iModel ： An Interactive 3D Crystal Structure Visualization Program

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1. Program Installation and Updates

1.1 System Requirements

Windows 10 and above.

1.2 Download and Installation

The installation steps will be continually optimized with the program's further development and updates. For specific installation instructions, please refer to the readme document at the download address https://github.com/iPowder/iModel.

1.3 Update

Download the update content from the program's release page and follow the instructions in the update notes。

2. Program Interface

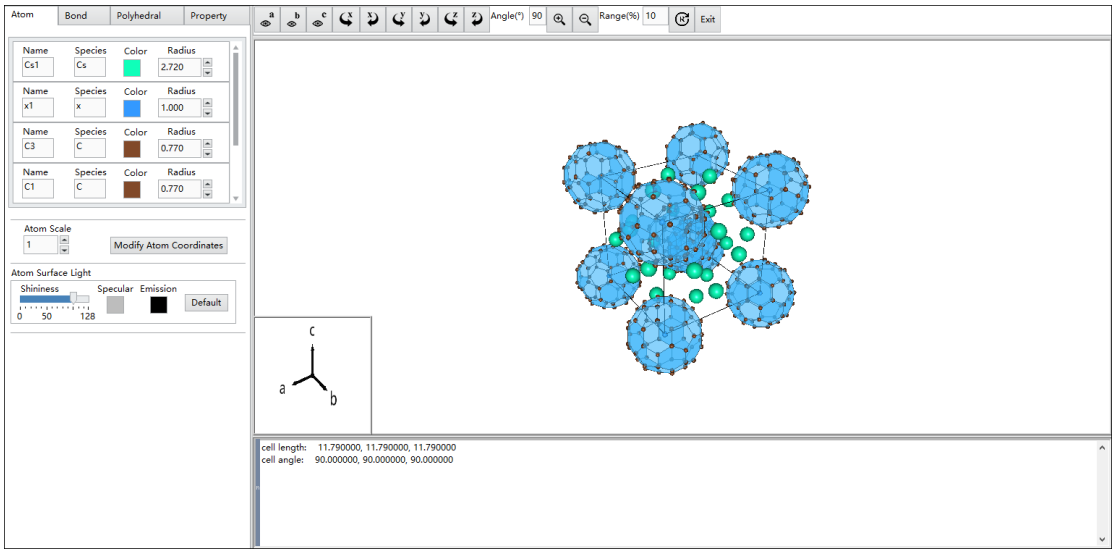


Figure 1: iModel program interface displaying the crystal structure of CSC_{10}.

The program interface is primarily divided into three windows, a toolbar, and a menu bar. The sizes of the three windows can be adjusted accordingly.

In Figure 1, the largest window is the structure model display window, where the display and manipulation of the crystal structure take place. Below this window is the structure information

output window, where crystal cell parameters, atomic coordinates upon mouse click, chemical bond names, and more will be displayed. The left window contains atoms, chemical bonds, polyhedral structures, and various other properties, along with related functional buttons.

The toolbar above the image is used to manipulate the structure model, enabling functions such as changing the viewing angle, rotating around a specific direction by a certain angle, zooming in and out, and resetting the image.

The menu bar includes three sections for file reading and writing, undo and redo operations, and help.

3. File Reading and Saving

3.1 Data File Reading and Writing

Click on the 'File-Open File' option in the menu bar to read crystal structure data files. Supported file formats include CIF, POSCAR/CONTCAR, CHGCAR, LOCPOT, vasprun.xml, CSSR, Netcdf, and pymatgen's JSON serialized structure files. Click on 'File-Save To File' in the menu bar to save the crystal structure as data files in formats such as CIF, POSCAR/CONTCAR, CHGCAR, etc. (refer to Table 1 for details).

Table 1: Data File Input and Output Formats

Input file formats	
1	*.cif
2	*.mcif
3	*POSCAR
4	*CONTCAR
5	*.vasp
6	CHGCAR
7	LOCPOT
8	vasprun
9	*.xml
10	*rndstr.in
11	*lat.in
12	*bestsqs
13	*.cssr
14	*.mson

Input file formats	
15	*.json
16	*.xsf
17	CTRL
18	*primatic
19	*.yaml
20	*.yml
21	*.in
22	*.res

Output file formats	
1	*.cif
2	*.mcif
3	*POSCAR
4	*.cssr
5	*.json
6	*.xsf
7	*rndstr.in
8	*lat.in
9	*bestsqs
10	*prismatic
11	*.yml
12	*.in
13	*.res

3.2 Save as Image File

Click on the File-Save As Image option in the menu bar to save the crystal structure as an image

file. Supported formats include jpg, jpeg, png, and bmp.

3.3 Project Files

You can save and load project files using the "Save As Project" and "Open Project" options in the menu bar, allowing you to pause and resume your work in the current state.

4. Structure Model Control

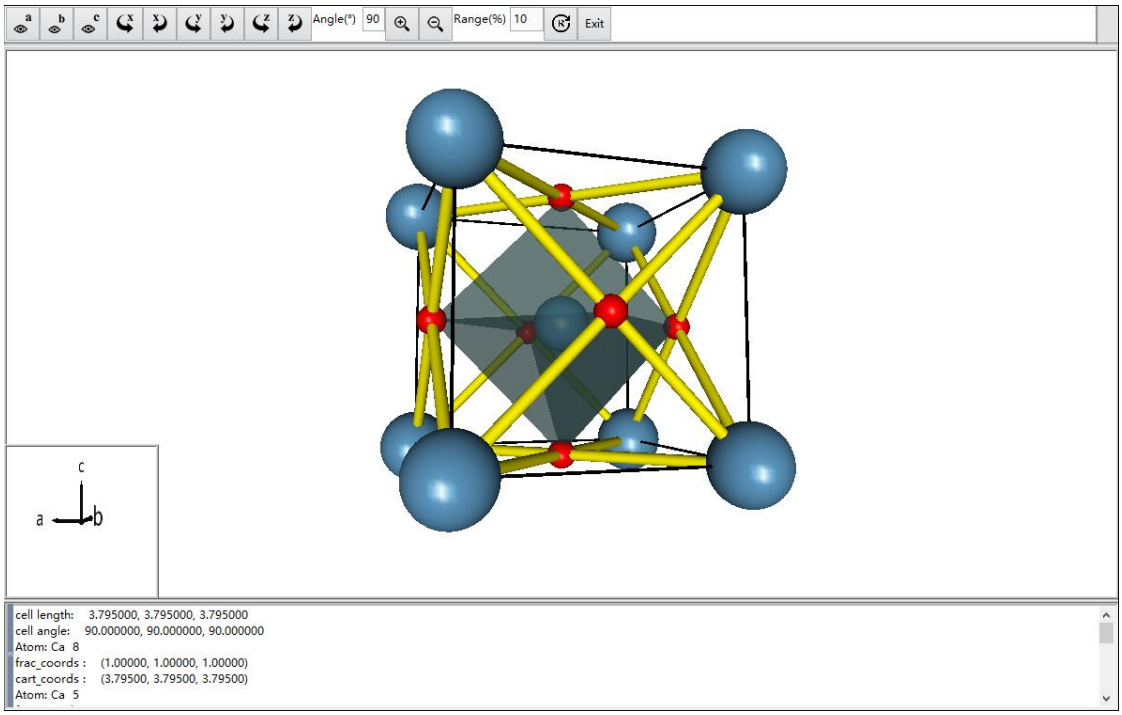


Figure 2: iModel program crystal structure display window showing the crystal structure of CaTiO3.

You can directly rotate the crystal structure by dragging with the left mouse button. The rotation center is the center of the display window, initially located at the origin (0,0,0).
Hold down the Shift key and simultaneously drag up or down with the left mouse button to zoom in or out on the crystal structure.

Hold down the Ctrl key and simultaneously drag with the left mouse button to freely move the structure model. After moving the structure model, the atomic coordinates remain unchanged; only the field of view is altered. Additionally, the rotation center will shift from the origin to the current center of the view.

Clicking on atoms, chemical bonds, or other objects in the structure with the left mouse button will display the selected object's name and coordinate-related properties in the structure information output window below.

Right-clicking on the structure display window with the mouse will bring up a prompt interface where you can view operation instructions and help.

5. Atom，Bond，Polyhedral，Property

5.1 Atom

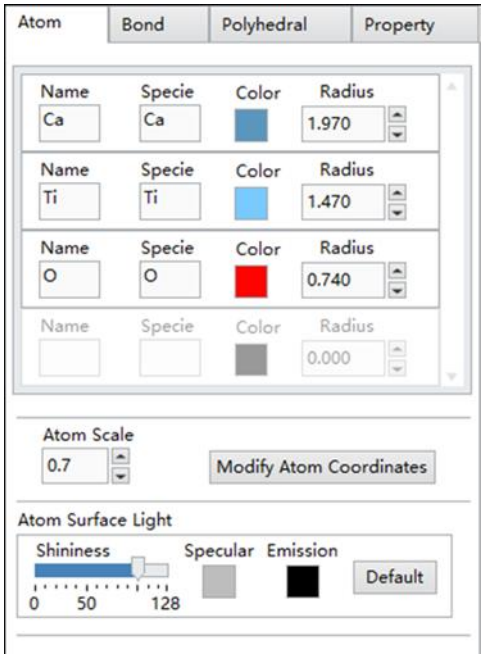


Figure 3: Atom Options Page

At the top of the page, the names, species, colors, and radius sizes of all types of atoms in the current structure are displayed. Users can freely adjust them within a suitable range.
The Atom Scale controls the current size ratio of all atoms. The 'Modify Atom Coordinates' button is used for precise adjustment of each atom's parameters. Clicking it will open a window displaying parameters such as color and radius size for all atoms. Right-clicking on an atom allows for its deletion.

The Atom Surface Light section is used to adjust the three-dimensional lighting effects on the surface of atoms, including parameters for emission, reflection, and diffuse light. It also includes a reset button.

5.2 Bond

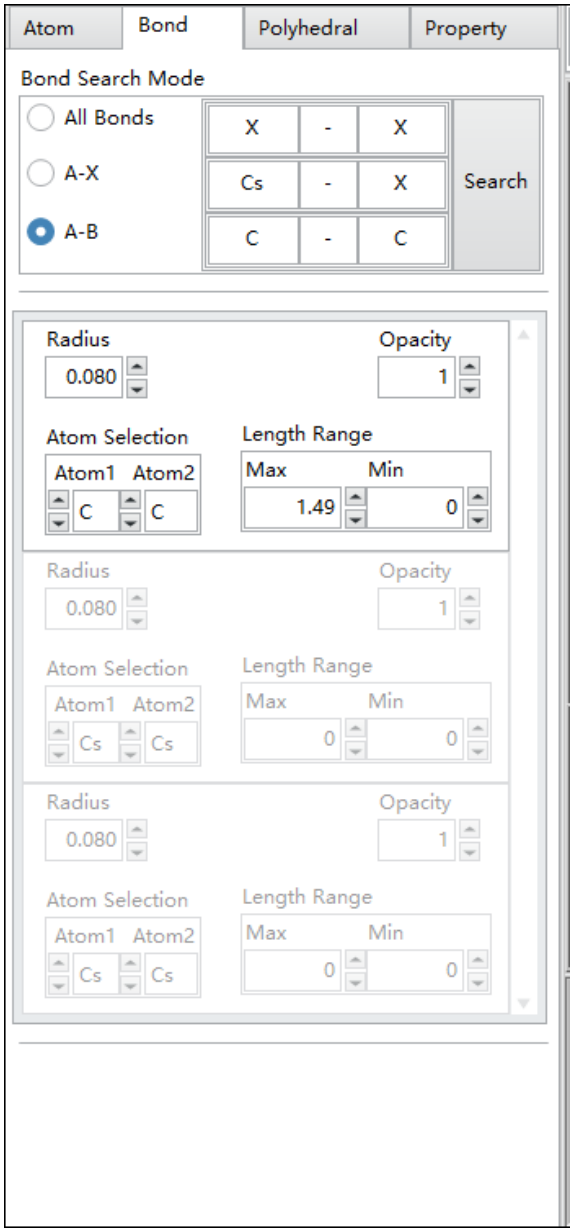


Figure 4: Bond Options Page

In the Bond Search Mode option, you can adjust the chemical bond search mode, which includes three modes. In the A-B mode, only the chemical bonds composed of atoms A and B are searched. In the A-X mode, chemical bonds formed by atom A with all types of atoms are searched. The All Bonds mode searches for all potentially existing chemical bonds in the structure.

Then, the page displays the names, radii, colors, transparency, and bond length search range of chemical bonds in the current structure. Users can add new chemical bonds for display by entering the information in the gray area below. Additionally, you can right-click to delete selected chemical bonds

5.3 Polyhedral

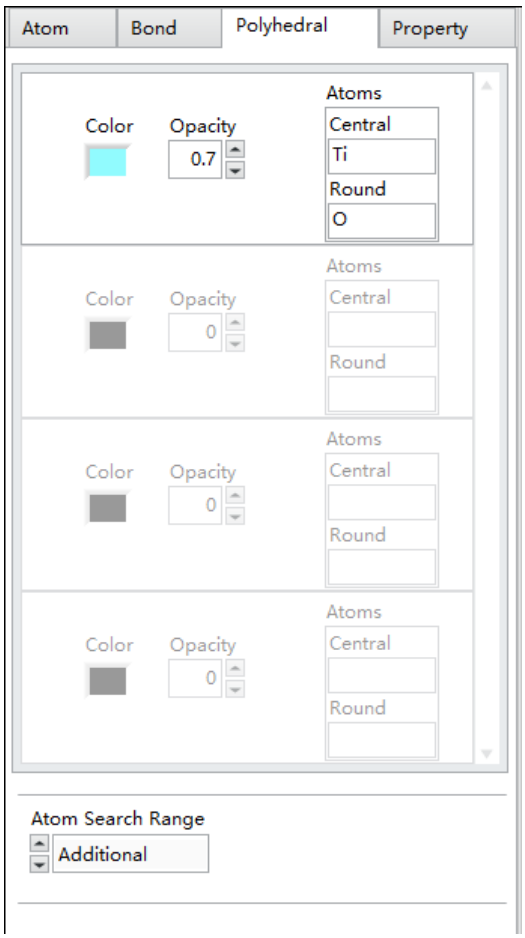


Figure 5: Polyhedral Options Page

At the top of the Polyhedral page, users can click the Search button in the Search Polyhedra window to automatically search for polyhedral structures. In the A-B field to the left of the button, A stands for the Central Atom, and B stands for the Round Atom.

In the Atom Search Range option, under the Inside the cell mode, only the polyhedral structures present in the current single unit cell are searched. In the Additional mode, atoms around the current unit cell are included in the search range and added to the crystal structure, displaying polyhedral structures collectively.

Then, the page displays the color, transparency, central atom, and surrounding atoms for the polyhedral structures being searched in the current structure. Users can add new polyhedral structures for display by entering information in the gray area below or right-click to delete polyhedral objects.

5.4 Property

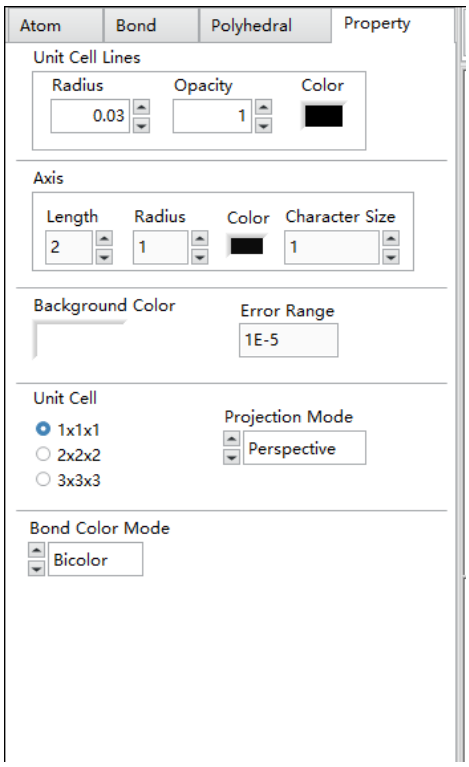


Figure 6: Property Options Page

Under this page, there are various options related to crystal structure properties. These include settings for the thickness, transparency, and color of cell indication lines, the length, thickness, color, and font size of coordinate axes, as well as the background color of the display window and the error range for program algorithm execution (such as atoms within the error range of atomic distances being considered as the same atom).

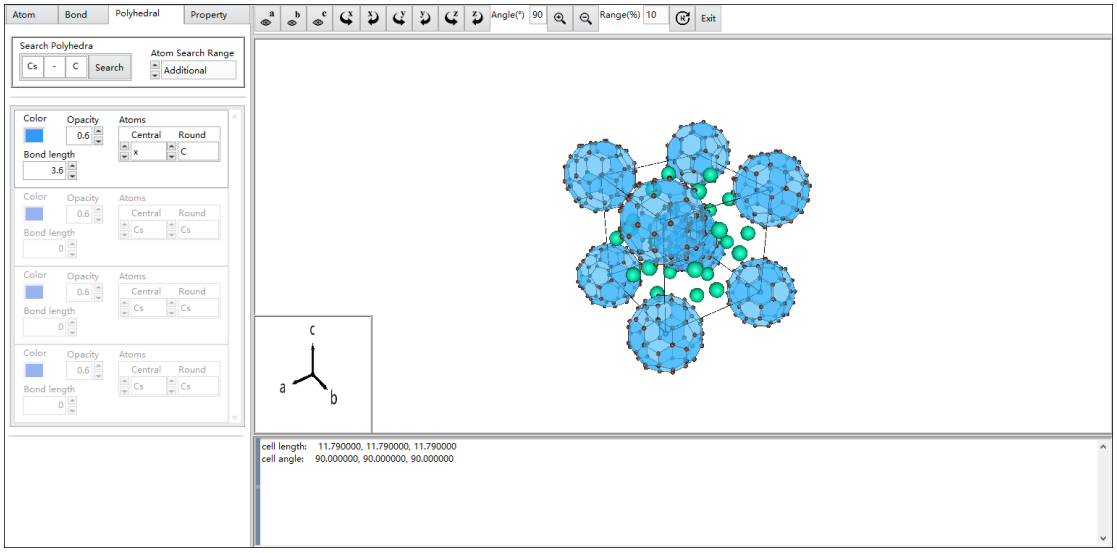
The 2x2x2 and 3x3x3 supercells can be displayed through the Unit Cell option, or revert to the initial single unit cell.

The Projection Mode is used to adjust the projection mode of the structure model and includes two options: Perspective Projection and Orthographic Projection.

The bond color display mode can be adjusted through the Bond Color Mode setting.

6. Example

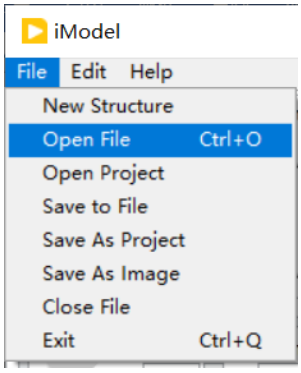
Structure of CSC_{10} with C60 polyhedron



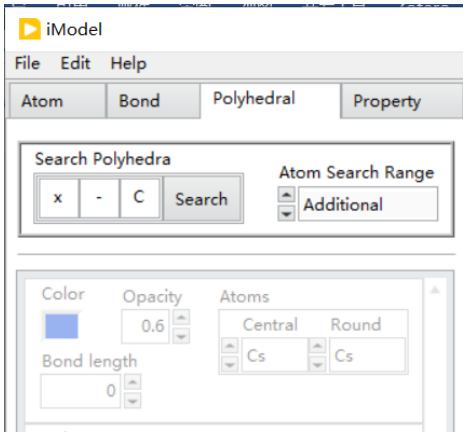
1. Open the CS10.cif file in the “example_files” folder of the program (using a text editor). At the bottom, add a line of data: "x1 H 0.0 0.0 0.0 1 0.0". This will add an H atom named 'x' (or any other name for different types of atoms) at the (0,0,0) position in the crystal structure.

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
Cs1 Cs 0.2781 0 0.5 1 0.0
C3 C 0.0611 0.1978 0.2212 1 0.0
C1 C 0 0.2968 0.0611 1 0.0
C2 C 0.1222 0.0989 0.259 1 0.0
x1 H 0.0 0.0 0.0 1 0.0
```

2. Run the iModel program and click the menu "File-Open File" to open the CS10.cif file from the first step.



3. Click the "Polyhydraulic" tab in the upper left corner to switch to the corresponding page. Click the drop-down box in "Search Polyhedra" and change the Central Atom and Round atom to x and C atoms. Then click the "Search button"



4. In the various attributes of the new polyhedron below, increase the "Bond Length" to 3.6 or above (because the C60 polyhedron of CSC10 recorded in the data file, There is a certain error in the distance between the C atom and the central x atom. The program searches according to the minimum chemical bond length, so the search range of bond length needs to be increased).