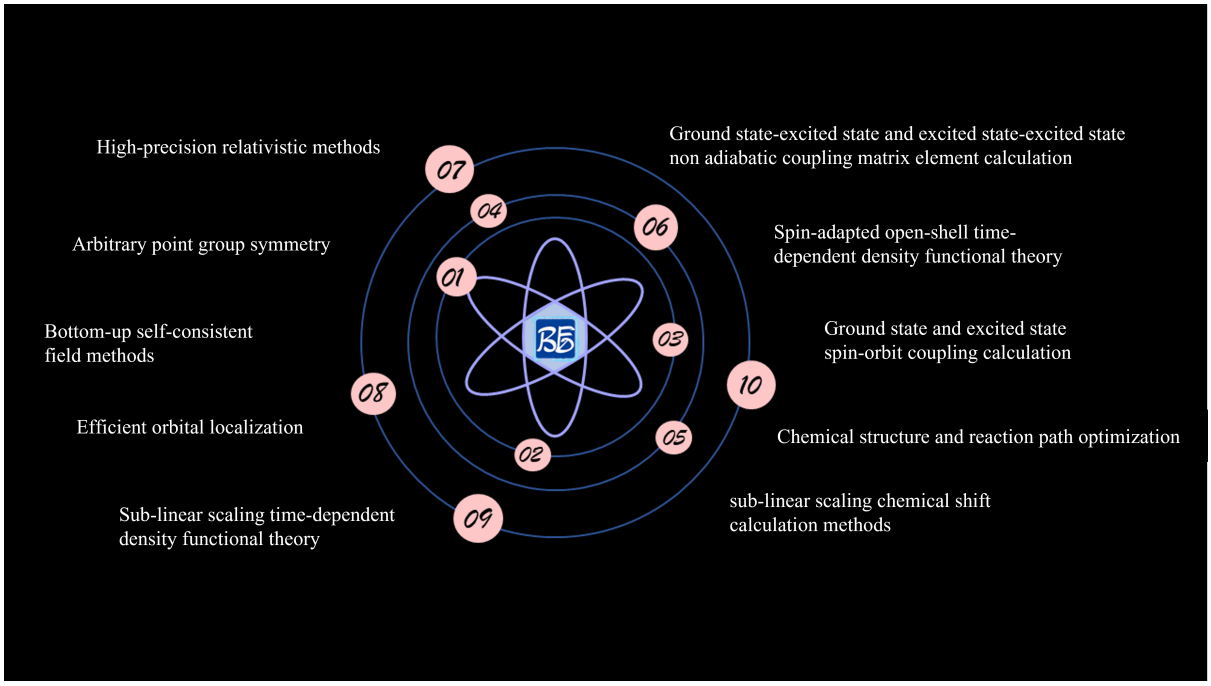


fig. 9.1: BDF Software Features Diagram

BDF Software Features:

1. High-precision relativistic methods.
2. Arbitrary point group symmetry.
3. Bottom-up self-consistent field methods.
4. Efficient orbital localization.
5. Sub-linear scaling time-dependent density functional methods.
6. Sub-linear scaling chemical shift calculation methods.
7. Spin-matched open-shell time-dependent density functional methods.
8. Ground state and excited state spin-orbit coupling calculations.
9. Ground state-excited state and excited state-excited state non-adiabatic coupling matrix elements.
10. Chemical structure and reaction path optimization.

Taking **ground state molecule CH2S sf-X2C/TDDFT-SOC spin-orbit coupling calculation** as an example to describe BDF application in Device Studio in detail.

9.1.1 BDF Development History

BDF development began in 1993 and was officially named in 1997. The initial idea was to **perform high-precision calculations on small molecular systems such as rare earths, actinides, transition metals, and superheavy elements**, examining relativistic effects in these systems, therefore initially adopting complete relativistic density functional theory (4C-DFT) based on Dirac operators and nearly complete basis functions "numerical basis + STO"(Slater-type orbital). Because of this, BDF's calculation results for rare earths, actinides, and superheavy elements have been used as benchmarks for testing other approximate relativistic methods. BDF's calculation results for electronic and molecular structures of heavy element systems have been verified by more than 20 subsequent experiments.

In 2009, **analytical integration based on Gaussian basis** was introduced, and BDF entered a new development stage.

Needless to say, BDF was initially positioned as a platform for developing new theories, new methods, and new algorithms, therefore it is a "research software". Theories and methods developed based on BDF include: relativistic time-dependent density functional theory (4C/ZORA/X2C-TDDFT), exact two-component (X2C) relativistic theory, quasi-four-component (Q4C) relativistic theory, spin-separated X2C relativistic theory (sf-X2C+so-DKHn), many-body effective quantum electrodynamics (eQED), relativistic nuclear magnetic theory (4C/X2C-NMR), relativistic nuclear spin-rotation theory (4C-NSR), relativistic band theory (X2C-PBC), X2C analytical gradients and Hessian; excited state HF/KS methods (mom); orbital localization scheme (FLMO) based on the idea of "synthesizing molecules from molecular fragments"(F2M), sub-linear scaling time-dependent density functional theory (FLMO-TDDFT), sub-linear scaling NMR methods (FLMO-NMR), iterative orbital interaction "bottom-up"self-consistent field methods (iOI); spin-matched open-shell time-dependent density functional theory (SA-TDDFT), spin-flip time-dependent density functional theory (SF-TDDFT), ground state/excited state-excited state non-adiabatic coupling time-dependent density functional theory (NAC-TDDFT), time-dependent density functional theory analytical energy gradients, arbitrary single-value/double-value point group symmetrization, etc.

Besides the above relativistic/non-relativistic density functional and time-dependent density functional theory, BDF also has wave function electron correlation methods based on the idea of "static then dynamic then static"(SDS), including SDSPT2SDSCI, iCI, iCIPT2, iCAS, iCISCF, SOC-iCI, iCI-SOC, and the iVI method for directly solving large matrix internal eigenstates, etc.

Given BDF's current status, the first commercial version will focus on fluorescence/phosphorescence material luminescence mechanism and material design as the main application targets, therefore it does not include 4C/X2C relativity, wave function electron

correlation, solid band/nuclear magnetic methods, etc. That is, the first commercialized BDF will mainly focus on DFT and TDDFT, including ground state and excited state KS, QM/MM, FLMO-TDDFT, SF-TDDFT, NAC-TDDFT, sf-X2C-SA-TDDFT/SOC, SA-TDDFT analytical energy gradients and numerical Hessian, stable structure and transition state optimization, reaction path optimization, implicit solvation models, FLMO-NMR, based on localized orbitals (FLMO) property calculations and analysis, and other special features.

9.1.2 BDF Calculation Process

The BDF calculation process in Device Studio is shown in fig. 9.2.

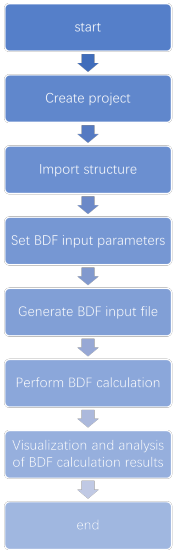


fig. 9.2: BDF Calculation Process

9.1.3 Creating a BDF Project

Double-click the Device Studio icon shortcut, log in and launch Device Studio. In the create or open project interface (*Graphical interface for selecting to create or open a project after starting the software*), according to the interface prompts, select to create a new project (*Create a new Project*) or open an existing project (*Open an existing Project*) button, then click the *OK* button in the interface. If you choose to create a new project, users can name the project as needed, such as naming this project `BDF`, or use the software's default project name.

9.1.4 Importing BDF Structure

In the Device Studio graphical interface, click *File* → *Import* → *Import Local*, which will pop up the interface for importing BDF structure files. According to the interface prompts, find the location of the `CH2S.hzw` structure file, select the `CH2S.hzw` structure file, click the *Open* button, and the Device Studio interface after importing the `CH2S.hzw` structure is shown in fig. 9.3. Other methods for importing structures in Device Studio are not explained in detail here, users can refer to the Import Structure section content.

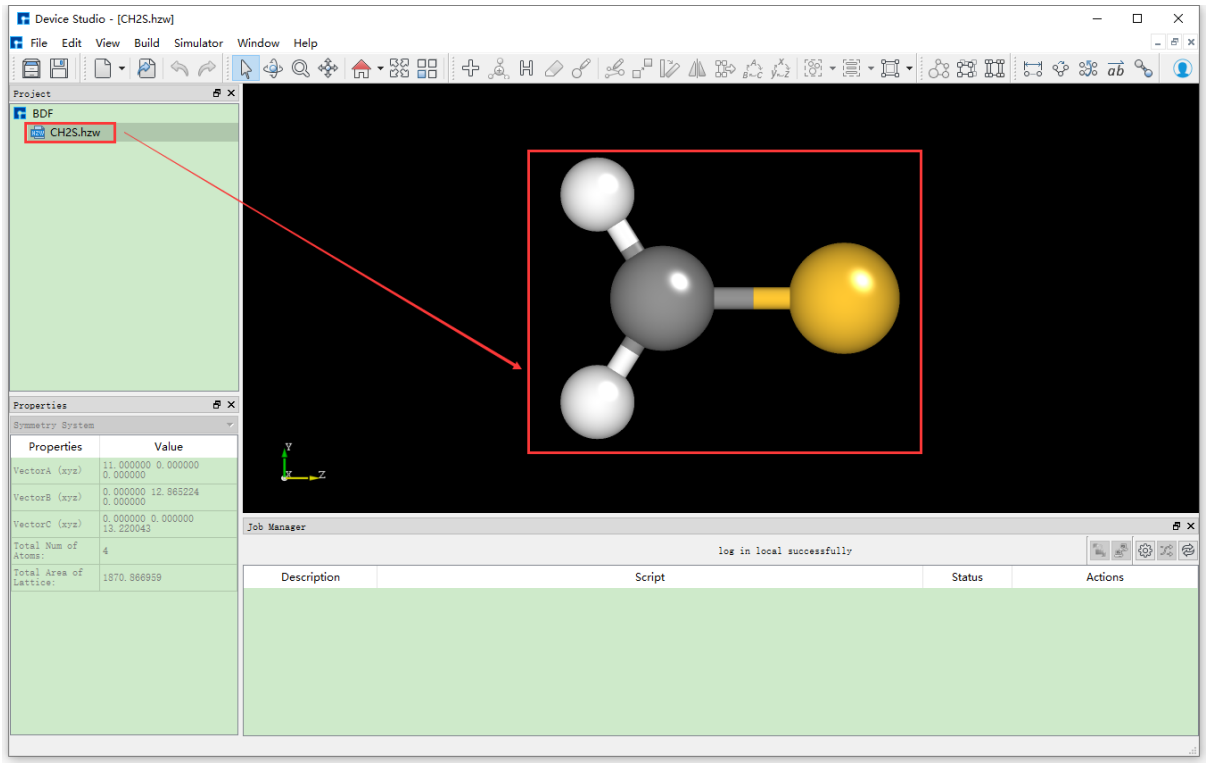


fig. 9.3: Device Studio graphical interface after importing the `CH2S.hzw` structure

9.1.5 Generating BDF Input Files

In the interface shown in fig. 9.3, select *Simulator* → *BDF* → *BDF*, which will pop up the BDF parameter settings interface BDF Job Setup as shown in fig. 9.4.

Taking the generation of input files for **ground state molecule CH2S sf-X2C/TDDFT-SOC spin-orbit coupling calculation** as an example, in the BDF Job Setup interface shown in fig. 9.3, according to calculation needs, select *Basic Settings*, *SCF Settings*, *TDDFT Settings* and *Preview Script* respectively, set parameters as shown in fig. 9.4, fig. 9.5, fig. 9.6 and fig. 9.7 respectively, then click the *Generate files* button in the interface to generate the input file `bdf.inp`.

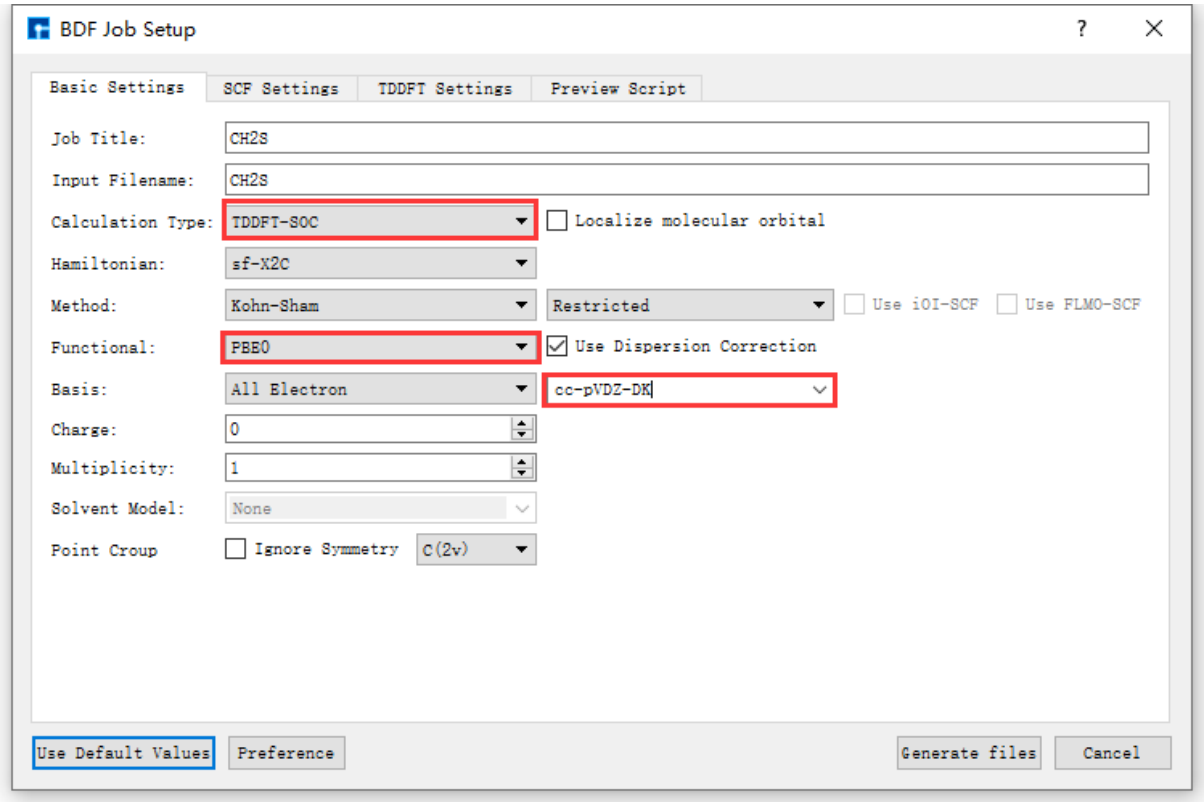


fig. 9.4: Basic Settings parameter settings interface

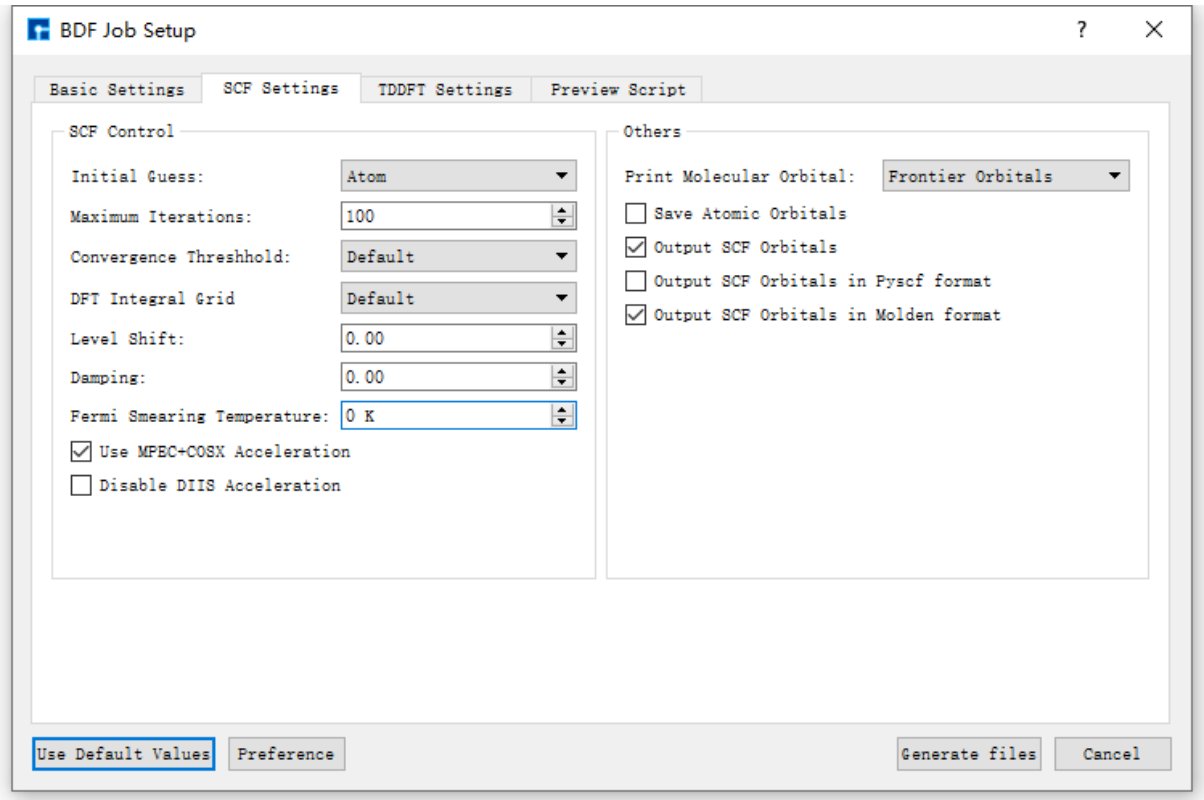


fig. 9.5: SCF Settings parameter settings interface

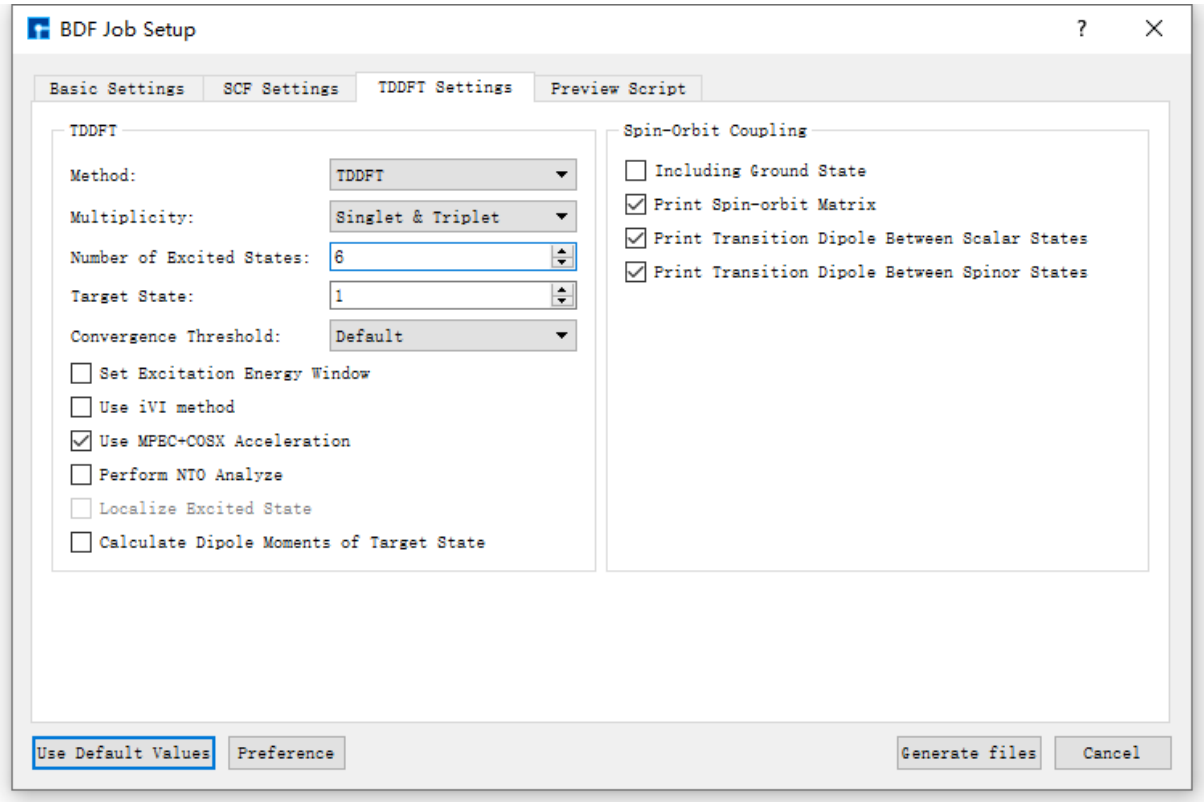


fig. 9.6: TDDFT Settings parameter settings interface

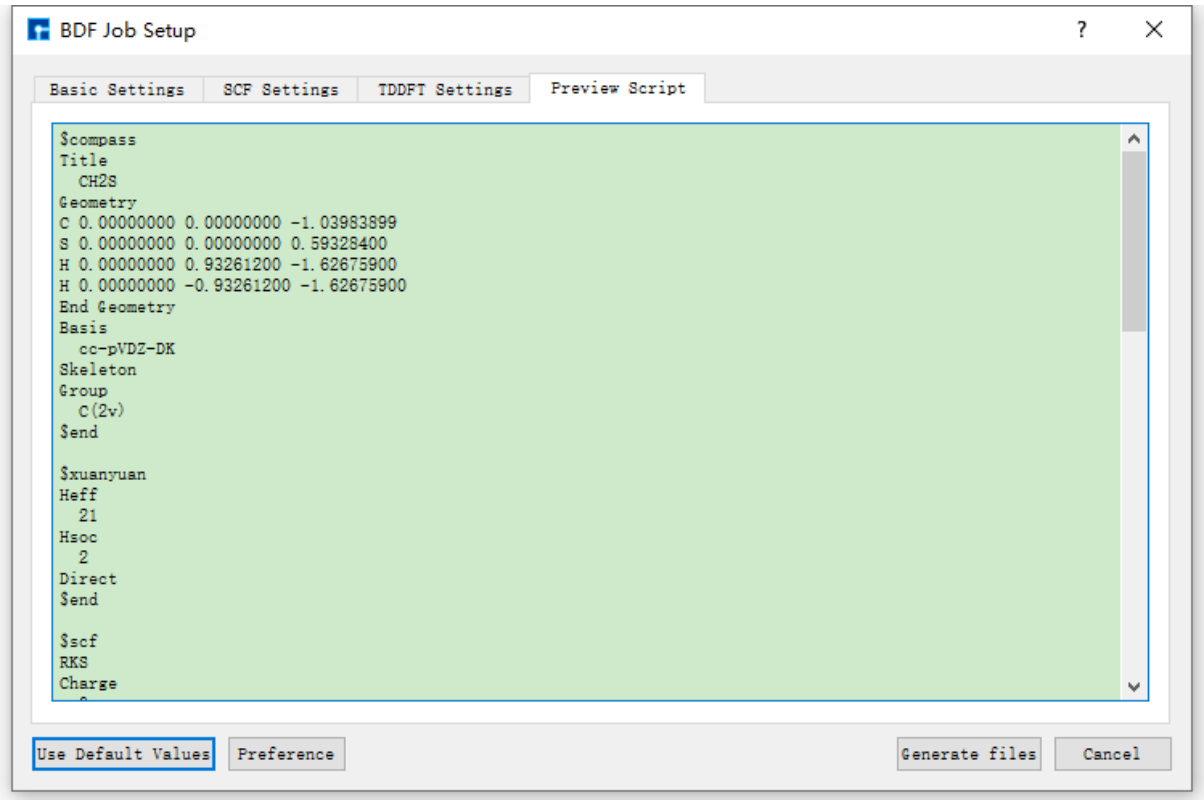


fig. 9.7: Preview Script parameter settings interface

The Device Studio interface for generating the input file `bdf.inp` for **ground state molecule CH2S sf-X2C/TDDFT-SOC spin-orbit coupling calculation** is shown in fig. 9.8.

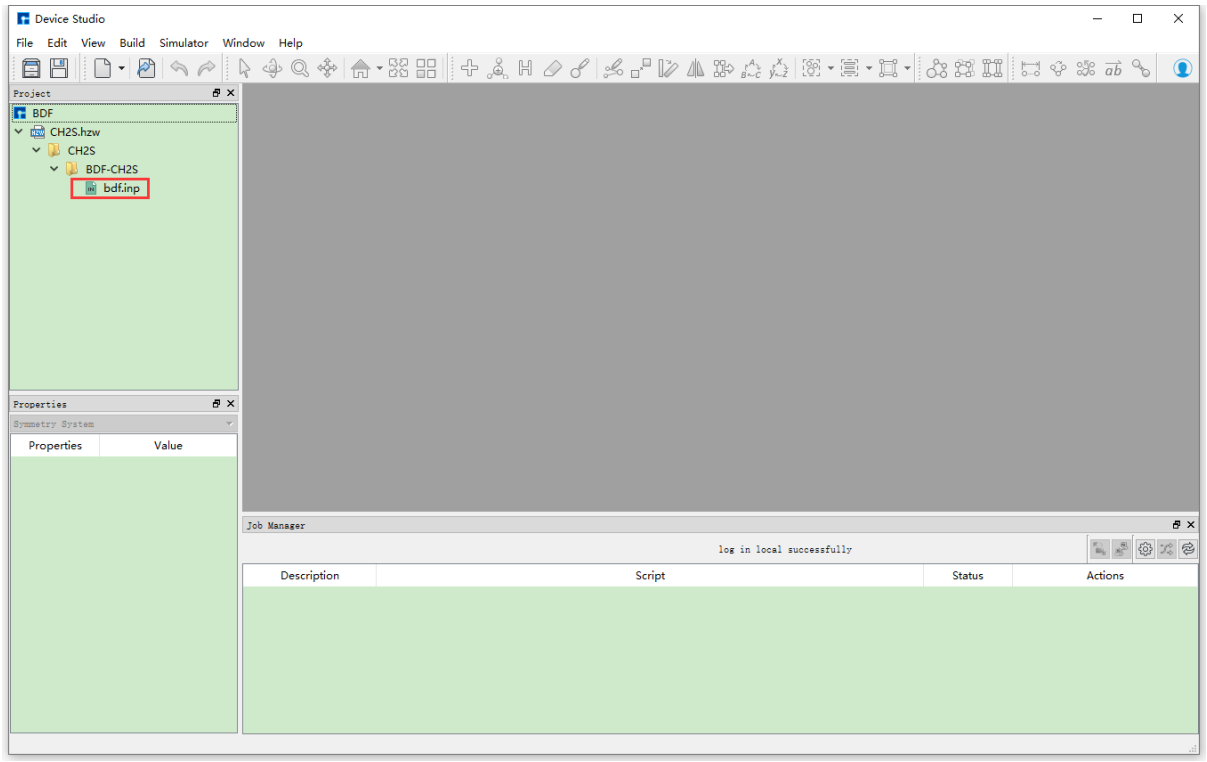


fig. 9.8: Device Studio interface for generating input files for **ground state molecule CH2S sf-X2C/TDDFT-SOC spin-orbit coupling calculation**

9.1.6 BDF Calculation

Before performing the **ground state molecule CH2S sf-X2C/TDDFT-SOC spin-orbit coupling calculation**, you need to connect to a server with BDF installed. The specific connection process is not explained in detail here, users can refer to the Nanodcal Connect to Server section content. After connecting to the server with BDF installed, before performing the calculation, users can open the input file and check if the parameter settings in the file are reasonable according to their needs. If not reasonable, they can choose to edit directly in the file or regenerate, and finally perform the BDF calculation (here BDF calculation refers to **ground state molecule CH2S sf-X2C/TDDFT-SOC spin-orbit coupling calculation**). For example, to open the `bdf.inp` file, in the Device Studio's Project Explorer area, select `bdf.inp` → right-click → *Open with* to view the `bdf.inp` file as shown below.

```
$compass
Title
  CH2S
```

(continues on next page)

(continued from previous page)

```
Geometry
C 0.00000000 0.00000000 -1.03983899
S 0.00000000 0.00000000 0.59328400
H 0.00000000 0.93261200 -1.62675900
H 0.00000000 -0.93261200 -1.62675900
End Geometry
Basis
  cc-pVDZ-DK
Skeleton
Group
  C(2v)
$end

$xuanyuan
Heff
  21
Hsoc
  2
Direct
$end

$scf
RKS
Charge
  0
SpinMulti
  1
DFT
  PBE0
D3
MPEC+COSX
Molden
$end

$tddft
```

(continues on next page)

(continued from previous page)

```
Imethod
  1
Isf
  0
Idiag
  1
Iroot
  6
MPEC+COSX
Istore
  1
$end

$tddft
Imethod
  1
Isf
  1
Idiag
  1
Iroot
  6
MPEC+COSX
Istore
  2
$end

$tddft
Isoc
  2
Nfiles
  2
Imatsoc
  -1
Imatrsf
```

(continues on next page)

(continued from previous page)

```
  -1
Imatrso
  -1
$end
```

note

During actual calculations, users can refer to the BDF **User Manual** to understand the detailed meaning of each parameter and set them appropriately according to calculation needs. To learn more about BDF, click on the corresponding purple or blue software name, or send an email to support@hzwtech.com for consultation.

In the interface shown in fig. 9.3, in the Device Studio's Project Explorer area, select `bdf.inp` → right-click → *Run*, which will pop up the Run interface. In the Run interface, click the *Run* button to perform the BDF calculation. Users can observe the BDF calculation status in the Job Manager area. When the BDF calculation task is in the queue, in progress, or completed, *Status* is Queued, Running, Finished respectively. After the calculation is completed, click the Actions button in the Job Manager area, which will pop up the Qsftp Explorer interface. In this interface, find the calculation result file, click the *Download* button to download the calculation result file from the server to the local, and the downloaded result file can be viewed in the Device Studio's Project Explorer area.

9.1.7 BDF results visualization

Currently, there is no visualization analysis function for BDF calculation results in Device Studio. Users can analyze them themselves. The specific analysis process can refer to the BDF user manual. The visualization analysis function of BDF will be integrated into the Device Studio in subsequent version updates.

9.2 DS-PAW Example

DS-PAW is a first-principles plane wave calculation software under the Device Studio platform, using plane waves as basis functions, and the pseudopotential is constructed using the Projector Augmented Wave method. DS-PAW is powerful and can be applied to different scenarios, such as metals, semiconductors, insulators, surfaces, magnetic, non-magnetic, lithium batteries, etc.; it can accurately predict material electron distribution; it can perform atomic geometric structure

optimization; it can be widely applied in materials science. DS-PAW has stable performance, having undergone millions of internal test cases on Intel chips and domestic Haiguang chips, including various functions and parallel efficiency.

As shown in fig. 9.9, DS-PAW 2021B version has implemented 28 calculation functions including **structure relaxation, electronic structure, mechanical properties, magnetic calculations, transition states, hybrid functionals, van der Waals corrections, optical properties, spin-orbit coupling, phonon calculations, strongly correlated calculations, first-principles molecular dynamics**, and more functions are still being added.

Taking **Si crystal structure hybrid functional band calculation** as an example to describe DS-PAW application in Device Studio in detail.

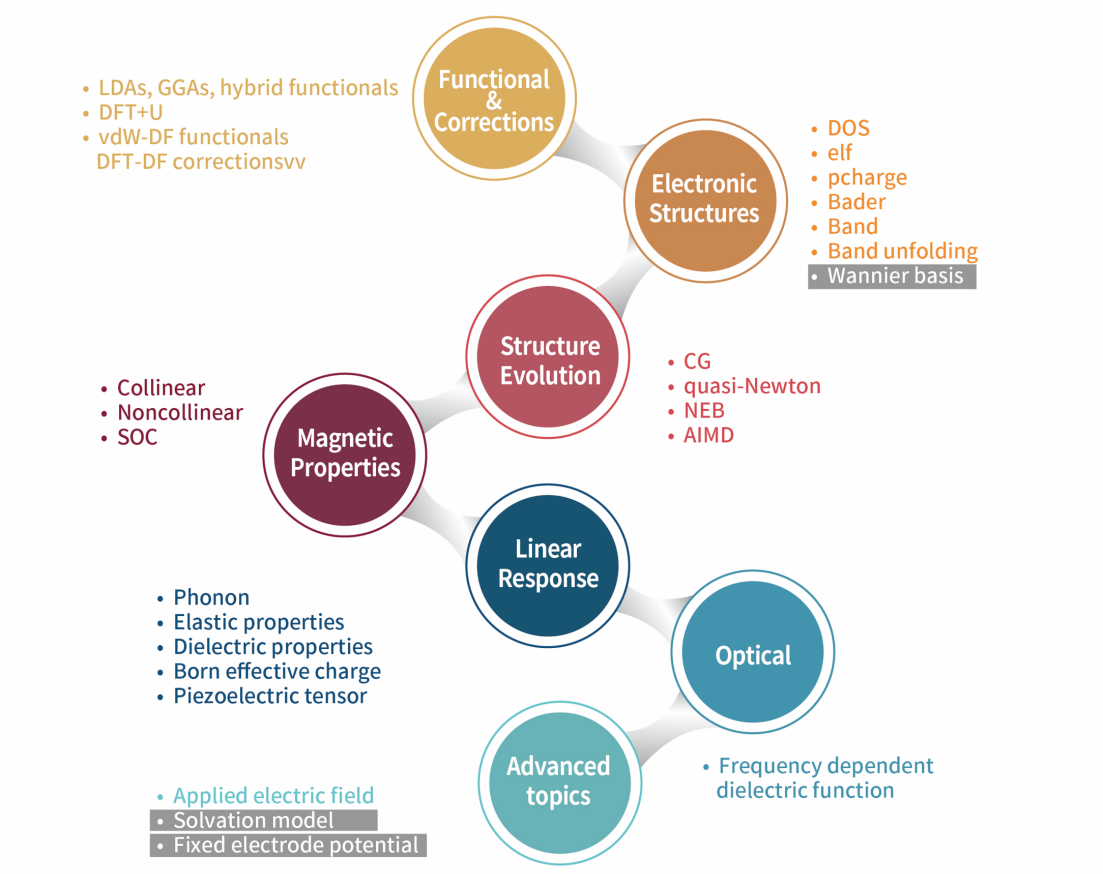


fig. 9.9: DS-PAW Software Function Diagram

9.2.1 DS-PAW Calculation Process

The DS-PAW calculation process in Device Studio is shown in fig. 9.10.

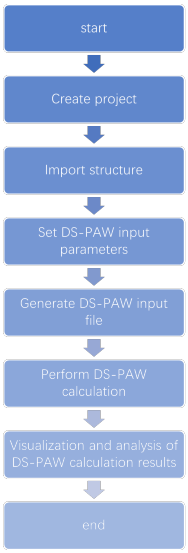


fig. 9.10: DS-PAW Calculation Process

9.2.2 DS-PAW Project Creation

Double-click the Device Studio icon shortcut, log in and start Device Studio. In the create or open project interface (*Graphical interface for selecting to create or open a project after starting the software*), according to the interface prompts, select the button to create a new project (*Create a new Project*) or open an existing project (*Open an existing Project*), then click the *OK* button in the interface. If choosing to create a new project, users can name the project according to their needs, such as naming this project `DS-PAW`, or use the software's default project name.

9.2.3 DS-PAW Structure Import

In the Device Studio graphical interface, click *File* → *Import* → *Import Local*, which will open the interface for importing DS-PAW structure files. According to the interface prompts, find the location of the `Si.hzw` structure file, select the `Si.hzw` structure file, click the *Open* button, then the Device Studio interface after importing the `Si.hzw` structure is shown in fig. 9.11. Other methods for importing structures in Device Studio are not detailed here, users can refer to the Import Structure section.

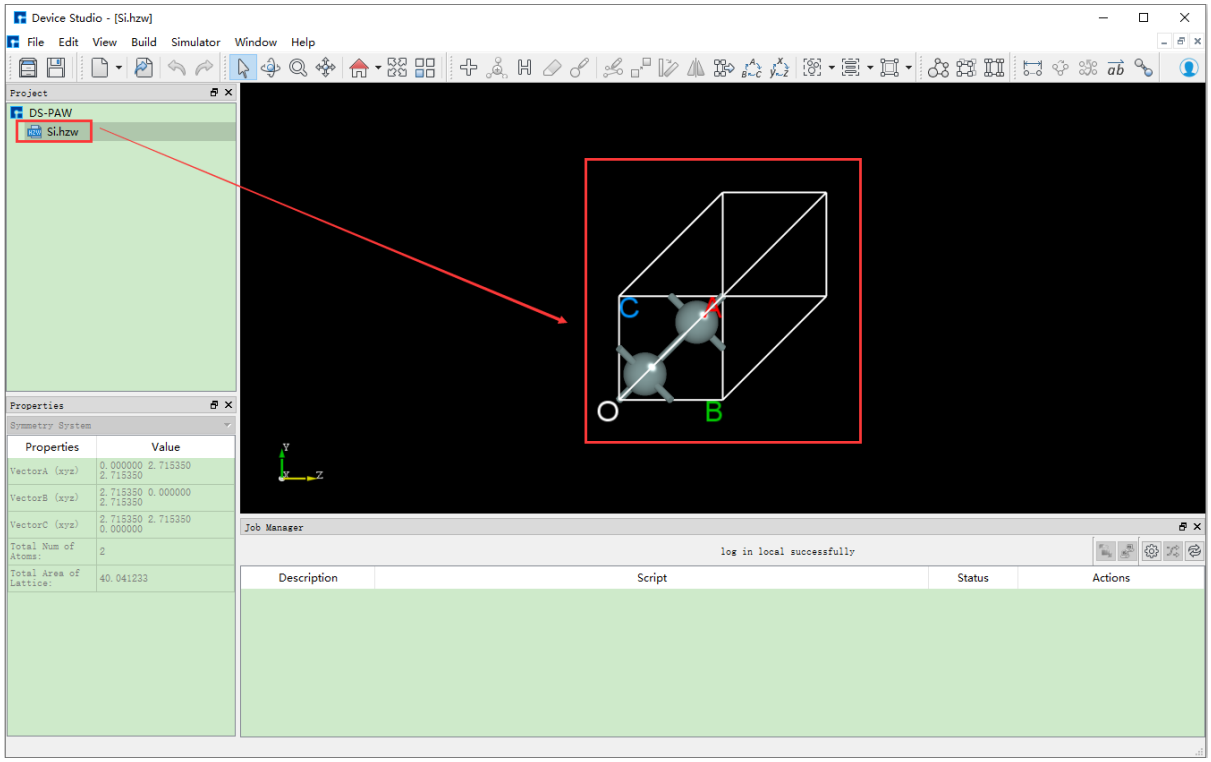


fig. 9.11: Device Studio Graphical Interface After Importing `Si.hzw` Structure

9.2.4 DS-PAW Input File Generation

In the interface shown in fig. 9.11, select *Simulator* → *DS-PAW* → *Electronic Structure*, which will open the DS-PAW parameter settings interface Electronic structure as shown in fig. 9.12. The Electronic structure interface is mainly divided into four modules: *Task*, *Solver setting*, *Physical setting*, and *Advanced*. Users can set parameters by clicking the four modules in sequence according to calculation needs, then click *Generate files* to generate the corresponding calculation input files.

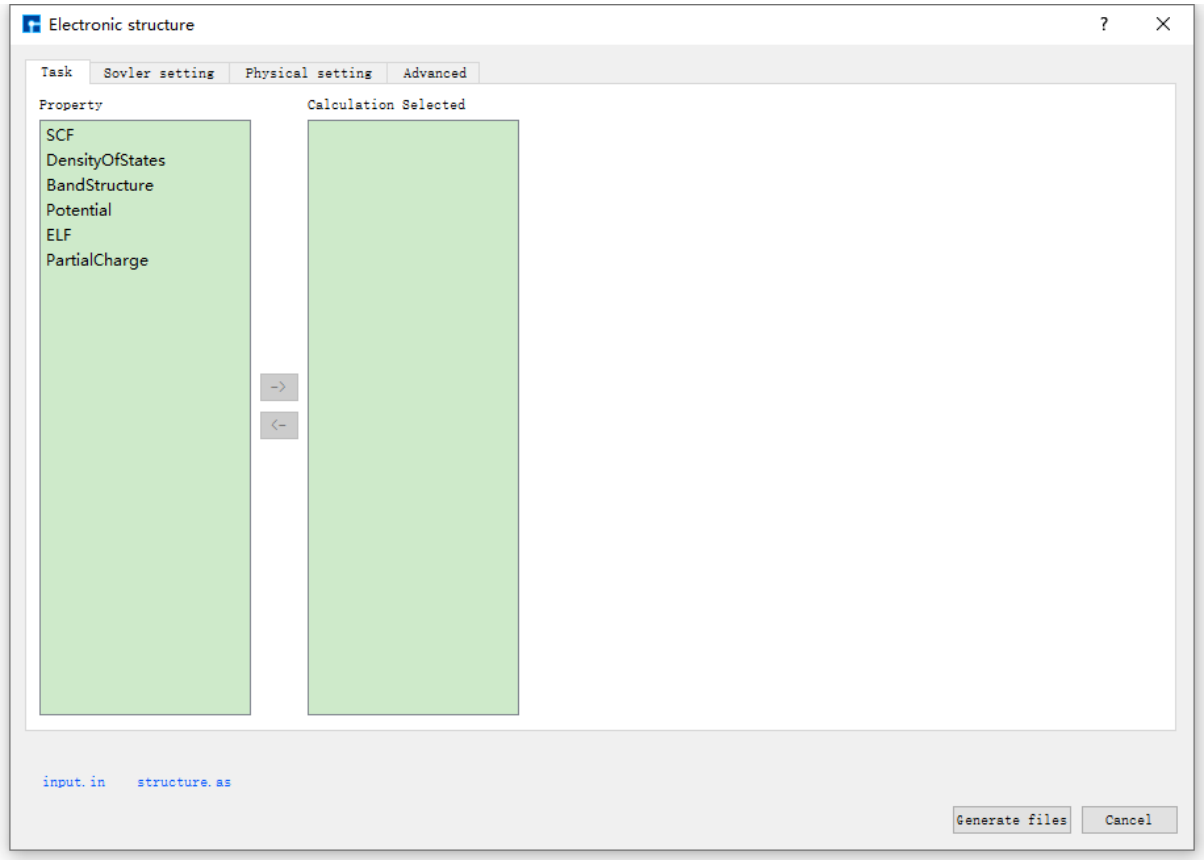


fig. 9.12: DS-PAW Parameter Settings Interface Electronic structure

Taking the generation of input files for **Si crystal structure hybrid functional band calculation** as an example, in the Electronic structure interface shown in fig. 9.12, according to calculation needs, select *Task*, *Solver setting*, *Physical setting*, and *Advanced* respectively, set parameters as shown in fig. 9.13, fig. 9.14, fig. 9.15, and fig. 9.16 respectively, then click *Generate files* in the interface to generate the input files `scf.in` and `structure`.

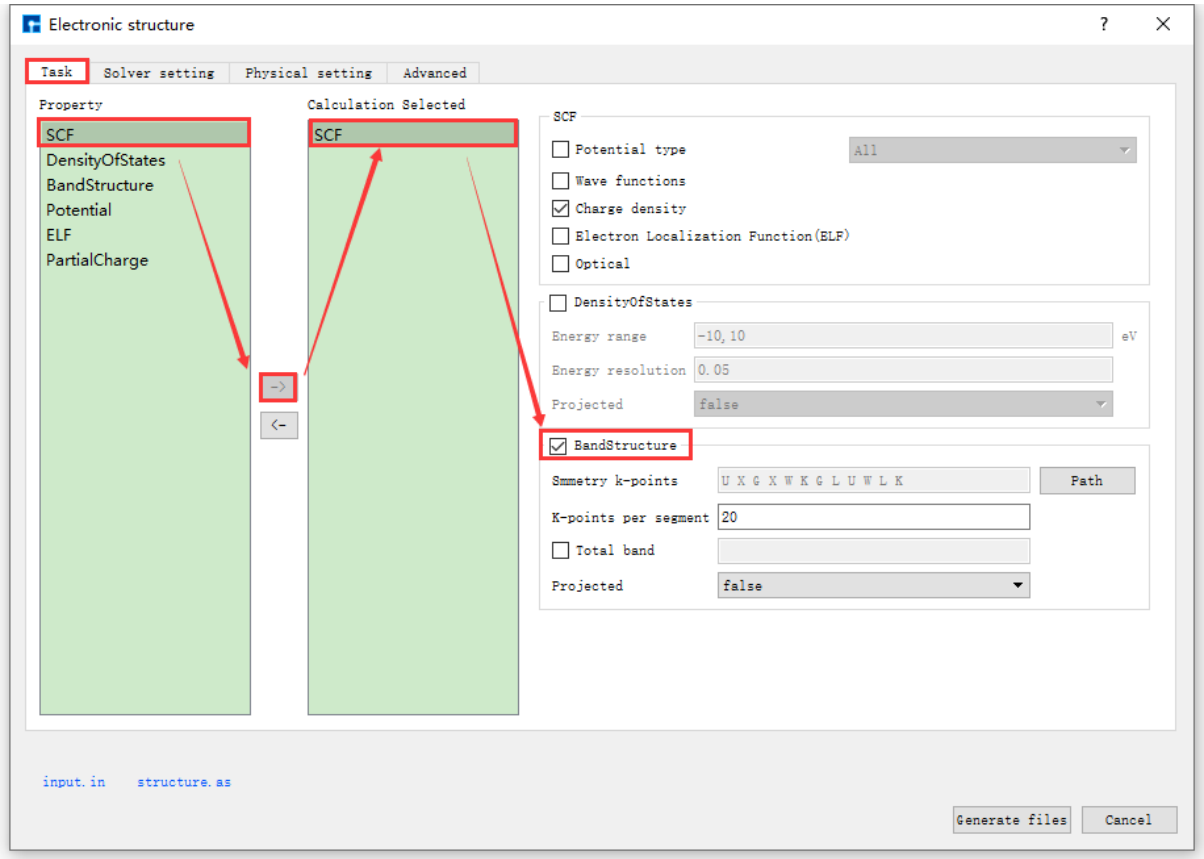


fig. 9.13: Task Parameter Settings Interface

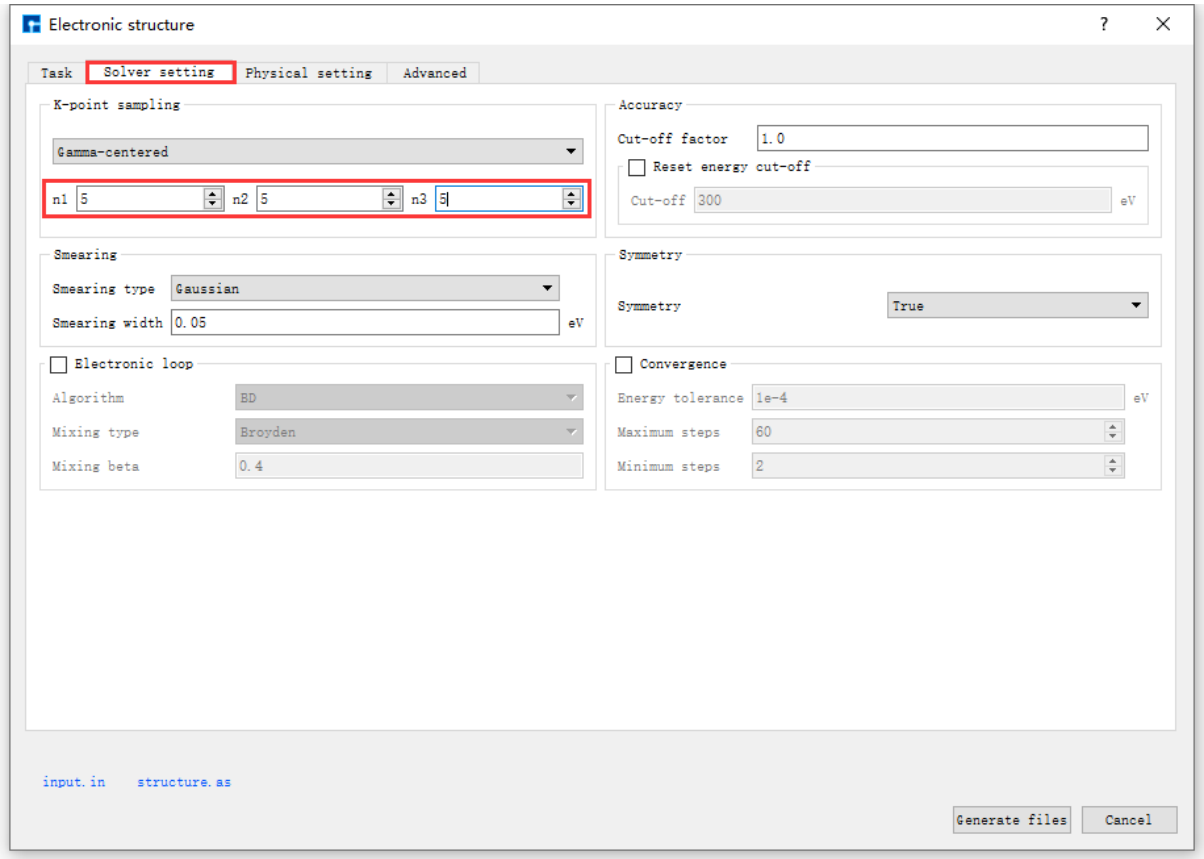


fig. 9.14: Solver Setting Parameter Settings Interface

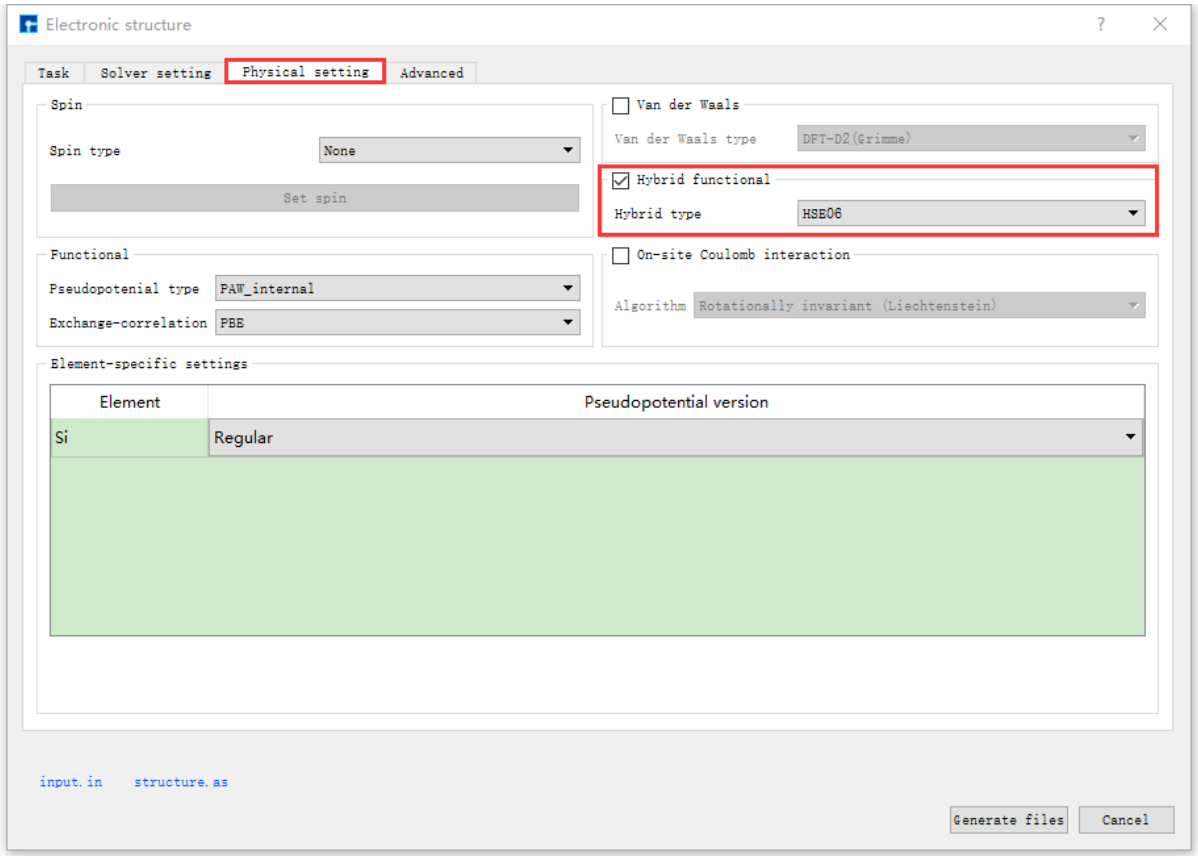


fig. 9.15: Physical Setting Parameter Settings Interface

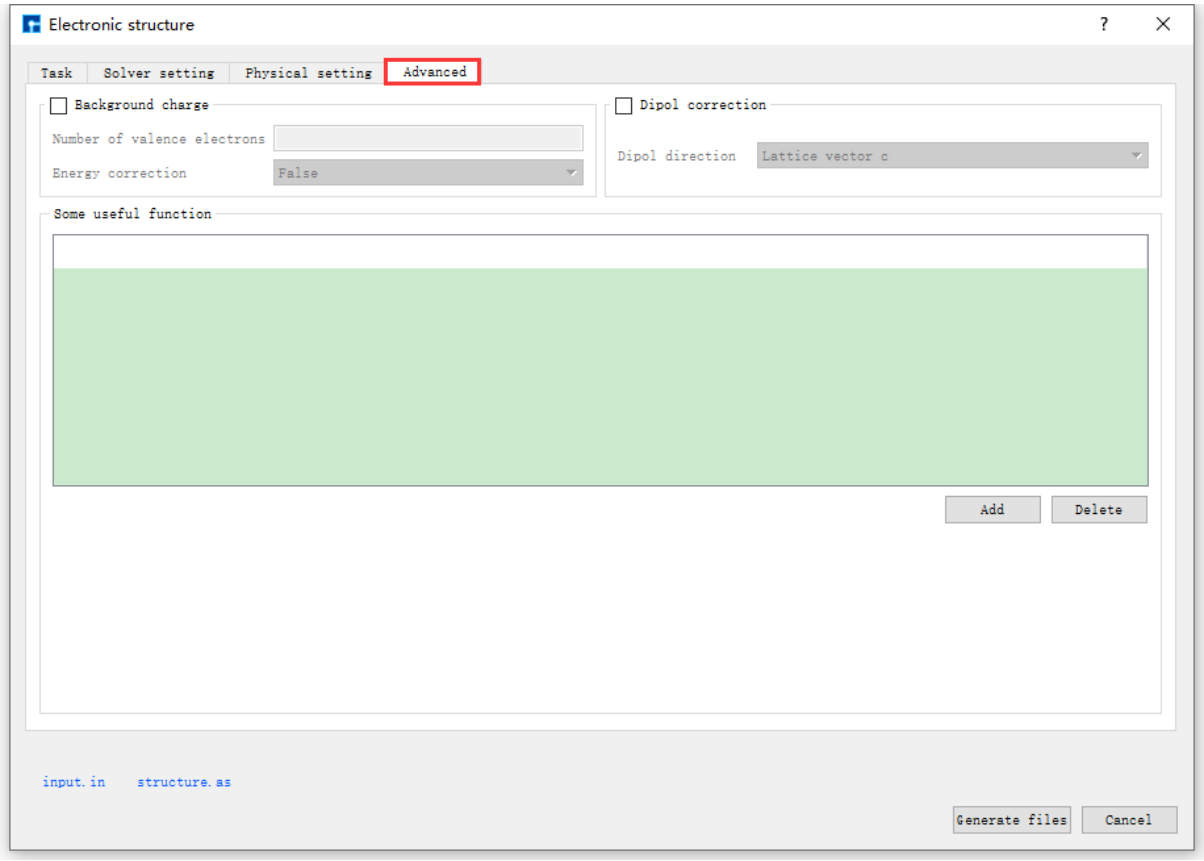


fig. 9.16: Advanced Parameter Settings Interface

The Device Studio interface for generating input files `scf.in` and `structure` for **Si crystal structure hybrid functional band calculation** is shown in fig. 9.17.

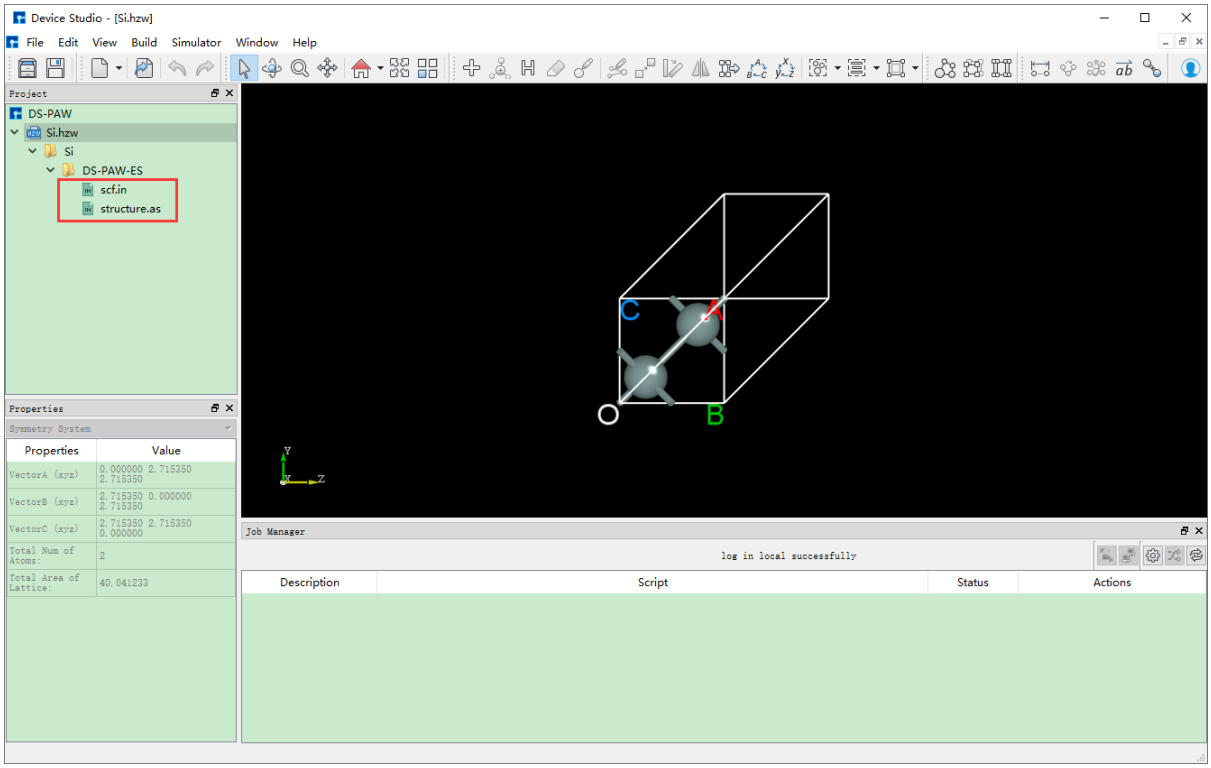


fig. 9.17: Device Studio Interface for Generating **Si crystal structure hybrid functional band calculation** Input Files

9.2.5 DS-PAW Calculation

Before performing the **Si crystal structure hybrid functional band calculation**, you need to connect to a local computer or server with DS-PAW installed. The specific connection process is not explained in detail here, users can refer to the Nanodcal Connect to Server section content. Taking calculation on a local computer as an example, after connecting to the local computer with DS-PAW installed, before performing the calculation, users can open the input files and check if the parameter settings in the files are reasonable according to their needs. If not reasonable, they can choose to edit directly in the files or regenerate, and finally perform the DS-PAW calculation. For example, to open the `scf.in` file, in the Device Studio's Project Explorer area, select `scf.in` → right-click → *Open with* to view the `scf.in` file as shown in fig. 9.18. For other input files, users can choose whether to open and view them according to their needs, which is not explained in detail here.

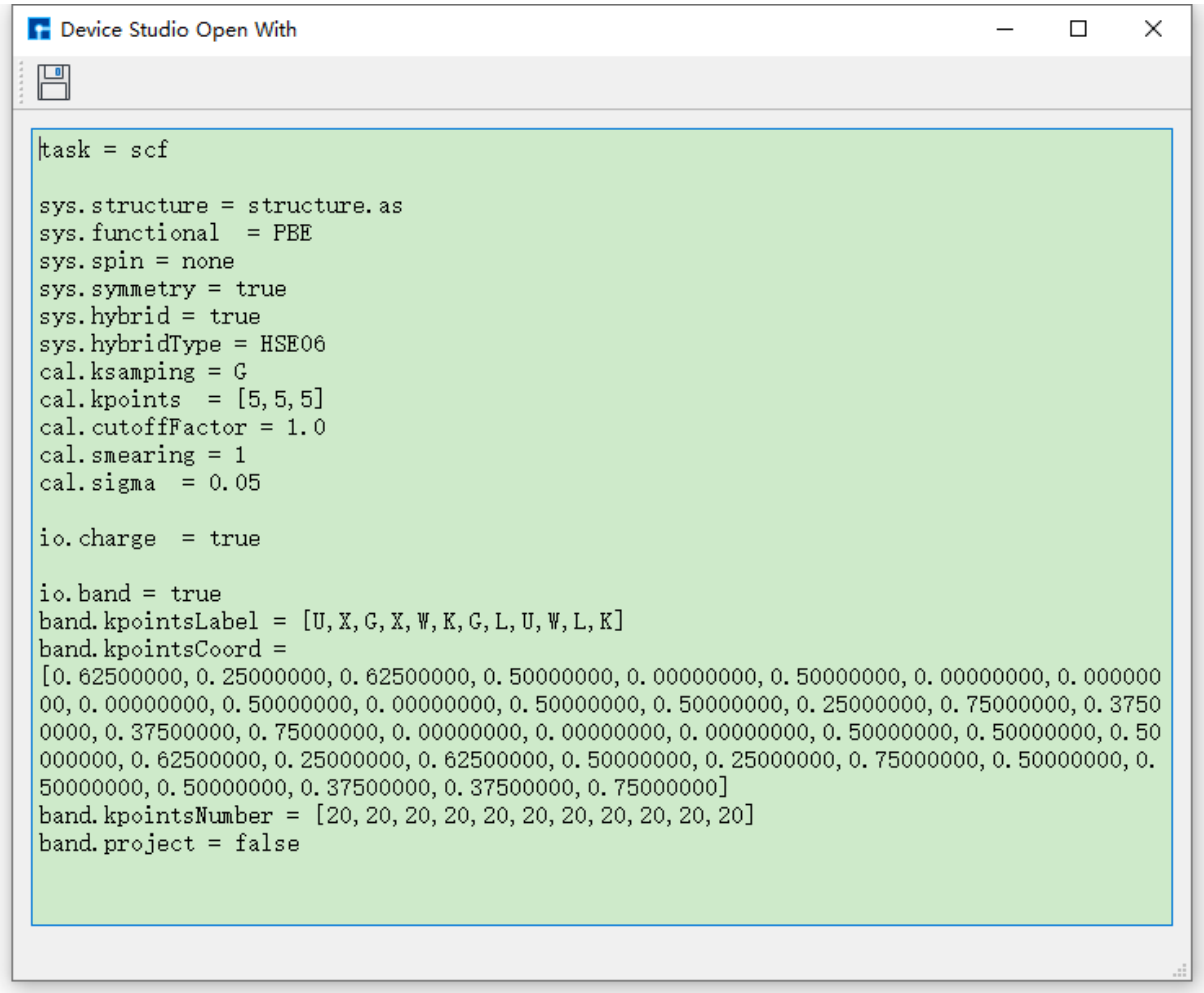


fig. 9.18: `scf.in` File

In the interface shown in fig. 9.17, in the Device Studio's Project Explorer area, select `scf.in` → right-click → *Run*, which will pop up the Run interface. In the Run interface, click the *Run* button to perform the DS-PAW calculation. Users can observe the DS-PAW calculation status in the Job Manager area. When the DS-PAW calculation task is in the queue, in progress, or completed, *Status* is Queued, Running, Finished respectively. After the calculation is completed, the result file `band.json` and log file `DS-PAW.log` can be seen in the Device Studio's Project Explorer area.

9.2.6 DS-PAW Results Visualization

In the Device Studio's Project Explorer area, select `band.json` → right-click → *Show View*, which will pop up the DS-PAW results visualization interface as shown in fig. 9.19.

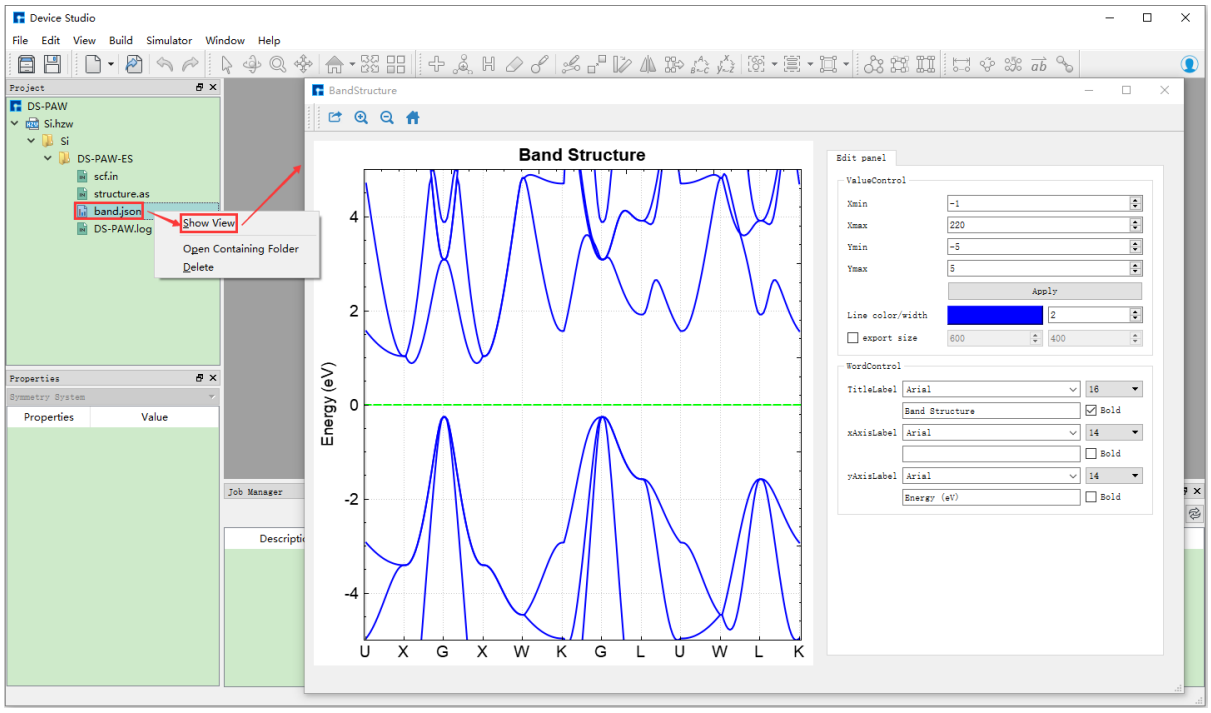


fig. 9.19: DS-PAW Results Visualization Interface

> **Note**
>
> DS-PAW calculation results are often stored in `.json` or `.h5` format. Currently, Device Studio supports visualization analysis of DS-PAW result files in `.json` format smaller than **68MB**. For `.json` files larger than **68MB**, it is recommended that users use the DS-PAW auxiliary toolkit dspawpy for data analysis.

CHAPTER

TEN

FREQUENTLY ASKED QUESTIONS AND SOLUTIONS

10.1 How to Find the Device Studio Shortcut?

Place the installation package `DeviceStudio***.zip` in an English-named directory on your local computer → Extract → Find the *DeviceStudio.exe* file in the **bin** directory → Right-click → *Send to (N)* → *Desktop shortcut*, then you will have a Device Studio shortcut on your desktop.

10.2 How to Cite Device Studio?

Device Studio has an article citation template. Users can refer to the Citation Instructions section.

10.3 How to Change Device Studio Background Color to White?

There are two ways to modify the Device Studio background color:

1. Modify the background color of the atomic structure display in the Device Studio main interface, i.e., modify the *Structure 3D Display Area (3D Viewer)* background color in Device Studio. Please refer to the Modify Device Studio Main Interface Background Color section.
2. Modify the background color in the atomic structure refinement module of Device Studio, i.e., modify the SRM Structure Display Area background color. Please refer to the Modify Atomic Structure Refinement Module Background Color section.