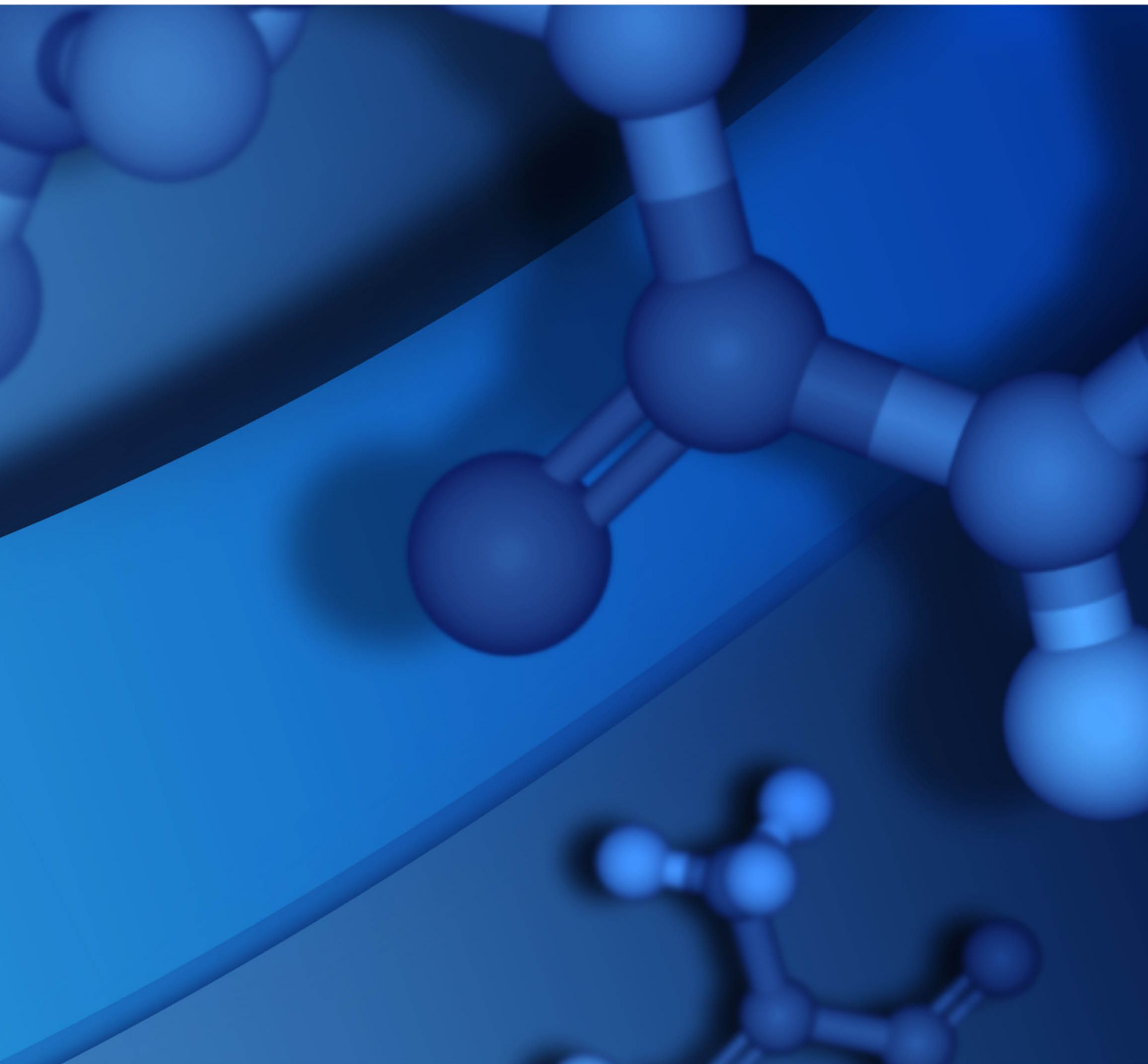


# SKETCHING AND EDITING STRUCTURES GUIDE

MATERIALS VISUALIZER  
8.0



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# Sketching and editing structures

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## Introduction

The following topics and their subtopics provide more details on sketching and general structure building:

- [Starting to sketch](#)
- [Creating atoms and bonds](#)
- [Creating rings](#)
- [Cleaning the structure](#)
- [Adjusting hydrogens](#)
- [Sketching with fragments](#)
- [Changing chemistry](#)
- [Organometallics, coordination complexes, and pi-bonds](#)

For more information on the [structure editing](#) features, the following topics and their subtopics are available:

- [Changing position and orientation](#)
- [Measuring and changing geometry](#)
- [Element Properties](#)
- [Atomic temperature factors](#)
- [Disorder](#)
- [Miller planes](#)

Materials Studio offers a number of features for building, exploring and viewing the symmetry of periodic and nonperiodic structures.

- [Symmetry in Materials Studio](#)
- [Symmetry constraints](#)
- [Tasks in symmetry](#)
- [Theory in symmetry](#)
- [Dialogs in symmetry](#)

## Further Information

For more information about the Materials Studio and other Accelrys software products, visit BIOVIA Support on the Web: <https://community.accelrys.com/index.jspa>

## General sketching

Almost every molecular modeling study begins with the construction of a model structure. A range of different classes of structure may be built and edited in Materials Studio, for example:

- Small molecules
- Macromolecules
- Molecular crystals
- Inorganic crystals
- Surfaces

The sketching tools in the Materials Visualizer allow you to both create new nonperiodic molecular structures and modify existing structures, simply by drawing atoms, bonds, and rings directly onto the structure document. In the case of crystal structures or macromolecules, it may be more convenient to use the crystal building and polymer building features, unless only modest changes to the structures are required.

### Starting to sketch

Prior to sketching, you must first either load a structure into the current project or create a new 3D Atomistic document. If the *Sketch* toolbar is not visible, select *View / Toolbars / Sketch* from the menu bar to display it.

The *Sketch* toolbar contains the following tools:

- *Sketch Atom*
- *Sketch Ring*
- *Sketch Fragment*
- *Measure/Change*
- *Create Centroid*
- *Clean*
- *Adjust Hydrogen*
- *Modify Element*
- *Modify Bond Type*
- *Modify Hybridization*

These tools provide most of the functionality you will need to create and modify structures. Other less commonly modified properties can be modified using the Properties Explorer.

### Sketching strategy

#### Why develop a strategy?

There are a variety of different approaches which can be adopted when constructing a structure, and it is often very useful to develop a strategy to improve the ease and efficacy of this process. There are many factors which might influence the strategy you ultimately adopt, for example:

- How complex is the structure?
- Does the structure contain symmetry or periodicity?
- How many similar structures will you create?
- Are there any common structural features?
- Does a similar structure already exist in a file?
- Is precise structural data available?

It is often wise to initially create a simplified version of the desired structure, then refine and modify it. If many analogous structures are to be generated, it may be prudent to save a template structure to be used as the basis for subsequent modifications.

If atom coordinates are known, you should consider adding the atoms explicitly at these sites, rather than sketching them. This is often the case for crystal structures, where detailed information may be available from crystallographic studies.

### Possible approaches

A few of the many possible approaches include:

- Sketch the basic framework of the structure using carbon atoms and rings, then edit the elements and bond orders as appropriate.
- Add hydrogens to the skeleton framework following completion, so the detail of the underlying structure does not become clouded. Alternatively, the hydrogens can be added during the process of sketching the structure.
- Keep the conformation and topology of the structure as correct as possible while building the structure, or build a topologically correct though distorted structure and then adjust its conformation later.
- Sketch small sections of the structure separately, then join the pieces together later.
- Sketch the basic backbone of the structure, then add functional groups from a fragment library.
- Load a similar structure from a file, then modify it.
- Create a library of small template structures. Load the structures, then cut and paste them into the relevant document and join them to create the target structure.

### 3D Sketcher

#### Why 3D ?

When sketching atoms, it is relatively easy to place them in two dimensions, the x and y directions of the plane of the screen. However, there is an infinite possibility of positions available to the third dimension, the z-direction, all of which are equally viable.

Traditional 2D sketching tools rely upon the user providing the basic topology of the structure, then use refinement techniques to convert the structure from 2D to 3D, affording little control over this third dimension. The 3D Sketcher, by utilizing rotatable bonds of fixed length, allows bonded atoms to be more precisely located, giving the user greater flexibility and control over the geometry of their structure. Complex or geometrically ambiguous three dimensional shapes can be easily constructed, for example, a square planar structure versus a tetrahedral, or square pyramidal versus trigonal bipyramidal.

#### Atom Sketcher, Ring Sketcher and Fragment Sketcher

The 3D Sketcher is comprised of three different tool modes - *Atom Sketcher*, *Ring Sketcher* and *Fragment Sketcher*. These tool modes are accessed by clicking on the relevant button in the *Sketch* toolbar.



Activating one of the tool modes changes the behavior of the mouse and certain keyboard keys. The status bar will indicate some of the common functions that are unique to these modes, and the mouse cursor will change to provide further visual cues to the mode of operation.

Though some of the mouse modes will differ from tool to tool, certain default modes are available globally, to allow model reorientation and selection.

The 3D Sketcher allows you to perform a variety of tasks.

The *Atom Sketcher* provides the capability to:

- create new atoms
- move existing atoms to different positions
- insert atoms into bonds
- create new bonds
- modify bond orders
- fuse atoms together to create a single atom
- replace an element with a different element

The *Ring Sketcher* allows you to:

- create rings in a variety of sizes, including aromatic rings
- fuse rings to atoms, and rotate them
- spiro-fuse rings to bonds, and rotate them

The *Fragment Sketcher* allows you to:

- add fragments to existing structures
- rotate fragments following addition
- fuse two existing fragments in a document, bonding and aligning them
- create new fragments and add them to existing or new (user-defined) libraries

Certain sketching operations are not allowed within periodic structures, such as crystals and surfaces. These operations would either require more precise ability to place atoms in three dimensions, or may be forbidden due to symmetry constraints, for example, attempting to move an atom away from a special position.

## Creating atoms and bonds

The *Atom Sketcher* provides the capability to:

- create new atoms
- move existing atoms to different positions
- insert atoms into bonds
- create new bonds
- modify bond orders
- fuse atoms together to create a single atom
- replace an element with a different element

The following topics include additional information about creating atoms and bonds.

## Sketching atoms and bonds

The simplest procedure for generating models is to draw them in the model window, manually placing atoms, connected by single bonds, at desired positions. The Sketcher can be used to create new structures, or modify existing ones.

## Beginning a sketch

Click the *Sketch Atom* button, and the cursor changes to a pencil shape.



Sketch Atom

Click on an empty spot in the 3D Viewer to begin sketching. An atom of the target element type is placed at the picked location. A pale yellow "virtual atom" with a bond attaching it to the first atom is connected to the cursor, ready to be placed at the click of the mouse.

**Note:** If the 3D Viewer contains a periodic structure such as a crystal, it is not possible to sketch a new structure, since such systems require greater control over placement in the z-direction. Atoms and bonds can, however, be added to existing atoms or bonds in the structure, subject to symmetry constraints.

## Placing subsequent atoms

The virtual atom represents the location of a subsequent atom. Moving the cursor about the 3D Viewer window will cause the virtual atom to track its movement. The bond to this atom is of fixed length, and the virtual atom is actually rotating about its bonded partner. Although the bond appears to shrink, in actuality the atom is being projected out of the plane of the screen, i.e., in the positive screen z-direction. The Sketcher is thus capable of sketching in three dimensions. When the virtual atom is at the desired location, a further click will cause it to be replaced by a real atom. A new virtual atom will be created, bonded to this newly created atom, and the process repeats.

## Placing the atom in the negative z-direction

By default, the virtual atom rotates in the positive z-direction, i.e., out of the plane of the screen. To place an atom behind the plane of the screen, hold down the ALT key and drag the mouse. Releasing the ALT key will cause the atom to shift to the positive direction once more.

## Modifying the default bond length

The default bond length is calculated as the sum of the covalent radii of the atoms involved in the bond. Hold down SHIFT + ALT, dragging the mouse to change the bond length. The bond length is reported in the status bar.

## Ending the sketching operation

Double-click to place one last atom and stop sketching. Or press ESC to cancel the sketching operation without placing another atom. The sketching operation is also canceled if the window loses focus, if a different window is picked, or if a command button is pressed.

## Sketching onto an existing atom

To sketch onto an existing atom, simply move the cursor over the target atom. The target atom changes color as the cursor passes over it. Click on the atom and a virtual atom appears, bonded to the existing atom. Proceed exactly as with a new structure.

## Inserting an atom into a bond

To insert an atom into a bond, move the cursor over the target bond. The target bond changes color as the cursor passes over it. Hold down the ALT key and click to insert an atom into the bond.

## Creating an isolated atom

To create an isolated atom, hold down the ALT key and click on an empty portion of the screen, or place the first atom then press ESC to cancel the sketching operation.

## Deleting atoms

To delete atoms, select the atoms and press the DELETE key.

## Creating a bond between two atoms

To create a bond between two existing atoms, sketch onto the first atom [as described above](#). As you move the cursor over the second atom, the virtual atom will "snap" to its coordinates. Click on the second atom to create the bond. If the cursor is moved away from the second atom before the bond is created, the virtual atom will return to its normal location.

## Changing the bond order of an individual bond

To change the bond order of an individual bond, move the cursor over the target bond and click. The bond is highlighted as the cursor passes over it. Bond order is incremented through the cycle: single to double to triple. If many bonds need to be changed, or if more complex bond orders are required, use the [bond editing commands](#).

## Changing the element type of an individual atom

To change the element type of an existing atom, move the cursor over the target atom, hold down the ALT key and click. If you need to change the element type of many atoms, or if Materials Studio is not in Sketcher mode, it is easier to use the [atom editing commands](#).

## Changing the position of an individual atom

To move an atom within the plane of the screen, position the cursor over the target atom, highlighting the atom. Hold down the left mouse button and drag the mouse. The cursor changes to the shape of a hand after the atom has been moved a short distance. The atom will track the movement of the cursor. If the atom has hydrogens bonded to it, the positions of the hydrogen atoms will also be reevaluated.

**Note:** If the structure is periodic and has symmetry, the motion of the atom may be constrained by the symmetry of the structure and it may not be possible to move it in the specified direction.

## Fusing atoms

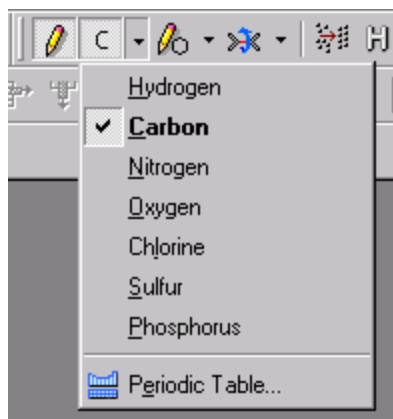
To fuse two atoms into a single atom, click and hold down the left mouse button over the first atom. Move the atom [as described above](#), until it is coincident with the target atom. The second atom's color will change to orange, indicating that the atoms are coincident. Release the left mouse button. The first atom will be fused with the second, i.e., the dragged atom will be deleted, and its bonds recreated with the second atom.

## Status bar

Useful information regarding Sketcher usage is presented in the status bar at the bottom of the Materials Studio frame. Certain diagnostic information may also be presented here.

## Selecting the element type

By default, the *Atom Sketcher* sketches carbon atoms. However any element can be used to sketch. A dropdown list, adjacent to the *Sketch Atom* button, contains a list of the most commonly used elements.



Element used to sketch

If the target element does not appear in this list, it can be selected from the [Periodic Table dialog](#), accessed at the bottom of the element list. When a new target element is selected, its atomic symbol is displayed next to the *Sketch Atom* button.

## Creating rings

The Sketch Ring tool is found on the *Sketch* toolbar.



Sketch Ring

Use the *Sketch Ring* tool to:

- Create rings in a variety of sizes, including aromatic rings
- Fuse rings to atoms, and rotate them
- Spiro-fuse rings to bonds, and rotate them

The following topics have information on working with rings.

## Sketching rings

Many structures, particular organic molecules, have substructures containing rings of varying sizes. The *Ring Sketcher* tool, located on the *Sketch* toolbar, allows rings to be easily created and added to structures. Since the majority of such rings primarily contain carbon, the rings created by the *Ring Sketcher* are composed of carbon atoms. These can easily be replaced by other elements later, if desired.



Sketch Ring

Click on the *Sketch Ring* tool to work in ring sketching mode.

## Creating an isolated ring

To create an isolated ring, click on an empty portion of the 3D Viewer window. A ring of the specified target size will be created.

**Note:** Creation of isolated rings is not possible in periodic symmetry systems, since the z-direction cannot be controlled.

## Creating an isolated aromatic ring

To create an isolated aromatic ring, hold down the ALT key and click on an empty portion of the 3D Viewer window. An aromatic ring of the target size will be created.

## Fusing a ring to an atom

To fuse a ring to an existing atom, move the cursor over the target atom. The target atom changes color as the cursor passes over it. Click on the atom and a ring of the specified target size will be fused to the target atom. The position and orientation of the ring will depend on the hybridization and number of bonds to the atom.

**Note:** It may not be possible to add a ring to certain atoms at special positions in periodic symmetry systems, due to symmetry constraints.

## Fusing an aromatic ring to an atom

To fuse an aromatic ring to an existing atom, move the cursor over the target atom. The target atom changes color as the cursor passes over it. Hold down the ALT key and click on the atom, and an aromatic of the specified target size will be fused to the target atom. The position and orientation of the ring will depend on the hybridization and number of bonds to the atom.

## Rotating a ring fused to an atom

To rotate a ring fused to an atom, position the cursor over the target atom. Hold down the left mouse button (plus the ALT key for an aromatic ring) and a ring will be created fused to the atom. Without releasing the mouse button, drag the mouse until the ring is in the desired orientation. The ring will be rotated about the axis between its center and the target atom.

**Note:** To rotate a ring that already exists in a structure, use the [Measure/Change tool](#) on the *Sketch* toolbar.

## Spiro-fusing a ring to a bond

To spiro-fuse a ring to a bond, position the cursor over the target bond. The target bond changes color as the cursor passes over it. Click on the bond and a ring will be fused to the bond. If the atoms of the ring coincide with any of the atoms of the structure, they will be automatically fused. The diameter and orientation of the ring depend on the bond length, number, position and hybridization of the bond atoms.

**Note:** It may not be possible to add a ring to certain atoms at special positions in periodic symmetry systems, due to symmetry constraints.

## Spiro-fusing an aromatic ring to a bond

To spiro-fuse an aromatic ring to a bond, position the cursor over the target bond. The target bond changes color as the cursor passes over it. Hold down the ALT key and click on the bond. An aromatic ring will be fused to the bond. If the atoms of the ring coincide with any of the atoms of the structure, they will be automatically fused. The diameter and orientation of the ring depend on the bond length, number, position and hybridization of the bond atoms.

## Rotating a ring spiro-fused to a bond

To rotate a ring spiro-fused to an atom, position the cursor over the target atom. Hold down the left mouse button (plus the ALT key for an aromatic ring) and a ring will be created fused to the atom. Without releasing the mouse button, drag the mouse until the ring is in the desired orientation. The ring

will be rotated about the bond vector. If the ring atoms are coincident with any other atoms in the structure, they will be automatically fused.

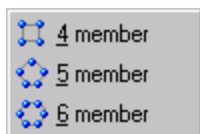
**Note:** To rotate a ring that already exists in a structure, use the *Measure/Change* tool on the *Sketch* toolbar.

## Selecting the ring type

By default, the *Ring Sketcher* creates 6-membered rings, but there are two ways to change the ring type.

### Selecting from the dropdown

The ring size can be changed by selecting the target ring size using the dropdown adjacent to the *Sketch Ring* tool.



Sketch Ring dropdown

Select 4-, 5-, or 6-membered rings. The cursor indicates the current ring size as an additional visual cue.

### Changing the ring size using keyboard accelerators

The ring size can be changed at any time during the sketching operation by pressing the keys 3 through 8 on the main keyboard, when in ring sketching mode. The cursor will change to indicate the current ring size.

**Tip:** The keys on the number keypad will *not* change the size of the ring.

## Cleaning the structure

The structure resulting from initial sketches is usually not chemically reasonable and needs to be "cleaned". In other words, its structure needs to be optimized. Initial optimization can be performed using the *Clean* button on the Sketch toolbar.



Clean

The *Clean* tool operates differently depending on nature of the current 3D model and what is selected.

- When no structure is selected, the geometries of all structures in the current 3D Viewer are cleaned. If multiple structures are present but none are selected, each structure in the view is cleaned in the presence of the other structures.
- If part of a structure is selected then only the selected portion is cleaned.
- *Clean* does not work for periodic systems. You can clean fragments of a crystal by turning the crystal into a nonperiodic superstructure, cleaning the fragments, and rebuilding the crystal.

## Adjusting hydrogens

Building or editing a structure often involves changes that might modify the chemistry of the structure. An element of a particular type may be replaced by a different element, the order of a bond may be changed, or an atom may be hybridized. Such changes may require a re-evaluation of the number of hydrogens bonded to a site; the number of hydrogens may no longer be appropriate, due to a change

in valence or formal charge, for example, or the position of the hydrogens may be incorrect due to changes in hybridization or the local geometry of the neighboring atoms.

The *Adjust Hydrogen* button on the Sketch toolbar provides a convenient mechanism for recalculating the number and positions of hydrogens on selected non-metal atoms.



Adjust Hydrogen

The number of hydrogens is calculated based on several factors:

- Common oxidation state
- Hybridization
- Formal charge
- Number and order of bonds

If the selected non-metal atom has too few hydrogens, additional hydrogens will be added. Existing hydrogens are retained, though their positions may change. If there are too many hydrogens, some of the existing hydrogens will be deleted. Heavy (non-hydrogen) atoms are never deleted.

The hydrogen position is controlled by the [hybridization](#) of the atom, and the number and positions of the heavy atoms to which it is bonded.

**Note:** The *Adjust Hydrogen* tool does not affect metal atoms. Only hydrogens attached to non-metal atoms, i.e., H, He, B, C, N, O, F, Ne, Si, P, S, Cl, Ar, As, Se, Br, Kr, Te, I, Xe, At, Rn, can be re-evaluated using the *Adjust Hydrogen* button.

## Auto-update hydrogen

The *Auto-update hydrogen* command causes hydrogens to be re-evaluated whenever a change to the chemistry of the structure occurs. Changes that will necessitate recalculation of the hydrogens include:

- Changing element
- Modifying bond order
- Deleting atoms
- Breaking or deleting bonds
- Modifying hybridization
- Modifying formal charge
- Creating new bonds
- Fusing atoms
- Moving atoms
- Sketching atoms
- Sketching rings

**Note:** Currently, if properties of atoms and bonds are changed using the Properties Explorer, automatic hydrogen adjustment will not be performed.

## Crystal structures

When modifying hydrogens in a crystal structure, symmetry becomes an important factor. If the non-metal atom is in a special position, it is not currently possible to calculate the hydrogen positions. However, hydrogens can be recalculated for atoms at general symmetry positions.

## Deleting hydrogens

### To delete all hydrogens

1. Double-click on a hydrogen while holding the ALT key to select all the hydrogens.
2. Delete the hydrogens using one of these methods:
  - Press the DELETE key
  - Right-click in the 3D structure document and choose *Delete* from the shortcut menu
  - Select *Edit / Delete* from the menu bar

## Sketching with fragments

The *Sketch Fragment* tool is found on the *Sketch* toolbar.



Sketch Fragment

Use the *Sketch Fragment* tool to:

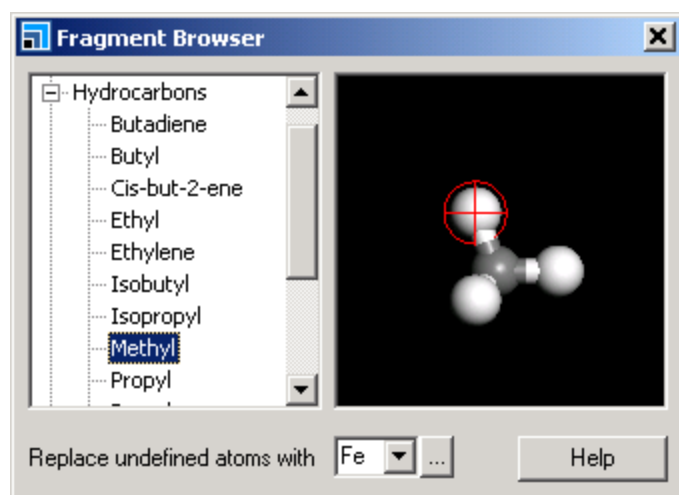
- Add fragments such as functional groups to documents
- Add fragments to existing atoms, and rotate them
- Align and merge two separate molecular fragments in a document
- Create organometallic compounds with pi-bonding schemes

### Selecting the fragment type

By default, the *Fragment Sketcher* sketches using a methyl fragment. The Fragment Browser allows different fragments to be selected.

### Fragment Browser

The Fragment Browser can be accessed by selecting the *Fragment Browser* menu item in the dropdown adjacent to the *Sketch Fragment* tool button.



Fragment Browser

The Fragment Browser consists of a tree view display, containing a list of available fragment libraries, and a fragment viewer.



## Opening a fragment library

A fragment library is opened by either clicking on the + icon adjacent to the library name, or by double-clicking on the library name. The library is similarly closed. To select a fragment within the library, click on the entry using the mouse button. The arrow keys, and alphanumeric short-cuts may also be used to select a fragment. When a fragment has been selected, it will be loaded into the fragment viewer. A red graphical object indicates the connection point. Selecting a new fragment will also cause the currently active view to change to *Fragment Sketch* mode.

## Reorienting the fragment display

The fragment may be zoomed, translated and rotated using the same controls available in the 3D Viewer.

## Changing the fragment connection point

The fragment connection point may be changed by double-clicking on any terminal atom in the fragment. The red graphical object will reflect the current connection point. Reloading the fragment will cause the change to be lost. The original fragment will be restored.

## Replacing undefined atoms

Certain fragments, such as the metal templates, contain undefined atoms. This provides a useful means of providing generic geometric templates which can be used for a variety of different structures. The undefined atoms will be replaced with a user-defined element when added to a structure. This may be selected either using the dropdown menu, or by selecting from the periodic table which is accessed by pressing the ... button.

## Adding fragments to your sketch


Many structures contain standard substructures such as functional groups, rings, or ligands. The *Fragment Sketcher* contains a library of such substructures which may be conveniently bonded to existing structures, without the need for explicitly sketching them atom by atom.



Sketch Fragment


Click on the *Sketch Fragment* tool to work in fragment sketching mode.

### Creating an isolated fragment

1. Select *File* / *New...* / *3D Atomistic* to create an empty 3D Atomistic document.
2. Select  / *Fragment Browser* from the toolbar to open the [Fragment Browser](#).
3. Select the fragment you wish to add from one of the libraries, a view of the highlighted fragment is displayed in the *Fragment Browser*.
4. Click in an empty space in the 3D Atomistic document. A fragment of the specified type will be created.

**Note:** Creation of isolated fragments is not possible in periodic symmetry systems, since the z-direction cannot be controlled.

### Bonding a fragment to an atom

1. Construct a fragment either by sketching with the *Atom Sketcher*, or by importing a saved file.
2. Select  / *Fragment Browser* from the toolbar to open the [Fragment Browser](#).
3. Select the fragment you wish to add from one of the libraries, a view of the highlighted fragment is displayed in the *Fragment Browser*.
4. Move the cursor over the target atom of the structure, which must be either an isolated or terminal atom. The target atom changes color as the cursor passes over it. The position and orientation of the fragment when it is added depends on the hybridization and number of bonds to the atom.

**Note:** It may not be possible to add a fragment to certain atoms at special positions in periodic symmetry systems, due to symmetry constraints.

5. Click on the atom and a fragment of the specified type will appear, fused to the target atom. Without releasing the mouse button, drag the mouse until the fragment is in the desired orientation. The fragment rotates about the axis between its center and the target atom, and a monitor displaying the dihedral angle will be shown.
6. Release the mouse button and the fragment will be fused to the target atom.

**Note:** To rotate a fragment that already exists in a structure, use the [Measure/Change tool](#) on the *Sketch* toolbar.



### Fusing two existing fragments

1. In a document containing two fragments, hold down the ALT key and click on a terminal atom of the first fragment. A small red cage is displayed indicating the position of the connection point.
2. Click on a terminal atom of the target structure. The first fragment will be moved so that it is aligned with the target structure. The red connection point object will be deleted. Holding the mouse button and moving the cursor while forming the connection allows you to rotate the fragment being added to the target.
3. To cancel the fusion operation once the first atom has been selected, press the ESC key.

### Defining Fragments


The *Define Fragment* command is located on the dropdown list adjacent to the *Sketch Fragment* tool on the *Sketcher* toolbar. This opens the [Define Fragment dialog](#) allowing you to define your own custom fragments and libraries, or modify existing fragments and libraries. To access the commands, a document must be currently active in the 3D Viewer.

## Creating a new fragment

1. Construct a fragment either by sketching with the *Atom Sketcher*, or by importing a saved file.
2. Select  / *Define Fragment* from the toolbar to open the [Define Fragment dialog](#).
3. Select a single terminal atom and click the *Define* button to create a connection point object to be created. This is displayed as a red cage. If a connection point is created on anything other than a terminal atom, the fragment will be invalid, and cannot be used for sketching.
4. Select the library to which you wish to add the new fragment, using the *Fragment Library* dropdown list.
5. Type a name for the new fragment into the *Fragment Name* box and click the *Add* button. The new fragment will be added to the selected library.
6. Select  / *Fragment Browser* from the toolbar. The new fragment will be listed in the specified library in the [Fragment Browser](#), and can be used in sketching operations.

The fragment will be saved with its current display style information. If you wish your fragment to be consistent with other fragments in the browser, you should change the display style before adding it to a library.

## Adding a fragment to a new library

1. Construct a fragment either by sketching with the *Atom Sketcher*, or by importing a saved file.
2. Select  / *Define Fragment* from the toolbar to open the [Define Fragment dialog](#).
3. Select a single terminal atom and click the *Define* button to create a connection point object to be created. This is displayed as a red cage. If a connection point is created on anything other than a terminal atom, the fragment will be invalid, and cannot be used for sketching.
4. Enter a name for the new library to which you wish to add the new fragment in the *Fragment Library* text box. Click *Yes* of the dialog asking if you would like to create a new library.
5. Type a name for the new fragment into the *Fragment Name* box and click the *Add* button. The new fragment will be added to the selected library, which can be viewed through the [Fragment Browser](#).

## Define Fragment dialog

The *Define Fragment* dialog can be used to [define](#) your own custom fragments and libraries, or modify existing fragments and libraries. To access the commands, a document must be currently active in the 3D Viewer.

## Connection Point

**Define:** Defines the single selected atom in a molecule in the currently active document to use as the connection point.

## Fragment Definition

**Fragment library:** Select the fragment library to which the fragment should be added. Options include:

- [Amino Acids](#)
- [Functional Groups](#)
- [Halogens](#)
- [Hydrocarbons](#)
- [Ligands](#)
- [Metal Templates](#)
- [Rings](#)
- [User](#) (default)

**Fragment name:** Enter the desired fragment name into the text box, or select a previously defined fragment to be overwritten. The name should not start nor end with a space.

**Add:** Adds the defined fragment to the selected library.

**Help:** Displays the Help topic in a browser.




#### Access methods



## Changing chemistry

The Sketch toolbar provides tools that enable you to create and modify structures. If the *Sketch* toolbar is not visible, select *View / Toolbars / Sketch* from the menu bar to display it.

The following tools on the *Sketch* toolbar allow you to change the chemistry of a structure:

-  Modify Element
-  Modify Bond Type
-  Modify Hybridization

Other less commonly modified chemical properties can be altered using the Properties Explorer.

## Changing element type

### To change element type via the Sketch toolbar

The *Modify Element* tool is found on the *Sketch* toolbar.



Modify Element

1. Select the atom or atoms you wish to edit.
2. Click the *Modify Element* button on the *Sketch* toolbar.
3. Select an element from the list or click on *Periodic Table* for a full listing.

### To change element type via the main menu

1. Select the atom or atoms you wish to edit.
2. Select *Modify | Modify Element* from the menu bar.
3. Select an element from the list or click on *Periodic Table...* for a full listing.

## Changing bond type

### To change the bond type of selected bonds

Use the Modify menu:

1. Choose *Modify | Modify Bond Type* from the menu bar.
2. Select the new bond type from the dropdown list.

Or use the Properties Explorer:

1. If not already open, open the Properties Explorer via *View | Explorers | Properties Explorer*.
2. Double-click on *BondType*.
3. Select the new bond type from the dropdown list.

Or use the *Modify Bond Type* tool on the Sketch toolbar:



Modify Bond Type

- Click on *Modify Bond Type* and select a new bond type from the dropdown list.

Or click on the bond in Sketch Atom mode:

1. If not already in Sketch Atom mode, click the *Sketch Atom* button.
2. Click on the bond one or more times, cycling through single, double and triple bonds.

You can assign the following types to a bond.

- [Single Bond](#)
- [Partial Double Bond](#)
- [Double Bond](#)
- [Triple bond](#)

There is also an option to break the bond.

## Formal charge

Formal charge is a theoretical number assigned to an atom on the basis that all bonds in a molecule are purely covalent. This means that each atom in the bonding pair is assigned one electron from the bond. This is the opposite extreme view of bonding to [oxidation state](#) which assumes 100% ionic character.

Formal charge values are used in typing for forcefield calculations and thereby affect classical simulations.

## Changing formal charge

### To change the formal charge of selected atoms

Either use the [Spin tab](#) of the Electronic Configuration dialog:

1. Make the 3D structure document containing the atom(s) to be modified the active document.
2. Select *Modify | Electronic Configuration* from the menu bar to display the [Electronic Configuration dialog](#).
3. Select the atom(s) for which you wish to alter the formal charge.
4. Enter the formal charge as a real or rational number in the *Formal Charge* field.

or use the Properties Explorer:

1. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
2. Make the 3D structure document containing the atom(s) to be modified the active document and select the atom(s) for which you wish to alter the formal charge.
3. Double-click on *FormalCharge* in the Properties Explorer to display the Edit Formal Charge dialog.
4. Uncheck the *Automatic* checkbox and enter the formal charge as a real or rational number.
5. Click the *OK* button.

**Tip:** If the *Automatic* checkbox is checked on either the Spin or the Edit FormalCharge dialog, Materials Studio will assign a formal charge to the atom on the basis of the typical chemistry of that particular element. This value is automatically updated as the bonding environment of the atom or its element type changes. As new atoms are sketched, they are created in this automatic formal charge assignment state so, under normal circumstances, there will be no need for you to explicitly assign another formal charge value to an atom.

If the *Automatic* checkbox is unchecked and the formal charge on an atom set to a particular value, that value will be fixed and independent of the bonding environment of the atom or any changes to its element type.

## Electronic Configuration

For some calculations more detailed information about electronic states for each ion can be specified. Currently [Formal spin](#), [Hubbard U](#), and [core hole](#) values can be adjusted through the [Electronic Configuration dialog](#).

Creation of core holes leads to excited electronic states, this is indicated in the electronic configuration reported. For example, for oxygen ([He] 2s<sup>2</sup> 2p<sup>5</sup>) creation of a 1s core hole will give the electronic configuration [He\*] 2s<sup>2</sup> 2p<sup>5</sup>.

## Atomic spin

Atomic spin is a measure of the spin, or magnetic moment, of an atom. Materials Studio deals with atom spins in two ways:

- *Formal spin* - This is an integral quantity, summing the spins of relevant electrons associated with an atom. The formal spin can be modified using the [Spin tab](#) of the Electronic Configuration dialog or the Properties Explorer.
- *Spin* - This is a floating point quantity that is set by computational servers, such as CASTEP or DMol<sup>3</sup>, indicating the net spin in the region around each atom. Spin is a read-only quantity and can be viewed using the Properties Explorer.

Typically, the formal spin is set when a structure is being prepared as input for a calculation using, for example, CASTEP or DMol<sup>3</sup>.

Using the ground-state electron configuration and formal charge of an atom, it is possible to predict its electron configuration. This electron configuration can then be used to calculate the magnitudes of the high and low spin states.

The high spin state is defined as the configuration where the spins of all the valence electrons are in parallel, resulting in a spin magnitude of zero or greater. Thus, the high spin magnitude reaches a maximum when a valence sub-shell is half-occupied. Conversely, the low spin state occurs when the spins of all the valence electrons are arranged so as to minimize the net spin, resulting in a spin

magnitude of zero or one. Thus, the low spin magnitude reaches a minimum when a valence sub-shell is either empty or fully occupied.

In order to calculate the high and low spin state magnitudes, a number of assumptions are made:

- High and low spin state magnitudes are calculated assuming that electrons in s and p orbitals do not contribute to the net spin of an atom.
- When deducing the electron configuration of an ion, electrons are removed from the highest energy s and p orbitals first.
- Certain exceptions for the first positive ionization are explicitly treated. Thereafter, second ionizations and beyond are assumed to follow the above rule.
- When permuting electrons to find high or low spin states, they are not moved from their initial orbitals.

The exceptions for the first positive ionization are noted in the following table:

Element	Atomic number	Electron configuration of first positive ionization
Vanadium	23	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^0 3d^4$
Cobalt	27	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^0 3d^8$
Nickel	28	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^0 3d^9$
Yttrium	39	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2$
Lanthanum	57	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^0 4f^0 5d^2$
Cerium	58	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^0 4f^1 5d^2$
Lutetium	71	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14}$
Hafnium	72	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^1$
Actinium	89	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2$
Protactinium	91	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2 5f^2$
Uranium	92	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2 5f^3$

### Changing atomic spin

To change the formal spin of selected atoms, use the [Spin tab](#) of the Electronic Configuration dialog or the Properties Explorer.

#### To use the Spin tab of the Electronic Configuration dialog

1. Make the 3D structure document containing the atom(s) to be modified the active document.
2. Select *Modify / Spins* from the menu bar to display the Spin dialog.
3. Select the atom(s) for which you wish to alter the formal spin. If the selected atoms are of the same element type and have the same electron configuration, the chemical symbol and electron configuration will be shown in the *Element* field and the magnitudes of the high and low spin states will be calculated and displayed in the *High spin* and *Low spin* fields, respectively.
4. Optionally, you can [modify](#) the *Formal Charge* of the selected atom(s).
5. Either choose a spin state for the selected atom(s) from the *Spin state* dropdown list or set the formal spin to the required value using the *Spin* control.
6. If you wish to specify a direction in which the formal spin should be considered, select either [Up](#) or [Down](#) from the *Direction* dropdown list.

**Note:** The *Spin state*, *Spin*, and *Direction* parameters are interdependent (i.e., altering the setting for one could result in the other parameters being updated so that the settings are chemically reasonable).

### To use the Properties Explorer

1. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
2. Make the 3D structure document containing the atom(s) to be modified the active document and select the atom(s) for which you wish to alter the formal spin.
3. Double-click on *FormalSpin* in the Properties Explorer to display the Edit FormalSpin dialog.
4. Enter the formal spin as a real or rational number and click the *OK* button.

### Hubbard U

Hubbard U is a parameter which allows correlation effects to be included in density functional calculations using the LDA+U approach. Materials Studio considers the *Hubbard U* value as a floating point quantity defined per valence orbital (of *s*, *p*, *d*, or *f* type) that is passed to the computational server such as CASTEP and used for electronic structure calculations.

Typically, the default values of Hubbard U are set when a structure is being prepared as input for a calculation, using for example CASTEP, according to the table below.

**Note:** Elements and angular momenta not mentioned here are assigned zero Hubbard U values by default.

Element Name	Atomic number	Angular Momentum	Hubbard U
Sc	21	d	2.5 eV
Ti	22	d	2.5 eV
V	23	d	2.5 eV
Cr	24	d	2.5 eV
Mn	25	d	2.5 eV
Fe	26	d	2.5 eV
Co	27	d	2.5 eV
Ni	28	d	2.5 eV
Cu	29	d	2.5 eV
Y	39	d	2.0 eV
Zr	40	d	2.0 eV
Nb	41	d	2.0 eV
Mo	42	d	2.0 eV
Tc	43	d	2.0 eV
Ru	44	d	2.0 eV



Element Name	Atomic number	Angular Momentum	Hubbard U
Rh	45	d	2.0 eV
Pd	46	d	2.0 eV
Ag	47	d	2.0 eV
Cd	48	d	2.0 eV
La	57	f	6.0 eV
Ce	58	f	6.0 eV
Pr	59	f	6.0 eV
Nd	60	f	6.0 eV
Pm	61	f	6.0 eV
Sm	62	f	6.0 eV
Eu	63	f	6.0 eV
Gd	64	f	6.0 eV
Tb	65	f	6.0 eV
Dy	66	f	6.0 eV
Ho	67	f	6.0 eV
Er	68	f	6.0 eV
Tm	69	f	6.0 eV
Yb	70	f	6.0 eV
Fr	87	f	2.0 eV
Ra	88	f	2.0 eV
Ac	89	f	2.0 eV
Th	90	f	2.0 eV
Pa	91	f	2.0 eV
U	92	f	2.0 eV
Np	93	f	2.0 eV
Pu	94	f	2.0 eV
Am	95	f	2.0 eV
Cm	96	f	2.0 eV
Bk	97	f	2.0 eV
Cf	98	f	2.0 eV

Element Name	Atomic number	Angular Momentum	Hubbard U
Es	99	f	2.0 eV
Fm	100	f	2.0 eV
Md	101	f	2.0 eV
No	102	f	2.0 eV

### Changing Hubbard U values

#### To change the Hubbard U values of selected atoms

1. Make the 3D structure document containing the atom(s) to be modified the active document.
2. Select *Modify | Electronic Configuration* from the menu bar to display the [Hubbard U](#) tab of the [Electronic Configuration dialog](#).
3. In the 3D structure select the atom(s) for which you wish to alter the Hubbard U values. If the selected atoms are of the same element type and have the same electron configuration, the chemical symbol and electron configuration will be shown in the *Element* field and current Hubbard U values will be displayed for all supported angular momenta (*s*, *p*, *d*, and *f*).
4. Change the values to those you require and close the dialog.

### Core Hole

For the vast majority of cases atomic core levels are fully occupied and are chemically inert. However, there are some cases where highly excited electronic states are important. A typical example is core level spectroscopy involving direct excitations of the core levels. To simulate such excited states the concept of the core hole (with an electron missing from one of the core shells) was introduced. Material Studio allows you to create a hole on one of the core levels of any atom, this core hole can then be used in quantum chemical calculations, for example using CASTEP.

### Changing Core Hole values

Creation of core holes leads to excited electronic states, this is indicated in the electronic configuration reported. For example, for oxygen ([He] 2s2 2p5) creation of a 1s core hole will give the electronic configuration [He\*] 2s2 2p5.

#### To change the Core Hole values of a selected atom

1. Make the 3D structure document containing the atom(s) to be modified the active document.
2. Select *Modify | Electronic Configuration* from the menu bar to display the [Core Hole](#) tab of the [Electronic Configuration dialog](#).
3. Select the atom for which you wish to alter the Core Hole parameters. The chemical symbol and electron configuration are shown in the *Element* field.
4. Choose the shell in which you wish to create a core hole from the *Shell* dropdown list.

### Electronic Configuration dialog

The Electronic Configuration dialog contains the following tabs:

- [Spin](#): Allows you to inspect and modify the electron configuration of atoms and groups of atoms.
- [Hubbard U](#): Allows you to view and change the Hubbard U parameter used in LDA+U calculations.
- [Core Hole](#): Allows you to view and alter the core level occupancy.

**Note:** Creation of core holes leads to excited electronic states, this is indicated in the electronic configuration reported. For example, for oxygen ([He] 2s<sup>2</sup> 2p<sup>5</sup>) creation of a 1s core hole will give the electronic configuration [He\*] 2s<sup>2</sup> 2p<sup>5</sup>.

**Help:** Displays the Help topic for the current tab.

### Access methods

Menu *Modify | Electronic Configuration*

### Spin tab

The Spin tab of the Electronic Configuration dialog allows you to inspect the electron configuration and modify the formal charge and spin of atoms and groups of atoms.

**Element:** Displays the chemical symbol and electron configuration, taking into account the formal charge, of the selected atom(s).

**Note:** If multiple element types are selected, no element symbol will be shown. Similarly, if the selected atoms have different electron configurations, the display changes to [multiple configurations](#).

**Formal charge:** Specify the [formal charge](#) of the selected atom(s).

**Automatic:** When checked, indicates that Materials Studio will automatically determine the formal charge of the selected atom(s).

**High spin:** Displays the calculated magnitude of the high spin state of the selected atom(s) based on the electron configuration.

**Low spin:** Displays the calculated magnitude of the low spin state of the selected atom(s) based on the electron configuration.

**Note:** If different high or low spin magnitudes are calculated for the selected atoms, no value will be shown.

**Tip:** The *High spin* and *Low spin* values are automatically updated as the number of unpaired electrons in the outer orbitals of the selected atom(s) changes.

**Spin state:** Select a spin state for the selected atom(s) from the dropdown list. Available options are:

- **High** - Changes the formal spin of the selected atom(s) to the value displayed in the *High spin* field and alters the spin direction, if necessary.
- **Low** - Changes the formal spin of the selected atom(s) to the value displayed in the *Low spin* field and alters the spin direction, if necessary.
- **Undefined** - Resets all the formal spin parameters to the default settings (i.e., no spin direction and a formal spin of zero).
- **Custom** - Leaves the spin parameter settings as they are. This option is automatically selected when the formal spin is changed manually.

**Direction:** Select the direction in which the formal spin should be considered. Available options are:

- **Up** - Positive formal spin.
- **Down** - Negative formal spin.

When a spin direction is specified, the spin state and formal spin are modified accordingly.

**Spin:** Specify the formal spin as the number of unpaired electrons of the selected atom(s). When a formal spin is specified, the spin state is set to **Custom** and the spin direction is modified accordingly.

## Access methods

Menu *Modify | Electronic Configuration | Spin*

### Hubbard U tab

The Hubbard U tab of the Electronic Configuration dialog allows you to inspect and modify the Hubbard U parameter used in LDA+U calculations.

**Element:** Displays the chemical symbol and electron configuration, taking into account the formal charge, of the selected atom(s).

**Note:** If multiple element types are selected, no element symbol will be shown. Similarly, if the selected atoms have different electron configurations, the display changes to [multiple configurations](#).

**s:** Specify a Hubbard U value in eV for the valence s shell.

**p:** Specify a Hubbard U value in eV for the valence p shell.

**d:** Specify a Hubbard U value in eV for the valence d shell.

**f:** Specify a Hubbard U value in eV for the valence f shell.

## Access methods

Menu *Modify | Electronic Configuration | Hubbard U*

### Core Hole tab

The Core Hole tab of the Electronic Configuration dialog allows you to inspect and modify the Core Hole parameters used in core level spectroscopy calculations.

**Element:** Displays the chemical symbol and electron configuration, taking into account the formal charge, of the selected atom(s).

**Note:** If more than one atom is selected the options on the Core Hole tab are not available.

Creation of core holes leads to excited electronic states, this is indicated in the electronic configuration reported. For example, for oxygen ([He] 2s<sup>2</sup> 2p<sup>5</sup>) creation of a 1s core hole will give the electronic configuration [He\*] 2s<sup>2</sup> 2p<sup>5</sup>.

**Shell:** Specify the shell for the electron loss.

## Access methods

Menu *Modify | Electronic Configuration | Core Hole*

### Hybridization

Hybridization describes the process of combining atomic orbitals of different types in order to simplify the description of molecular orbitals in a molecule. For example, the C-H bond in the tetrahedral molecule methane is most simply described in terms of an sp<sup>3</sup> hybrid orbital (a linear combination of s and 3 p orbitals) on C whereas the C-H bond in the linear molecule ethyne is most simply described in terms of an sp hybrid orbital (a linear combination of s and 1 p orbital) on C. The hybridization is thereby connected to the preferred geometry of the bonded atoms.

In Materials Studio, hybridization values are used in typing for forcefield calculations and thereby affect the clean tool and classical simulations.

In Materials Studio you can assign the following hybridizations to an atom.

- None: Unhybridized atomic orbitals
- Sp (Linear), Sp<sup>2</sup> (Trigonal), Sp<sup>3</sup> (Tetrahedral): These involve combinations of an s orbital and (1, 2, or 3 respectively) p orbitals. Typical of non-metal atoms.
- Square planar, Trigonal bipyramidal, Square pyramidal, Octahedral: These hybridizations involve combinations of s, p and d atomic orbitals and are therefore relevant only for transition metal atoms.
- Trigonal prismatic, Trigonal anti-prismatic, Pentagonal bipyramidal, Square anti-prismatic: These hybridizations can only be assigned using the Properties Explorer.
- Auto-detect: The hybridization will be determined based upon the coordination of the atom, or its default assignment.

## Changing hybridization

### To change the hybridization of selected atoms

Use the *Modify* menu:

1. Choose *Modify* / *Modify Hybridization* from the menu bar.
2. Select the new hybridization from the dropdown list.

Or use the Properties Explorer:

1. If not already open, open the Properties Explorer via *View* / *Explorers* / *Properties Explorer*.
2. Double-click on *Hybridization*.
3. Select the new hybridization from the dropdown list.

Or use the *Modify Hybridization* tool on the Sketch toolbar:



Modify Hybridization

1. Click on the triangle next to *Modify Hybridization*.
2. Select the new hybridization from the dropdown list.

You can assign the following hybridizations to an atom:

- None
- Sp (Linear)
- Sp<sup>2</sup> (Trigonal)
- Sp<sup>3</sup> (Tetrahedral)
- Square planar
- Trigonal bipyramidal
- Square pyramidal
- Octahedral
- Trigonal prismatic\*
- Trigonal anti-prismatic\*
- Pentagonal bipyramidal\*
- Square anti-prismatic\*
- Automatic

\* These values can only be assigned using the Properties Explorer.

When you choose *Automatic*, Materials Studio assigns the hybridization of an atom on the basis of the typical chemistry of that element. This value changes automatically as the bonding environment or element type changes. As new atoms are sketched, they are created in this automatic state so under

normal circumstances there will be no need for you to explicitly assign another hybridization value to an atom.

**Note:** When you change an atom's hybridization, the new value is fixed and independent of the atom's bonding environment or changes to the atom's element type.

## Oxidation state

Oxidation states are theoretical numbers assigned on the basis that all bonds in a molecule or fragment are purely ionic. This means that the electrons in each bond are assigned to the most electronegative element in the bonding pair, and the oxidation number is given by [number of valence electrons in the pure atom](#) minus [number of valence electrons in the pseudo-ion](#). This view is the opposite extreme of bonding in [formal charge](#), which assigns charges assuming all bonds are purely covalent.

Oxidation states affect the ionic radius of the atom in Materials Studio.

### Changing oxidation state

#### To change the oxidation state of selected atoms

1. If not already open, open the Properties Explorer via *View | Explorers | Properties Explorer*.
2. Double-click on *OxidationState*.
3. Enter the oxidation state as an integer. Default = 0. Range = -5 to +8.

## Isotopes

An isotope of a given element is defined by its mass number, which is the total number of protons and neutrons in the nucleus. Only a few isotopes are physically stable for each element.

In Materials Studio the mass number affects the mass of the atom. Materials Studio knows about some of the more important isotopes and their masses, in particular for the lighter elements. Note however that any mass number can be assigned to an atom. If the mass number is that of a known isotope, the mass of the element will be the appropriate isotopic mass. If the mass number is not a known isotope the atom will exhibit a mass equal to the mass number.

It is possible to view and edit the list of known isotopes, including adding new isotopes, using the [Element Properties](#) dialog.

### Changing isotope

By default atoms in Materials Studio are considered to be a natural abundance mixture of isotopes for the specific element. This condition is indicated by a value of **No** for the *IsIsotope* property in the Properties Explorer. The *MassNumber* property shows the most common mass number for the element.

#### To change the isotope of selected atoms

1. Open the Properties Explorer by selecting *View | Explorers | Properties Explorer* from the menu bar.
2. Double-click on *MassNumber*.
3. Enter the mass number as an integer.

At this point the *IsIsotope* property should show the value **Yes**.

#### To set selected atoms back to natural abundance

1. Open the Properties Explorer by selecting *View | Explorers | Properties Explorer* from the menu bar.
2. Double-click on *IsIsotope*.
3. Set the value to **No**.

The *MassNumber* property should now show the most common mass number.

**Note:** If an atom is a mixture atom then any changes to the mass number of an atom will apply only to the main component of the mixture.

## Organometallics, coordination complexes, and pi systems

The term "organometallic" describes compounds in which carbon atoms or organic groups are bonded to metal or metalloid atoms. For the more general case of a metal center bonding to inorganic groups, or ligands, the term "coordination complex" is adopted.

In some instances, where an organometallic involves bonding between a metal atom and a ligand containing a resonant or partially filled system of pi-orbitals, it may be more convenient to describe the bonding in terms of a single bond between metal and pi-system rather than as numerous bonds between metal and individual ligand atoms.

In Materials Studio, this case is described by bonding the metal atom to a pi-system object which lies at the center of the non-metal atoms that form the extent of the resonant pi-system. Pi-systems are present in certain libraries provided via the Fragment Browser. Additionally, they are created when importing .msi files that contain Cp dummy atoms.

Note that pi-systems created through the import of an .msi file lie at the location in Cartesian space defined by the file, rather than strictly at the geometric center of the system. This behavior can subsequently be customized using the *HasDynamicPosition* property exposed in the Properties Explorer for pi-systems.


Note that it is not currently possible to create dummy atoms other than by importing an .msi file or using the template libraries. Dummy atoms cannot be created via the Atom Sketcher.

### Building organometallics and coordination complexes

Organometallic compounds, or coordination complexes in general, can be most easily constructed using the *Fragment Sketcher* tool, located on the Sketcher toolbar, and the *Fragment Browser*, accessed via the dropdown menu adjacent to the *Fragment Sketcher* button.

#### Selecting a metal template

The *Fragment Browser* contains several libraries useful for creating and modifying structures. One such library is the "Metal Templates" library, which contains structures in a variety of different coordinations, and geometries. Each structure contains a central, undefined atom, which can be replaced with the element of your choice. To select the template, click on the + icon alongside the Metal Templates library. Select the desired template, which will be displayed in the browser viewer. The *Replace undefined atoms* command lists the element which will be used to replace the unassigned metal center. To select an

element, either select from the dropdown list, or click the  button to display a periodic table, from which the element can be selected. By default, Fe will be used to replace undefined template atoms. The dropdown list contains elements of the first row transition metals, plus the three most recently selected elements.

Click in empty space in the viewer and the fragment will be placed there, with the central atom appropriately replaced.

#### Adding ligands

The *Fragment Browser* also contains a "Ligands" library which contains many commonly occurring ligand structures. To access this library, click on the + icon next to the library name, or double-click on the library name itself, then select the desired ligand. The ligand's connection point is indicated by a red marker. If desired, this can be changed by double-clicking on any terminal atom.

To bond the ligand to the metal center added above, click on the terminal atom you wish to replace. The terminal atom will be deleted, and the ligand bonded to the metal center.

### **Pi systems**

Several of the ligands, such as the cyclopentadienyl ligand, contain pi-systems. These fragments will be bonded to the metal center via a central pi-bond. It is not advised to change the connection point on these structures, since it may lead to incorrect bonding.

Any of the fragment libraries may be used for such building operations. Further, these building operations are not dependent on order. The previously described procedure could just as easily have been reversed, i.e., a ligand sketched first, then a metal center bonded to it.



## Structure editing

This section describes specialized tools and options that give control over specific aspects of a structure and tend to be less commonly used than the sketching and structure manipulation tools detailed in the [General sketching](#) section.

The advanced building and editing tools allow you to edit element properties that are used in calculations and for displaying structures. You can also automatically calculate bonds, hydrogen bonds, and close contacts using a range of criteria and options. The effects of thermal vibrations can be simulated using temperature factors and disorder can be introduced into crystal structures by defining mixture atoms and partial atomic occupancy.

### Changing position and orientation

The 3D Movement and 3D Viewer toolbars provide tools that enable you to move and align objects and to align the view with respect to the objects in scope. If the *3D Movement* or *3D Viewer* toolbar is not visible, select *View / Toolbars* and the appropriate toolbar from the menu bar to display it.

**Note:** You can also change the position of atoms and centroids using the Properties Explorer.

The *3D Viewer Recenter* tool on the *3D Viewer* toolbar allows you to recenter the current view or align the current view in relation to selected objects or particles.



3D Viewer Recenter

The following topics and their subtopics provide more details on moving and aligning objects.

### Moving structures

The [Movement dialog](#), accessible via the *Movement* button on the 3D Movement toolbar, allows you to move selected objects by precise regular displacements.



Movement

The *Move To* tool on the *3D Movement* toolbar allows you to move objects to specific locations.



Move To

The following topics provide more details on moving atoms, structures, and other objects in 3D structure documents.

### Changing positions

The positions of groups of selected atoms or beads can be changed, regardless of the currently active tool mode, using various mouse and key combinations.

#### To translate selected particles in the x or y direction

1. Hold down the SHIFT key and middle mouse button.
2. Without releasing the mouse button or the SHIFT key, drag the particles to the desired location.

or:

1. Hold down the SHIFT and ALT keys and the right mouse button.
2. Without releasing the mouse button or the SHIFT and ALT keys, drag the particles to the desired location.

**or:**

1. Hold down the SHIFT and ALT keys.
2. Without releasing the SHIFT and ALT keys, use the cursor arrow keys to move the selected particles to the desired location.

#### **To translate selected particles in the z direction**

1. Hold down the SHIFT and Z keys and the middle mouse button.
2. Without releasing the mouse button or the SHIFT and Z keys, drag the particles to the desired location.

**or:**

1. Hold down the SHIFT, ALT, and Z keys and the right mouse button.
2. Without releasing the mouse button or the SHIFT, ALT, and Z keys, drag the particles to the desired location.

#### **To rotate selected particles about their center in x and y**

1. Hold down the SHIFT key and the right mouse button.
2. Without releasing the mouse button or the SHIFT key, drag the mouse near the view center to rotate the selected particles.

**or:**

1. Hold down the SHIFT key.
2. Without releasing the SHIFT key, use the cursor arrow keys to rotate the selected particles.

#### **To rotate selected particles about their center in z**

1. Hold down the SHIFT and Z keys and the right mouse button.
2. Without releasing the mouse button or the SHIFT key, drag the mouse near the view edge to rotate the selected particles.

#### **To set the coordinates of a selected atom or bead**

1. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
2. Set the *Filter* on the Properties Explorer to [Atom](#) or [Bead](#) using the dropdown list.
3. Double-click on XYZ in the Properties Explorer to display the Edit XYZ dialog.
4. Enter the required coordinates in the appropriate fields on the dialog, then click the *OK* button.

**Note:** In structures possessing symmetry, it may not be possible to set the coordinates to the values specified due to symmetry constraints. In such cases, Materials Studio will attempt to modify the coordinates to values consistent with the symmetry of the structure.

### **Using Move To mode to place fragments**

You can move objects to a specific location using the *Move To* tool on the 3D Movement toolbar.



Move To

The *Move To* tool can be used to move fragments. For example, you can:

- Move a [centroid](#) defined on a fragment to a centroid defined by a pore boundary, thus centering the fragment in the pore.
- Move a fragment atom to a centroid defined by a pore boundary, thus centering the atom in the pore.
- Move a centroid defined on an open cage structure to an atom, thus centering the cage around the atom.
- Move a fragment atom in one physical system to an atom in another physical system in a 3D Atomistic Collection document, thus aligning the overlaid structures.
- Move a fragment atom or centroid onto a [plane](#) defined on another fragment, thus lining up the two fragments.
- Move a fragment atom or centroid onto a [line](#) defined on another fragment, thus lining up the two fragments.

### To move an object

1. Click the *Move To* button on the *3D Movement* toolbar to enter Move To mode.
2. Move the cursor over the object you wish to move. When it changes color, left-click with the mouse.
3. Move the cursor over the object at the location you wish to move to. When it changes color, left-click with the mouse.

**Note:** When you use the *Move To* tool on an atom, the whole fragment that the atom is part of moves with the atom to the new location.

In structures possessing symmetry, it may not be possible to move to the specified location due to symmetry constraints. In such cases, a message detailing the nature of the constraint will be displayed in the status bar.

## Movement dialog

The Movement dialog allows selected objects to be moved by precise regular displacements.

### Translation



**Move Left:** Translates selected objects to the left by a fixed amount.



**Move Right:** Translates selected objects to the right by a fixed amount.



**Move Up:** Translates selected objects up the screen by a fixed amount.



**Move Down:** Translates selected objects down the screen by a fixed amount.



**Move In:** Translates selected objects directly away from the viewer by a fixed amount.



**Move Out:** Translates selected objects directly toward the viewer by a fixed amount.

**Distance:** When selected, indicates that displacements will be made in terms of a specific fixed distance. Specify the fixed distance, in structural Å units, in the associated text box.

**Screen:** When selected, indicates that displacements will be made in terms of the view size. Specify the displacement, as a percentage of the view size, in the associated text box.

**Note:** For translations defined as a percentage of the view size, the distance moved is based upon the smallest dimension of the viewer.

## Rotation



**Move Around X:** Rotates selected objects clockwise by a fixed amount around an axis passing through the center of geometry of the fragment and parallel with the screen x-axis.



**Move Around-X:** Rotates selected objects counterclockwise by a fixed amount around an axis passing through the center of geometry of the fragment and parallel with the screen x-axis.



**Move Around Y:** Rotates selected objects clockwise by a fixed amount around an axis passing through the center of geometry of the fragment and parallel with the screen y-axis.



**Move Around-Y:** Rotates selected objects counterclockwise by a fixed amount around an axis passing through the center of geometry of the fragment and parallel with the screen y-axis.



**Move Around Z:** Rotates selected objects clockwise by a fixed amount around an axis passing through the center of geometry of the fragment and parallel with the screen z-axis.



**Move Around-Z:** Rotates selected objects counterclockwise by a fixed amount around an axis passing through the center of geometry of the fragment and parallel with the screen z-axis.

**Angle:** Specify the angular displacement rate, in degrees. Default = 45°.

**Note:** In structures possessing symmetry, it may not be possible to move in the chosen direction due to symmetry constraints. In such cases, Materials Studio will attempt to modify the coordinates to values consistent with the symmetry of the structure.

## Access methods

Toolbar



## Aligning structures

The *Align Onto View* tool on the 3D Movement toolbar allows you to align objects in relation to the current viewing direction.

Using the *Align Onto View* tool you can:

- Align a set of atoms or beads
- Align periodic cell vectors
- Align a best fit line, a best fit plane, or principal axes
- Simultaneously align multiple structures in a 3D Atomistic Collection document

**Note:** In structures possessing symmetry, it may not be possible to align to the specified direction due to symmetry constraints. In such cases, a message detailing the nature of the constraint will be displayed in the status bar.

The *3D Viewer Recenter* tool on the *3D Viewer* toolbar allows you to align the view in relation to selected objects.

## Aligning atoms and beads

You can align selected atoms or beads to the current viewing direction using the *Align Onto View* tool on the 3D Movement toolbar.



Align Onto View

### To align a fragment with the view

1. Select the particles you wish to align.
2. Click the *Align Onto View* button on the *3D Movement* toolbar. The selected particles will be rotated rigidly about their center so that they move into a plane parallel to the screen, with their longest axis lying horizontally across the screen.

### To align a rod-like fragment with the view

1. Select the particles you wish to align.
2. Click on the options arrow associated with the *Align Onto View* tool on the *3D Movement* toolbar and select *Align Left/Right* from the dropdown list. The selected particles will be rotated rigidly about their center so that their longest axis lies horizontally across the view.

### To align a planar fragment with the view

1. Select the particles you wish to align.
2. Click on the options arrow associated with the *Align Onto View* tool on the *3D Movement* toolbar and select *Align With Screen* from the dropdown list. The selected particles will be rotated rigidly about their center so that they move into a plane parallel to the screen.

### To align a rod-like part of a fragment with the view

1. Select the particles you wish to align.
2. [Create a best fit line](#) for the selected particles.
3. Select the best fit line object.
4. Click on the options arrow associated with the *Align Onto View* tool on the *3D Movement* toolbar and select *Align Left/Right* from the dropdown list. The whole fragment will be rotated rigidly about the center of the rod-like part, so that the rod axis lies horizontally across the screen.

### To align a planar part of a fragment with the view

1. Select the particles you wish to align.
2. [Create a best fit plane](#) for the selected particles.
3. Select the best fit plane object.
4. Click on the options arrow associated with the *Align Onto View* tool on the *3D Movement* toolbar and select *Align With Screen* from the dropdown list. The whole fragment will be rotated rigidly about the center of the planar part, so that the plane lies parallel to the screen.

**Note:** When you use the *Align Onto View* tool directly on a selection, the rest of the fragment is neither considered nor affected. The selected part is rotated around its own center to produce the alignment, based upon its own principal axes.

In structures possessing symmetry, it may not be possible to align to the specified direction due to symmetry constraints. In such cases, a message detailing the nature of the constraint will be displayed in the status bar.

## Aligning a periodic lattice

You can align a crystal or surface lattice to the current viewing direction using the *Align Onto View* tool on the 3D Movement toolbar.



Align Onto View

### To align a crystal with the view

1. Select the lattice of the crystal you wish to align.
2. Click the *Align Onto View* button on the *3D Movement* toolbar. The lattice will be rotated so that the a-axis lies horizontally and runs from left to right across the screen, with the  $c^*$  reciprocal vector pointing in the direction of the view.

### To align a cleaved surface with the view

1. Select the lattice of the surface you wish to align.
2. Click the *Align Onto View* button on the *3D Movement* toolbar. The lattice will be rotated so that the u-axis lies horizontally and runs from left to right across the screen, with the plane of the surface parallel to the screen.

### To realign a crystal according to one of its planar fragments

1. Select the atoms you wish to align.
2. Additionally, select the lattice of the crystal by holding the SHIFT key and clicking on the lattice.
3. Click on the options arrow associated with the *Align Onto View* tool on the *3D Movement* toolbar and select *Align With Screen* from the dropdown list. The lattice will be rotated so that the planar fragment moves into a plane parallel to the screen. The bulk crystal will remain otherwise unaffected.

## Aligning structures in a collection document

You can simultaneously align multiple structures to the current viewing direction using the *Align Onto View* tool on the 3D Movement toolbar.



Align Onto View

### To align all physical systems with the view

1. Make the 3D Atomistic Collection document containing the physical systems to be aligned the active document and press CTRL + A to select all the physical systems in the document.
2. Click the *Align Onto View* button on the *3D Movement* toolbar. The atoms in each physical system will be rotated independently about their centers so that they each move into a plane parallel to the screen, with their longest axes lying along the screen x direction.

### To align a rod-like feature common to multiple fragments with the view

1. Create a pattern document containing a fragment with the rod-like feature that you wish to align to and select all the atoms that comprise this rod-like feature (i.e., not all the atoms in the entire fragment).
2. [Create a best fit line](#) for the selected atoms.
3. Select the best fit line object.
4. Choose *Edit / Find Patterns* from the menu bar to display the Find Patterns dialog. Click on *Pattern document* and select the pattern document from the dropdown tree view of the current project.
5. Make the 3D Atomistic Collection document containing the physical systems to be aligned the active document and click the *Find* button on the Find Patterns dialog.
6. Providing that only one pattern match was found in each physical system, click on the options arrow associated with the *Align Onto View* tool on the *3D Movement* toolbar and select *Align Left/Right* from the dropdown list. The whole fragment in each physical system will be rotated independently about the center of the rod-like part, so that the rod axis lies along the screen x direction.

## Measuring and changing geometry

The Sketch toolbar provides tools that enable you to measure and change the geometry of structures. If the *Sketch* toolbar is not visible, select *View / Toolbars / Sketch* from the menu bar to display it.

### Using Measure/Change mode to adjust geometry

The *Measure/Change* tool on the Sketch toolbar allows you to measure and alter distances, angles, and torsions for atoms, bonds, beads, bead connectors, hydrogen bonds, and close contacts.

Monitors on distances, angles, and torsions can be deleted in much the same way as other objects in 3D structure documents.

#### To delete measurements

1. Select the measurement you wish to delete. While in a tool mode (such as the *Measure/Change* tool mode), you can select objects by using one of the special mouse actions (for example, CTRL + left-click for single selection or ALT + left double-click to select all objects of a given type). Measurements can be selected by clicking on the label or on one of the solid lines comprising the monitor.
2. Delete the restraint using one of these methods:
  - Press the DELETE key
  - Right-click in the 3D structure document and choose *Delete* from the shortcut menu
  - Select *Edit / Delete* from the menu bar.

If you have a lot of measurements defined, you may not wish to see all of them at the same time. You can hide measurements or their numeric labels using the controls on the Measurement tab of the Display Style dialog.

#### To control the visibility of measurements and measurement labels

1. Make the 3D structure document containing the measurement(s) to be modified the active document and select the measurement(s)/measurement label(s) that you wish to hide.
2. Right-click in the active document and select *Display Style* from the shortcut menu to display the Display Style dialog.
3. Select the *Measurement* tab.
4. To make selected measurement(s) invisible, select *None* in the *Display style* section. To make selected measurement label(s) invisible, uncheck the *Label measurement* checkbox.

## Measuring distances

You can measure bond, hydrogen bond and bead connector lengths, close contact distances, or the distance between any two atoms or beads using the *Measure/Change Distance* tool on the Sketch toolbar.



Measure/Change Distance

### To measure bond or bead connector lengths

1. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Distance* from the dropdown list to enter Measure/Change Distance mode.
2. Move the cursor over the bond or bead connector whose length you wish to measure and when the connector changes color, click on it. A dashed line appears on top of the linkage and a label indicating the bond or bead connector length, in Å, is shown.

### To measure hydrogen bond lengths

1. Use the Calculate Hydrogen Bonds tool on the *Atoms & Bonds* toolbar to generate and display hydrogen bonds in a 3D periodic structure.
2. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Distance* from the dropdown list to enter Measure/Change Distance mode.
3. Move the cursor over the hydrogen bond whose length you wish to measure and when the bond changes color, click on it. A dashed line appears on top of the hydrogen bond and a label indicating the bond length, in Å, is shown.

### To measure close contact distances

1. Use the Calculate Close Contacts tool on the *Atoms & Bonds* toolbar to generate and display close contacts.
2. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Distance* from the dropdown list to enter Measure/Change Distance mode.
3. Move the cursor over the close contact whose length you wish to measure and when it changes color, click on it. A dashed line appears on top of the close contact and a label indicating the contact length, in Å, is shown.

### To measure arbitrary distances between points

1. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Distance* from the dropdown list to enter Measure/Change Distance mode.
2. Move the cursor over the first atom or bead and when it changes color, click on it.
3. Click on the second atom or bead. A dashed line appears between the two and a label indicating the distance, in Å, is shown.

### To measure arbitrary distances from a plane

1. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Distance* from the dropdown list to enter Measure/Change Distance mode.
2. Move the cursor over the plane and when it changes color, click on it.
3. Click on a second object, defining a point. A dashed line appears between the two and a label indicating the distance, in Å, is shown. The projection of the point onto the plane is also shown.

## Measuring angles

You can measure angles between any three atoms or beads using the *Measure/Change Angle* tool on the Sketch toolbar.





#### Measure/Change Angle

##### To measure angles

1. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Angle* from the dropdown list to enter Measure/Change Angle mode.
2. Move the cursor over the first atom or bead and when it changes color, click on it.
3. Click on the second atom or bead and then the third. Dashed lines appear between the three centers and the angle is indicated by an arc. A label giving the magnitude (0 - 180°) of the angle in degrees is shown.

##### To measure arbitrary angles between planes

1. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Angle* from the dropdown list to enter Measure/Change Angle mode.
2. Move the cursor over the first plane and when it changes color, click on it.
3. Click on the second plane. Dashed lines appear indicating the directions of the planes and the angle is indicated by an arc. A label giving the magnitude (0 - 90°) of the angle in degrees is shown.

#### Measuring torsions

You can measure bond torsion angles and dihedral angles between any four atoms or beads using the *Measure/Change Torsion* tool on the Sketch toolbar.



#### Measure/Change Torsion

##### To measure bond torsion angles

1. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Torsion* from the dropdown list to enter Measure/Change Torsion mode.
2. Move the cursor over the bond or bead connector whose torsion angle you wish to measure and when the linkage changes color, click on it.
3. The *Measure/Change* tool will arbitrarily pick two additional particles that are bonded to the atoms or beads at either end of the selected linkage to create the torsion measurement. Dashed lines appear on top of the linkages connecting the four particles and the torsion angle is indicated by three solid lines. A label giving the magnitude (-180 - +180°) of the torsion angle in degrees is shown.

##### To measure arbitrary dihedral angles

1. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Torsion* from the dropdown list to enter Measure/Change Torsion mode.
2. Move the cursor over the first atom or bead and when it changes color, click on it.
3. Click on the second atom or bead, then the third, and then the fourth. Dashed lines appear between the four particles and the dihedral (torsion) angle defined by these centers is indicated by three solid lines. A label giving the magnitude (-180 - +180°) of the dihedral angle in degrees is shown.

#### Changing distances

You can dynamically adjust bond and hydrogen bond lengths, close contact distances, or the distance between any two atoms or beads using the *Measure/Change Distance* tool on the Sketch toolbar. A distance monitor must be created before a bond length or distance can be altered.



#### Measure/Change Distance

### To change a bond or bead connector length or distance

1. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Distance* from the dropdown list to enter Measure/Change Distance mode.
2. If one is not already present, [create a distance monitor](#) on the bond or distance you wish to change.
3. Click on the distance monitor to make it active. The currently active monitor is colored red. If you are in a Measure/Change mode other than the Distance mode, the mode will automatically change to the Measure/Change Distance mode.
4. With the distance monitor active and the mouse pointer in empty space, click and hold the left mouse button and drag the mouse up or to the right to increase the length of the bond or bead connector or distance; drag down or left to decrease it. If the monitor is constrained by geometry or symmetry, the cursor will change to a 'forbidden' sign and a message detailing the nature of the constraint will be displayed in the status bar.

**Tip:** You can invert the motion of the monitor (i.e., the opposite particles will move) by pressing and holding the ALT key when dragging the mouse. Releasing the ALT key while dragging restores the original behavior.

### To set a bond or bead connector length or distance to a precise value

1. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
2. If one is not already present, [create a distance monitor](#) on the bond or distance you wish to change.
3. Select the distance that you wish to alter by pressing and holding the CTRL key and clicking on the monitor.

**Note:** Monitors are colored yellow upon selection. This is NOT the same as making a monitor active, in which case it is colored red and can be dynamically altered using the mouse. Even when selected, an active monitor also remains active, although its color will be changed. Upon deselection, the original red color is restored. Only a single monitor can ever be active at any given time, while multiple monitors can be selected simultaneously.

4. Set the *Filter* on the Properties Explorer to *Distance* using the dropdown list.
5. Double-click on *Distance* in the Properties Explorer to display the Edit Distance dialog.
6. Enter the required distance and click the *OK* button.

**Note:** In structures possessing symmetry, or if the distance corresponds to a bond within a ring, it may not be possible to set the distance to the value specified due to constraints. In such cases, the distance will not be changed.

**Tip:** You can also adjust a monitor for a [distance from a plane](#).

### Changing angles

You can dynamically adjust angles between any three atoms or beads using the *Measure/Change Angle* tool on the *Sketch* toolbar. An angle monitor must be created before an angle can be altered.



Measure/Change Angle

### To change an angle

1. Click on the options arrow associated with the *Measure/Change* tool on the *Sketch* toolbar and select *Angle* from the dropdown list to enter Measure/Change Angle mode.
2. If one is not already present, [create a monitor](#) on the angle you wish to change.
3. Click on the angle monitor to make it active. The currently active monitor is colored red. If you are in a Measure/Change mode other than the Angle mode, the mode will automatically change to the Measure/Change Angle mode.
4. With the angle monitor active and the mouse pointer in empty space, click and hold the left mouse button and drag the mouse up or to the right to increase the angle; drag down or left to decrease it. If the monitor is constrained by geometry or symmetry, the cursor will change to a 'forbidden' sign and a message detailing the nature of the constraint will be displayed in the status bar.

**Tip:** You can invert the motion of the monitor (i.e., the opposite particles will move) by pressing and holding the ALT key when dragging the mouse. Releasing the ALT key while dragging restores the original behavior.

### To set an angle to a precise value

1. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
2. If one is not already present, [create a monitor](#) on the angle you wish to change.
3. Select the angle that you wish to alter by pressing and holding the CTRL key and clicking on the monitor.

**Note:** Monitors are colored yellow upon selection. This is NOT the same as making a monitor active, in which case it is colored red and can be dynamically altered using the mouse. Even when selected, an active monitor also remains active, although its color will be changed. Upon deselection, the original red color is restored. Only a single monitor can ever be active at any given time, while multiple monitors can be selected simultaneously.

4. Set the *Filter* on the Properties Explorer to [Angle](#) using the dropdown list.
5. Double-click on *Angle* in the Properties Explorer to display the Edit Angle dialog.
6. Enter the required angle and click the *OK* button.

**Note:** In structures possessing symmetry, or if the angle forms part of a ring, it may not be possible to set the angle to the value specified due to constraints. In such cases, the angle will not be changed.

**Tip:** You can also adjust a monitor for an [angle between planes](#).

### Changing torsions

You can dynamically adjust bond torsion angles and dihedral angles between any four atoms or beads using the *Measure/Change Torsion* tool on the *Sketch* toolbar. A torsion monitor must be created before a torsion angle can be altered.



Measure/Change Torsion

### To change a torsion angle

1. Click the *Measure/Change* arrow on the *Sketch* toolbar and select *Torsion* from the dropdown list to enter Measure/Change Torsion mode.
2. If one is not already present, [create a torsion monitor](#) on the angle you wish to change.
3. Click on the torsion monitor to make it active. The currently active monitor is colored red. If you are in a Measure/Change mode other than the Torsion mode, the mode will automatically change to the Measure/Change Torsion mode.
4. With the torsion monitor active and the mouse pointer in empty space, click and hold the left mouse button and drag the mouse up or to the right to increase the torsion angle; drag down or left to decrease it. If the monitor is constrained by geometry or symmetry, the cursor will change to a 'forbidden' sign and a message detailing the nature of the constraint will be displayed in the status bar.

**Tip:** You can invert the motion of the monitor (i.e., the opposite particles will move) by pressing and holding the ALT key when dragging the mouse. Releasing the ALT key while dragging restores the original behavior.

### To set a torsion angle to a precise value

1. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
2. If one is not already present, [create a torsion monitor](#) on the angle you wish to change.
3. Select the torsion angle that you wish to alter by pressing and holding the CTRL key and clicking on the monitor.

**Note:** Monitors are colored yellow upon selection. This is NOT the same as making a monitor active, in which case it is colored red and can be dynamically altered using the mouse. Even when selected, an active monitor also remains active, although its color will be changed. Upon deselection, the original red color is restored. Only a single monitor can ever be active at any given time, while multiple monitors can be selected simultaneously.

4. Set the *Filter* on the Properties Explorer to *Torsion* using the dropdown list.
5. Double-click on *Angle* in the Properties Explorer to display the Edit Angle dialog.
6. Enter the required torsion angle and click the *OK* button.

**Note:** In structures possessing symmetry, or if the torsion angle forms part of a ring, it may not be possible to set the torsion to the value specified due to constraints. In such cases, the torsion will not be changed.

### Measuring averaged geometries

The *Create Centroid* tool on the Sketch toolbar allows you to create various measurements that describe the averaged geometry of a structure or set of atoms or beads.

The centroid is defined as the average of the position vectors of the selected particles - that is, atoms or beads. The best fit line and plane are defined as a line/plane where the (mass weighted) root mean square distances from the line/plane to the selected particles are minimized. The principal axes are defined as a set of axes for which the inertial tensor is diagonal. Each axis is displayed scaled by the corresponding principal moment.

**Note:** When any of the above averaged geometry measurements is created, it is defined in terms of a mass-weighted average of the particle coordinates. You may switch to a geometric average by setting the *IsWeighted* property of the measurement using the Properties Explorer.

Averaged geometry measurements can be deleted in much the same way as other objects in 3D structure documents.

### To delete averaged geometry measurements

1. Select the averaged geometry measurement you wish to delete. Averaged geometry measurements can be selected by clicking on the label or on one of the lines or planes comprising the measurement.
2. Delete the restraint using one of these methods:
  - Press the DELETE key
  - Right-click in the 3D structure document and choose *Delete* from the shortcut menu
  - Select *Edit / Delete* from the menu bar.

**Note:** An averaged geometry measurement is automatically deleted when any of the particles defining its position are deleted.

### Creating centroids

You can create a centroid object marking either the center of mass or the geometric center of a set of atoms or beads using the *Create Centroid* tool on the Sketch toolbar. The centroid is defined as the average of the position vectors of the selected atoms or beads. By default, the coordinates are weighted by the mass of the particle, but you can also choose a purely geometric average.



Centroid

A centroid object can be used as an aid in measuring or modifying a structure. For example, you can:

- View or specify the position of a centroid by setting the *CentroidXYZ* property (and also the *FractionalXYZ* property for periodic structures) using the Properties Explorer.
- Use the [Measure/Change](#) tool to create distance, angle, and torsion measurements between centroids or between particles and centroids.
- Use the [Move To](#) tool to move a centroid or to move particles to a position defined by a centroid.

**Note:** When the position of a centroid is modified, the coordinates of the particles used to define the centroid and all other particles in the same fragment are shifted rigidly.

### To create a centroid

1. Select the atoms or beads for which you wish to create the centroid.
2. Click the *Create Centroid* button on the *Sketch* toolbar or click on the options arrow associated with the *Create Centroid* tool and select *Centroid* from the dropdown list. The centroid is shown as a sphere and dashed lines appear between the selected particles and the centroid object.

**Note:** For 3D periodic systems, the creation of a centroid may cause not only the desired centroid to be displayed, but also periodic images. Similarly, for systems which exhibit symmetry, creating a centroid may cause symmetric images of the centroid to be displayed. Occasionally, the display of periodic or symmetric centroid images can be excessive. This can be addressed by selecting (CTRL + left-click) the centroid images that you do not wish to see and setting the *IsVisible* property to **No** using the Properties Explorer.

When a centroid is created, it is defined in terms of a mass-weighted average of the particle coordinates. You can switch to a geometric average using the Properties Explorer.

#### To switch to a geometric average for a centroid

1. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
2. Make the 3D structure document containing the centroid to be modified the active document and select the centroid that you wish to recalculate.
3. Set the *Filter* on the Properties Explorer to **Centroid** using the dropdown list.
4. Double-click on *IsWeighted* in the Properties Explorer to display the Edit *IsWeighted* dialog.
5. Select **No / False** and click the **OK** button to recalculate the selected centroid using the geometric average.

#### Creating best fit lines

You can create a best fit line object for a set of atoms or beads using the *Best Fit Line* option on the dropdown list associated with the *Create Centroid* button on the Sketch toolbar. The best fit line is defined as a line where the (mass weighted) root mean square distances from the line to the selected particles are minimized.



Best Fit Line

A best fit line object can be used as an aid in visualizing or modifying a structure. For example, you can:

- Use the [Movement dialog](#) and associated tools on the 3D Movement toolbar to modify the position and orientation of a best fit line and its associated particles.
- Use the [Align Onto View](#) tool to align a best fit line and its associated particles with the view.

**Note:** When the position or orientation of a best fit line is modified, the coordinates of the particles used to define the best fit line and all other particles in the same fragment are shifted rigidly.

#### To create a best fit line

1. Select the atoms or bead for which you wish to create the best fit line.
2. Click on the options arrow associated with the *Create Centroid* tool on the *Sketch* toolbar and select *Best Fit Line* from the dropdown list. The best fit line object is shown as a dashed line.

When a best fit line is created, it is defined in terms of a mass-weighted average of the selected particle coordinates. You can switch to a geometric average using the Properties Explorer.

### To switch to a geometric average for a best fit line

1. If the Properties Explorer is not visible, select *View / Explorers / Properties Explorer* from the menu bar to display it.
2. Make the 3D structure document containing the best fit line to be modified the active document and select the line that you wish to recalculate.
3. Set the *Filter* on the Properties Explorer to **Best Fit Line** using the dropdown list.
4. Double-click on *IsWeighted* in the Properties Explorer to display the Edit IsWeighted dialog.
5. Select *No / False* and click the *OK* button to recalculate the selected best fit line using the geometric average.

### Creating best fit planes

You can create a best fit plane object for a set of particles using the *Best Fit Plane* option on the dropdown list associated with the *Create Centroid* button on the Sketch toolbar. The best fit plane is defined as a plane where the (mass weighted) root mean square distances from the plane to the selected atoms or beads are minimized.



Best Fit Plane

A best fit plane object can be used as an aid in visualizing or modifying a structure. For example, you can:

- Use the [Movement dialog](#) and associated tools on the 3D Movement toolbar to modify the position and orientation of a best fit plane and its associated particles.
- Use the [Align Onto View](#) tool to align a best fit plane and its associated atoms with the view.

**Note:** When the position or orientation of a best fit plane is modified, the coordinates of the atoms or beads used to define the best fit plane and all other particles in the same fragment are shifted rigidly.

### To create a best fit plane

1. Select the particles for which you wish to create the best fit plane.
2. Click on the options arrow associated with the *Create Centroid* tool on the *Sketch* toolbar and select *Best Fit Plane* from the dropdown list. The best fit plane object is shown as a semi-transparent surface with an arrow normal to the plane indicating its orientation. The best fit plane object can be selected by clicking on this arrow.

When a best fit plane is created, it is defined in terms of a mass-weighted average of the selected particle coordinates. You can switch to a geometric average using the Properties Explorer.

### To switch to a geometric average for a best fit plane

1. If the Properties Explorer is not visible, select *View / Explorers / Properties Explorer* from the menu bar to display it.
2. Make the 3D structure document containing the best fit plane to be modified the active document and select the plane that you wish to recalculate.
3. Set the *Filter* on the Properties Explorer to **Best Fit Plane** using the dropdown list.
4. Double-click on *IsWeighted* in the Properties Explorer to display the Edit IsWeighted dialog.
5. Select *No / False* and click the *OK* button to recalculate the selected best fit plane using the geometric average.

## Creating principal axes

You can create a principle axes object for a set of particles using the *Principal Axes* option on the dropdown list associated with the *Create Centroid* button on the Sketch toolbar. The principal axes are defined as a set of axes for which the inertial tensor is diagonal. Each axis displayed is scaled by the corresponding principal moment.



Principal Axes

A principal axes object can be used as an aid in visualizing or modifying a structure. For example, you can:

- View or specify the position of principal axes by setting the *CentroidXYZ* property (and also the *FractionalXYZ* property for periodic structures) using the Properties Explorer.
- Use the [Movement dialog](#) and associated tools on the 3D Movement toolbar to modify the position and orientation of principal axes and their associated atoms or beads.
- Use the [Align Onto View](#) tool to align principal axes and their associated particles with the view.

**Note:** When the position or orientation of a principal axes object is modified, the coordinates of the atoms or beads used to define the principal axes and all other particles in the same fragment are shifted rigidly.

### To create principal axes

1. Select the particles for which you wish to create the principal axes.
2. Click on the options arrow associated with the *Create Centroid* tool on the *Sketch* toolbar and select *Principal Axes* from the dropdown list. The principal axes object is shown as two arrows.

**Note:** For 3D periodic systems, the creation of principal axes may cause periodic images of the desired set of principal axes to be displayed. Similarly, for systems that exhibit symmetry, symmetric images of the principal axes may also be displayed. Occasionally, the display of periodic or symmetric images can be excessive. This can be addressed by selecting the images of the principal axes that you do not wish to see, choosing [Principal Axes](#) from the *Filter* dropdown list on the Properties Explorer, and changing the *IsVisible* property setting to [No](#).

When principal axes are created, they are defined in terms of a mass-weighted average of the selected particle coordinates. You can switch to a geometric average using the Properties Explorer.

### To switch to a geometric average for principal axes

1. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
2. Make the 3D structure document containing the principal axes to be modified the active document and select the axes that you wish to recalculate.
3. Set the *Filter* on the Properties Explorer to [Principal Axes](#) using the dropdown list.
4. Double-click on *IsWeighted* in the Properties Explorer to display the Edit *IsWeighted* dialog.
5. Select *No / False* and click the *OK* button to recalculate the selected principal axes using the geometric average.

## Element properties

Each atom in a structure acquires a number of properties from its associated element. Element properties may be edited using the [Element Properties dialog](#), in which case any modifications apply to



the current project.

The editable element properties include the following.

**Color.** An atom typically takes its color from its associated element.

**Radii.** Each element has several radii, including covalent radius, Slater radius, van der Waals (VDW) radius and metallic radius. In addition, ionic radii may be defined for any known oxidation states of an element.

The covalent radius is used in bonding calculations.

The van der Waals radius is used by the *CPK* display style.

**Masses.** For each element, an atomic mass is defined. This corresponds to the averaged mass for the natural abundance of isotopes. In addition, any number of isotopes may be defined for an element. Each isotope has an isotopic mass defined. Typically, the mass of an atom will be this natural abundance mass of the element. However, if an atom has been assigned as a particular isotope, the appropriate isotopic mass will be used.

## Viewing and editing element properties

The Element Properties dialog allows you to view and edit the properties of elements including the display color, the radius, and the mass.

### To edit element properties

1. Choose *Modify | Element Properties* from the menu bar.
2. Select the element you want to edit in the *Element* dropdown list.
3. Modify the properties as desired:
  - To edit the color, click *Color* and select a color from the palette.
  - To edit a radius double-click on it in the *Radii* list, or select it and click the *Edit...* button.
  - To add a new oxidation state with its ionic radius click the *Add...* button.
  - To delete an oxidation state and its radius click the *Delete* button.
  - To edit a mass value double-click on it in the *Masses* list, or select it and click the *Edit...* button.
  - To add a new isotope with its isotope mass click the *Add...* button.
  - To delete an isotope and its mass click the *Delete* button.
4. *Reset* returns the properties of the selected element to their default values.

## The periodic table

Materials Studio handles atomic numbers up to 118, the highest atomic number reported experimentally at the time of writing. For each element the symbols and element names assigned by IUPAC are used. Hence S = sulfur, Al = aluminum. Note that atomic numbers 110-118 have yet to be assigned names and symbols by IUPAC.

More information about the periodic table and about individual elements can be obtained from a number of web sites around the world, for example WebElements Periodic Table (<http://www.webelements.com>).

## Element Properties dialog

The Element Properties dialog allows you to view and edit the properties of elements, including the display color, atomic radii and atomic masses. The values you enter apply to all structures in the current project and any modifications you make will be saved as part of the current project.

**Element:** Displays the specified element's properties and allows you to edit them. To view or edit the properties of an element, enter the element symbol (or its atomic number) in the textbox, select it from

the dropdown list, or select it from the [periodic table](#) by clicking the  button.

**Color:** Specifies the display color for the element. All atoms of this type will appear with the chosen color unless explicitly modified (for example, by using the atom coloring functionality on the Atom tab of the Display Style dialog).

**Radii:** Specifies the radius (in Å) used for the element type in atom bonding calculations. The values of the various atomic radii, including ionic radii for the known oxidation numbers, are listed.

**Edit...:** Opens the [Edit Radius](#) dialog for the selected item.

**Add...:** Opens the [Add Oxidation State](#) dialog.

**Delete:** Removes the selected item from the list of radii.

**Masses:** Displays the natural abundance mass and the isotopic masses (in atomic mass units) of the known isotopes.

**Edit...:** Opens the [Edit Mass](#) dialog for the selected item.

**Add...:** Opens the [Add Isotope](#) dialog.

**Delete:** Removes the selected item from the list of isotopes.

**Reset:** Resets all the element properties for the current element to the default values.

**Help:** Displays the Help topic in a browser.

#### Access methods

Menu	<i>Modify / Element Properties</i>
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#### Edit Radius dialog

The Edit Radius dialog allows you to edit the defined radii of an element as selected on the [Element Properties](#) dialog.

**Radius:** The radius being edited is reported and its value can be changed. Range = 0.0 to 10.0 Å.

**OK:** Updates the settings with any changes and closes the dialog.

**Cancel:** Closes the dialog without updating any settings.

**Help:** Displays the Help topic in a browser.

#### Access methods

Menu	<i>Modify / Element Properties / Edit...</i>
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#### Add Oxidation State dialog

The Add Oxidation State dialog allows you to add further oxidation states to the element selected on the [Element Properties](#) dialog. The radius of the new oxidation state can be defined.

**Oxidation Number:** The oxidation number of the new state being added. This is automatically set to one more than the previous highest state. Both positive and negative oxidation states can be defined.

**Ionic Radius:** The ionic radius of the element when it is in this oxidation state. Range = 0.0 to 10.0 Å.

**OK:** Updates the settings with any changes and closes the dialog.

**Cancel:** Closes the dialog without updating any settings.

**Help:** Displays the Help topic in a browser.

### Access methods

Menu	<i>Modify / Element Properties / Add...</i>
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### Edit Mass dialog

The Edit Mass dialog allows you to edit the mass of the isotope selected on the [Element Properties](#) dialog.

**Element:** The mass of the isotope being edited (in amu). The mass must be a positive value.

**OK:** Updates the settings with any changes and closes the dialog.

**Cancel:** Closes the dialog without updating any settings.

**Help:** Displays the Help topic in a browser.

### Access methods

Menu	<i>Modify / Element Properties / Edit...</i>
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### Add Isotope dialog

The Add Isotope dialog allows you to add further isotopes to the element selected on the [Element Properties](#) dialog. The mass number and exact mass of the isotope can both be specified.

**Mass Number:** The mass number of the new isotope being added. This is automatically set to one more than the previous highest mass.

**Isotope Mass:** Specifies the absolute mass of the isotope in amu. The mass must be a positive value.

**OK:** Updates the settings with any changes and closes the dialog.

**Cancel:** Closes the dialog without updating any settings.

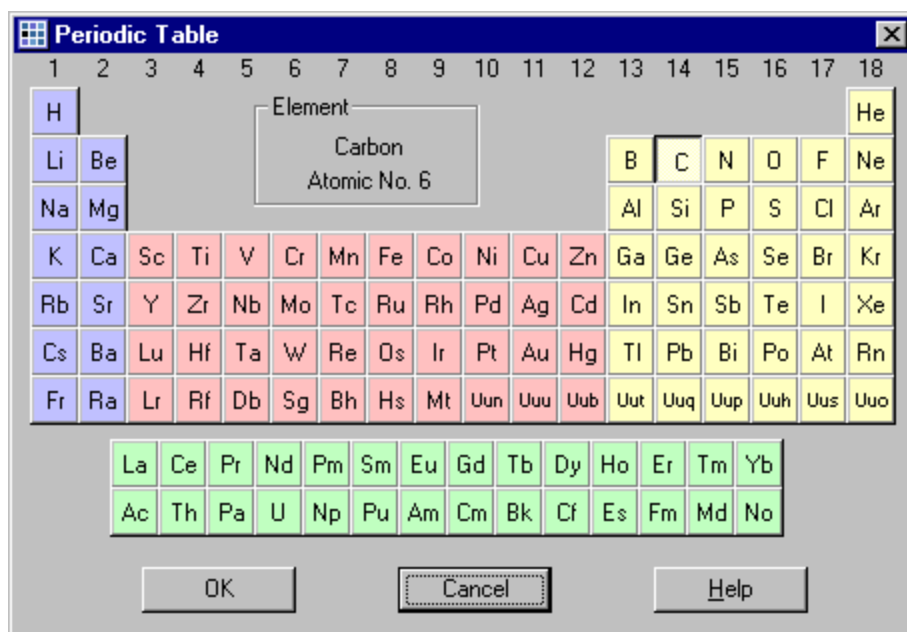
**Help:** Displays the Help topic in a browser.

### Access methods

Menu	<i>Modify / Element Properties / Add...</i>
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### Periodic Table dialog

The Periodic Table dialog allows you to select an element (or in some cases several elements) from the periodic table display.



**[element symbols]:** Click an element symbol to select that element for use.

**Element:** the text displayed here describes the currently selected element by its name and atomic number.

The periodic table is used by several applications in Materials Studio. Depending on the application it may appear in "single select" mode or in "multiple select" mode.

When selecting an element type for sketching or adding atoms, or when changing element type, use the periodic table to select a single element ("single select" mode).


In "multiple select" mode any number of elements may be selected by pressing the CTRL key and clicking to toggle element selection. This mode is used, for example, when editing the Donor-Acceptor list for H-bond calculation.

**OK:** Updates the settings with any changes and closes the dialog.

**Cancel:** Closes the dialog without updating any settings.

**Help:** Displays the Help topic in a browser.

#### Access methods

Menu	<i>Modify   Modify Element   Periodic Table...</i>
Toolbar	 / <i>Periodic Table...</i>

## Atomic temperature factors

Temperature factors are used to represent the effects of individual atomic vibrational motions within a crystal.

### Setting temperature factors

You can use the Properties Explorer to assign isotropic and anisotropic temperature factors to individual atoms in a structure.

### To assign temperature factors

1. Choose *View | Explorers | Properties Explorer* from the menu bar.
2. Select an atom in the structure.
3. In the *Properties Explorer*, double-click on the *Temperature Factors* property to display the Atomic Temperature Factors dialog.
4. Using the option buttons, choose the type of temperature factor that you wish to apply - *Anisotropic*, *Isotropic*, or *None*.
5. Select a unit format from the dropdown list.
6. Enter the value(s) for the temperature factor(s) and click *Apply*. Materials Studio automatically applies any necessary symmetry constraints and the temperature factor values are displayed in the applied units.

**Tip:** You can also specify temperature factors for a structure when you are adding atoms by choosing *Build | Add Atoms*.

### Theory of temperature factors

Atomic vibrations are described in the lowest order by their temperature factors. If the deviation of an atom from its Cartesian equilibrium position is  $\mathbf{r}=(x,y,z)$ , the vibration is characterized by the matrix:

#### Eq. 1 The vibration matrix

$$\mathbf{H} = \begin{bmatrix} \langle x^2 \rangle & \langle xy \rangle & \langle xz \rangle \\ \langle yx \rangle & \langle y^2 \rangle & \langle yz \rangle \\ \langle zx \rangle & \langle zy \rangle & \langle z^2 \rangle \end{bmatrix}$$

Where  $\langle xy \rangle$  represents the average over many vibrations.  $\mathbf{H}$  is symmetric and contains six independent quantities. If the atomic vibration is isotropic, then  $\mathbf{H}$  reduces to the form  $\langle x^2 \rangle \mathbf{I}$  and only one number is required to describe it:

#### Eq. 2 Isotropic vibration

$$\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{\langle r^2 \rangle}{3}$$

### The effects of vibration on x-ray scattering

Temperature factors are commonly used to describe the effect of vibration on X-ray, electron, and neutron scattering. For the first-order amplitude of scattering from an atom at  $\mathbf{q} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$  in reciprocal space, the scattering amplitude is multiplied by:

#### Eq. 3a Isotropic vibration

$$T(\mathbf{q}) = e^{-2\pi^2 \langle x^2 \rangle q^2}$$

#### Eq. 3b Anisotropic vibration

$$T(\mathbf{q}) = e^{-2\pi^2 \mathbf{q}^T \mathbf{H} \mathbf{q}}$$

## Temperature factor conventions

**Eq. 3a** and **3b** are general but not very usable as they depend explicitly on the orientation of the reciprocal lattice vectors in Cartesian space. It is conventional to express temperature factors in an alternative form that are defined relative to the crystal lattice.

If an atom has coordinates  $(x,y,z)$  with respect to the Cartesian axial system and  $(u,v,w)$  with respect to the lattice system so that:

### Eq. 4 Cartesian and fractional coordinates

$$x\hat{i} + y\hat{j} + z\hat{k} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

then  $(x,y,z)$  and  $(u,v,w)$  can be interconverted by multiplying by a matrix  $(x,y,z)^T = \mathbf{A}(u,v,w)^T$  where  $\mathbf{A}=(\mathbf{a}, \mathbf{b}, \mathbf{c})$ . It may be shown that  $\mathbf{A}^{-1}=(\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*)^T$ . This allows **Eq. 3b** to be rewritten:

### Eq. 5 Anisotropic vibration

$$T(\mathbf{q}) = e^{-2\pi^2 \mathbf{q}^T \mathbf{H} \mathbf{q}} = e^{-2\pi^2 (hkl) \mathbf{A}^{-1} \mathbf{M} (\mathbf{A}^{-1})^T (hkl)^T} = e^{-(hkl) \boldsymbol{\beta} (hkl)^T}$$

Thus by expressing the temperature factor as  $\boldsymbol{\beta}=2\pi^2 \mathbf{A}^{-1} \mathbf{H} (\mathbf{A}^{-1})^T$  a temperature factor form is obtained that allows the effect of atomic vibration on scattering to be expressed in terms of the miller index of the reflection only. Other forms for temperature factors are shown in **Table 1** below:

**Table 1. Temperature factor forms**

Temperature factor form	Scattering amplitude multiplied by
$U_{iso} = \langle x^2 \rangle$	$T_{hkl} = e^{\frac{-8\pi^2 U_{iso} \sin^2 \theta}{\lambda^2}}$
$B_{iso} = 8\pi^2 \langle x^2 \rangle$	$T_{hkl} = e^{\frac{-B_{iso} \sin^2 \theta}{\lambda^2}}$
$\beta_{ij} = 2\pi^2 \mathbf{A}^{-1} \mathbf{H} (\mathbf{A}^{-1})^T$	$T_{hkl} = e^{-(\beta_{11}h^2 + 2\beta_{12}hk + 2\beta_{13}hl + \dots)}$
$U_{ij} = \frac{\beta_{ij}}{2\pi^2  \mathbf{a}_i^*   \mathbf{a}_j^* }$	$T_{hkl} = e^{-2\pi^2 (U_{11}h^2 a^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + \dots)}$
$B_{ij} = 8\pi^2 U_{ij}$	$T_{hkl} = e^{-\frac{1}{4}(B_{11}h^2 a^{*2} + 2B_{12}hka^*b^* + 2B_{13}hla^*c^* + \dots)}$

## Thermal ellipsoid scaling

Thermal ellipsoids are scaled using the *Scale factor* on the Temperature Factor tab. A scale factor of **1.0** corresponds to an ellipsoid whose radius in any direction is equal to the *rms* atomic vibration in that direction. The atom actually has a fairly low probability of lying in this ellipsoid.

This table lists other scale factors together with the probability of finding the atom within the ellipsoid.

Scale factor	Probability
1.54	50%
2.02	75%
2.50	90%
2.80	95%
3.37	99%

## Atomic Temperature Factors dialog

You can use the Atomic Temperature Factors dialog to set temperature factors on atoms and groups of atoms. You can choose *None*, *Isotropic*, or *Anisotropic* factors, select a unit format in the list box, and enter appropriate numerical values for the temperature factor(s).

**None/Isotropic/Anisotropic:** Sets the type of temperature factor to be applied. The choice of unit formats and the number of values you can enter depends on the type of factor you select.

**Isotropic/Anisotropic value:** Specifies the numerical value(s) of the temperature factor.

**Units:** Sets the unit format to be used. The temperature factor values are displayed in the applied units.

Option	Unit format	Number of values
Isotropic	U, B	1
Anisotropic	Uij, Bij, $\beta_{ij}$	6

**OK:** Updates the settings with any changes and closes the dialog.

**Apply:** Applies the unit format to the existing temperature factor values. The matrix entered may also be modified so that it obeys the site symmetry of the selected atom(s).

**Cancel:** Closes the dialog without updating any settings.

**Help:** Displays the Help topic in a browser.

### Access methods

Properties Explorer	<i>TemperatureFactor</i>
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## Disorder

Disorder may be introduced into a structure in Materials Studio in one of two ways:

- **Mixture atoms** may be used to simulate the case where one atomic site is randomly occupied by two or more different types of atom. Materials Studio allows you to create mixtures of different elements, oxidation states and isotopes.
- **Atom occupancy** may be used to simulate vacancies which are randomly distributed through a structure.

### Creating and editing mixture atoms

Mixture atoms may be used to simulate the case where one atomic site is randomly occupied by two or more different types of atom. Materials Studio allows you to create mixtures of different elements, oxidation states and isotopes.

### To edit the selected atoms as mixture atoms

1. Choose *View | Explorers | Properties Explorer* and select one or more atoms.
2. Double-click on the *IsMixtureAtom* property to display the Edit Mixture Atom dialog.

### To edit a component of the mixture atom

1. Highlight the appropriate component in the list and click the *Edit* button to display the Edit Mixture Component dialog.
2. To change the element type you may either type the element symbol directly into the box, select an element from the dropdown list, or click the button to display the periodic table.
3. To change the isotope, select the desired mass number from the list of known isotope in the dropdown list. *Natural* refers to the element having an isotopic mixture in naturally occurring abundances.
4. To change the composition, enter a value between 0.0 and 100.0 in the box. Note that the total composition of all components must add up to 100% and so it may be necessary to adjust the compositions of other components. Materials Studio will perform a scaling for you, but the results may be undesirable.
5. To change the oxidation state, enter the value between -5 and +8 in the box, or use the spin control.

### To add a component to the mixture atom

Click the *Add* button to display the Edit Mixture Component dialog and follow steps 2-5 above.

### To delete a component of the mixture atom

Select the component to be deleted in the list, and then click the *Delete* button.

## Changing atom occupancy

Atom occupancy may be used to simulate vacancies which are randomly distributed through a structure.

### To change the occupancy of selected atoms

1. Choose *View | Explorers | Properties Explorer* and select one or more atoms.
2. Double-click on *Occupancy*.
3. Enter the occupancy as a real number between 0.0 and 1.0. Materials Studio assigns a default value of 1.0 for new atoms.

## Dialogs for disorder

### Edit Mixture Atom dialog

You can use the Edit Mixture Atom dialog to create and edit mixture atoms to simulate disorder in a structure.

**Name:** Specify a new name for the selected atom(s).

All the components that make up the selected atom(s) are shown in the list. The component list contains the following columns:

- *Element* - Shows the element type of the component
- *Ox. State* - Shows the oxidation state of the component
- *Composition* - Shows the percentage of the whole atom that is represented by the component

Double-clicking on an entry in the list displays the [Edit Mixture Component dialog](#), which allows you to edit the properties of a component.

**Add...:** Displays the Edit Mixture Component dialog to enable you to add a new component to the mixture.



**Edit...:** Displays the Edit Mixture Component dialog to enable you to edit an existing component.

**Delete:** Deletes the currently selected component from the component list.

**Note:** This button is disabled if the mixture atom contains only one component.

**OK:** Implements the changes to the composition mixture atom and closes the Edit Mixture Atom dialog.

**Cancel:** Closes the dialog without updating any settings.


**Help:** Displays the Help topic in a browser.

#### Access methods

Properties Explorer	<i>Composition</i>
Properties Explorer	<i>IsMixtureAtom</i>

### Edit Mixture Component dialog

The Edit Mixture Component dialog allows you to edit the individual components of the selected mixture atom.

**Element:** Changes the element of the component. Type an element symbol or atomic number in the *Element* list or click the  button next to the list and choose an element from the Periodic Table dialog.

**Isotope:** Selects the isotope of the component from a list of known isotopes.

**Composition:** Sets the percentage of the whole that the component makes up.

**Oxidation state:** Sets the oxidation state of the component. You can enter the new oxidation state by typing directly into the box or by using the spin control.

**OK:** Updates the settings with any changes and closes the dialog.

**Cancel:** Closes the dialog without updating any settings.

**Help:** Displays the Help topic in a browser.

#### Access methods

Properties Explorer	<i>IsMixtureAtom</i> / <i>Edit/Add</i>
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### Miller planes

Miller planes in crystals refer to sets of planes in the crystal lattice defined by a set of Miller indices (*h k l*), where *h*, *k*, and *l* are integers.

A set of such planes is defined (using fractional coordinates *x*, *y*, and *z*) by the equation:

$$hx + ky + lz = m$$

where *m* is an integer. Varying *m* generates a set of parallel planes, with that corresponding to *m* = 0 passing through the lattice origin. This set of planes is known as a *family* of Miller planes with Miller indices (*h k l*). All planes of this form pass through lattice points.

The plane corresponding to *m* = 1 has intercepts of 1/*h*, 1/*k*, and 1/*l* with each of the lattice axes. A value of 0 for *h*, *k*, or *l* indicates that the plane intersects that axis at infinity, i.e., it is parallel to that axis. Hence, *h*, *k* and *l* cannot all be 0.

More generally, the family of Miller planes with Miller indices (*h k l*) can be translated to pass through any point in the crystal lattice. This then corresponds to planes with the equation:

$$hx + ky + lx = d + m$$

where  $d$  is the distance from one plane to the lattice origin (not necessarily an integer) and  $m$  takes all integer values.

The sets of planes produced by the operation of all the elements of a crystallographic point group on the Miller planes with indices  $(h\ k\ l)$  is known as a *form* and is denoted by the presence of braces around the indices, i.e.,  $\{h\ k\ l\}$ . Materials Studio allows the creation of such families of planes, including the  $\{h\ k\ l\}$  form generated from symmetry images.

In addition, Materials Studio extends the concept of Miller planes from crystals to surfaces. In this case, the basic equation reduces to:

$$hx + ky = m$$

As  $m$  varies, this defines a set of parallel lines in the surface mesh, each line passing through mesh points. The Materials Studio implementation then generates a set of planes perpendicular to the surface with an extent determined by the extent of the atomistic structure perpendicular to the surface.

## Creating Miller planes

The [Miller Planes dialog](#) allows you to add Miller planes to crystal lattices or surface meshes. Multiple Miller planes with different Miller indices may be added to the same lattice.

### To create Miller planes

1. Either import the structure from a pre-existing file or construct a new periodic system using the tools for building crystals, surfaces, and single-wall nanotubes in the Materials Visualizer.
2. Make the 3D structure document containing the crystal lattice or surface mesh the active document.
3. Choose *Tools | Miller Planes* from the menu bar to display the Miller Planes dialog.
4. Enter the Miller indices for the plane(s) you wish to create in the *Miller indices (h k l)* text box.
5. If you wish to display the entire family of parallel planes with the specified Miller indices, check the *Show set of parallel planes* checkbox.
6. If you wish to display symmetry images of the specified plane(s), check the *Show symmetry images of form* checkbox.

**Tip:** After you have created Miller plane(s) you can toggle the display of parallel planes and symmetry images on and off using the Miller Plane tab of the Display Style dialog.

7. Set the position of the plane (or of a representative if you are displaying the set of parallel planes) either by specifying the fractional coordinates of a point in the plane using the *Point in plane* text box or by entering a value in one of the *Distance from origin* text boxes to indicate the perpendicular distance of the plane from the lattice origin either in fractional units (as a fraction of the  $d$ -spacing of the specified family of planes) or in Å.
8. Click the *Create* button to generate Miller planes with the specified properties in the 3D crystal lattice or 2D surface mesh in the currently active 3D structure document. Planes will be created using your default settings for the color, the transparency, and the extent of the display halo. These properties subsequently can be modified using the *Miller Plane* tab of the Display Style dialog.

## Working with Miller planes

Once you have created Miller planes in a 3D crystal lattice or a 2D surface mesh, you can manipulate them using the tools in the Materials Visualizer, just as with other objects in 3D structure documents.

### Miller planes display attributes

You can use the Miller Plane tab on the Display Style dialog to change the appearance and display properties of Miller planes.

The *Display style* and *Coloring* controls on the *Miller Plane* tab of the Display Style dialog apply to individual planes, parallel sets of planes, or entire families of Miller planes, depending on the scope of the current selection in the active document. The *Editing* field shows the number of objects that are in scope in the currently active document. When nothing is selected, all the families and the planes in the current display range in the document are deemed to be in scope.

If a Miller family is selected for editing, any changes will apply to that family, including all parallel sets and all planes within that family, whether or not they are currently visible. If one or more parallel sets of Miller planes (but not the corresponding families) are selected for editing, then any changes will apply just to those parallel sets of planes, and all Miller planes within those parallel sets, whether currently visible or not. Changes will not apply to unselected families or sets that are not currently visible. If one or more Miller planes (but not the corresponding parallel set or families) are selected for editing, then any changes will apply just to those selected planes. If other planes are brought into view (for example, due to lattice display range changes or [repositioning](#)), they will not exhibit the new parameters.

The *Show periodic images*, *Show symmetry images*, and *Halo size* controls on the *Miller Plane* tab of the Display Style dialog all act on the complete family or families to which the selected planes belong. The former two controls govern the visibility of periodic images within parallel sets of planes and of symmetry replicate sets of parallel planes, respectively. The *Halo size* control governs the extent by which the display of each plane exceeds its intersection with the visible lattice range.

### **Positioning Miller planes**

The position of a family of Miller planes can be set precisely using the Properties Explorer.

### To set the precise position of Miller planes using the Properties Explorer

1. If the currently active 3D structure document contains more than one Miller family, select the family that you wish to move. You can select a Miller family by selecting a single plane in the family and then double-clicking twice on the plane to select first the parent *Miller Parallel Planes* object and then the parent of that object in turn, which is *Miller Family*. Alternatively, select a single Miller plane in the family you wish to move, right-click and choose *Select Miller Parallel Planes* from the shortcut menu, then right-click again and choose *Select Miller Family* from the shortcut menu.
2. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
3. You can set the position of a family of Miller planes either by adjusting the properties of a plane in that family or by altering the properties of the entire family.

To position a Miller plane, select **Miller Plane** from the *Filter* dropdown list in the Properties Explorer, then carry out one of the following operations:

- Double-click on *DistanceFromOrigin* in the *Property* column of the Properties Explorer to display the Edit DistanceFromOrigin dialog and specify the distance, in Å, from the lattice origin of the plane, then click the *OK* button.
- Double-click on *FractionalDistanceFromOrigin* in the *Property* column of the Properties Explorer to display the Edit FractionalDistanceFromOrigin dialog and specify the distance, as a fraction of the d-spacing of the Miller family, from the lattice origin of the plane, then click the *OK* button.
- Double-click on *FractionalPointInMillerPlane* in the *Property* column of the Properties Explorer to display the Edit FractionalPointInMillerPlane dialog and specify the fractional coordinates for a representative point in the plane, then click the *OK* button.
- Double-click on *PointInMillerPlane* in the *Property* column of the Properties Explorer to display the Edit PointInMillerPlane dialog and specify the Cartesian coordinates for a representative point in the plane, then click the *OK* button.

To position a Miller family, select **Miller Family** from the *Filter* dropdown list in the Properties Explorer, then carry out one of the following operations:

- Double-click on *MillerFamilyFractionalDistance* in the *Property* column of the Properties Explorer to display the Edit MillerFamilyFractionalDistance dialog and specify the distance, as a fraction of the d-spacing of the Miller family, from the lattice origin of the plane, then click the *OK* button.
- Double-click on *PointInMillerFamily* in the *Property* column of the Properties Explorer to display the Edit PointInMillerFamily dialog and specify the fractional coordinates for a representative point in the plane, then click the *OK* button.

Alternatively, the position of a selected Miller plane (but not multiple planes) can be adjusted manually, regardless of the currently active tool mode, using various mouse and key combinations.

**Note:** The movement operations described below can be performed only if a single Miller plane is selected. Sets or families of planes, or multiple selected planes cannot be translated using the mouse and keyboard. Use the Properties Explorer to [position](#) multiple Miller planes.

### To translate a selected Miller plane using the mouse and keyboard

1. Hold down the SHIFT key and middle mouse button.
2. Without releasing the mouse button or the SHIFT key, drag the plane to the desired location.

or:

1. Hold down the SHIFT and ALT keys and the right mouse button.
2. Without releasing the mouse button or the SHIFT and ALT keys, drag the plane to the desired location.

or:

1. Hold down the SHIFT and ALT keys.
2. Without releasing the SHIFT and ALT keys, use the cursor arrow keys to move the selected plane to the desired location.



All other planes in the same family as the selected plane will move accordingly and their visibility will be adjusted as they move in or out of the lattice display range.



## Orientation and alignment using Miller planes

As with many other objects in the 3D Viewer, Miller planes can be used to orient the view of a crystal or surface.

**Note:** The orientation and alignment operations described below can be performed only if a single Miller plane is selected. Sets or families of planes, or multiple selected planes cannot be used to orient the view or align a structure.


### To orient the view of a structure using Miller planes

1. [Create](#) the appropriate Miller plane(s) in the structure that you wish to align.
2. Select a single Miller plane.
3. If you wish to orient the view so that the selected Miller plane is parallel to the screen, click on the options arrow associated with the *3D Viewer Recenter* button  on the 3D Viewer toolbar and select *View Onto*  from the dropdown list.

If you wish to orient the view so that the selected Miller plane is perpendicular to the screen, click the *3D Viewer Recenter* button  on the *3D Viewer* toolbar and select *View Across*  from the dropdown list.

Miller planes can be used to align a crystal lattice or surface mesh relative to the Cartesian coordinate system.

### To align a crystal or surface using Miller planes

1. [Create](#) the appropriate Miller plane(s) in the structure that you wish to align.
2. Select a single Miller plane, then press and hold CTRL while selecting the crystal lattice.
3. Click the *Align Onto View* button  on the 3D Movement toolbar. The lattice as a whole will be rotated rigidly relative to the Cartesian coordinate system so that the selected Miller plane is oriented parallel to the view.

## Miller Planes dialog

The Miller Planes dialog allows you to create Miller planes for addition to crystals or surfaces.

**Miller indices (h k l):** Specify the indices of the plane to be created, using spaces to separate each entry.

**Note:** If the currently active 3D structure document contains a surface, then the third index must be zero, otherwise all the other controls on the Miller Planes dialog will be disabled. Planes in two-dimensional nets are defined by two indices only, so a third index would have no meaning in this scenario.

**Show set of parallel planes:** When checked, indicates that the entire family of Miller planes with the specified index will be displayed when the *Create* button is pressed.

**Show symmetry images of form:** When checked, indicates that all planes of the specified form, i.e., all symmetry images of the plane specified in the *Miller indices (h k l)* text box, will be displayed when the *Create* button is pressed.

**Note:** If either *Show set of parallel planes* and *Show symmetry images of form* is checked, the set of planes that are visible will be those that intersect with the visible lattice display range. Similarly, it is possible for the specification to be such that no planes with the desired indices and position will be visible.

If *Show set of parallel planes* and *Show symmetry images of form* are both checked, then, for each plane in the specified form, a family of parallel planes will be shown.

Miller planes can be positioned using one of two methods. You can either specify a point that the plane should include or you can specify the distance from the origin to the plane.

**Point in plane (a b c):** Specify the fractional coordinates of a point in the Miller plane that you wish to create.

**Distance from origin:** Specify the perpendicular distance from the origin to the desired plane either in fractional units, which will be a multiple of the d-spacing of the desired family of planes, or in units of Å.

**Note:** When you specify coordinates in the *Point in plane (a b c)* text box the distances in the *Distance from origin* text boxes will be updated automatically with the appropriate values. Similarly, altering either of these distance values will cause the other distance setting and the point coordinates to be updated accordingly.

**Create:** Creates a set of Miller planes with the specified parameters to add to the crystal or surface in the currently active 3D structure document.

The visibility of the individual planes is determined by the *Show set of parallel planes* and *Show symmetry images of form* settings. If *Show set of parallel planes* is checked, then all those members of the family of parallel planes that intersect the current lattice display range will be displayed. If *Show symmetry images of form* is checked, all the families of planes of the specified form containing the symmetry images will be displayed. If both checkboxes are checked, all the parallel planes in the specified Miller family and all their symmetry images will be displayed.

**Tip:** Use the Miller Plane tab on the Display Style dialog to change the appearance and display properties of Miller planes.

**Help:** Displays the Help topic in a browser.

#### Access methods

Menu *Tools | Miller Planes*

## Symmetry

Symmetry and periodicity are fundamental concepts for the treatment of extended systems on an atomistic scale. Macroscopically, symmetry manifests itself in many different ways, for example in the shapes of crystallites or the diffraction pattern from an X-ray diffraction experiment.

When a system is symmetric or periodic, it means that atom positions and properties within that system repeat themselves regularly. Thus, it is possible to map the structure onto itself by the application of a set of symmetry operations, such as rotations, reflections, and translations (or combinations thereof).

If a system is symmetric or periodic, it follows that all atoms (or more generally, all of the potentially infinite number of objects) within the system are generated from a finite and often small number of independent objects (the [asymmetric unit](#)) by the application of these symmetry operations. Materials Studio automatically performs these operations and thus allows you to interact easily with infinite symmetric or periodic models.

Symmetry and periodicity generally simplify the physical description of a material significantly and symmetry relationships are therefore invariably exploited in molecular modeling. This is why symmetry and periodicity are built into the Materials Visualizer data structures at a very fundamental level. It is possible to query the symmetry relationships between atoms, bonds, or other objects. Many atom properties, such as charge and atomic mass, are automatically forced to obey the symmetry relationships imposed by the crystal structure. A wealth of crystallographic information for the structure under consideration is also available and is dynamically updated throughout your Materials Studio session.

Conceptually, Materials Studio classifies systems according to their translational symmetry (periodicity). There are three main classes: systems without translational symmetry (0D), such as molecules; systems that periodically repeat themselves in two dimensions and which are referred to as 2D lattices or surfaces; systems that periodically repeat themselves in three dimensions and which are called 3D lattices or crystals. The common method of visualization for all of these structures is via the 3D Viewer. Many properties of a symmetric or periodic system can also be examined and edited in the Properties Explorer.

All symmetry-related information associated with a given structure can be saved and reloaded in Materials Studio's native XSD file format. In addition, as much of the symmetry information as possible is imported from/exported to any of the supported non-native file formats. In particular, symmetry information can be easily transferred to and from Materials Studio using the MSI file format.

The following sections discuss symmetry in Materials Studio in more detail and explain the symmetry-related functionality of the Materials Visualizer.

### Symmetry in Materials Studio

One of the most important features of the Materials Visualizer is its ability to import, build, visualize, and modify symmetric and periodic systems.

This functionality makes it possible for applications to compute the properties of such systems in accordance with all the rules imposed by the symmetry groups to which they belong. As a user, you can interact easily with both finite and infinite systems. Any change to a part of a symmetric system is automatically propagated to all the periodic or symmetric copies.

You are generally prohibited from making changes to the system which would violate symmetry relationships. If you want to reduce the symmetry or periodicity of the system, you have to specify this

explicitly. Of course, the Materials Visualizer also allows you to deal with completely non-symmetric systems, such as molecules.

A few of the features of the symmetry implementation in Materials Studio are:

- The symmetry system is truly symmetric.  
In symmetric or periodic systems, symmetric objects such as atoms or bonds never deviate from the specified symmetry.
- Periodicity is infinite.  
From the user's perspective, it seems as if all possible symmetry images exist and are treated equally. Operations are carried out on the full infinity of objects, whether currently visible or not. For example, if you delete an atom, all of its symmetry images are also deleted.
- The asymmetric unit is not 'special'.  
No preference is given to a particular set of atoms over others. The [asymmetric unit](#) is not treated as unique (see also [Crystal systems and space group operators](#)).
- All objects can have symmetry images.  
All physical entities (atoms, molecules, thermal ellipsoids, etc.) may have some or all of their properties (such as position, charge, mass, etc.) constrained by symmetry.

The *Build / Symmetry* menu commands, the Symmetry toolbar and the Properties Explorer allow you to view and modify many attributes related to the symmetry of systems. The following topics describe a number of important concepts specific to the implementation of symmetry in Materials Studio.

## Symmetry system

In Materials Studio, a symmetry system is any molecular system whose constituent parts (atoms, bonds, etc.) are related to one another by the symmetry operators of a particular symmetry group. 3D crystals, 2D surfaces, and [nonperiodic systems with point group symmetry](#) are all examples of symmetry systems.

As a consequence of the [symmetry relationships](#) that exist in symmetry systems, certain properties of the objects they contain (for example, position, charge, etc.) are also related. However, these relationships are not always trivial.

Information about the properties of the current symmetry system is accessible from the Properties Explorer. Selecting [Symmetry System](#) from the *Filter* dropdown list enables you to view a number of properties of the current symmetry system, the values of which are dynamically updated whenever a change is made to the system. These properties are:

**CellFormula:** The number of atoms of each element type that are unique with regard to periodic translations. For crystals and surfaces, this corresponds to the number of atoms of each element type in the unit cell. In nonperiodic symmetry systems, this is the total number of atoms of each element type.

**Density:** The density of the system in  $\text{g cm}^{-3}$  (for crystals only).

**Name:** The name of the system.

**NumberOfAtoms:** The number of atoms which are unique with regard to periodic translations. For crystals and surfaces, this corresponds to the number of atoms in the unit cell. In nonperiodic symmetry systems, this is the total number of atoms.

**Volume:** The unit cell volume in  $\text{\AA}^3$  (for crystals only).

## Lattice

A [symmetry system](#) which possesses translational symmetry, or periodicity, is known as a lattice. Atoms in a lattice are arranged regularly in 2D (a surface) or 3D (a crystal). Lattice vectors determine how each



atom is repeated. The sizes and relative orientation of the lattice vectors are given by the lattice parameters.

Lattices are displayed in the 3D Viewer. The view can be modified using the *Lattice* options on the Display Style dialog.

The current lattice parameters can be [viewed and modified](#) using the [Lattice Parameters dialog](#). In addition, you can [view symmetry information](#) for the current lattice in the [Show Symmetry dialog](#).

More detailed information about the lattice and its symmetry is accessible from the Properties Explorer.

Selecting [Lattice 2D](#) (for surfaces) or [Lattice 3D](#) (for crystals) from the *Filter* list enables you to view many properties of the lattice, the values of which are dynamically updated whenever a change is made to the system. These properties are:

**AngleAlpha, AngleBeta, AngleGamma:** The current values of the  $\alpha$   $\beta$   $\gamma$  crystal [lattice parameters](#).

**AngleTheta:** The current value of the  $\vartheta$  surface lattice parameter.

**BravaisLattice:** The [Bravais lattice](#) of the system.

**CellVolume:** The unit cell volume in  $\text{\AA}^3$  (for crystals only).

**CellArea:** The unit cell area in  $\text{\AA}^2$  (for surfaces only).

**CenteringType:** The centering type of the system. Available options are:

- [3D Primitive-Centered](#)
- [3D Body-Centered](#)
- [3D Face-Centered](#)
- [3D A-Centered](#)
- [3D B-Centered](#)
- [3D C-Centered](#)
- [3D Rhombohedral-Centered](#)
- [3D Unclassified Centering](#)
- [2D Primitive-Centered](#)
- [2D Centered](#)
- [2D Unclassified Centering](#)
- [0D No Centering](#)

**GroupName:** The short form of the Hermann-Mauguin symbol (see International tables, Hahn 1983).

**LatticeOrigin:** The position of the lattice origin, with respect to the [Cartesian](#) origin in  $\text{\AA}$ .

**LatticeRepresentation:** The lattice representation of the system. Available options are:

- 3D Triclinic
- 3D Monoclinic-A
- 3D Monoclinic-B
- 3D Monoclinic-C
- 3D Orthorhombic
- 3D Tetragonal
- 3D Hexagonal
- 3D Rhombohedral
- 3D Cubic
- 3D mCPrimitive
- 3D oCPrimitive
- 3D olPrimitive
- 3D oFPrimitive
- 3D tIPrimitive
- 3D cIPrimitive
- 3D cFPrimitive
- 3D Unclassified
- 2D Oblique
- 2D Rectangular
- 2D Square
- 2D Hexagonal
- 2D rCPrimitive
- 2D Unclassified
- 0D No Lattice

**LengthA, LengthB, LengthC:** The current values of the  $a$ ,  $b$ , and  $c$  crystal lattice parameters.

**LengthU, LengthV:** The current values of the  $u$  and  $v$  surface lattice parameters.

**Name:** An editable name, identical to the *GroupName* by default.

**NumOperators:** The total number of symmetry operators of the space group.

**OrientationConvention:** The [Orientation standard](#), or rule used for the alignment of the crystal lattice with respect to the Cartesian axes.

**SpaceGroupCrystalClass:** The space group crystal class (see International tables, Hahn 1983).

**PlaneGroupCrystalClass:** The space group crystal class for surfaces (see International tables, Hahn 1983).

**SpaceGroupCrystalSystem:** The [space group crystal system](#) (see International tables, Hahn 1983).

**PlaneGroupCrystalSystem:** The space group crystal system for surfaces (see International tables, Hahn 1983).

**SpaceGroupITNumber:** The International Tables number of the space group (Hahn 1983).

**LaueClass:** The Laue Class (Patterson symmetry) of the space group, which is important in determining the symmetry of X-ray diffraction patterns.

**SpaceGroupLongName:** The long form of the Hermann-Mauguin symbol (see International tables, Hahn 1983).

**PlaneGroupLongName:** The long form of the Hermann-Mauguin symbol for surfaces (see International tables, Hahn 1983).

**SpaceGroupQualifier:** The space group qualifier.

**SpaceGroupSchoenfliesName:** The [Schoenflies name](#) of the space group.

**VectorA, VectorB, VectorC:** The Cartesian coordinates of the crystal lattice vectors in Å.

**VectorU, VectorV:** The Cartesian coordinates of the surface lattice vectors in Å.

## Asymmetric unit

The asymmetric unit of a crystal or surface is defined as the largest subset of atoms which can be chosen such that no two atoms are related to each other by a symmetry operator or by a periodic translation. As discussed [elsewhere](#), the choice of asymmetric unit atoms is not unique.

In Materials Studio, the concept of the asymmetric unit encompasses not just atoms, but all symmetry objects for which a [symmetry relationship](#) is defined.

Any object in an infinite [symmetry system](#) can be generated from the asymmetric unit atoms by symmetry operators, such as rotations or mirror planes.

Materials Studio does not currently provide an option to visualize the asymmetric unit, as it is not unique. However, the choice of asymmetric unit does determine which atoms are visible when you choose certain [lattice display styles](#). In particular, if the **Original** display style is chosen from the options on the Lattice tab of the Display Style dialog, the objects shown in the display will be derived from a particular asymmetric unit by application of all symmetry operators of the current symmetry group. The asymmetric unit chosen in this case is obtained arbitrarily from the original objects that were present before the current crystal or surface was built.

## Symmetry-related objects and properties

In 3D model documents containing a [symmetry system](#), each atom in the [asymmetric unit](#) is related to an infinite number of symmetry-equivalent atoms that are generated by the application of the operators and translations of the symmetry group to which the system belongs.

The most obvious consequence of this is that the atoms in the system are positioned regularly throughout the model. This regular arrangement of atoms can be seen in the 3D Viewer and inspected, for individual atoms, in the Properties Explorer (XYZ property).

Changes to the position of any one atom cause corresponding changes to the position of each of its symmetry equivalents. Similarly, other atom properties have relationships that are imposed by symmetry.

In Materials Studio, these symmetry relationships are strictly maintained for all atom properties with physical meaning. However, other properties that merely facilitate user interaction with objects are not subject to such symmetry relationships. For example, objects can be colored or selected individually without affecting the color or selection status of symmetrically related objects.

Atoms are not the only objects within 3D model documents that have symmetry relationships. Bonds, molecules, linear chains, repeat units, dendrimers, dendrimer repeat units, linkages, and charge groups are handled in the same way. However, some types of objects, such as labels, have no symmetry images and behave in the same way, whether or not symmetry is present.

**Tip:** You can select all the objects in a 3D Viewer that are related by symmetry to the current selection by right-clicking and choosing Select Symmetry Images from the shortcut menu.

Objects that do possess symmetry relationships have the following additional properties in the Properties Explorer:

**SymmetryDerivationSymbol:** A [shorthand notation](#) for the matrix of the symmetry operator used to generate the symmetry equivalent from the corresponding asymmetric unit object. The notation

describes how a given asymmetric unit coordinate value  $x,y,z$  is transformed by the symmetry operator. Simple examples are:  $-x;y;z$  - a mirror image about  $x = 0$ ;  $x+1;y;z$  - a translation by one cell repeat unit (along the A vector in a crystal);  $-x;-y;z$  - a dyad image about  $x = y = 0$ .

**SymmetryDerivationType:** Describes the geometric character of the symmetry operator used to generate the symmetry equivalent from the corresponding asymmetric unit object. The types include: [Lattice Vector](#), [Mirror Plane](#), [Rotation Axis](#), [Inversion Center](#), [Glide Plane](#), [Screw Axis](#), [Roto Inversion](#), and [Identity](#).

**SymmetryMultiplicity:** The number of symmetry equivalents of the current object that are unique with regard to periodic translations. For crystals and surfaces, this corresponds to the number of symmetry equivalents per unit cell. In the case of nonperiodic systems, this is the total number of equivalents. The maximum value is the number of operators in the symmetry group. For an object subject to a [symmetry constraint](#), the value will be lower in proportion to the [SpecialPositionOrder](#) property.

**Note:** Although the *SymmetryMultiplicity* property is defined as the number of symmetry equivalents per unit cell, Materials Studio treats objects in periodic systems as if they have an infinite number of symmetry equivalents, only a subset of which are visible or selected at any one time.

## Fractional and Cartesian coordinates

In [lattices](#), atom positions may be described using two different coordinate systems, Cartesian or fractional.

Cartesian coordinates are defined in the usual way using 3 orthogonal unit vectors **i**, **j** and **k**.

In Materials Studio, Cartesian coordinates are used to describe the positions of objects in nonperiodic structures and the absolute positions of objects in a lattice.

Fractional coordinates are used to describe the positions of objects in a lattice relative to the unit cell. For crystals they are defined in terms of the lattice vectors **a**, **b** and **c**. For surfaces they are defined in terms of **u** and **v** and a third vector **w** which is a unit vector normal to both **u** and **v**.

Fractional coordinates indicate where objects are in the unit cell. For example, in a crystal an atom lying at (0.5,0.5,0.5) in fractional coordinates will be directly in the middle of the unit cell.

In a surface an atom lying at (0.5,0.5,0.5) in fractional coordinates will be 0.5 Å from the surface plane directly above the middle of the unit cell. Likewise a second atom lying at (0.5,0.5,4.5) in fractional coordinates will be 4.5 Å from the surface plane directly above the middle of the unit cell, and will have no periodic relationship to the first.

## Interconversion of fractional and Cartesian coordinates

If you have a point  $xi+yj+zk$  in Cartesian space which corresponds to  $ua+vb+wc$  in fractional space, then the fractional coordinates may be converted to Cartesian using a  $3 \times 3$  matrix and an offset to account for a possible change in origin:

$$(x,y,z)^T = A(u,v,w)^T + p$$

where **A** = (**a**,**b**,**c**) is a matrix whose columns indicate the Cartesian coordinates of the lattice vectors, and **p** is the origin of the unit cell in Cartesian coordinates.

## Properties

Cartesian coordinates may be found in the Properties Explorer as *XYZ* and fractional coordinates as *FractionalXYZ*.

## Conventional and primitive representations

The set of symmetry operators that define the symmetry of a crystal categorize it into one of [seven crystal systems](#).

The conventional cell used to describe the crystal [lattice](#) is determined by rules relating to the symmetry operators it contains. For example, in an orthorhombic system, the lattice vectors **a**, **b** and **c** are assumed to lie along the three perpendicular two-fold axes present in orthorhombic crystals. It is these lattice vectors that define the unit cell.

Lattice points are points in the lattice which have identical environments.

Some crystals contain lattice points that cannot be described by integral combinations of lattice vectors. In these crystals the unit cell may contain two, three or four lattice points. Unit cells that contain multiple lattice points are called centered cells.

Combining the seven crystal systems with the various centering possibilities for each system yields 14 different types of lattice. These are known as the [Bravais lattices](#).

If a conventional cell contains multiple lattice points, it is possible to define another cell such that it contains just a single lattice point. Such a cell is called a primitive cell.

**Note:** Conventional cells that contain just one lattice point are also primitive.

The use of primitive cells that are not also conventional cells has some advantages and several disadvantages. The main advantage is that primitive cells are smaller by a factor of 2, 3 or 4, making some calculations faster. The main disadvantage is that primitive unit cells have inconvenient shapes making visualization difficult and complicating the description of the relationships that exist between the lattice vectors.

In general the disadvantages outweigh the advantages and non-conventional primitive representations of crystal lattices are rarely used.

For most space groups listed in the International Tables (Hahn 1983), the symmetry operators are listed only in relation to the conventional cell. This means that when the operators are described relative to the primitive cell the space group is not recognized as one of the standard settings of the group as listed in the Tables. The exception to this concerns rhombohedral settings of hexagonal space groups, which are also listed in the International Tables. This is primarily because the rhombohedral cell has simple relationships between the lattice vectors.

In certain calculations, for efficiency reasons, it is desirable to use a non-conventional primitive unit cell. In these situations it is normal to convert to the primitive representation immediately before the calculation and back to a conventional representation immediately afterward.

## Converting between conventional and primitive representations

Commands are provided for converting between the conventional representation and the primitive representation of a crystal unit cell. In the case of trigonal crystals, these commands get renamed to reflect the special relationships that exist between the rhombohedral and hexagonal settings.

## Symmetry constraints

### Symmetry constraints within the lattice

In [lattices](#), [symmetry relationships](#) exist between objects. As a result of these relationships, certain constraints are imposed on the properties of the objects. For example, it is not possible to arbitrarily change the distance between two atoms which are related by a translation, because this would violate the periodicity of the system.

Materials Studio automatically ensures that such constraints are imposed. Consequently, you cannot make changes to a structure that would break the current symmetry, unless you first redefine the symmetry or remove it altogether.

**Note:** It may be possible to make changes to objects in the [asymmetric unit](#). However, if you attempt to apply symmetry-inconsistent changes to an asymmetric unit object and one (or more) of its symmetry equivalents, there is a risk that a symmetry constraint will be violated and the operation will be prohibited.

## Symmetry constraints within the asymmetric unit

Sometimes, asymmetric unit objects themselves are subject to symmetry constraints.

If an asymmetric unit object can be mapped onto itself by a symmetry operator other than the identity, then it is symmetry constrained. Symmetry-constrained atoms are called [special position](#) atoms.

The symmetry constraint of an object is defined as the [point group](#) of symmetry operators which map the object onto itself. The point group must be a subgroup of the overall symmetry group.

In practical terms, this means that certain geometric and physical properties of the object must satisfy particular conditions. For example, the position of an atom may be constrained by a point group consisting of the identity operator  $(x,y,z)$  and the mirror operator  $(-x,y,z)$ . The atom must have an  $x$  coordinate of zero because that is the only value of  $x$  for which  $x = -x$ . Restricting the atom position such that  $x = 0$  satisfies the condition of equivalence of the atom with itself through the application of either symmetry operator. In this case, the restriction on the possible coordinates of the atom is represented by  $(0,y,z)$ , which describes a plane.

For any object which may possess symmetry equivalents, the Properties Explorer shows properties related to symmetry constraints:

**SymmetryConstraintType:** Describes the geometric character of the restrictions imposed on the position of this object by virtue of its symmetry constraints. Available options include: [Plane](#), [Axis](#), [Point](#), and [Identity](#) (unconstrained).

**SymmetryConstraintSymbol:** A shorthand notation for a matrix describing the locus of points satisfying the symmetry constraint of this object. Available options include: [0,y,z](#) - constrained to lie on plane  $x = 0$ ; [0,1,0](#) - constrained totally to position  $(0,1,0)$  in [fractional coordinates](#).

**SpecialPositionOrder:** The number of operators in the point group of the symmetry constraint on this object.

Symmetry constraints are discussed in more detail in the following topics:

- For a discussion of how symmetry constraints relate to the symmetry group as a whole, see the [Special positions](#) topic.
- For a discussion of how symmetry relationships between atoms further constrain possible rigid body motions, see the [Motion constraints](#) topic.
- For a discussion of how symmetry constraints affect scalar, vector, and tensor (matrix) properties of objects, see the [Constrained properties](#) topic.

## Motion constraints

In Materials Studio it is possible to move atoms in a variety of ways. For example, you can select and drag atoms directly using the mouse. Alternatively, you can move an atom by changing the value of a [geometry monitor](#).

When you attempt to move atoms in a [lattice](#) and particularly when you attempt to move several atoms together, it is possible that the movement will violate the [symmetry](#) of the structure. In such situations, Materials Studio will prevent you moving the atoms and report the constraint giving rise to the

restriction in the status bar. If you are moving the atoms directly using the mouse and the motion is not fully constrained, then Materials Studio will move the atoms in a manner which does not violate the symmetry constraints but which is as close as possible to the intended, unconstrained motion.

## Property constraints

As a consequence of the [symmetry relationships](#) that exist in [symmetry systems](#), certain properties of the objects they contain (for example, position, charge, etc.) are also related.

Materials Studio automatically ensures that these relationships are maintained. When a property is assigned to an object on a [special position](#), this may mean that constraints are imposed on the values of the property by the symmetry of the structure.

Such constraints will mainly affect vector and tensor properties. For example, if an anisotropic [temperature factor](#) (which is a second rank tensor quantity) is applied to an atom lying on a special position in a crystal with cubic symmetry, Materials Studio will modify the temperature factor such that it is transformed onto itself under the symmetry operations defined by the [symmetry constraint](#) of the special position.

## Special positions

A special position is a point in the coordinate space of a [lattice](#) which is mapped onto itself under the application of a symmetry operation other than the identity.

Typically, atoms in Materials Studio that lie on one of these special positions are given a [symmetry constraint](#).

Symmetry constraints work by reducing the number of symmetry generated images of an atom. So, if the application of a symmetry operator other than the identity on an atom would put another atom on top of it, no new atom is created and instead the original atom is marked as a special position atom.

The atoms which would have been generated by the application of the operators of the point group but which were omitted, would have had identical properties to the original atom.

The omitted atoms are accounted for by a reduction in the *SymmetryMultiplicity* of the atom in proportion to the number of operators in the point group of the special position.

Atoms on special positions are detected either when a document is imported or during a crystal or surface build operation.

Materials Studio automatically ensures that any conditions imposed by the symmetry constraints of the special position atom are met. So, for example, an atom which is constrained by a point group consisting of the identity operator  $(x,y,z)$  and the mirror operator  $(-x,y,z)$  must have an x coordinate of zero and can therefore only be moved in the plane  $(0,y,z)$ .

For any object which possesses symmetry equivalents, the Properties Explorer shows the following properties related to special positions:

**SpecialPositionOrder:** The number of operators in the point group of the [symmetry constraint](#) on the object. For example, an atom on the special position arising from a mirror operator gives a value of 2, and an atom lying on a tetrad axis gives a value of 4. An atom with no constraint has a value of 1.

**SymmetryMultiplicity:** The number of symmetry images of the object which are generated per unit cell. This value is the total number of operators in the symmetry group divided by the SpecialPositionOrder property.

**IsOverspecified:** This property indicates whether the imposed constraint on an atom is consistent with its current location in space. An atom which has a location away from a special position at the time of building a crystal may subsequently be moved close to the special position site. In these circumstances, the atom and some of its equivalents will overlap. This is shown by a [Yes](#) value for this property.

## Tasks in symmetry

Materials Studio offers a number of features for building, exploring, and viewing the symmetry of periodic and nonperiodic structures.

The following sections discuss how to use the symmetry tools in the Materials Visualizer in more detail.

### Finding and imposing symmetry


When viewing the symmetry properties of a structure, it is important to remember that the symmetry details shown may not necessarily correspond to the highest possible symmetry of that structure. Instead, they correspond to the symmetry properties which Materials Studio uses to build the complete [lattice](#) from an [asymmetric unit](#).

For example, you may have imported a 3D model document which is identified as being periodic, using a simple space group setting such as P1. However, there may be an alternative higher symmetry representation which could be adopted, reducing the number of atoms in the asymmetric unit.

Alternatively, you might have performed tasks that required you to create a supercell, and you now want to reimpose symmetry.

The *Find Symmetry* tool determines the symmetry present in the current structure using the positions and element types of each of the atoms. It also allows you to impose the results of the search on the structure, which will then exhibit all the attributes of the symmetry group that was found. Further details on the [algorithm](#) used by the *Find Symmetry* tool are given in the [theory](#) section.

#### To find symmetry

1. Choose *Build | Symmetry | Find Symmetry*, or click the *Find Symmetry*  button on the Symmetry toolbar.
2. Select a *tolerance* from the dropdown list, or enter a numeric value. This value determines how closely atoms in the symmetrized structure should match atoms in the original structure.
3. In the Find Symmetry dialog, click the *Find Symmetry* button to find symmetry and show any results in the *Results* list. If the structure is a crystal, *Find Symmetry* will look for [space group symmetry](#); if the structure is nonperiodic, it will look for [point group](#) symmetry.

**Note:** It is not possible to use *Find Symmetry* to search for symmetry in surfaces.

**Tip:** In some cases, usually when a large tolerance is used and there is some degree of positional disorder, the *Find Symmetry* tool generates unreliable results. This is characterized by the reported *Max. deviation* being greater than the *Tolerance*, and in this case a message is shown at the bottom of the *Results* list. If this happens you are recommended to look for symmetry using different *Tolerance* values. Smaller tolerance values will be more reliable, but occasionally better results can be obtained by using a larger value for the tolerance.

#### For periodic structures

- Click the *Impose Symmetry* button to redefine the symmetry of the structure so that it matches the symmetry found, then close the dialog.

**Note:** Impose Symmetry is enabled only if some of the current symmetry settings are different from those shown in the *Results* list.

Subsequently, it will not be possible to move atoms in a way which would violate the [symmetry constraints](#) imposed by the space group found.



### For nonperiodic structures

- Click the [Snap to Symmetry button](#) to reset the coordinates of the atoms in the structure so that they are exactly consistent with the symmetry found.

**Note:** *Snap to Symmetry* is enabled only if a non-trivial point group is shown in the *Results* list.

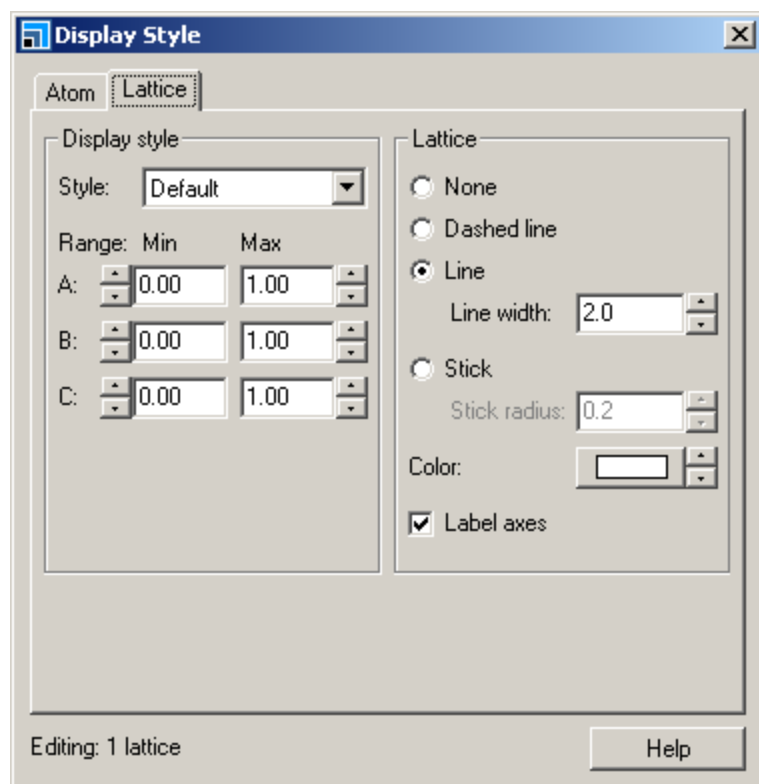
*Snap to Symmetry* does not define any symmetry relationships between objects. As a result, no symmetry constraints are imposed for nonperiodic systems. So it will still be possible to move atoms in ways which violate the symmetry of the point group found.

### Setting the lattice display style

Crystals and surfaces are infinite so there are many different ways of looking at them. The view you choose depends on what you are interested in. For example, to explore hydrogen bonding motifs, it may be better to view many adjacent cells in the lattice. On the other hand, to modify or analyze the structure of individual molecules, it may be less confusing to display only a single unit cell.


The Lattice tab on the Display Style dialog allows you to control how a crystal or surface lattice is displayed. You can specify the display style and the range of visible atoms, and determine how the lattice is drawn.

**Note:** You are not restricted to viewing multiples of complete unit cells. Fractional display ranges can be specified and result in only part of a unit cell being shown.



Display Style dialog, Lattice tab

## To set the lattice display

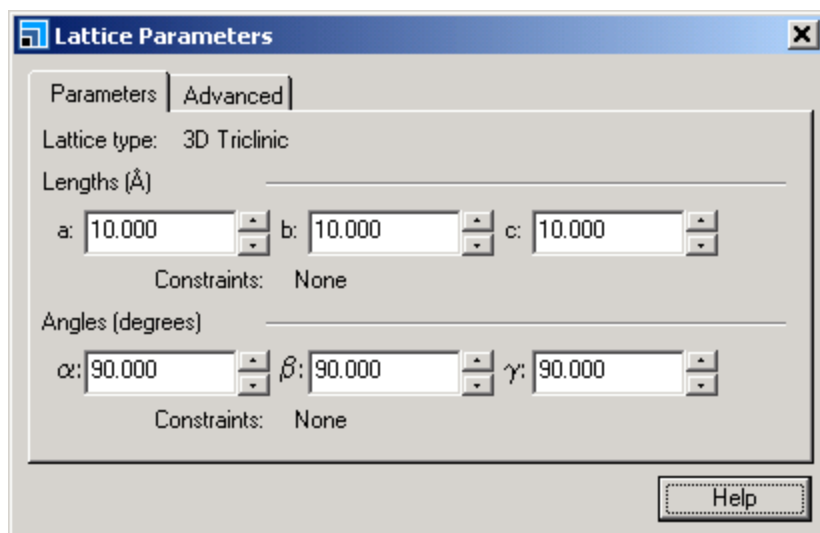
1. Choose *View / Display Style* from the menu bar, click the *Display Style* button  on the 3D Viewer toolbar, or right-click in the 3D structure document and select *Display Style* from the shortcut menu to display the Display Style dialog.
2. Select the *Lattice* tab and choose a display style from the *Style* dropdown list.
3. Use the *Range* controls to specify minimum and maximum values for the A, B, and C crystallographic directions in fractional units. The C direction controls are disabled if the structure is a surface.
4. Choose how the lattice is to be represented. It can be drawn with lines, dashed lines, or sticks, or not drawn at all. The color, line thickness, and stick radius for the lattice can be adjusted using the appropriate controls.
5. If you want the axes to be labeled (where displayed), check the *Label axes* checkbox.

## Viewing or changing the lattice parameters

Lattice parameters determine the length and relative orientation of the lattice vectors in space. In crystals and surfaces, these lattice vectors control how each atom is repeated periodically.


The [Lattice Parameters dialog](#) allows you to set the lattice parameters. The [Parameters tab](#) allows you to inspect and modify the values of the lengths and angles of the lattice vectors of the current crystal or surface. The [Advanced tab](#) allows you to set the lattice origin and orientation.

Any changes you make to the values have an immediate effect.



Setting the lattice parameters

## To view or change the lattice

1. Select *Build | Symmetry | Lattice Parameters* or click the *Lattice Parameters* button  on the Symmetry toolbar.

The lattice type of the structure is shown. The labels on the length and angle boxes change depending on whether the current structure is a crystal or a surface. The dialog can remain open while you work with other Materials Studio modules.

2. Use the [Parameters tab](#) to specify the cell *Lengths*  $a$ ,  $b$  and  $c$  (crystal) or  $u$  and  $v$  (surface) and *Angles*  $\alpha$ ,  $\beta$  and  $\gamma$  (crystal) or  $\vartheta$  (surface), either directly into the boxes or by using the spin controls.

If the lattice parameters are constrained to certain values by the specified symmetry, these constraints are shown and the appropriate text boxes are disabled. So, in a cubic crystal, for example, where  $a = b = c$  and  $\alpha = \beta = \gamma = 90^\circ$ , only a value for  $a$  is required.

**Note:** For some complex constraint relationships, the text boxes are not disabled, although assignment remains automatic.

3. Use the [Advanced tab](#) to:
  - Set a new cell origin.
  - Set the rule for the lattice alignment.
  - Force a realignment of the lattice.
  - Control the behavior of coordinates when a change is made.

**Note:** You can also view and change the lattice parameters in the Properties Explorer. They are shown as properties of the [Lattice 2D](#) and [Lattice 3D](#) objects.


## Viewing symmetry

When viewing the symmetry properties of a structure, it is important to remember that the symmetry details may not necessarily correspond to the highest possible symmetry of that structure. Instead, they correspond to the symmetry properties which Materials Studio uses to build the complete [lattice](#) from an [asymmetric unit](#).

For example, you may have imported a 3D model document which is identified as being periodic, using a simple space group setting such as P1. However, there may be an alternative higher symmetry representation which could be adopted, reducing the number of atoms in the asymmetric unit.

You can either view the symmetry of the current structure, or you can obtain information on a particular symmetry group regardless of which structure is currently open.

### To view the symmetry of the current structure

1. Choose *Build | Symmetry | Show Symmetry* or click the *Show Symmetry* button  on the Symmetry toolbar.
2. The [Symmetry Group tab](#) shows the general details of the group. The [Operators tab](#) shows the details of the individual operators with the position and description of each symmetry element in shorthand notation.
3. The [Show Symmetry dialog](#) can remain open while you work with other modules in Materials Studio.

**Note:** Alternatively, the Properties Explorer provides the capability for you to view and edit a more comprehensive [list of parameters](#) relating to the symmetry/lattice of the current system.

### To view the symmetry of a space group

1. Choose *Build | Crystals | Build/Rebuild Crystal...* to display a description of the space group and its properties (name, symbol, etc).
2. Click the *Details* button on the Space Group tab to display the *Show Symmetry* dialog, which contains further details about the current space group.

This dialog closes when the *Build Crystal* dialog closes.

### To view the symmetry of a plane group

1. Choose *Build | Surfaces | Build/Rebuild Surface...* to display a description of the plane group and its properties (name, symbol, etc).
2. Click the *Details* button on the Plane Group tab to display the *Show Symmetry* dialog, which contains further details about the current plane group.

This dialog closes when the *Build Surface* dialog closes.

## Theory in symmetry

When moving atoms or altering atom parameters in a crystal, any changes are propagated through the structure by the space group symmetry.

Materials Studio allows you to move atoms or alter their parameters using full space group symmetry relationships, using only translational symmetry, or without using any symmetry information. In the latter two cases full space group symmetry can be restored later on in the session.

### Crystal systems and space group operators

Crystalline materials have both translational periodicity and space group symmetry. The building blocks for the description of a crystal structure include a collection of 'parent' atoms called the [asymmetric unit](#), a 3D reference system called a [lattice](#) (whose basis is called the [unit cell](#)) and a space group that comprises a set of symmetry operators.

The asymmetric unit of a crystal or surface is defined as the largest subset of atoms which can be chosen such that no two atoms are related to each other by a symmetry operator or by a periodic translation. The choice of asymmetric unit atoms is not unique. In fact, there are an infinite number of possibilities for choosing an asymmetric unit. For convenience, the asymmetric unit is usually chosen as a contiguous set of neighboring atoms, enclosed by a finite asymmetric volume. Again, the choice of this asymmetric volume is not unique.

The symmetry operators and the unit cell translations act on this asymmetric volume to generate the complete crystal structure. Any choice of asymmetric unit will result in the same crystal structure being generated. Each atom is derived from a unique asymmetric 'parent' by applying a symmetry operation on the coordinates of the 'parent' atom.

The unit cell basis vectors, **a**, **b**, and **c**, are not necessarily orthogonal and are determined by the characteristics of the given material. The unit cell is usually described by the axial lengths, *a*, *b*, and *c*, and the interaxial angles  $\alpha$  (the angle between *b* and *c*),  $\beta$  (*a* and *c*), and  $\gamma$  (*a* and *b*).

The space group symmetry that is present imposes constraints on the interaxial angles and on the relative axial lengths (see [Table 1](#)). Thus, the three non-parallel three-fold axes present in a cubic system determine that  $a = b = c$  and  $\alpha = \beta = \gamma = 90^\circ$ . These geometrical constraints are a consequence of rather than a definition of the crystal symmetry. These constraints serve to divide crystal structures into seven crystal systems which, when combined with the possible centering operations, yield 14 types of Bravais lattice (see [Figure 1](#)).

**Table 1. The seven crystal systems**

Symmetry requirement	Crystal system	Symmetry constraints on unit cell parameters	Types of Bravais Lattices
1(E) or 1(i)	Triclinic	no conditions	P
2(C <sub>2</sub> ) or -2(m)	Monoclinic	$\alpha=\gamma=\pi/2$ (1st setting)	P, B
		$\alpha=\beta=\pi/2$ (2nd setting)	P, C
		$\beta=\gamma=\pi/2$ (3rd setting)	P, A
Three perpendicular 2-fold axes or mirror planes, or two mirror planes and one 2-fold axis	Orthorhombic	$\alpha=\beta=\gamma=\pi/2$	P, I F, C
4(C <sub>4</sub> ) or -4(S <sub>4</sub> )	Tetragonal	$a=b$ $\alpha=\beta=\gamma=\pi/2$	P, I
3(C <sub>3</sub> ) or -3(S <sub>6</sub> )	Trigonal	$a=b$ $\alpha=\beta=\pi/2$ $\gamma=2\pi/3$	P, R
	Rhombohedral*:		
	i) on Rhomb. axes	$a=b=c$ $\alpha=\beta=\gamma$	R
	ii) on Hex. axes	$a=b$ $\alpha=\beta=\pi/2$ $\gamma=2\pi/3$	
6(C <sub>6</sub> ) or -6(S <sub>3</sub> )	Hexagonal	$a=b$ $\alpha=\beta=\pi/2$ $\gamma=2\pi/3$	P
Four 3-fold axes	Cubic	$a=b=c$ $\alpha=\beta=\gamma=\pi/2$	P, I F

\* Rhombohedral: hexagonal cell centered at (2/3,1/3,1/3) obverse or at (1/3,2/3,1/3) reverse.

Figure 1. The fourteen Bravais lattices

The symmetry elements present may include point operations such as 1-, 2-, 3-, 4- or 6-fold proper rotations or -1, -2, -3, -4, or -6 rotary inversion operations or operations that entail an additional translation like screw rotations,  $M_n$  (which involve a  $360/M$  rotation and a shift of  $n/M$  times the unit cell length along the rotation axis) or  $a_n^-$ ,  $b_n^-$ ,  $c_n^-$ ,  $n^-$  or  $d$ -glide planes (which involve reflection through a mirror plane combined with a translation parallel to that plane). Cell centerings  $A$ ,  $B$ ,  $C$ ,  $R$ ,  $F$ , or  $I$  may also be present.

There are two conventions for describing such symmetry operations: the *Schoenflies* notation, used mainly by optical spectroscopists and the *Hermann-Mauguin* notation, preferred by crystallographers. As well as the symbols used (for example, the Schoenflies symbol for space group number 227 is  $O_h^7$ , the Hermann-Mauguin symbol is  $Fd-3m$ ) the systems differ in the definition of improper rotations.

In the Hermann-Mauguin notation, which is used predominantly to describe the space group symmetry of the point operations listed above, a 1-fold rotation corresponds to the identity operation, a -1 rotary inversion is a strict inversion and a -2 rotary inversion is identical with a mirror plane.

Both conventions are listed in the International Tables for Crystallography (Hahn 1983).

The symmetry operators describe the effect of a given symmetry element on a general position,  $xyz$ . They are  $3 \times 4$  matrix transformations expressed in terms of the unit cell, which map each of the atoms in the asymmetric unit onto other equivalent positions. Application of all of the symmetry operators to all

of the asymmetric unit atoms (with appropriate translations) generates a full unit cell from which the entire crystal structure can then be generated by translations alone.

The space group symmetry operators play a central role in crystal structure representation. The subsequent sections provide a more detailed discussion of the space group symmetry operators, the practical aspects of generating standard symmetry operators, and generation of extensions to the standard symmetry forms to provide more convenient and comprehensive use. Much of the following material is based on the International Tables for Crystallography (Hahn 1983) which is the reference standard for specific space group symmetry information.

### Space group definitions and conventions

A crystal can be constructed by applying the space group symmetry operators and lattice translations to those atoms comprising the asymmetric unit. The symmetry operators are conveniently expressed in matrix form. Each operation comprises a rotation or linear component and a translation component. The linear component describes one of the point operations (a 1-, 2-, 3-, 4-, or 6-fold proper rotation or a -1, -2, -3, -4, or -6 rotary inversion operation) and it is written as a  $3 \times 3$  matrix. The translation component can be expressed as a vector of order 3, representing the relative shifts along the crystallographic  $a$ ,  $b$ , and  $c$  directions. For a pure point operation, the translation components are all zero. For a screw-rotation or glide operation, one or more translation components will be non-zero.

The matrix and vector parts can conveniently be combined into a single, augmented  $4 \times 4$  pre- or left-multiplier matrix that combines the  $3 \times 3$  rotation/reflection matrix with the  $3 \times 1$  translation vector. A fourth row of leading zeros and a 1 are added to provide  $4 \times 4$  multiplier compatibility. Standard matrix multiplication can then be used to map point column vectors, also with an added row containing a 1, and to concatenate operators. Thus the new coordinates  $x'$  produced from the original coordinates  $x$  by the operation  $O$  are obtained by  $x' = Ox$ .

As an example, consider the atom that is located at  $(1/4, 1/4, 1/4)$  and the operator,  $O$ , which reflects this point through the  $y=0$  plane followed by translations of  $a/2$  and  $c/2$  (an  $n$ -glide operation perpendicular to  $b$ , as is found in space group  $P2_1/n$ ).

Let:

#### Eq. Th-1

$$O = \begin{bmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

#### Eq. Th-2

$$\begin{bmatrix} 3/4 \\ -1/4 \\ 3/4 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1/4 \\ 1/4 \\ 1/4 \\ 1 \end{bmatrix}$$

The symmetry operator matrices can be written in a shorthand xyz notation that is the augmented matrix mapping on the arbitrary point  $(x, y, z)$ . For the example above:

### Eq. Th-3

$$\begin{bmatrix} x + 1/2 \\ -y \\ z + 1/2 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1/2 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix}$$

Then by transposing the result and dropping the augmented 1:

### Eq. Th-4

$$(x + 1/2, -y, z + 1/2)$$

This is the form in which symmetry operators are presented in the International Tables.

A space group is a collection of symmetry operators that meets the four criteria necessary for forming a mathematical group:

- The set is closed. That is, the product of any two symmetry operator matrices in the space group is also a symmetry operator matrix in the space group.
- There is an identity operator. In this case the augmented matrix is just  $(x, y, z)$  in  $xyz$  notation.
- For each operator there is an inverse operator whose product is the identity operator. In other words, for every motion there is an equal but opposite motion.
- Operator multiplication is associative. This means that, while the order of the operators for multiplication is significant, the order in which the multiplications are performed is not.

Although any arbitrary set of symmetry operators can be collected, if the set does not form a group by satisfying these four criteria, it cannot be a sensible basis for constructing a crystal structure. The fact that the symmetry operators do form a group can be utilized in a number of ways. For example, this property permits generation of the full set of group members from a small subset of operators called the *generator set*, which can be defined in a variety of ways.

The properties of a group also limit the number of distinct ways in which the possible symmetry elements can be combined. There are only 230 distinct space groups. The symmetry in any given crystal structure can be assigned to one of these 230 space groups. In practice, many of the space groups are described in different settings, which represent different choices of labeling the three crystal axes  $a$ ,  $b$ , and  $c$  or a different choice of origin within the lattice.

## Symmetry group data

Three types of symmetry are handled in Materials Studio.

**Space groups** represent symmetry in structures that are periodic in 3 dimensions, i.e. crystals. There are 230 different space groups, although each one can be described in a number of ways (settings) according to the particular choice of lattice.

**Plane groups** represent symmetry in structures that are periodic in 2 dimensions, i.e. surfaces. There are 17 different plane groups. These can also be described in a number of different ways, although the use of different settings is less common than it is with space groups.

**Point groups** represent symmetry in structures that are nonperiodic. Point groups can be further subdivided.

**Crystallographic point groups** are those point groups that can transform an infinite set of lattice points (as used to describe a crystal lattice) into themselves.

**General point groups** include operations such as 5-fold rotations that cannot keep an infinite lattice invariant. These together with the crystallographic point groups form the more general complete set of point groups. There are 32 crystallographic point groups, some of which can have alternative settings if different reference systems are used. There are an infinite number of non-crystallographic point groups. Each of these types of symmetry will be described in more detail below.

## Space Group data

### General provision of data

The ability to model a full range of crystalline materials requires a comprehensive, general, and flexible treatment of space group symmetry. The long form of the Hermann-Mauguin symbol contains sufficient information to generate a full set of symmetry operators appropriate for the space group.

Unfortunately this decomposition treatment has its drawbacks. First, this symbol does not convey information about the location of the origin, preventing simple access to the different choices of origin either listed explicitly in the International Tables For Crystallography (Hahn 1983) or desired in a special application. Furthermore, the long form of the Hermann-Mauguin symbol is generally not used in publications and the short form is insufficient to specify several of the monoclinic settings unambiguously. Finally, a consistent derivation of the operators from the long form of the Hermann-Mauguin symbol would sometimes not yield the set of operators in the order in which they appear in the International Tables, even for certain standard space group settings. For example, compare space groups Fd-3 and Fd-3m.

To allow full generality while avoiding the three deficiencies of a decomposition method described above, sufficient information is provided for each space group in the form of a set of generators. A "composition series" (Ledermann 1976) is then used to generate the full set of operators for the given space group. This process involves the following:

1. The list of generators,  $\{G\}_n$ , appropriate for each space group is provided (see the Positions heading in the International Tables for the standard setting of any given space group).
2. An operator set,  $\{O\}_m$ , is built by adding a given generator, say  $G_i$ , to the current end of the operator set.
3. The generator entry is then multiplied by all its predecessors in the operator set and all new unique products are added to the end of the operator set. For example, if  $O_k = G_i O_l$  and  $O_k$  is not contained in  $O_{k-1}$  then  $O_k$  is added to the list.
4. Steps 2 and 3 are repeated until all generators are processed.
5. If the product of a generator with itself, say  $G_i^2$ , has not appeared previously as a distinct generator, then  $G_i^2$  is treated as a new generator upon addition to the operator list. It is multiplied by all predecessors, with unique products also being added to the operator list.

Each operator in the space group can then be specified in terms of an appropriate combination of the generators:

### Eq. Th-5

$$O_i = G_k G_j G_i \dots$$

where  $k \geq j \geq i$ .

By selecting and ordering the generators appropriately, the symmetry operators for each space group can be produced, referenced to the same origin, and placed in the order given in the International Tables.



## Alternative settings

For many centrosymmetric space groups, the International Tables provide two choices of origin. Invariably the second choice of origin has the inversion center(s) at the origin; the first choice has the inversion center(s) at some other position within the unit cell. Both choices of origin are provided here by explicit specification of the appropriate generators.

In monoclinic and orthorhombic space groups, different symmetry settings are possible based on alternative choices or labeling of axes. The long forms of the Hermann-Mauguin symbols are different in such cases and these alternative symbols are often encountered, particularly in the earlier crystallographic literature. For all alternative settings of the monoclinic space groups, the appropriate generator sets have been provided explicitly. For the orthorhombic family, space groups 16 to 74, the symmetry operators corresponding to the alternative settings can be generated from a new set of generators derived by appropriate transformation of those given for the standard setting (see, for example, International Tables, section 2.6, p. 18).

Each orthorhombic space group has six possible alternative settings, not all necessarily unique. Thus, the first axis can be labeled  $a$ ,  $b$  or  $c$ , and the second can be either of the two labels not chosen for the first. This *relabeling* amounts to a change of basis of the axis system to which the symmetry operators are referred. The International Tables represent the six alternative settings with the symbols:  $abc$ ,  $b-ac$ ,  $a-cb$ ,  $-c-ab$ ,  $-cba$ , and  $bca$ .

Diagrams are provided for each, but only for the standard setting,  $abc$ , are symmetry operators explicitly listed for the given space group number. The setting symbols are shorthand notation for the change of basis map necessary to convert from the standard setting basis vectors to the vectors of the new setting. Thus  $-c-ab$  implies that  $-z$  goes to  $x$ ,  $-x$  goes to  $y$  and  $y$  goes to  $z$ .

In those cases where fewer than six distinct alternative settings exist, the first symbol in this list which matches the input label is used. For example, if Bm2m (an alternative setting for space group number 35) is input then  $a-cb$  is used rather than  $bca$  which also corresponds to Bm2m.

## Plane group symmetry data

The 17 plane groups are listed in the International Tables in the same manner as the space groups. However the listings do not include the different settings that are available for many of the space groups.

Within Materials Studio, the plane groups are each derived from a list of generator operators, in the same manner as for space groups.

## Point group symmetry data

The 32 crystallographic point groups are each derived from a list of generator operators in a manner similar to that for space groups and plane groups. This is also the case for the two icosahedral point groups. Other groups of the general form  $C_n$ ,  $S_n$ ,  $C_{nh}$ ,  $C_{nv}$ ,  $D_n$ ,  $D_{nh}$ ,  $D_{nd}$  (where  $n$  is not 1, 2, 3, 4 or 6) are derived as required, as the required generators are easily determined from the name of the group.

## Systems with point group data

A point group is a set of symmetry operations, all of which leave at least one point unmoved. Thus, operations involving translations are excluded. There are two types of systems with point group symmetry.

Nonperiodic structures with symmetry relationships between atoms (or other objects in the structure). These symmetry relationships can include rotations about an axis (with any order of rotation, although 2, 3, 4, 5 and 6 are the most common), rotary inversions and reflections. There are also special cases of cylindrical and spherical symmetry which will be described briefly below.

Periodic structures in which the symmetry of the lattice points (other than those with translational components) can be described by point group symmetry. In these cases, the symmetry operations described by the point group must transform the infinite set of lattice points onto itself. As a result, a more restricted set of symmetry operations are permitted, with only 2-, 3-, 4- and 6-fold rotations being allowed, along with equivalent rotary inversions and reflections. This set of point groups is known as the set of Crystallographic point groups.

### General point groups

Point groups consist of sets of symmetry operations. There are two conventions for describing such symmetry operations: the *Schoenflies* notation, used mainly by optical spectroscopists and the *Hermann-Mauguin* notation, preferred by crystallographers. The following is a list, with brief descriptions, of the various types of point groups and point group operations that have been implemented.

1. *N*-Fold Rotation ( $n$  or  $C_n$ ; the Hermann-Mauguin symbol appears first, then the Schoenflies symbol). These symmetry sets are generated by specifying a rotation axis and angular rotation increment  $360^\circ/n$ .  
The result is a set of  $n$  rotation matrices (including the identity) which correspond to the  $n$  incremental positions. For example, specifying an  $n=3$  rotation about the z-axis would generate an identity matrix, plus a  $120^\circ$  rotation, plus a  $240^\circ$  rotation about z.
2. *N*-Fold Rotary Inversion ( $-n$  or  $S_n$ ). These symmetry sets are generated using a single *N*-fold rotation as described above and then adding another operation to each operator matrix (or position).  
For  $-n$  (Hermann-Mauguin notation), point inversion is applied and for  $S_n$  (Schoenflies), mirror reflection is applied to each operation. Input here consists of  $n$ , the rotation axis, and either an inversion point or mirror plane. Generally,  $n > 1$ , and for  $S_n$ ,  $n$  must also be even.
3. *N*-Fold Rotation with a Perpendicular Reflection ( $n/m$  or  $C_{nh}$ ). These symmetry sets are generated using *N*-fold rotation as described above and adding a mirror reflection perpendicular to the rotation axis for each operation (or position). Thus,  $C_{nh}$  is  $C_n$  with an additional mirror plane.
4. *N*-Fold Rotation with a Parallel Reflection ( $nm$  or  $C_{nv}$ ). These symmetry sets are generated using *N*-fold rotation as described above, combined with a mirror reflection containing the rotation axis for each operation (or position).
5. *N*-Fold Rotation with a Perpendicular 2-Fold Rotation ( $n_2$  or  $D_n$ ). These symmetry sets are generated using *N*-fold rotation as described above, combined with a 2-fold rotation perpendicular to the main rotation axis for each operation (or position).
6. *N*-Fold Rotation with a Perpendicular 2-Fold Rotation and a Perpendicular Reflection ( $n_2m$  or  $D_{nh}$ ). These symmetry sets are generated using *N*-fold rotation as described above, combined with a 2-fold rotation perpendicular to the main rotation axis as well as reflection in a mirror plane perpendicular to the main rotation axis.
7. *N*-Fold Rotation with a Perpendicular 2-Fold Rotation and a Parallel Reflection ( $-n_2m$  or  $D_{nd}$ ). These symmetry sets are generated using *N*-fold rotation as described above, combined with a 2-fold rotation perpendicular to the main rotation axis and a mirror reflection in a plane containing the main rotation axis, but perpendicular to the  $C_2$  axis.
8. Icosahedral Point Groups ( $235$  or  $I$ ,  $m-3-5$  or  $I_h$ ). There are two types which correspond to the non-crystallographic platonic solids, the regular icosahedron with 20 faces and 12 vertices and the related pentagonal-dodecahedron with 12 faces and 20 vertices. See International Tables, section 10.4, p. 779 for further details.
9. Cylindrical Point Groups ( $8m$  or  $C_{8v}$ ,  $8/mm$  or  $D_{8h}$ , etc.). These have circular symmetry about a rotation axis, and may also have a mirror plane perpendicular to the axis. Any molecules having cylindrical symmetry must be completely linear.

10. The Spherical Point Group (28 or  $K$ ,  $m-8$  or  $Kh$ ). This has spherical symmetry about a point. Any molecular structure having spherical symmetry must have just a single atom at the center of symmetry.

### Crystallographic point groups

Point group symmetry data is an intrinsic part of 3D crystal structure definition as described previously. Point groups have no translational periodicity or any symmetry operations that involve translations. There are 32 distinct crystallographic point groups. Each of these will transform a particular type of crystal lattice onto itself. Because the types of crystal lattice are described by the crystal system from which they are derived, the crystallographic point groups are often classified in the same manner.

The descriptive label of such a point group consists of either the Hermann-Mauguin or the Schoenflies point group label. Each of these labels effectively corresponds to a primitive space group whose symmetry operators can be returned in the same format as for the [space groups](#). However, for point groups the translation components of the  $4 \times 4$  augmented matrix will always be zero.

The labels and the corresponding space group numbers for the 32 crystallographic point groups are given in [Table 2](#) (see Burns and Glazer 1990 for more details).

**Table 2. Crystallographic point group labels**

Schoenflies	Hermann-Mauguin	Space Group Number
<b>Triclinic</b>		
C1	1	1
S2(Ci)	1	2
<b>Monoclinic</b>		
C2	2	3
C1h(Cs)	m	6
C2h	2/m	10
<b>Orthorhombic</b>		
D2	222	16
C2v	mm2	25
D2h	mmm	47
<b>Tetragonal</b>		
C4	4	75
S4	4	81
C4h	4/m	83
D4	422	89
C4v	4mm	99
D2d	-42m	111
D4h	4/mm	123

Schoenflies	Hermann-Mauguin	Space Group Number
<b>Trigonal</b>		
C3	3	143
S6(C3i)	3	147
D3	32 (312)	149
C3v	3m (3m1)	156
D3d	-3m (-31m)	162
<b>Hexagonal</b>		
C6	6	168
C3h	6	174
C6h	6/m	175
D6	622	177
C6v	6mm	183
D3h	-6m2	187
D6h	6/mmm	191
<b>Cubic</b>		
T	23	195
Th	m-3	200
O	432	207
Td	-43m	215
Oh	m-3m	221

### Surface systems and plane group operators

Crystalline materials have both translational periodicity in three dimensions and space group symmetry. The building blocks for the description of a crystal structure include a collection of "parent" atoms called the asymmetric unit, a 3D reference system called a lattice (whose basis is called the unit cell) and a space group that comprises a set of symmetry operators.

For some types of modeling, it is desirable to represent just a layer of the structure, as would be seen at the surface of a crystal. This can be represented by using surfaces, which are structures in Materials Studio which have periodicity in two dimensions, and which can also have symmetry. The symmetry within a two dimensional surface structure is known as plane group symmetry. Various tools, such as Cleave Surface and Build Vacuum Slab Crystal, are provided to allow the user to switch between a crystal and a surface representation of a structure.

Within Materials Studio, plane group symmetry is generated and processed in a manner identical to that used for space group symmetry.

The unit cell basis vectors, **u**, and **v**, are not necessarily orthogonal and are determined by the characteristics of the given material. The unit cell is usually described by the axial lengths, *u*, and *v*, and the interaxial angle  $\vartheta$  (the angle between *u* and *v*).

The plane group symmetry that is present imposes constraints on the interaxial angle and on the relative axial lengths (see [Table 1](#)). These geometrical constraints are a consequence of rather than a definition of the symmetry. The constraints serve to divide surface structures into four surface systems which, when combined with the possible centering operations, yield five types of lattice.

**Table 1. The four surface systems**

Symmetry requirement	Surface system	Symmetry constraints on unit cell parameters	Types of Lattices
None	Oblique	no conditions	P
A mirror or glide plane	Rectangular	$\vartheta = \pi/2$	P, C
A three-fold axis	Hexagonal	$u = v, \vartheta = 2\pi/3$	P
Two mirror or glide planes	Square	$u = v, \vartheta = \pi/2$	P

The symmetry elements present may include the point operations 1-, 2-, 3-, 4- or 6-fold rotations, mirror or glide operations, or C cell centering.

## Finding space group symmetry

The Materials Visualizer [Find Symmetry](#) function identifies space group symmetry operations in crystal lattices and classifies them according to the conventions described in the International Tables for Crystallography (Hahn 1983). It does this using the following procedure:

1. It establishes the point group symmetry of the 3D lattice, using a quaternion-based representation of proper and improper rotations in 3D space. You can specify a capture distance for lattice points in real space, and then force low symmetry lattices into higher symmetry.
2. It identifies the space group operators, and for each point group operation identified in step 1, attempts to find a translational vector such that the combination of point group operation and translational vector is a valid space group operation within the capture distance.
3. It classifies the space group, in two steps. First, it identifies the actual point group of the unit cell including the unit cell contents. Second, it determines the transformation into a conventional setting, including any origin shift.

## Dialogs in symmetry

Most symmetry tasks in Materials Studio can be performed using dialogs which can be accessed from the Build menu or the Symmetry toolbar.

### Find Symmetry dialog

The Find Symmetry dialog allows you to find symmetry and apply it to the current crystal or nonperiodic structure.

**Note:** It is not possible to use *Find Symmetry* to search for symmetry in surfaces.

If the current structure is a crystal, you can also redefine the symmetry so that it matches the space group found.

If the current structure is nonperiodic, you can reset the coordinates of the atoms and beads so that they are exactly consistent with the symmetry found.

The Find Symmetry dialog contains the following tabs:

- [Find](#): Allows you to search for symmetry and display details of the symmetry group located.
- [Options](#): Allows you to control the behavior of the *Find Symmetry* tool.

**Impose Symmetry:** Redefines the symmetry of the current structure to match that located by the *Find Symmetry* operation and displayed in the *Results* pane, then closes the dialog.

*Impose Symmetry* is enabled only if some or all of the current symmetry settings are different from those located by *Find Symmetry*.

After pressing *Impose Symmetry* you will not be able to move atoms in ways which would violate the [symmetry constraints](#) of the new symmetry group.

**Note:** The *Impose Symmetry* button is visible only when the current 3D model is a periodic structure.

**Snap to Symmetry:** Resets the coordinates of the atoms in the current structure such that they are consistent with the symmetry located by the *Find Symmetry* operation.

*Snap to Symmetry* is enabled only if a non-trivial point group is located by *Find Symmetry*.


In the present implementation, *Snap to Symmetry* does not define any symmetry relationships between objects and consequently, no symmetry constraints are imposed. Therefore after pressing the *Snap to Symmetry* button you will be able to move atoms in ways which would violate the new symmetry.

**Note:** The *Snap to Symmetry* button is visible only when the current 3D model is a nonperiodic structure.

**Cancel:** Closes the dialog without updating the symmetry.

**Help:** Displays the Help topic for the current tab.

### Access methods

Menu	Select <i>Build</i>   <i>Symmetry</i>   <i>Find Symmetry</i>
Toolbar	

### Find tab

The *Find* tab allows you to search for symmetry and display details of the symmetry group located.


**Find Symmetry:** Searches for symmetry in the current 3D model document using the specified *Tolerance* and displays any results in the *Results* pane.

**Find Symmetry | Copy Script:** Converts the current settings to a script and copies the script to the clipboard. Refer to the *Generating scripts* topic for more information on using sections of scripts generated from a dialog.

**Tolerance:** Specify how closely the positions of atoms and beads in the symmetrized structure must match those in the original structure.

**Results:** Displays brief details of the symmetry group located, the deviation from that symmetry, and other relevant information. For periodic structures, the new lattice is also shown.

## Access methods

Menu	<i>Build   Symmetry   Find Symmetry   Find</i>
Toolbar	 / <i>Find</i>

## Options tab

The *Options* tab allows you to control the behavior of the Find Symmetry tool.

**Re-orient structure after update:** When checked, indicates that after a *Find Symmetry* operation, the updated structure will be reoriented so that the symmetry axes are aligned with the Cartesian axes, according to the *Orientation standard* specified on the [Lattice Parameters dialog](#). Default = **unchecked**.

**Re-generate display visibility after update:** When checked, indicates that after the symmetry has been imposed, the appearance of the atoms and beads will be updated so that the view is consistent with the current display options. Default = **checked**.

**Force to standard setting:** When selected, indicates that the Find Symmetry tool will only use the standard setting of the located space group.

**Attempt to maintain current lattice alignment:** When selected, indicates that the Find Symmetry tool will use any setting of the located space group that allows the alignment of the current lattice to be retained.

**Note:** The *Force to standard setting* and *Attempt to maintain current lattice alignment* options are enabled only if the current structure is a crystal.

**Use these properties to distinguish symmetry images:** Select the set of properties that the Find Symmetry tool will use to distinguish symmetry images by checking the appropriate checkboxes in the list. Available options are:

- *Composition* - The component elements present in a mixture atom or, for normal/pure atoms, the element type or, for beads, the bead type


**Note:** This option is always selected and cannot be deselected. For beads this is the only distinguishing property that is used.

- *Occupancy\** - The degree to which a location in space is occupied
- *ForcefieldType* - The type ascribed to the atom for use with a forcefield, such as Forcite
- *FormalSpin* - An integral count of unpaired electrons that contribute to the net magnetic moment of an atom
- *Spin\** - A value set by computational servers that indicates the net spin in the region around an atom
- *FormalCharge\** - The charge on an atom assuming that all bonds to the atom are purely covalent
- *Charge\** - A value set by computational servers that indicates the point charge at an atom
- *MassNumber* - The isotope mass of an atom
- *OxidationState* - A value assigned to an atom assuming that all bonds to the atom are purely ionic
- *Hybridization* - The hybridization of the valence orbitals of an atom
- *NumBonds* - The number of bonds connecting to an atom
- *CoreShellWithHole* - A hole in one of the core shells of an atom
- *HubbardU* - A parameter which allows [correlation effects](#) to be included in density functional calculations

All the properties listed above can also be viewed (and, in some cases, edited) via the Properties Explorer when the relevant atoms are selected.

**Tip:** The properties marked with \* are floating point quantities. When these properties are used to distinguish candidate symmetry images, atoms with values differing by more than 0.05 are deemed to be inequivalent.

### Access methods

Menu	<i>Build   Symmetry   Find Symmetry   Options</i>
Toolbar	 / Options

## Lattice Parameters dialog

Lattice parameters determine the length and relative orientation of the lattice vectors in space. In crystals and surfaces, these lattice vectors determine how each atom is repeated periodically.


The Lattice Parameters dialog allows you to inspect and modify the values of the lengths and angles of the lattice vectors of the current crystal or surface. The dialog can remain open while you work with other Materials Studio modules.

The Lattice Parameters dialog contains the following tabs:

- [Parameters](#): Allows you to inspect and modify the values of the lengths and angles of the lattice vectors of the current crystal or surface.
- [Advanced](#): Allows you to set the lattice origin and orientation.

**Help:** Displays the Help topic for the current tab.

### Access methods

Menu	<i>Build   Symmetry   Lattice Parameters</i>
Toolbar	

## Parameters tab

The *Parameters* tab allows you to inspect and modify the values of the lengths and angles of the lattice vectors of the current crystal or surface.

**Lattice type:** Displays the lattice type of the selected symmetry group.

If the lattice parameters are constrained to certain values by the specified symmetry, these constraints are shown and the appropriate text boxes are disabled.

**Lengths:** Specify the values of the lattice parameters  $a$ ,  $b$  and  $c$  (crystal) or  $u$  and  $v$  (surface) which determine the lengths of the lattice vectors.


The spin controls beside each text box change the current values by 0.2 Å.

**Angles:** Specify the values of the lattice parameters  $\alpha$ ,  $\beta$  and  $\gamma$  (crystal) or  $\vartheta$  (surface), which determine the relative orientation of the lattice vectors.

The spin controls beside each text box change the current values by 1.0 degree.



## Access methods

Menu	<i>Build   Symmetry   Lattice Parameters   Parameters</i>
Toolbar	 / <i>Parameters</i>

### Advanced tab

The *Advanced* tab allows you to set the lattice origin and orientation.

**Cell Origin:** Specify the origin of the lattice.

When a new origin is specified a bulk move of the symmetry system will be performed. The fractional coordinates will remain unchanged, however the Cartesian coordinates will be affected.

**Orientation standard:** Specify the rule used to align the lattice with respect to the Cartesian axes. The *Orientation standard* determines how changes to the cell parameters are interpreted.

**Note:** Changing the *Orientation standard* does not affect the current orientation of the lattice. Thus, there is no guarantee that the lattice will actually be aligned according to the current value of the *Orientation standard*, unless the *Reorient to standard* button is pressed.


**Note:** The *Cerius<sup>2</sup> standard* is [C along Z, B in YZ plane](#) and the *Insight II standard* is [A along X, B in XY plane](#).

**Re-orient to standard:** When pressed, realigns the lattice to match the *Orientation standard*.

**Keep fractional coordinates fixed during changes to the lattice:** When checked, indicates that the [fractional coordinates](#) of objects in the asymmetric unit will remain unchanged when changes are made to the lattice parameters. Default = [checked](#).

**Note:** If *Keep fractional coordinates fixed during changes to the lattice* is unchecked the Cartesian coordinates of all objects in the asymmetric unit will be fixed and the coordinates of any symmetry copies will be recalculated. In addition, certain changes to cell parameters may not be allowed for some structures, due to symmetry constraints. In these situations Materials Studio displays a warning message.

## Access methods

Menu	<i>Select Build   Symmetry   Lattice Parameters   Advanced</i>
Toolbar	 / <i>Advanced</i>

### Redefine Lattice dialog

The Redefine Lattice dialog allows you to define new lattice vectors for the current crystal or surface in terms of the existing ones.

**Note:** Redefining the lattice removes all symmetry relationships within the unit cell. As a result, the new structure will have P1 (crystal) or p1 (surface) symmetry.

**Tip:** To convert the current lattice to its [primitive or conventional representation](#) without losing any symmetry information, select *Build | Symmetry | Primitive Cell* or *Conventional Cell* from the menu bar.

The Redefine Lattice dialog contains the following tabs:

- [New Lattice](#): Allows you to specify new lattice vectors for the current crystal or surface in terms of the existing ones.
- [Options](#): Allows you to control how the new lattice will be oriented after redefinition.

**Redefine:** Performs checks to ensure that the vectors specified on the [New lattice](#) tab:

- are lattice vectors of the current lattice
- are independent of each other
- form a right-handed set (if the layered structure is to be a crystal)

If the specified vectors are acceptable, the lattice is then redefined. If the specified vectors fail any of the checks, the *Redefine* operation is canceled and you are prompted to specify alternative vectors.

**Note:** When the lattice is redefined all symmetry relationships within the unit cell are removed. As a result the new lattice will have P1 (crystal) or p1 (surface) symmetry.

**Help:** Displays the Help topic for the current tab.

#### Access methods

Menu *Build | Symmetry | Redefine Lattice*

#### New Lattice tab

The *New Lattice* tab allows you to specify new lattice vectors for the current crystal or surface in terms of the existing ones.

**Enter new lattice parameters in terms of old:** Specify new lattice vectors *A*, *B* and *C* (crystal) or *U* and *V* (surface) separated by spaces, in terms of the existing ones. For example, to transpose the *a* and *b* axes in a crystal type:

*a: 0 1 0, b: -1 0 0, c: 0 0 1*

**Note:** It is necessary to invert one of the axes in order to generate a right-handed set of lattice vectors.

The values of the new lattice parameters and the volume of the new lattice, relative to the old one, are also displayed.

**Note:** The new lattice vectors must be lattice vectors of the existing lattice. However, in [lattices with centering](#), the new lattice vectors can refer to centering points. In such lattices, the new lattice vectors can be specified using non-integer values.

#### Access methods

Menu *Build | Symmetry | Redefine Lattice | New lattice*

#### Options tab

The *Options* tab allows you to control how the new lattice will be oriented after redefinition.

**Re-orient structure after redefinition:** When checked, indicates that after the lattice has been redefined, the new lattice will be reoriented to match the *Orientation standard* of the original lattice. Default = [unchecked](#).

### Access methods

Menu	<a href="#">Symmetry</a>   <a href="#">Redefine Lattice</a>   <a href="#">Options</a>
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## Show Symmetry dialog

The Show Symmetry dialog displays information about the symmetry of the current structure.

The information displayed depends on the context in which you open the dialog. The label changes to reflect the context:

If you open the Show Symmetry dialog from the *Symmetry* menu or the Symmetry toolbar, the symmetry information displayed relates to the current structure. The dialog can remain open while you work with other Materials Studio modules.

If you open the Show Symmetry dialog using the *Details* buttons on the Space Group or the Plane Group tabs of the crystal or surface builders, a separate instance of the dialog appears and the details displayed relate to the currently selected symmetry group. In this case, the dialog closes when the parent Build Crystal or Build Surface dialog is closed.


The Show Symmetry dialog contains the following tabs:

- [Symmetry Group](#): Displays general information about the current symmetry group.
- [Operators](#): Displays details of the individual operators of the current symmetry group with the position and description of each symmetry element in [shorthand notation](#).

**Note:** A more comprehensive list of [parameters](#) relating to the symmetry of the current system can be displayed and edited with the Properties Explorer.

**Help:** Displays the Help topic for the current tab.

### Access methods


Menu	<a href="#">Build</a>   <a href="#">Symmetry</a>   <a href="#">Show Symmetry</a>
	<a href="#">Build</a>   <a href="#">Crystals</a>   <a href="#">Build/Rebuild Crystal...</a>   <a href="#">Space Group</a>   <a href="#">Details</a>
	<a href="#">Build</a>   <a href="#">Surfaces</a>   <a href="#">Build/Rebuild Surface...</a>   <a href="#">Plane Group</a>   <a href="#">Details</a>
Toolbar	

## Symmetry Group tab

The *Symmetry Group* tab displays general information about the current symmetry group.

**Note:** A more comprehensive list of [parameters](#) relating to the symmetry of the current system can be displayed and edited with the Properties Explorer.

## Access methods


Menu	<i>Build   Symmetry   Show Symmetry   Symmetry Group</i> tab
	<i>Build   Crystals   Build/Rebuild Crystal...   Space Group   Details   Symmetry Group</i>
	<i>Build   Surfaces   Build/Rebuild Surface...   Plane Group   Details   Symmetry Group</i>
Toolbar	 / <i>Symmetry Group</i>

## Operators tab

The *Operators* tab displays details of the individual operators of the current symmetry group with the position and description of each symmetry element in [shorthand notation](#).

**Note:** A more comprehensive list of [parameters](#) relating to the symmetry of the current system can be displayed and edited with the Properties Explorer.

## Access methods

Menu	<i>Build   Symmetry   Show Symmetry   Operators</i>
	<i>Build   Crystals   Build/Rebuild Crystal...   Space Group   Details   Operators</i>
	<i>Build   Surfaces   Build/Rebuild Surface...   Plane Group   Details   Operators</i>
Toolbar	 / <i>Operators</i>

## Supercell dialog

The *Supercell* dialog allows you to create a supercell from the current crystal or surface. A supercell has lattice vectors which are integral multiples of their equivalents in the original lattice. Supercells always have P1 (crystal) or p1 (surface) symmetry.

**Supercell range:** Specify the size of the superlattice to be created.

**Note:** The text box labels depend on the structure in focus. For a crystal the directions are labeled *A*, *B*, and *C*. For a surface the directions are labeled *U* and *V*.

When you open the dialog or change the current structure, the values of the superlattice vectors are set to the integer equivalents of the display range for the structure.

**Create Supercell:** Creates supercell of the size specified in *Supercell range*.

**Create Supercell | Copy Script:** Converts the current settings to a script and copies the script to the clipboard. Refer to the Generating scripts topic for more information on using sections of scripts generated from a dialog.

All symmetry relationships within the cell of a crystal or surface are removed. The resultant structure has P1 (crystal) or p1 (surface) symmetry.

**Note:** The *Create Supercell* button is enabled only if the current structure is a crystal or a surface.

**Help:** Displays the Help topic in a browser.

## Access methods

Menu	<i>Build   Symmetry   Supercell</i>
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