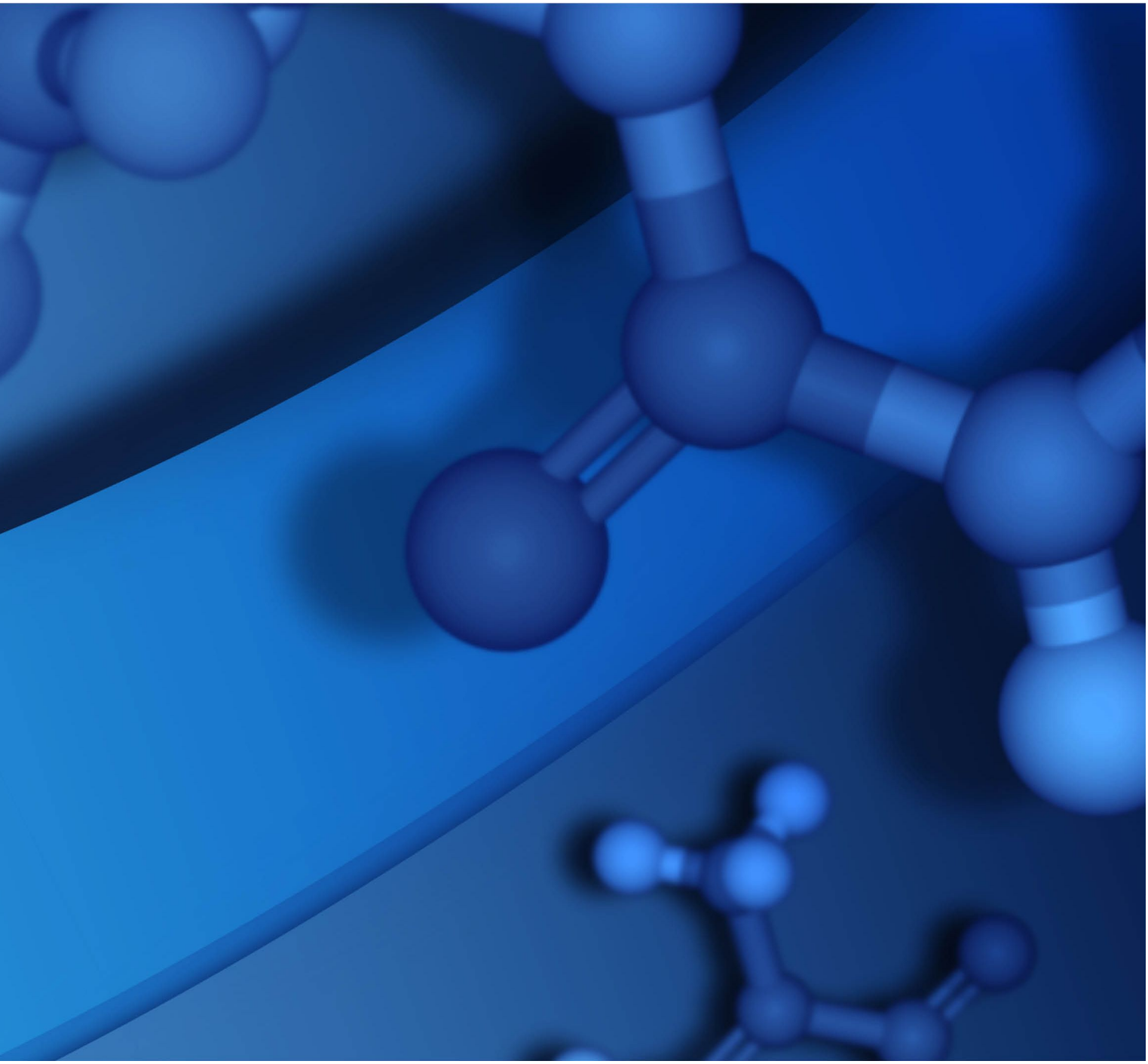
DASSAULT SYSTEMES

BIOVIA

VISUALIZER TUTORIALS

MATERIALS STUDIO

8.0



Acknowledgments and References

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Contents

Tutorials

This section contains tutorials for the products you have installed. The Quick start tutorials provide an overview of the functionality available in the Materials Visualizer. For a more in-depth introduction to the basic features of the Materials Visualizer, see the Visualizer tutorials.

Note: Numbers in the tutorials are shown in American English format. If your system is configured for a different locale, you should "translate" the numbers to the format appropriate to your locale before entering them.

For example, if your system is configured for the German locale, and a tutorial asks you to enter a value of 5,000 (five thousand), you should enter 5.000.

Quick start tutorials

The Quick start tutorials introduce you to some of the basic features of Materials Studio. After reading or working through these tutorials, you will be prepared to start working with Materials Studio.

Quick start covers the following tasks:

- Creating a project
- Opening and viewing 3D documents
- Sketching a benzamide molecule
- Viewing and working with study table and chart documents
- Working with a molecular crystal: studying urea
- Building an α-quartz crystal
- Building poly(methyl methacrylate)
- Saving a project and finishing up

Note: These instructions assume that you will run through all the Quick start tutorials from start to finish without closing and reopening Materials Studio. If you do wish to close Materials Studio, it is recommended that when you start the program again, you load the my quickstart project created in the Creating a project tutorial.

Note: All numbers given in the tutorial are in American English format. See the Localization topic for more information.

Creating a project

Purpose: Provides an introduction to the concept of a project in Materials Studio.

Modules: Materials Visualizer

Time:

Prerequisites: None

Introduction

To make the management of documents and workflow as easy as possible, Materials Studio uses the concept of projects. You can view and manage your project data during your Materials Studio session by using the Project Explorer. This system allows you to save, reload, and share Materials Studio projects and to send data and results to other users, either in the form of individual documents or as complete projects.

This tutorial shows you how to start a new project. The project you create can then be used for all the other tutorials in the Quick start section.

This tutorials covers:

- To start Materials Studio
- To create a project
- To restore default projects settings

Note: You cannot work within Materials Studio without either creating a new project or opening an existing one.

More detailed instructions on how to use the Project Explorer can be found in the Project management tutorial.

1. To start Materials Studio

Select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

If you have a Materials Studio icon on your desktop, you can also start Materials Studio by double-clicking on this icon.

When you start Materials Studio, it opens with a dialog called Welcome to Materials Studio. You must either create a new project or load an existing project from this dialog.

Note: If you are starting Materials Studio for the first time, you may see a dialog called Materials Studio File Associations. If this is the case, follow the instructions in this dialog and click the *OK* button.

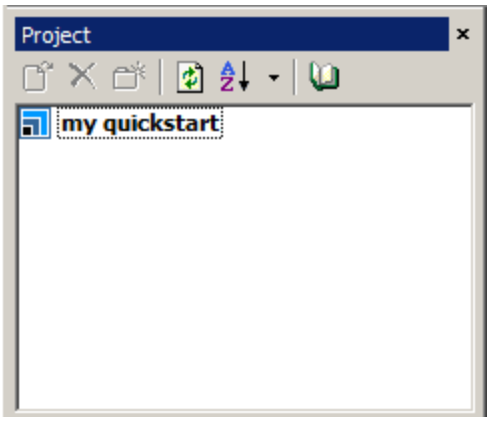
2. To create a project

On the Welcome to Materials Studio dialog, select **Create a new project** and then click the **OK** button.

This opens the New Project dialog.

Select a file location where the project will be stored and enter **my quickstart** in the **File name** field, then click the **OK** button.

This starts your Materials Studio session, working with a project called my quickstart. The Project Explorer should now look like this:



Project Explorer showing the my quickstart project

You have created a new Materials Studio project.

3. To restore default project settings

By default, every new project you create uses the settings defined in the template project that is automatically created by Materials Studio in your Windows user profile, for example, `C:\Users\[user name]\AppData\Roaming\Accelrys\Materials Studio\8.0\Templates\Normal.stp` on

Windows. For the purposes of these tutorials, you need to ensure that all the settings in the my quickstart project are set to their Accelrys default values.

Select **Tools | Settings Organizer** from the menu bar to display the Settings Organizer dialog.

The Settings Organizer dialog allows you to define a template project containing default settings for Materials Studio modules and various tools in the Materials Visualizer. You can also use the Settings Organizer dialog to exchange settings from external projects into the current project or to restore any of the settings in the current project to their Accelrys default values.

On the Settings Organizer dialog, click on the Materials Studio icon at the top of the tree view in the **All settings in current project** window to select all the modules and Visualizer tools. Click the **Reset** button.

All the default settings for the selected Materials Studio modules and Materials Visualizer tools are reset to their Accelrys default values.

Opening and viewing 3D documents

Purpose: Provides an introduction to the concept of documents in Materials Studio.

Modules: Materials Visualizer

Time:

Prerequisites: Creating a project

Introduction

Materials Studio employs a variety of different document types - 3D Atomistic and Mesoscale, text, chart, HTML, study table, grid, script, and forcefield documents. In the Quick start tutorials, you will work primarily with the 3D Atomistic document type. Documents are managed within projects, which record the general workflow as documents are created and saved.

This tutorial covers:

- To import a structure
- To adjust display styles
- To change the view of 3D structures
- To select various types of objects

You should carry out this tutorial in the **my quickstart** project you created in the Creating a project tutorial.

1. To import a structure

The Materials Visualizer enables you to open a document in the 3D Viewer and adjust the graphical display style of the structure that you are viewing using an array of convenient tools.

Select **File | Import...** from the menu bar.

The Import Document dialog is displayed.

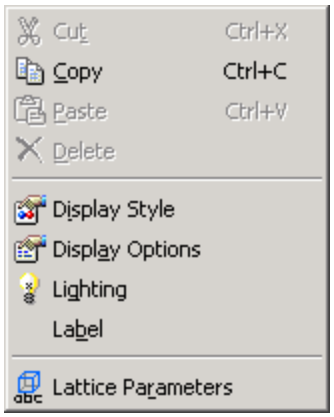
Note: This dialog can also be opened using the *Import* button  on the *Standard* toolbar.

Navigate to and select **Examples/Documents/3D Model/TON.msi**, then click the **Open** button.

A 3D Viewer containing the conventional zeolite Theta-1 unit cell is displayed. A document called `TON.xsd` is now shown as part of the my quickstart project in the Project Explorer. Note that the file extension has changed from `.msi` to `.xsd`, the XML-based native Materials Studio format for 3D structures.

2. To adjust display styles

Right-click in the 3D Viewer to display the shortcut menu, select **Display Style** from the list.



Shortcut menu

This opens the Display Style dialog.

On the **Atom** tab, click on each option in the **Display style** section to view the structure using the **Line**, **Stick**, **Ball and stick**, **CPK**, and **Polyhedron** display styles. When you have finished, return to the **CPK** display style.

Select the **Lattice** tab of the Display Style dialog.

The *Lattice* tab contains controls for changing the periodic lattice display style.

In the **Lattice** section, select the **None**, **Dashed line**, **Line**, and **Stick** styles in turn. Note their effect on how the lattice is displayed in the 3D Viewer.

Make sure that the lattice display style is set to **Line**.

The tabs available on the Display Style dialog are dependent on the type of objects present in the active document.

Right-click in the 3D Viewer and select **Lighting** from the shortcut menu.

This opens the Lighting dialog. The *Preview* box on the left-hand side of the dialog displays a sphere with an arrow on its surface. You can use this control to change the settings for up to three light sources.

Hover the mouse cursor over the sphere until the cursor changes to a hand. Click and drag over the sphere to change the direction of the incoming light, indicated by the arrow.

The lighting in the 3D view of TON.xsd responds interactively as you move the arrow.

Close the Lighting dialog by clicking on the **Close** button in the top right.

On the **Atom** tab of the Display Style dialog, select the **Ball and stick** option. Click the **Close** button to close the Display Style dialog.

3. To change the view of 3D structures

3D structures can be manipulated in a variety of different ways using the buttons on the *3D Viewer* toolbar.

3D Viewer toolbar

You can perform simple manipulations of a structure in the 3D Viewer by choosing the rotation, zoom, and translation mode buttons on this toolbar. Clicking on any of these and then left-clicking and dragging in the 3D Viewer causes an associated transformation of the view.

Click each of the tools associated with the following actions and drag the cursor around inside the 3D Viewer:

3D Viewer Rotation Mode: Rotates the view of the structure.

3D Viewer Zoom Mode: Dragging the cursor upward or to the right enlarges the view of the structure (zooms in); dragging the cursor downward or to the left decreases the structure's visual size (zooms out).

3D Viewer Translation Mode: Moves the structure to different points in the plane of your computer screen.

Mouse and key combinations are provided to enable you to rotate, zoom, or translate in any mode. The right mouse button can also be used for rotation in any mode. Materials Studio employs trackball rotation. Moving the cursor over the middle of the 3D Viewer causes the structure to rotate in the direction of cursor motion and moving the cursor at the edge of the 3D Viewer causes the structure to rotate in the plane of the screen.

While in **3D Viewer Translation** mode, right-click and drag the mouse. This will rotate the view.

A full list of mouse and key operations can be found in the Mouse and keyboard actions help topic.

Try the following tools to change the position of the structure in the 3D Viewer:

 **3D Viewer Reset View:** Resets the view to its original position and orientation within the window.

 **3D Viewer Recenter:** Recenters the current view with respect to selected atoms or the entire structure.

 **3D Viewer Fit to View:** Chooses an appropriate size for the structure based on the size of the window.

4. To select various types of objects

The selection mode enables you to select objects in the 3D Viewer.

On the **3D Viewer** toolbar, click the **3D Viewer Selection Mode** button  and then select a single atom in the TON structure by clicking on it.

The atom changes color to yellow to show it has been selected.

Click on any bond.

The bond changes color to yellow to show it has been selected.

Left click and drag diagonally over an area of the structure.

This draws a selection box and selects any objects (atoms and bonds in this case) inside the box.

Double-click on any atom or bond in the TON structure.

This selects the whole structure.

Click or double-click anywhere in the 3D Viewer away from the structure to deselect everything.

Click the **Close** button  to close the 3D Viewer. When you are prompted to save the document as part of the project, click the **Yes** button.

Sketching a benzamide molecule

Purpose: Provides an introduction to the sketching tools available in the Materials Visualizer.

Modules: Materials Visualizer

Time: 

Prerequisites: Creating a project

Introduction

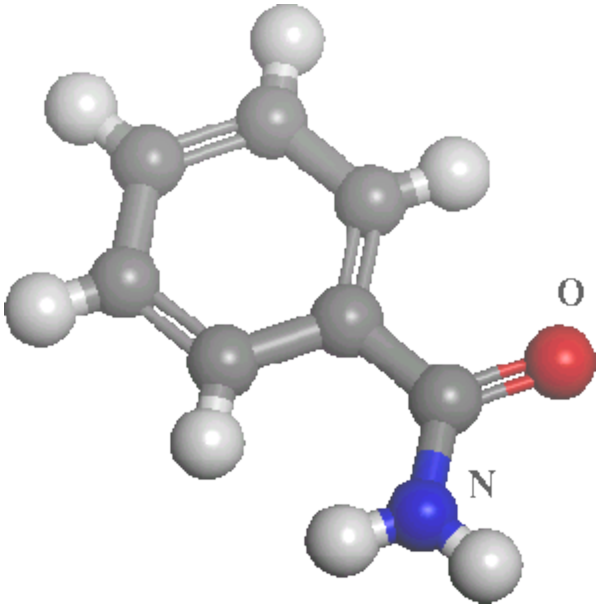
Chemists have to deal with a wide range of small molecules and chemical intermediates on a daily basis. To be able to easily create models of such molecules is important in any molecular modeling environment. Benzamide is a typical example of a small molecule that might be created and studied with Materials Studio.

This tutorial covers:

- To create a new 3D Atomistic document
- To change to ball and stick default display style
- To sketch the ring and atom chain
- To sketch with oxygen
- To edit the element type
- To edit the bond type
- To adjust Hydrogen and Clean
- To convert from Kekulé to resonant bond representation
- To monitor and adjust distances

You should carry out this tutorial in the **my quickstart** project you created in the Creating a project tutorial.

This is the structure of benzamide that you will be building:



Benzamide

1. To create a new 3D Atomistic document

Select **File | New...** from the menu bar to open the New Document dialog. Select **3D Atomistic** and click the **OK** button.

This opens a new 3D Viewer. A corresponding item called 3D `Atomistic.xsd` is shown in the Project Explorer.

Right-click on the **3D Atomistic.xsd** item in the Project Explorer and select **Rename** from the shortcut menu. Type **my_benzamide** and press the **ENTER** key.

Select **File | Save** from the menu bar or click the **Save** button  on the **Standard** toolbar.

You have created a new 3D Atomistic document called `my_benzamide.xsd` in the my quickstart project.

2. To change to ball and stick default display style

Materials Studio's versatile sketching tools allow you to sketch in any display style. For this example, you will use ball and stick as the default display style.

Select **Modify | Default Atom Style** from the menu bar.

This opens the Default Atom Style dialog.

Select the **Ball and stick** option from the **Display Style** section. Click the **Close** button  in the top right corner to close the Default Atom Style dialog.

The default display style for this project is set to ball and stick.

3. To sketch the ring and atom chain

Click the **Sketch Ring** button  on the **Sketch** toolbar. Move the mouse cursor to the 3D Viewer.

The cursor now looks like a pencil to show that you are in sketching mode. The number next to the cursor indicates the size of the ring about to be sketched. You can change the ring size by pressing any number key on the main keyboard from 3 to 8.

Check that the number beside the cursor is **6**. Left-click in the 3D Viewer.

A six-membered carbon ring is sketched. Note that holding down the ALT key and clicking the left mouse button sketches an aromatic ring with resonant bonds.

Click the **Sketch Atom** button  on the **Sketch** toolbar.

You have chosen the general atom sketching tool, which can sketch with any element. By default, it sketches with carbon. You will attach a two-carbon side chain to the ring.

Hover the cursor over one of the carbons in the ring until it is highlighted in blue, then left-click to anchor the bond to this carbon. Move the cursor and left-click again to sketch a carbon atom, then move the cursor again and double-click to terminate the two-carbon chain attached to the carbon ring.

Another way of terminating the chain would be to click once to sketch the final carbon atom and then press the ESC key. Notice that bonds are added automatically between the newly sketched atoms.

Note: You can undo any mistakes that you make by clicking the *Undo* button  on the *Standard* toolbar.

4. To sketch with oxygen

On the **Sketch** toolbar, click on the options arrow  associated with the **Sketch Atom** button  to show a list of alternative elements for sketching.

Select **Oxygen**. Hover the cursor over the first carbon of the side chain and, when it is highlighted in blue, left-click to anchor the bond to this carbon. Now move the cursor away from this point and double-click to sketch an oxygen atom and terminate the chain.

Click the **3D Viewer Selection Mode** button  on the **3D Viewer** toolbar. (If the **3D Viewer** toolbar is not displayed, select **View | Toolbars** from the menu bar and choose **3D Viewer**).

You are now in selection mode.

5. To edit the element type

Click on the end carbon in the side chain to select it.

When selected correctly, it is highlighted in yellow.

Click on the options arrow associated with the **Modify Element** button  on the **Sketch** toolbar to show a list of elements. Choose **Nitrogen**.

Click anywhere in the 3D Viewer to deselect the atom.

The carbon atom has changed to a nitrogen atom.

6. To edit the bond type

In the 3D Viewer, click the center of the **C-O** bond to select it.

When the bond is selected, it is highlighted in yellow.

Hold down the **SHIFT** key and then click on three alternate bonds in the carbon ring.

You should now have four bonds selected: three C-C bonds in the carbon ring and the C-O bond.

Click on the options arrow associated with the **Modify Bond Type** button  on the **Sketch** toolbar and select **Double Bond** from the dropdown list.

All four selected bonds change to double bonds.

Deselect everything by clicking anywhere away from the structure in the 3D Viewer.

7. To adjust Hydrogen and Clean

Now you can add hydrogens automatically to the structure, without having to sketch them individually.

Click the **Adjust Hydrogen** button on the **Sketch** toolbar to add the appropriate number of hydrogen atoms to the structure.

Tidy the geometry of the structure by clicking the **Clean** button on the **Sketch** toolbar.

This modifies the geometry of the structure so that bond lengths, angles, and torsions are chemically reasonable.

8. To convert from Kekulé to resonant bond representation

Materials Studio's Bond Calculation tool allows easy conversion of the bonding representation between Kekulé and resonant.

Select **Build | Bonds** from the menu bar.

This opens the Bond Calculation dialog.

In the **Options** section of the **Bonding Scheme** tab, make sure that **Convert representation to** is checked and click on the options arrow associated with the list box to the right (which is set to **Kekule** by default).

Select **Resonant** from the dropdown list and click the **Calculate** button. Clicking the **Close** button to close the Bond Calculation dialog.

The bonds in the phenyl ring are now displayed as resonant. In this example, however, you will retain the Kekulé bonding representation.

Select **Edit | Undo Calculate Bonds** from the menu bar or, alternatively, click the **Undo** button on the **Standard** toolbar.

The bond calculation is undone and the bonding in the phenyl ring reverts to the Kekulé representation.

Note: You can undo multiple steps by clicking on the options arrow associated with the *Undo* button .

9. To monitor and adjust distances

You can monitor and adjust distances, angles, and torsions in any structure in Materials Studio using the *Measure/Change* tool on the *Sketch* toolbar.

Measure/Change tool

Click on the options arrow associated with the **Measure/Change** button  . Select **Distance** from the dropdown list.

Hover the cursor over the oxygen atom until it is highlighted in blue and then left-click with the mouse. Repeat this action on the carbon atom to which the oxygen atom is bonded.

A distance monitor appears, with the distance displayed in Å.

With the cursor in the 3D Viewer, away from the molecule, left-click and drag the cursor upwards to increase the C-O bond length. Click the **Clean** button  .

The numerical display of the distance monitor changes to reflect the increase in bond length and the decrease as a result of the cleaning process.

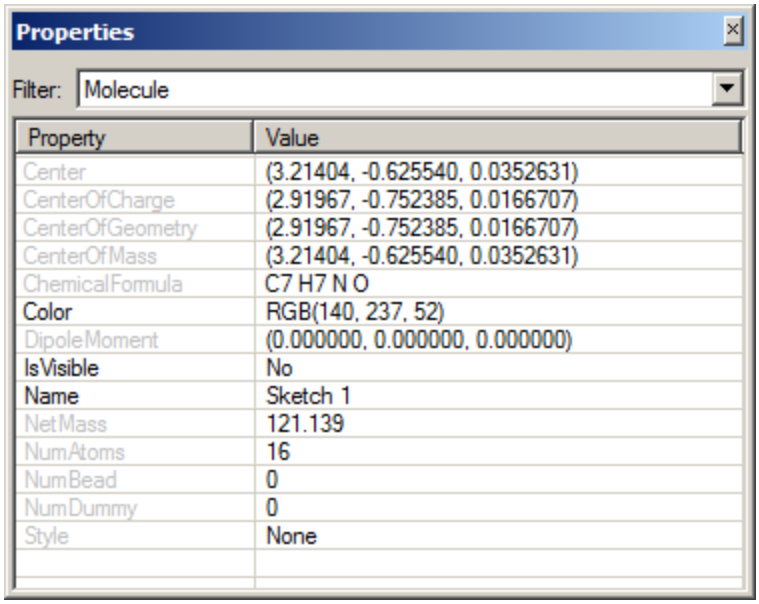
Click the **3D Viewer Rotation Mode** button  on the **3D Viewer** toolbar. Click and drag in the 3D Viewer to rotate the model and view it from different angles.

Note that the color of the distance monitor changes from red to green when it becomes inactive. You can now use the context-sensitive Properties Explorer to view information about the model you have created.

Select **View | Explorers | Properties Explorer** from the menu bar.

This opens the Properties Explorer, which is automatically docked to the left-hand side of the Materials Studio window. You can undock this and any other explorer by clicking on its title bar and dragging to another position in the window, including the bottom of the screen, where it will dock again.

Click the options arrow associated with the **Filter** list box in the Properties Explorer and select **Molecule** from the dropdown list to display a list of the properties of the molecule.



Properties Explorer with values for benzamide

The value of the centroid vector will vary, depending on where in the 3D Viewer you started to sketch the molecule. You can change the width of the *Property* and *Value* columns by clicking and dragging on the separator line between the two column headings.

Click on any atom in the benzamide molecule to select it.

The atom appears highlighted in yellow to show it is selected.

Note: The Properties Explorer is context sensitive and automatically displays the properties of the selected atom.

Click on any single bond in the benzamide molecule to select it.

When selected correctly, the bond is highlighted in yellow and the atom previously selected should be deselected; the Properties Explorer now displays the properties of the selected bond.

You can directly edit certain properties of the structure through the Properties Explorer.

In the Properties Explorer, double-click on **BondType**.

This opens the Edit BondType dialog.

Click on the options arrow associated with the list box to display a list of different bond types and select **Double**, then click the **OK** button.

The single bond changes to a double bond.

Click the **Undo** button  on the **Standard** toolbar to return the bond type to single bond.

Close the 3D view of the **my_benzamide.xsd** document by clicking on the **Close** button  . When prompted to save the document, click the **Yes** button.

Viewing and working with study table and chart documents

Purpose: Provides an introduction to the concepts of study tables and charts in Materials Studio.

Modules: Materials Visualizer, QSAR

Time: 

Prerequisites: Creating a project

Introduction

Study tables are an important part of the workflow in Materials Studio. These documents (.std files) are displayed as a spreadsheet, combining mathematical expression evaluation and data control with chemical awareness. The cells of a study table can contain alphanumeric strings, 3D structures, or charts.

This tutorial shows you how to open a study table, import molecular structures, and calculate some basic properties of the imported molecules:

Note: In order to complete this tutorial, you will need a QSAR license.

You should carry out this tutorial in the **my quickstart** project you created in the Creating a project tutorial.

1. To open a new study table document

Select **File | New...** from the menu bar to open the New Document dialog. Select **Study Table** and click the **OK** button.

Note: There are several other ways to create a new study table document, for example, click the *New* button  or the options arrow associated with it on the *Standard* toolbar and select *Study Table Document* from the New Document dialog or from the dropdown list. You can also right-click on the project name in the Project Explorer and select *New | Study Table Document* from the shortcut menu.

The new study table document, in the form of a spreadsheet, is displayed in the Study Table Viewer. The next section describes how to insert molecules into this table.

2. To insert molecular structures into a study table

With the study table document as the active document, choose **Edit | Insert From...** from the menu bar or click the **Insert From File** button  on the **Standard** toolbar.

This opens the Insert Into Active Document dialog.

You will insert molecules from the library of organic molecules into the study table.

Navigate to the **Structures\organics** folder. Select all the **.msi** files in this folder, then click the **Open** button.

The ten molecules are inserted into the study table.

3. To view structures in the study table

Column *A* of the table is populated with the names and 3D Atomistic document icons of the molecules. To see the structure of a molecule, simply double-click on the appropriate cell.

Double-click on the cell containing **135benz**.

A Study Table Detail View is displayed, containing the 3D structure of 1,3,5-trimethylbenzene. You can manipulate this structure in the usual ways, for example, edit, zoom, translate, rotate, and so on.

Change one of the benzene hydrogen atoms into another methyl group.

Click on one of the three hydrogen atoms on the benzene ring to select it. Click on the options arrow associated with the **Modify Element** button on the **Sketch** toolbar to show a list of elements. Choose **Carbon**.

The hydrogen atom changes to a carbon.

Click the **Adjust Hydrogen** button to attach three hydrogen atoms to the new carbon atom. Click the **Clean** button.

Click the **Commit Edit To Study Table** button. Close the Study Table Detail View by clicking on the **Close** button.

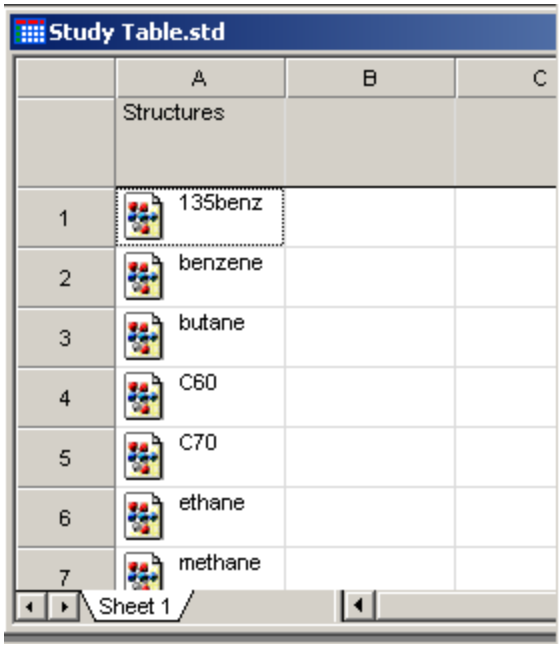
4. Other types of structures supported by the study table

The study table also supports 3D periodic systems, for example crystals or Amorphous Cell constructions, and chart documents. 3D Atomistic Trajectory documents (`.xtd`) can also be inserted, with each frame of the trajectory file being placed in its own row in the study table. These structures can either be inserted as before or directly inserted from the Project Explorer.

Note: Only charts and 3D atomistic structures and trajectories are supported by the study table document type.

5. To calculate basic descriptors

A view of part of the study table is shown below.



Study table document containing structures

Note: The cells in the top row of the study table, containing column labels *A*, *B*, etc., are known as "column headings". The cells in the second row, containing descriptions of column content, for example, *Structures*, are called the "column descriptions".

The value of a study table becomes apparent when calculating properties of multiple structures.

In the Study Table, click on the column heading **A**.

The entire column turns blue, indicating that it is selected.

Note: You can deselect at any time (cancel the current selection) by pressing the ESC key.

Click the **Models** button  on the **QSAR Models** toolbar to display the Models dialog.

From the **Output** column, select **Element count**. Hold down the **CTRL** key and also select **Atom count** and **Non bond energy**. Click the **Run** button and click the **Close** button  to close the Models dialog.

Note: Default behavior for an *Element count* is to count the number of carbon atoms. You can use the *Edit Model* tools  on the Models dialog to change this.

Wait for the job to finish; it should take only a few seconds.

A job completion message will appear when the calculation is over. The results of the calculation are reported in columns *B* to *G*.

Click the **OK** button to close the Job Completed dialog.

6. To manipulate data shown in the Study Table Viewer

Several tools on the *Study Table Viewer* toolbar become useful now.

Select column **B**, containing the atom count data. Click the **Filter Selection** button  on the **Study Table Viewer** toolbar.

A second data sheet, comprising part of the same study table, is created. The other columns are not displayed in this view. This option can be helpful when large sets of data are involved. Now remove the filtering from the new sheet.

Click on the options arrow associated with the **Filter Selection** button  and select **Show All** from the dropdown list.

All columns are now displayed.

Note: Similar filtering can also be performed on rows.

Select column **B**, containing the atom count data. Click the **Sort Ascending** button  .

The data are sorted in order of ascending numbers of atoms.

With column **B** selected, click the **Quick Plot** button  on the **Study Table Viewer** toolbar.

A chart document (`.xcd`) containing a plot of Atom count vs. Row Number is generated.

Click anywhere in the Study Table to make it the active document. Select the empty column **H**. Click the **Define Function** button  to open the Define Function dialog.

In the **Expression** text box, enter **C/B**. In the **Name** text box, enter **Ratio**. In the **Description** text box, enter **Fraction of carbon**. Click the **OK** button.

The fraction of atoms in each molecule which are carbon is calculated and displayed in column *H*.

7. To plot multiple data in a chart

Select columns **B, D, F, and G** selected, click on the options arrow associated with the **Plot Graph** button  on the **Study Table Viewer** toolbar and select **Plot Graph**.

The Plot Graph dialog is displayed.

Select **Scatter (2-D)** from the **Graph Type** dropdown list. Select **B** as the X-axis variable and click the **Plot** button.

A chart document (`.xcd`) containing a plot of non bond contribution vs. atom count is generated. Below the X-axis legend of the chart document there are number of check boxes.

Uncheck and check the legend check boxes, to hide or display the corresponding data.

Right-click in the chart document to open the chart shortcut menu, select **Show Crosshair**.

You can use the crosshair to get information about individual data points.

Select **Window | Close All** to close all of the windows. When prompted to save, click the **Yes to All** button.

This is the end of the tutorial.

Working with a molecular crystal: studying urea

Purpose: Provides an introduction to the crystal building tools available in the Materials Visualizer.

Modules: Materials Visualizer

Time: 

Prerequisites: Creating a project

Introduction

Pharmaceuticals, agrochemicals, pigments, dyes, specialty chemicals, and explosives are all, at some stage during the manufacturing process, crystalline materials. Being able to model such structures can extend your understanding of them and, ultimately, help to control properties such as solubility, shelf life, morphology, bioavailability, color, shock sensitivity, vapor pressure, and density. Urea, used in this exercise, is a simple example of a molecular crystalline material.

This tutorial covers:

- To open a molecular crystal document
- To calculate hydrogen bonds
- To adjust the display range for the crystal cell
- To change the lattice display style
- To examine the structure's hydrogen bonding

You should carry out this tutorial in the **my quickstart** project you created in the Creating a project tutorial.

1. To open a molecular crystal document

Select **File | Import...** from the menu bar.

This opens the Import Document dialog.

Navigate to and select **Examples/Documents/3D Model/urea.msi**, then click the **Open** button.

A window containing a 3D view of one unit cell of the crystalline phase of urea is displayed. A document called `urea.xsd` is now shown in the Project Explorer. Note that the file extension has changed from `.msi` to `.xsd`, the XML-based native Materials Studio format for 3D structures.

2. To calculate hydrogen bonds

Select **Build | Hydrogen Bonds** from the menu bar.

This opens the Hydrogen Bond Calculation dialog. Note that you can apply a number of different schemes and bond geometry parameters for calculating hydrogen bonds or create and save your own schemes.

For the purposes of this example, leave the default values and click the **Calculate** button.

Hydrogen bonds appear as blue dashed lines in the unit cell.

Note: A hydrogen bond calculation can also be carried out by pressing the *Calculate Hydrogen Bonds* button  on the Atoms & Bonds toolbar.

Close the Hydrogen Bond Calculation dialog by clicking on the **Close** button  .

3. To adjust the display range for the crystal cell

Right-click in the 3D Viewer and select **Display Style** from the shortcut menu.

This opens the Display Style dialog.

Select the **Lattice** tab on the Display Style dialog to display the options for changing the lattice display style. In the **Display style** section, change the **Max** value in the **A** row to **2.00**. Do the same for the **Max** value in the **B** and **C** rows.

The *Display style* controls give the option to display a user-defined range and number of unit cells, including the ability to input fractions of unit cell lengths. You should now have a 2 × 2 × 2 lattice of urea that shows the hydrogen bonding scheme more clearly.

4. To change the lattice display style

In the **Lattice** section, select **None**. Close the Display Style dialog by clicking the **Close** button.

5. To examine the structure's hydrogen bonding

Rotate the view to study the hydrogen bonding network. To help you see the hydrogen bonding clearly, click the **Reset View** button on the **3D Viewer** toolbar. Use the **up**, **down**, **right**, and **left** arrow keys to rotate the model by 45° increments.

Close **urea.xsd** by clicking the **Close** button. When prompted to save, click the **Yes** button.

Building an α-quartz crystal

Purpose: Provides an introduction to the crystal building tools available in the Materials Visualizer.

Modules: Materials Visualizer

Time:

Prerequisites: Creating a project

Introduction

Modeling of inorganic crystalline materials is a very important area, particularly relevant to applications such as the design of heterogeneous catalysts, for example zeolite catalysts, or analysis of mineral samples during oil and gas exploration. This tutorial shows you how to build an α-quartz crystal and, in doing so, introduces you to some of Materials Studio's crystal building functionality.

This tutorial covers:

- To build the α-quartz crystal
- To add silicon and oxygen atoms
- To compare two versions of the crystal

You should carry out this tutorial in the **my quickstart** project you created in the Creating a project tutorial.

1. To build the α-quartz crystal

Select **File | New...** from the menu bar to open the New Document dialog. Select **3D Atomistic** and click the **OK** button.

This opens a new 3D Viewer. A corresponding item called 3D Atomistic.xsd is shown in the Project Explorer.

Right-click on **3D Atomistic.xsd** in the Project Explorer and select **Rename** from the shortcut menu. Type **my_quartz_alpha** and press the **ENTER** key.

Select **File | Save** from the menu bar or click the **Save** button  on the **Standard** toolbar.

You have now created a 3D Atomistic document called my_quartz_alpha.xsd in the my quickstart project.

Select **Build | Crystals | Build Crystal...** from the menu bar to open the Build Crystal dialog. On the **Space Group** tab, click on the **Enter group** text box, type **p3221**, and press the **TAB** key.

Instead of manually entering the space group, you could also scroll down the *Enter group* dropdown list of space groups and select the one you want.

On the **Lattice Parameters** tab, enter the **a** and **c** lattice parameters of α-quartz in the appropriate text boxes: **a** = **4.910** Å, **c** = **5.402** Å.

Note that once the space group information has been entered on the *Space Group* tab, the *b*, *α*, *β*, and *γ* lattice parameter values are set automatically according to the constraints imposed by the symmetry of the p3221 space group.

Click the **Build** button.

An empty unit cell with the defined lattice parameters is displayed in the 3D Viewer.

2. To add silicon and oxygen atoms

Now you will add Si and O atoms. Because the symmetry of the system has already been defined, you only need to add one Si and one O atom; symmetry copies will be generated automatically throughout the unit cell.

Select **Build | Add Atoms** from the menu bar.

This opens the Add Atoms dialog. You can also open this dialog by clicking on the *Add Atoms* button  on the *Atoms and Bonds* toolbar.

Select the **Options** tab. Make sure that the **Test for bonds as atoms are created** checkbox is checked.

When this option is enabled, Materials Studio will automatically create appropriate bonds during the crystal building process. Materials Studio also has a versatile Bond Calculation tool, accessible from the *Build* menu, which allows you to select, edit, and define appropriate bonding schemes, but in this case, choosing the automatic option is sufficient.

On the **Options** tab, make sure that the **Coordinate system** is set to **Fractional**. Select the **Atoms** tab. Choose **Si** from the **Element** dropdown list and enter the following values for **a** and **b** on the right-hand side of the dialog: **a** = **0.480781**, **b** = **0.480781**. Click the **Add** button.

A silicon atom and its symmetry copies are added to the unit cell.

On the **Atoms** tab, select **O** from the **Element** dropdown list and enter the following values for **a**, **b**, and **c**: **a** = **0.150179**, **b** = **0.414589**, **c** = **0.116499**. Click the **Add** button. **Close** the Add Atoms dialog.

An oxygen atom and its symmetry copies are added to the unit cell, and bonds are automatically calculated and drawn.

3. To compare two versions of the crystal

Next, you will compare the structure of α-quartz from Materials Studio's structure library with the structure you just built.

Select **File | Import...** from the menu bar.

This opens the Import Document dialog.

Navigate to and select **Examples/Documents/3D Model/quartz_alpha.msi**, then click the **Open** button.

This opens a new 3D Viewer containing one unit cell of α-quartz. A document called `quartz_alpha.xsd` is now shown as part of the my quickstart project in the Project Explorer. Note that the file extension has changed from `.msi` to `.xsd`, the XML-based native Materials Studio format for 3D structures. Materials Studio provides a document for displaying groups of atoms or molecules that do not physically interact. These are called 3D Atomistic Collection documents.

Select **File | New...** from the menu bar to open the New Document dialog, select **3D Atomistic Collection** and click the **OK** button.

In the Project Explorer, right-click on **my_quartz_alpha.xsd** and select **Insert Into** from the shortcut menu. Repeat this for **quartz_alpha.xsd**. Use the **up**, **down**, **right**, and **left arrow** keys to view the structures in corresponding orientations to check that they are identical.

Note: The newly built structure `my_quartz_alpha.xsd` shows atoms which would be located in neighboring unit cells in order to illustrate the bonding topology of the SiO_2 structure.

Right-click in the 3D Atomistic Collection document and choose **Display Style** from the shortcut menu to open the Display Style dialog.

On the **Lattice** tab, select **In-Cell** from the **Style** dropdown list, then **close** the dialog.

The atoms in the neighboring cells are now removed from the 3D view of `my_quartz_alpha.xsd` and the two structures are now displayed in identical fashion.

Note: This can also be achieved by selecting *Build | Crystals | Rebuild Crystal* from the menu bar and clicking the *Rebuild* button on the Rebuild Crystal dialog.

Select **File | Save Project** from the menu bar.

This saves the project settings and all documents in it.

Finally, close all documents by selecting **Window | Close All** from the menu bar.

This is the end of the tutorial.

Building poly(methyl methacrylate)

Purpose: Provides an introduction to the polymer building tools available in the Materials Visualizer.

Modules: Materials Visualizer

Time:

Prerequisites: Creating a project

Introduction

Poly(methyl methacrylate), or PMMA, is important as a commercial thermoplastic material, particularly for glazing applications. It is typically produced by free radical polymerization of methyl methacrylate using peroxide or azo initiators, or by thermal or photochemical initiation. In this example, you will use Materials Studio's polymer building features to build a 20-mer of isotactic PMMA, which could then be used for further simulation and study of the structure and properties.

This tutorial covers:

- To build isotactic PMMA
- To select and label an individual repeat unit
- To study the structure

You should carry out this tutorial in the **my quickstart** project you created in the Creating a project tutorial.

1. To build isotactic PMMA

Materials Studio gives you the option of building homopolymers, block copolymers, random copolymers, and dendrimers.

Select **Build | Build Polymers | Homopolymer** from the menu bar.

This opens the Homopolymer dialog.

On the **Polymerize** tab, select **acrylates** from the **Library** dropdown list. Select **methyl_methacrylate** from the **Repeat unit** dropdown list. Examine the **Tacticity** dropdown list.

It is possible to build polymers in isotactic, syndiotactic, or atactic form. You are going to build an isotactic methylmethacrylate polymer.

The **Tacticity** should be set to **Isotactic**. Set the **Chain length** to **20**.

On the **Advanced** tab and set the **Torsion** to **60**.

You have now set up the Polymer Builder to build isotactic PMMA with 20 repeat units in the molecule.

Click the **Build** button and **close** the dialog.

A new 3D Atomistic document called `Polymethyl_methacrylate.xsd` is created containing your constructed PMMA molecule and is displayed in the 3D Viewer.

Click the **Clean** button  on the **Sketch** toolbar to rearrange the structure to a more reasonable geometry.

Normally, further geometry optimization would be necessary, the Forcite module can be used to achieve this.

2. To select and label an individual repeat unit

First you will change the display style of the structure.

Right-click in the 3D Viewer and select **Display Style** from the shortcut menu to open the Display Style dialog. On the **Atom** tab, ensure that the **Line** option is selected in the **Display style** section.

The display style of the whole structure is set to line.

Click on an atom anywhere in the PMMA molecule (you may need to zoom in to be able to do this easily).

The selected atom is highlighted in yellow.

Right-click anywhere in the 3D Viewer to display the shortcut menu, choose **Select Repeat Unit methyl_methacrylate** from the shortcut menu.

The whole of a single methyl methacrylate repeat unit is selected and highlighted in yellow.

On the **Atom** tab of the Display Style dialog, select the **Ball and stick** option. Close the Display Style dialog by clicking on the **Close** button  .

The selected repeat unit is now displayed in the ball and stick style.

With the repeat unit selected, right-click in the 3D Viewer and choose **Label** from the shortcut menu to open the Label dialog.

Select **Repeat Unit** from the **Object Type** dropdown list, and in the **Properties** field, select **Name**. In the **Font** section of the dialog, change the font size to **24** and the **Color** to green through the color chooser.

Click the **Apply** button and **close** the Label dialog. Click anywhere in the **Polymethyl_ methacrylate.xsd** 3D view to deselect the repeat unit.

A green label with the name of the repeat unit is added next to the selected repeat unit.

3. To study the structure

Rotate, zoom, and translate to study the structure, either by selecting different modes using the buttons on the **3D Viewer** toolbar or by using the mouse and keyboard shortcuts detailed in the Opening and viewing 3D documents tutorial.

Close **Polymethyl_methacrylate.xsd** by clicking on the **Close** button  . When prompted to save the document, click the **Yes** button.

Saving a project and finishing up

Purpose: Illustrates how to save documents and close projects in Materials Studio.

Modules: Materials Visualizer

Time:

Prerequisites: Creating a project

You have now created your first Materials Studio project.

1. To save the project

Double-click on each of the following items in the Project Explorer: **my_benzamide.xsd**, **urea.xsd**, **my_quartz_alpha.xsd**, **Polymethyl_methacrylate.xsd**.

The four documents are opened in the Materials Studio workspace.

Select **Window | Tile Horizontally** from the menu bar.

The 3D views of the four documents are tiled within the Materials Studio workspace.

Select **File | Save Project** from the menu bar.

You have now reached the end of these Quick start tutorials. The project settings and all the documents are now saved in the project my quickstart. If you open this project again, it will automatically open with the same four 3D Viewers displayed and the same items showing in the Project Explorer. You can now either create a new project, load another existing project (both using the appropriate options on the *File* menu), or exit Materials Studio.

To exit Materials Studio, select **File | Exit** from the menu bar.

Visualizer tutorials

The following tutorials illustrate how to utilize the Visualizer's capabilities.

- Project management: Introduces projects in Materials Studio and illustrates how to use them to manage workflow.
- Sketching simple molecules: Introduces basic sketching tools for drawing chains and rings, editing bond order and element type, and measuring different geometrical properties.
- Sketching a porphyrin: Shows how to manipulate fragments and use the Display Style dialog.
- Sketching organometallic structures: Introduces the Fragment Browser and illustrates the use of the Find Symmetry tool.
- Overlaying and aligning molecules: Introduces the collection document and demonstrates how it can be used to overlay and align molecules.
- Precise positioning and movement of atoms: Illustrates the use of the Move to, precise Movement tools, and alignment tools.
- Docking molecules on surfaces: Introduces the Surface Builder for cleaving crystal structures.
- Using the polymer builder: Introduces the Polymer Builder for constructing various types of polymer structures.
- Using the layer builder: Shows how to use the Layer Builder to construct an interface and a metal-polymer-metal layered structure.
- Using the crystal builder: Introduces the Crystal Builder for constructing and visualizing 3D periodic structures.
- Library enumeration using the analog builder: Illustrates the use of the Analog Builder to enumerate libraries of molecules.
- Building mesoscale molecules: Illustrates how to use the mesomolecule builder to build bead representations of molecules.
- Building bulk mesostructures: Introduces the mesostructure template builder and mesostructure builder
- Coarse graining atoms to beads: Demonstrates how to use the coarse graining tools
- Working with isosurfaces and slices: Introduces the isosurfaces and slices tools available in the Materials Visualizer.
- Field segregation and analysis: Demonstrates how to perform field segregation on an Atom Volumes Field.
- Building transport devices for electron transport calculations: Introduces the building of electrodes and transport devices.

Note: All numbers given in the tutorial are in American English format. See the Localization topic for more information.

Project management

Purpose: Introduces the concept of a Project in Materials Studio and illustrates how they are used to manage your workflow.

Modules: Materials Visualizer, Reflex

Time:

Prerequisites: None

Background

When you are running advanced operations such as Forcite and CASTEP jobs, many different documents with a number of different document types can be generated. To make the management of these documents simpler, Materials Studio has a feature called the Project Explorer. This is similar to the document management systems seen in advanced programming language packages such as Visual C++®. As well as the folders and documents automatically created by the program, you can create your own folders to customize the document organization and your own documents to help you track what you are doing.

Introduction

This tutorial is split into two parts. The first section describes a sample project, in which you can see how performing calculations such as energy minimizations affects the structure of your project. The later sections guide you through creating your own project. As working with projects is an essential part of using Materials Studio, references are also made to the Project Explorer in other tutorials.

This tutorial covers:

- Illustrated breakdown of a sample project
- Getting started
- To use Autosave
- To import a structure
- To generate a chart document
- To create a new folder and move documents
- To add and rename an HTML document
- To import into a pre-defined folder
- To copy and paste
- To save a project
- To sort the project
- To change focus
- To remove documents

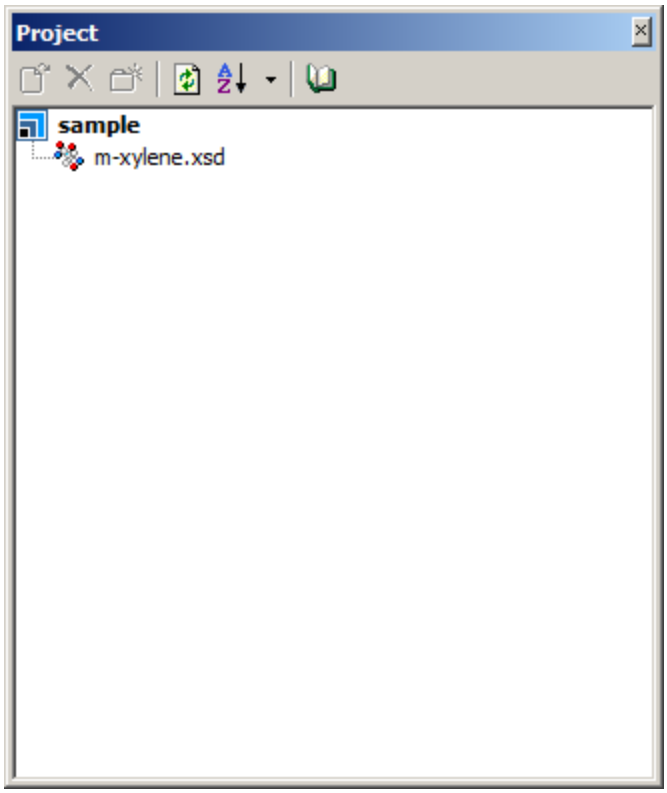
Note: Sections of this tutorial require use of the Reflex module.

1. Illustrated breakdown of a sample project

This section of the tutorial consists of a breakdown of a sample project. It is used for illustrative purposes only and does not include any work for you to complete. In this sample project, a molecule of m-xylene has been loaded and minimized, then a dynamics run has been performed and the results of

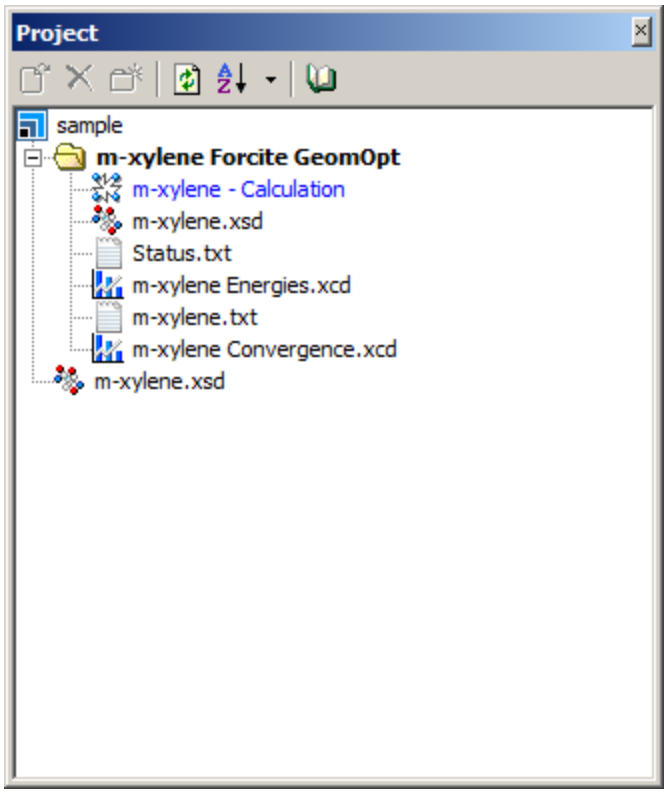
the dynamics run have been analyzed. It has been broken down to reflect the changes to the Project Explorer after each step.

1. The initial project called *sample* with a m-xylene structure imported.

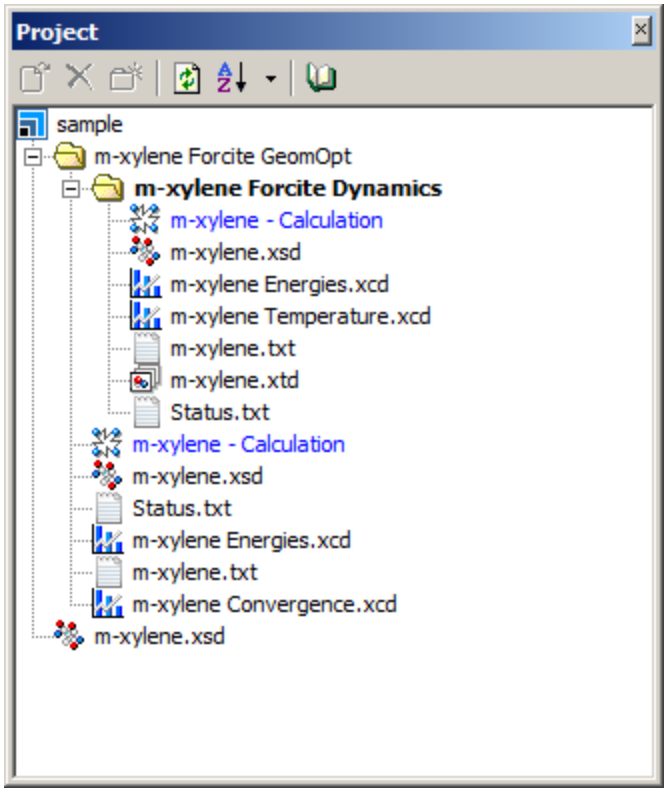


2. After a Forcite geometry optimization run, a new folder called m-xylene Forcite GeomOpt is created and the minimized structure is placed in that folder. The `m-xylene.txt` document contains information from the Forcite

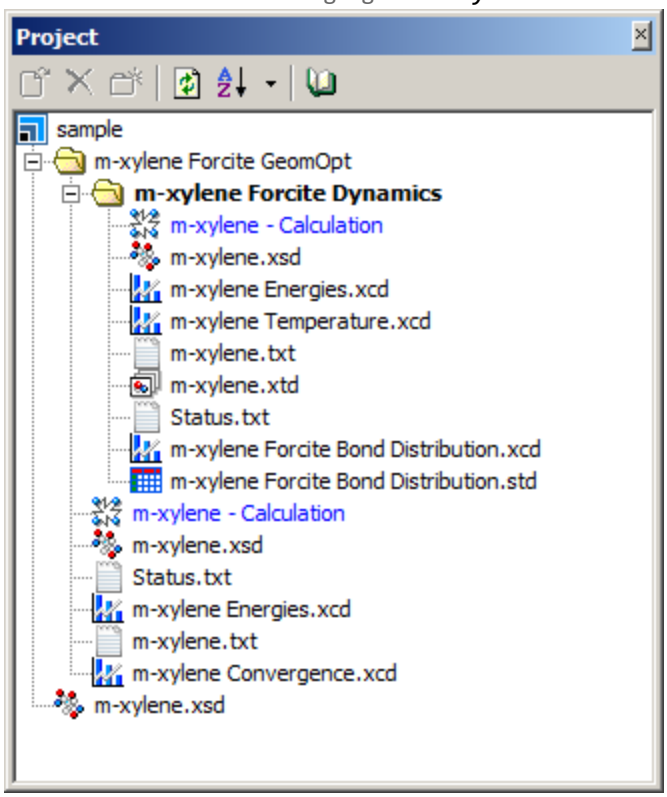
calculation.



3. A Forcite dynamics calculation has been performed and the data are placed in the `m-xylene Forcite Dynamics` folder. The document `m-xylene.xtd` is the trajectory document that contains the dynamics simulation.



4. Analysis has been performed to assess the distribution of bond lengths throughout the dynamics run. This information is stored in the highlighted `m-xylene Forcite Bond Distribution.xcd` document.



This is the layout of a standard calculation. As each new calculation is performed on the results from a previous calculation, a new subfolder is added to the tree. This allows you to follow the path of an experiment from the directory tree. If you were to construct and minimize a second molecule in the same project, you would see a second tree appearing from the *sample* root project.

Note: The folder containing the active document is displayed in bold.

Now you can proceed and create a small project of your own.

2. Getting started

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

When Materials Studio has started, this opens the Welcome to Materials Studio dialog, asking if you want to open an existing project or create a new one.

Click the **Create a new project** radio button and then the **OK** button.

This opens the New Project dialog. You will create a project called `Management`.

Delete the text **Untitled** and type **Management**. Click the **OK** button.

If Materials Studio is already open:

Choose **File | New Project...** from the menu bar to open the New Project dialog. In the **File name** text box, type **Management** and click the **OK** button.

You have now created a Materials Studio project. Materials Studio will open with a menu bar and toolbars along the top, the Project Explorer on the left side and a large gray area in the center, known as the workspace. The Project Explorer window, called Project, contains the title of the project, Management, in bold next to the Materials Studio icon.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

3. To use Autosave

Materials Studio includes an *Autosave* feature which automatically writes changes to documents in the current project to disk at specified intervals during a session. If you want *Autosave* to operate during a session, you should ensure that it is switched on and, if necessary, adjust the interval between updates.

Select **Tools | Options...** from the menu bar to open the Options dialog. On the **General** tab, check the **Enable Autosave** checkbox and set the update interval to **10** minutes.

If a Materials Studio session ends unexpectedly, because of a loss of power or a computer failure, for example, before you have an opportunity to save your work, when you restart, you will be given the opportunity to restore the latest autosaved versions of the documents in the current project.

Note: The option to recover files is only offered once. If you decline to restore autosaved files, then the versions on disk will be deleted.

Alternatively, you can recover the autosaved documents manually from the location specified on the *Locations* tab of the Options dialog.

Choose the **Locations** tab on the Options dialog. Inspect the default location of the **Autosave** folder. Click the **OK** button to close the Options dialog.

Tip: Autosave is not a replacement for regularly saving the documents in your project.

4. To import a structure

The next step is to import a structure to see where it fits into the Project Explorer hierarchy.

Click the **Import** button  on the **Standard** toolbar.

This opens the Import Document dialog. You should import the MnO structure that is located in the 3D `Model` folder.

Navigate to the **Examples\Documents\3D Model** folder on the Import Document dialog. Select the **MnO.xsd** document and click the **Open** button.

The `MnO.xsd` document is displayed in the Project Explorer in the first level under the Materials Studio icon and opened in a 3D Viewer in the workspace.

5. To generate a chart document

In order to see the practical applications of the Project Explorer, you need to generate some documents to work with. This can be achieved quickly by calculating a powder pattern. You will not be analyzing this data, since you are generating it solely for the purposes of document manipulation.

Powder diffraction patterns are generated using the Reflex module. This can be accessed using the *Modules* menu or toolbar.

Click on the **Reflex** arrow  on the **Modules** toolbar or choose **Modules | Reflex** from the menu bar, then select **Powder Diffraction** from the dropdown list.

This opens the Reflex Powder diffraction dialog. As you are not using these results for any scientific analysis, you do not need to change any of the settings.

Click the **Calculate** button.

A chart is displayed, showing a simulated powder diffraction pattern.

Click the  button to close the Reflex Powder Diffraction dialog.

In the Project Explorer window, there are now two documents, one called `MnO.xsd`, a 3D Atomistic document, and the other called `MnO.xcd`, a chart document. Later, you are going to generate a chart for a different structure, so you should place the current structure and chart in a new folder to keep the Project Explorer tidy.

6. To create a new folder and move documents

Click on the root icon  in the Project Explorer.

The buttons highlighted on the *Project Explorer* toolbar change so that the new folder button is now active.

Click the **New Folder** button  on the **Project Explorer** toolbar.

A new folder is created with the default name, `New Folder` available for editing. You should change this name to something more appropriate.

Type **MnO** and press the **ENTER** key.

You now have a new folder in the management project called `MnO` and you can move the chart and structure documents into it.

Move the cursor over **MnO.xcd** in the Project Explorer, then click and hold the left mouse button and drag the document onto the **MnO** folder, release the mouse button. Repeat this procedure for the **MnO.xsd** document.

7. To add and rename an HTML document

Materials Studio also features the ability to add HTML documents to projects. These can be very useful for adding experimental notes or calculation settings for reference as you work. HTML documents have advantages over plain text documents, as they allow text formatting that can be loaded into any word processor that supports HTML and they are easy to share.

If you create a new document, it is added to the folder that is currently selected. For example, if the MnO folder is selected and you create a new document, it is automatically placed in the MnO folder. As you want this HTML document to be in the root folder, you need to select the Management project icon.

Click on **Management** in the Project Explorer.

Now create a new document.

Select **File | New...** from the menu bar.

This opens the New Document dialog, which allows you to choose from the different document types that can be added to the current project. You will select the HTML document type from the options available.

Select **HTML** and click the **OK** button.

A new window appears, entitled HTML. This is a basic HTML text editor that can be used in conjunction with the *HTML Formatting* toolbar to create standard HTML text with features such as bold and italic text, and justification. It is used in much the same way as a word processing package.

Select **View | Toolbars | HTML Formatting** from the menu bar.

The HTML formatting tool bar is displayed, now you can format the text you are going to add.

Type the following in the HTML text editor window:

This is the first project I have created and it contains:

Click the **Number List** button  and type:

MnO Folder - holds the MnO structure document and results from a powder diffraction calculation with default values.

Now give the document a more informative name.

Select **HTML.htm** in the Project Explorer. Right-click and select **Rename** from the shortcut menu. Type **Project Information** and press the **ENTER** key.

8. To import into a pre-defined folder

As well as importing documents into the Project Explorer, you can direct them into a specific folder. You do this by selecting the folder before you import the structure. To demonstrate this, you are going to import another metal oxide structure called CeO2.msi. First, you will create a new folder called CeO2.

Select the root icon and right-click, select **New | Folder** from the shortcut menu. Change the name of the folder to **CeO2** and press the **ENTER** key.

You have now created the folder into which you are going to import your documents. The new folder should already be selected but if not, you should select it.

Click on the **CeO2** folder to select it.

Now you can import the document.

Select **File | Import...** from the menu bar to open the Import Document dialog. Navigate to the **Examples\Documents\3D Model** directory. Select **CeO2.xsd** from the list of documents and click the **Open** button.

Note: The text box at the bottom of the Import Document dialog indicates where the document will be imported.

The structure is imported into the CeO2 folder. Now, you will use Reflex again to calculate a powder diffraction pattern.

Click the **Reflex** arrow  or choose **Modules | Reflex** from the menu bar, then select **Powder Diffraction** from the dropdown list.

This opens the Reflex Powder Diffraction dialog. Before you calculate the diffraction pattern, you must change an option on the *Display* tab.

Select the **Display** tab of the Reflex Powder Diffraction dialog. In the **View management** section, click on the **Chart view** dropdown list and change the option from Replace to **New**.

Now when you calculate a new diffraction pattern, it will be written to a new chart document rather than replacing the original chart, which is the default behavior.

Click the **Calculate** button and **close** the dialog.

A chart document, `CeO2.xcd`, is displayed in the CeO2 folder in the Project Explorer. You should update the `Project Information` HTML document.

Double-click on **Project Information.htm** in the Project Explorer. On a new line, type the following:

CeO2 Folder - contains CeO2 structure and results from a powder diffraction calculation with default values.

9. To copy and paste

As well as importing documents into folders you can make copies of other project documents. You will place all your diffraction charts together in a folder. First, you will create a new folder called `Charts`.

Select the root icon and right-click, select **New | Folder** from the shortcut menu. Change the name of the folder to **Charts** and press the **ENTER** key.

You have now created the folder into which you are going to copy your chart documents.

Note: You can also copy documents or folders to the project root.

First, copy the CeO2 chart.

Select the **CeO2.xcd** document, right-click and choose **Copy** from the shortcut menu.

Select the **Charts** folder, right-click and select **Paste** from the shortcut menu.

Now, copy the MnO chart using an alternative method.

Select the **MnO.xcd** document, hold down the **CTRL** key and drag the chart document onto the **Charts** folder.

Tip: Either of these methods can be used to make copies of folders or of several selected documents in a single step. If you copy more than one item a dialog will check that you want to copy all the selected items to the specified folder, click *Yes* to make copies.

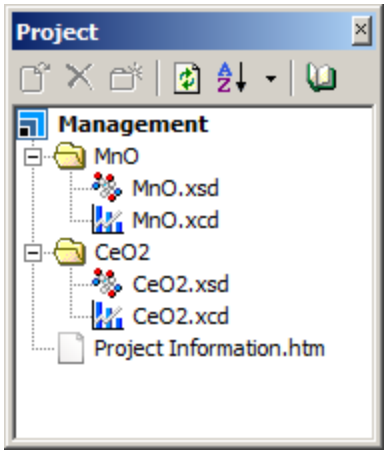
10. To save a project

Now that you have some results, you should save the project.

Select **File | Save Project** from the menu bar.

All the documents have been saved into the project and they have all been saved in their current state. If you are working on a large project with many documents and want to save selected documents occasionally as you proceed, you can do this by selecting *File | Save* from the menu bar.

The Project Explorer should now look like this.

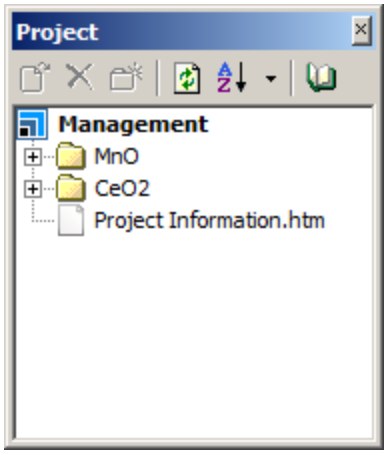


Project Explorer with expanded nodes

You can compress the nodes to hide the folder contents. This may make it easier to navigate large projects.

Click on the - symbols next to the folder icons to collapse the nodes.

Only the items at the top level of the project are displayed.



Project Explorer with collapsed nodes

11. To sort the project

The files and folders listed in the Project Explorer can be sorted to make it easier to locate particular files if there are many available.

If you click the *Sort* button both the files and folders will be sorted according to the type of sorting requested, but the folders will always be listed first in the Project Explorer - before any files.

Click the **Sort** button on the Project Explorer toolbar.

The folders and files are sorted by name, so that the *CeO2* folder is listed before the *MnO* folder.

Click on the **Sort** arrow on the Project Explorer toolbar and choose **Date Created** from the dropdown list.

The folders and files are sorted by the time and date when they were created, so that the *MnO* folder is listed before the *CeO2* folder because it was created first in the steps you have carried out so far.

12. To change focus

Using focus is a very important part of the Materials Studio experience. If you have many documents open in the workspace area, it can sometimes be unclear which document belongs to what folder. However, using the Project Explorer, you can easily navigate around. The active document in the workspace area is highlighted in gray in the Project Explorer and the folder containing the document is displayed in bold.

If you double-click on a document name in the Project Explorer, it becomes the active document in the workspace area.

Double-click on **MnO.xsd** in the Project Explorer.

The 3D Atomistic document is brought to the front of the workspace area and the document name is highlighted in gray.

Double-click on **MnO.xcd** in the Project Explorer.

The MnO chart document becomes active and is highlighted in gray in the Project Explorer. It is also possible to change the focus in the workspace area.

Click on the title bar or frame of any of the Viewers that are visible in the workspace area.

The document you selected becomes active and the document name in the Project Explorer is highlighted in gray. This is just a simple example of the use of changing focus. When you perform experimental calculations using the other modules, a good knowledge of the way focus works will be invaluable.

13. To remove documents

You can remove individual documents from the project. This is done by selecting the document you wish to remove in the Project Explorer and clicking the *Delete* button. Now remove the HTML Document from the current project.

In the Project Explorer, select the **Project Information.htm** document and click the **Delete** button  on the **Project Explorer** toolbar.

This opens a dialog asking if you are sure that you want to remove the document.

Click the **Yes** button.

The HTML document window will disappear from the workspace area and the document will be removed from the Project Explorer. This means that you have completely erased the HTML document from the project.

However, if you want to remove a document from the workspace area, but not remove the document from the project, you can do this by clicking the *Close* button on the window you wish to close. If the project is saved and no further alterations have been made, this will remove the document from the workspace area, but not from the project.

Close the **MnO.xcd** chart document.

The chart will disappear from the workspace area, but not from the Project Explorer window. It is very easy to redisplay the chart.

Double-click on **MnO.xcd** in the Project Explorer.

The chart document is re-displayed in the workspace area.

As well as removing single documents from the Project Explorer, you may also need to remove entire folders. This task is performed in a similar way.

Select the **CeO2** folder in the Project Explorer and press the **DELETE** key. A dialog box is displayed asking if you want to remove the folder. Click the **Yes** button.

Now you can shut down Materials Studio.

Select **File | Exit** from the menu bar. At the prompt, click the **Yes** button to save the project.

This is the end of the tutorial.

Sketching simple molecules

Purpose: Introduces the basic sketching tools that allow you to sketch chains and rings, edit bond type, edit element type, and measure different geometrical properties.

Modules: Materials Visualizer

Time:

Prerequisites: Project management

Introduction

In this tutorial, you will learn how to sketch structures in Materials Studio. Using the different visualization techniques available in Materials Studio, you can create high quality graphics that can be easily pasted into other Windows-based software programs or saved as bitmaps. You will build a variety of simple organic compounds by following the detailed instructions provided. At the end of the tutorial, there are some additional structures for you to build on your own.

In many cases, there is more than one way to modify a structure. This tutorial introduces you to various different methods so that you can determine which is best in a given situation.

This tutorial covers:

- Getting started
- To sketch phenol
- To sketch dicyclopentadiene
- To sketch a pyridine
- To sketch methyl methacrylate
- To add lighting effects

1. Getting started

Begin by starting Materials Studio and creating a new project called Sketching. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Sketching** as the name and click the **OK** button.

The new project is created with *Sketching* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

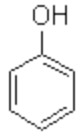
2. To sketch phenol

The first task is to open a new 3D Atomistic document in which to sketch a structure.

Choose **File | New...** from the menu bar to open the New Document dialog. Select **3D Atomistic** from the options and click the **OK** button.

A new 3D Atomistic document is created and displayed in a 3D Viewer in the workspace.

The structure of phenol is shown below.



Structure of phenol

First, you must draw the phenyl ring. Four-, five-, and six-membered rings are provided as templates in Materials Studio and can be sketched easily using the *Sketch Ring* tool.

Click the **Sketch Ring** button on the **Sketch** toolbar.

The cursor will change to the sketching cursor, with a number 6 in the center of a ring denoting that a six-membered ring will be drawn when you click in the new document. The next step is to place the phenyl ring in the 3D Atomistic document.

By default, the *Sketch Ring* tool generates a ring of carbons connected by single bonds. So, for a six-membered ring, it typically produces a cyclohexane ring minus the hydrogen atoms. However, you can add an aromatic ring directly.

Hold down the **ALT** key and click in the 3D Viewer.

A phenyl ring, with no hydrogen atoms, is sketched in the 3D Atomistic document, with the aromatic partial double bonds represented by dotted lines. Now, you need to sketch an oxygen atom and link it to the ring using the *Sketch Atom* tool. The default sketching element is carbon, so you need to specify that you wish to sketch with oxygen.

Select the **Sketch Atom** tool on the **Sketch** toolbar. Click the **Element used to sketch** arrow C and select **Oxygen** from the dropdown list.

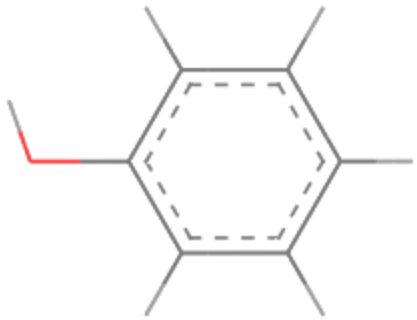
Because the phenyl ring is symmetrical, you can attach the oxygen to any of the carbon atoms.

Move the cursor over one of the carbon atoms in the 3D Viewer. When the atom changes color to light blue, click on it. Move the cursor away to sprout a bond. Click again to place the oxygen atom. Press the **ESC** key to cancel further drawing.

The change in color of the carbon atom as the cursor moves over it indicates that you can select it. You should now have a structure containing a red oxygen atom attached to a gray carbon ring. The final step is to add the hydrogen atoms. The *Adjust Hydrogen* tool automatically fills up any empty valences in a structure with hydrogen atoms.

Click the **Adjust Hydrogen** button on the **Sketch** toolbar.

Hydrogen atoms are attached to the carbon atoms and the oxygen atom to satisfy the empty valences, producing a structure that looks similar to this.



Initial 3D structure of phenol

Now that you have sketched the structure, you should use the *Clean* tool to tidy up the geometry. This is not an energy minimization, but uses a look-up table of standard bond lengths and angles to give a first approximation to the correct geometry.

Note: The *Clean* operation should not be a replacement for geometry optimization with a good Hamiltonian or forcefield.

Click the **Clean** button  .

The cleaning operation begins. The progress of the procedure is displayed in the status bar at the bottom right of the screen and disappears on completion. This may happen so quickly that the progress bar disappears as soon as it is created.

You will save the structure in the project.

Select **File | Save As...** from the menu bar to open the Save As dialog. Enter **phenol** as the **File name** and click the **Save** button.

The structure is saved in `.xsd` format. This is a native Materials Studio file format based on XML (extensible markup language) and is very flexible, allowing future changes, such as hierarchical searching.

The structure you have drawn can be rotated and translated in three dimensions using the right mouse button.

Hold down the right mouse button and move the cursor in the center of the 3D Viewer.

Moving the mouse up, down, left, and right rotates the molecule in the x and y planes.

Move the cursor to the edge of the 3D Viewer. Hold down the right mouse button and move the cursor along the edge.

The molecule rotates in the z plane.

The structure can be translated along the x and y axes using the *3D Viewer Translation Mode* tool.

Click the **3D Viewer Translation Mode** button  on the **3D Viewer** toolbar. Click and hold down the left mouse button in the 3D Viewer and drag the cursor around the screen.

The structure follows the movements of the mouse. After performing translations or rotations, you may wish to adjust the original view. There are three buttons on the *3D Viewer* toolbar that enable you to adjust the view of a 3D model document.

3D Viewer Reset View - Resets the 3D view to the original orientation.

3D Viewer Recenter - Recenters the 3D view with respect to selected atoms or the entire structure and provides access to the view alignment dropdown list, which allows you to orient the view so that it is either parallel or perpendicular to the plane of a near-planar object or the major axis of a near-linear object.

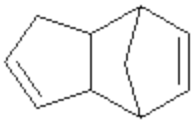
3D Viewer Fit to View - Rescales the current view so that the entire contents of the 3D Viewer fit on screen.

Click the **3D Viewer Reset View** button on the **3D Viewer** toolbar.

The structure is returned to its original orientation prior to the rotation and translation moves you carried out.

3. To sketch dicyclopentadiene

The structure of dicyclopentadiene is shown below.



Structure of dicyclopentadiene

It is used as an intermediate in the synthesis of insecticides and herbicides.

Open a new document in which to draw the model.

Click the **New** button on the **Standard** toolbar to open the New Document dialog, double-click on **3D Atomistic**.

Now draw a six-membered ring.

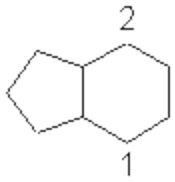
Click the **Sketch Ring** button. In the empty 3D Viewer, click once to place a six-membered ring.

Next, you will fuse a five-membered ring to the six-membered ring.

Click on the **Sketch Ring** arrow and select **5 Member** from the dropdown list. Hover the cursor over the middle of one of the bonds in the six-membered ring. When it changes color to light blue, click to fuse a five-membered ring to the bond.

A five-membered ring is fused to the six-membered ring. Now, you will add the bridging carbon atom. You can do this using the *Sketch Atom* tool.

Click the **Sketch Atom** button. Check that **C** is the **Element used to sketch**. If it is not, click the **Element used to sketch** arrow and choose **Carbon** from the dropdown list.



Adding the bridging carbon atom

Move the cursor over atom 1 in the diagram above. When the atom changes color to light blue, click on it. Move the cursor to the center of the ring and click again to place the bridging atom. Move the cursor to atom 2 and, when its color changes to orange, click a final time.

You have now created a bridging carbon atom between two carbon atoms in the six-membered ring.

If you make a mistake, you can go back one step by pressing the *Undo* button, selecting *Edit | Undo* from the menu bar, or pressing CTRL + Z.

To undo the last action, click the **Undo** button  on the **Standard** toolbar.

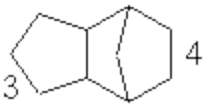
In addition, the *Undo* button provides access to the Undo dropdown list, which allows you to undo up to 20 previous actions in a single step.

If you undo too many steps, you can redo them using the *Redo* button, selecting *Edit | Redo* from the menu bar, or pressing CTRL + Y.

To redo the last action, click the **Redo** button  .

Similarly, the dropdown list for the *Redo* button allows you to redo up to 20 previous undone actions in a single step.

To complete the structure, you must add double bonds to the two rings using the *Modify Bond Type* tool. The first step is to select the two bonds you wish to modify.



Modifying the bond type

Click the **3D Viewer Selection Mode** button  on the **3D Viewer** toolbar. Select bond 3 in the diagram above.

A yellow square will appear in the middle of the bond, indicating that it has been selected. You can increase the bond order of both bonds at the same time.

Hold down the **SHIFT** key and move the cursor over bond 4, click on the middle of the bond.

A yellow square appears on the second bond, indicating that it too has been selected. Now you can change the bond order.

Click on the **Modify Bond Type** arrow  on the **Sketch** toolbar and select **Double Bond** from the dropdown list.

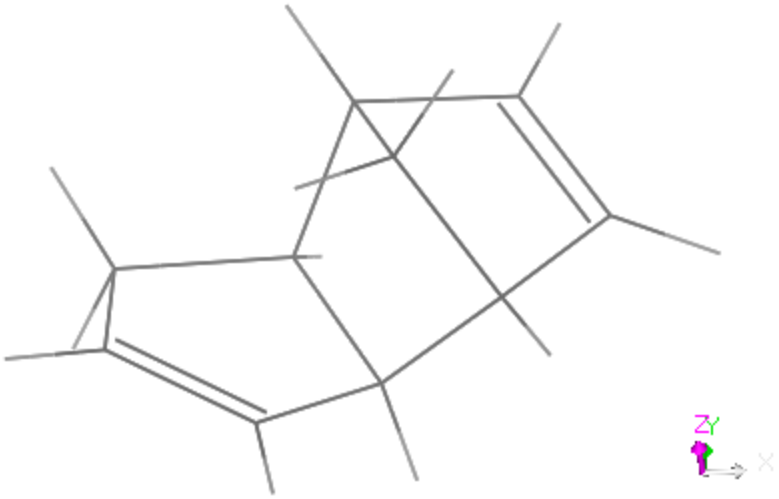
The selected bonds in the structure change to become double bonds.

Now deselect the bonds by clicking anywhere in **3D Viewer** so that the next action affects all of the atoms.

The final step is to add hydrogens and clean the structure.

Click the **Adjust Hydrogen** button  , and then the **Clean** button  .

The final structure will look similar to this.



3D structure of dicyclopentadiene

Now you will save the structure in the project.

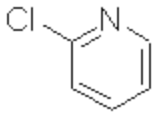
Click the **Save** button  on the **Standard** toolbar.

This saves the structure with the default document name. If you are constructing a project with multiple structures, it is simpler to use the *Save As...* command, as this allows you to specify the model name that appears in the Project Explorer. You can also change the name of the document.

In the Project Explorer, right-click on **3D Atomistic.xsd** and select **Rename** from the shortcut menu. Enter **Dicyclopentadiene** and press the **ENTER** key.

4. To sketch a pyridine

The next structure you are going to construct is 2-chloropyridine.



Structure of 2-chloropyridine

Click on the **New** arrow  on the **Standard** toolbar and select **3D Atomistic Document** from the dropdown list.

Before sketching, you should rename the empty 3D Atomistic document.

In the Project Explorer, right-click on **3D Atomistic.xsd** and select **Rename** from the shortcut menu. Type **2-chloropyridine** and press the **ENTER** key.

To begin, you will sketch a phenyl ring in the new 3D Atomistic document.

Click on the **Sketch Ring** arrow and select **6 Member** from the dropdown list. Hold down the **ALT** key and click once in the 3D Atomistic document.

A phenyl ring is drawn in the 3D Atomistic document. Now, you should edit one of the carbon atoms to change it to a nitrogen atom. This time, you will make the change using the Properties Explorer.

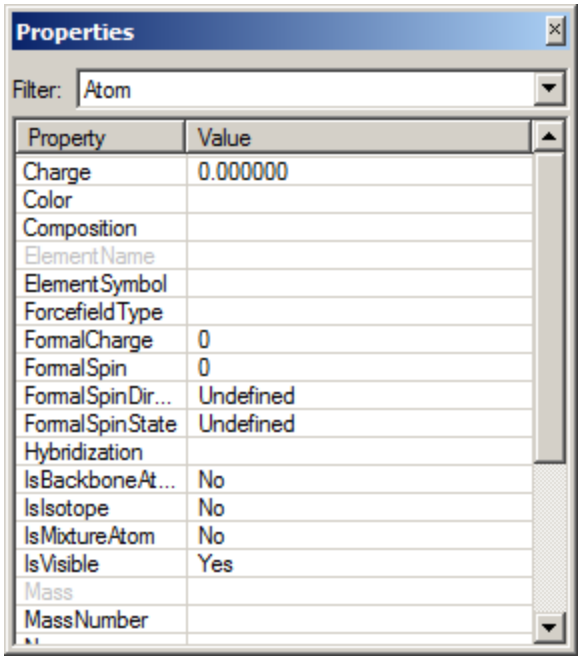
Select **View | Explorers | Properties Explorer** from the menu bar.

This opens the Properties Explorer on the left side of the screen under the Project Explorer. It contains a grid view with two columns labeled *Property* and *Value*.

Click the **3D Viewer Selection Mode** button  and select any atom in the 3D Viewer.

The Properties Explorer will update with information about the selected atom. The first few items in the list are *Charge*, *Color*, *Composition*, *ElementName*, and *ElementSymbol*.

The Properties Explorer can be enlarged and reduced by moving the cursor to the top of the explorer and, when the icon changes to a standard enlarge icon, clicking and holding and moving the top of the explorer up. In common with other explorers in Materials Studio, the Properties Explorer can be undocked from its location and repositioned in the window by clicking on the header bar and dragging.



Properties Explorer

Now you will change the selected atom from carbon to nitrogen.

Double-click on **ElementSymbol** in the **Property** column of the Properties Explorer.

This opens the Edit ElementSymbol dialog, containing the periodic table.

Select **N** and click the **OK** button.

The selected atom will change color from gray to blue. Other parameters in the Properties Explorer, such as the *MassNumber*, will also be updated.

Scroll down the list of **Properties** to see what else has changed.

Note: The given *Name* of the atom is not important in this context. Changing the *Name* does not change the element type.

Click in the 3D Viewer to deselect all the atoms.

The next step is to connect a chlorine atom to the ring using the *Sketch Atom* tool.

Select the **Sketch Atom** tool  . Click the **Element used to sketch** arrow  and choose **Chlorine** from the dropdown list.

Click on one of the carbon atoms adjacent to the nitrogen in the ring, move the cursor away to sprout a bond, and double-click to add the Cl atom and stop sketching.

A green chlorine atom is attached to the ring at the 2-position.

Next, you need to add the hydrogens.

Click the **Adjust Hydrogen** button  .

Before you clean the structure, look at some of the measurement tools included in Materials Studio. You will set up bond length and bond angle measurements and monitor these before and after the structure is cleaned by writing the values in an HTML document.

Click on the **Measure/Change** arrow  on the **Sketch** toolbar. Select **Distance**  from the dropdown list.

Hover the cursor over the middle of the bond connecting the chlorine and carbon atoms and, when it changes color to light blue, click on it.

A set of red dashes appears on the bond and a number is displayed in red. This is the C-Cl bond length and its value is dependent on how you drew the structure.

Instead of recording information on paper, Materials Studio provides you with the facility to add HTML documents to your projects. This allows you to track any settings or results as you change the parameters of your calculations.

In the Project Explorer, right-click on the project root and select **New | HTML Document** from the shortcut menu.

An HTML view opens, into which you can enter information. This new HTML document is also shown in the Project Explorer.

Click in the HTML document and type **C-Cl bond length before cleaning is:** then enter the value from the distance measurement.

Now you will measure the bond angle between the chlorine atom and the ring.

Double-click on **2-chloropyridine.xsd** in the Project Explorer to make it the active document. Click on the **Measure/Change** arrow  and select **Angle**  from the dropdown list.

Click on the connected chlorine, carbon, and nitrogen atoms in sequence to measure the **Cl-C-N** bond angle.

The bond angle is displayed in red with a dotted red line indicating the measured angle. The distance monitor has changed to green. You should record the value of the angle in the HTML document.

Double-click on **HTML.htm** in the Project Explorer to make it the active document. On a new line, type **Cl-C-N bond angle is:**, followed by the value obtained from the bond angle measurement.

Return to **2-chloropyridine.xsd** by double-clicking on the filename in the Project Explorer.

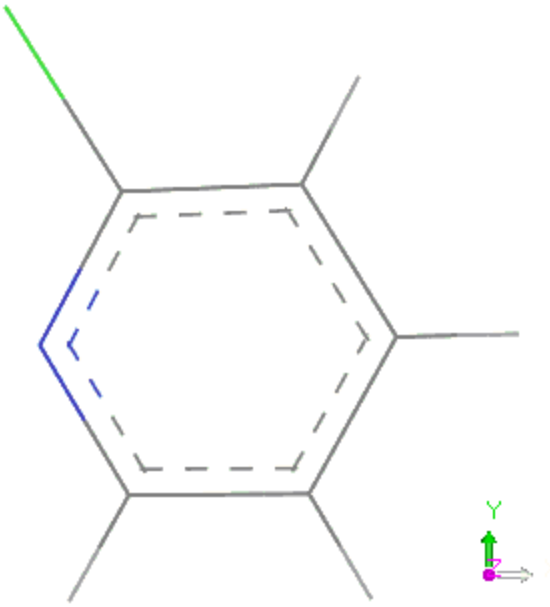
Now clean the structure.

Click the **Clean** button.

The values of the bond angle and bond length will change after the cleaning process, indicating the improvement in the geometry provided by the *Clean* tool.

The new bond lengths and angles can be recorded in the HTML document.

The final structure should look like this.



3D structure of chloropyridine

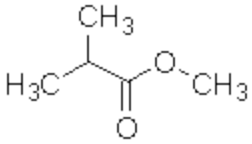
Select the HTML Viewer window and enter the new values.

Select **File | Save Project** from the menu bar.

You have saved the project, along with all the files it contains.

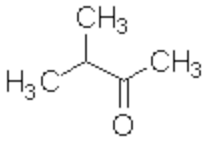
5. To sketch methyl methacrylate

The structure of methyl methacrylate is shown below.



Structure of methyl methacrylate

You will not draw this structure initially, as this is a good example of how to add atoms to an existing structure. First, you will create 3-methyl butan-2-one.



Structure of 3-methyl butan-2-one

Then you will add the second linking oxygen atom to convert the ketone into an ester.

The first stage is to construct the carbon chain.

Create a new **3D Atomistic Document** and rename it **Methylmethacrylate.xsd**.

You now have a new document in which to sketch the structure.

Click the **Sketch Atom** button  . Make sure that the **Element used to sketch** is **C**.

Click in the new 3D Viewer to draw a carbon atom. Move away and click again. Repeat this until you have drawn four carbon atoms, forming the backbone of the molecule. Press the **ESC** key to cancel the sketching action.

The next step is to add a methyl group to one of the carbon atoms to form the branched carbon chain.

Move the cursor over the second carbon atom in the chain. When it changes color to light blue, click on it and move the cursor away to sprout a bond. Double-click to place the carbon atom and stop sketching.

Now you need add to add the carbonyl oxygen to the chain.

Click on the **Element used to sketch** arrow  and select **Oxygen** from the dropdown list. Move the cursor over the third carbon along the chain and click on it. Move the cursor away to sprout a bond and click to place the oxygen atom. Press the **ESC** key to cancel the sketching action.

Having added the oxygen, you must change the bond type, using the *Sketch Atom* tool.

With the **Sketch Atom** tool selected, move the cursor so that it is over the middle of the carbon-oxygen bond. When the bond changes color to light blue, click on it.

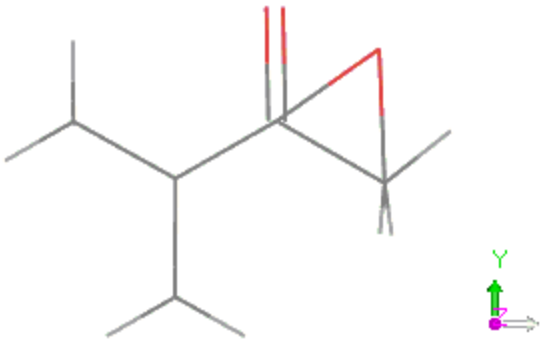
The bond type will change to be a double bond. Now you just need to add hydrogens and clean the structure.

Click the **Adjust Hydrogen** button and then the **Clean** button.

You have now sketched 3-methyl butan-2-one. However, to obtain methyl methacrylate, you must modify the structure. An esteric oxygen must be added. You can do this by adding an oxygen atom in between the carbonyl carbon and the terminal carbon and then deleting the carbon-carbon bond.

Click on the **Sketch Atom** tool. In the 3D Viewer, click on the terminal carbon atom and move the cursor away to sprout a bond. Click again to place an oxygen atom, then move to the carbonyl carbon and click on it.

You should now have a structure that looks similar to that shown below.



The intermediate structure

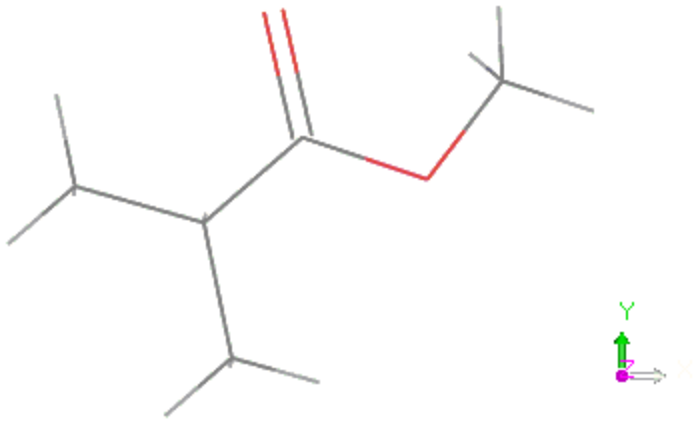
The next step is to delete the bond joining the two carbon atoms so that the oxygen bridge is the only link between the methyl and carbonyl groups.

Hold down the **SHIFT** key to use the selection mode and select the bond joining the two carbon atoms. Press the **DELETE** key.

The carbon-carbon bond disappears leaving only the oxygen atom joining the carbonyl and methyl groups. The last step is to add hydrogens and clean the structure.

Click the **Adjust Hydrogen** button and then the **Clean** button.

The final structure of methyl methacrylate should look like that shown below.



3D structure of methyl methacrylate

6. To add lighting effects

The ability to control lighting effects is often overlooked, but can be used to produce some impressive images. In this section, you are going to change the position of the first light and add a second light to enhance the image. The Lighting dialog can be accessed from the *View* menu or through the shortcut menu displayed when you right-click in a 3D Atomistic document.

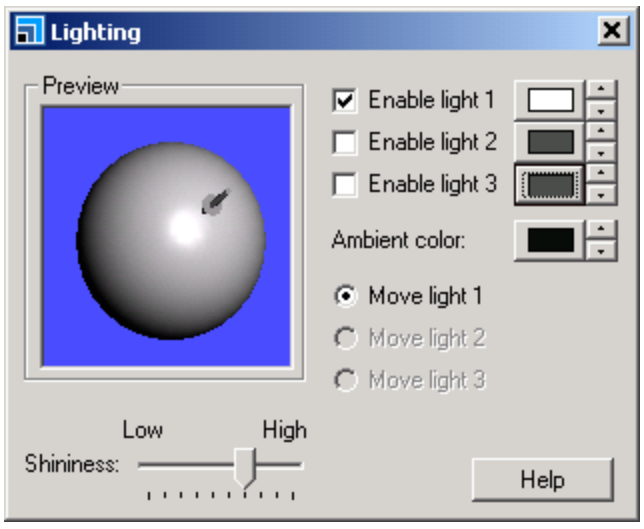
First you will change the display style of the structure as the line style does not show the lighting effects.

Make **2-chloropyridine.xsd** the active document. Right-click in the 3D Viewer and select **Display Style** from the shortcut menu to open the Display Style dialog. On the **Atom** tab, select the **CPK** option in the **Display style** section.

The display style of atoms changes to large CPK (Corey-Pauling-Koltun) spheres with their radii dependent on the van der Waals radius of the element they represent.

Right-click in the 3D Viewer and select **Lighting** from the shortcut menu.

This opens the Lighting dialog.



Lighting dialog

This dialog controls the presence of up to three lights, their colors and positions. You will move *Light 1* so that it is at the top right-hand corner of the ball.

Click on the ball and move your mouse up and to the right.

The lighting on the molecule changes as the light is moved. When you have the light in the correct position, it will look similar to this:

Preview ball with one light

Now you can add a second light into the display.

Check the **Enable Light 2** checkbox to add a second light.

A second light is displayed in the *Preview* box and the position of the first light is fixed. The second light is light gray, but this can be changed to a more suitable color.

Click the gray color indicator associated with **Enable Light 2**.

This displays the color palette. For this tutorial, you will select light blue.

Click the light blue color box in the top row, then click the **OK** button.

The light changes to light blue and the 3D Viewer is updated. Now you can move the light into the position you require.

Click and move the light to the bottom of the ball and close the Lighting dialog.

The preview ball should now look like this:

Preview ball with two lights

Now you can change the display styles and the quality of the image until you get one you are satisfied with.

You should save all the structures and documents you have generated in the project.

Select **File | Save Project** from the menu bar or click the **Save Project** button  on the **Project** toolbar.

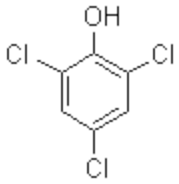
The project is saved.

Additional structures

Now you should be able to sketch molecules quite easily using different methods for selecting and changing bond type and atom type. Below are a few structures that you can build by yourself. There are hints with each structure to help you work out how to build them.

Trichlorophenol (TCP)

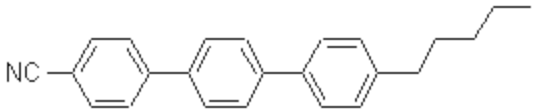
An antiseptic liquid.



- Make a copy of *phenol.xsd* (from step 2) and save it with a new filename.
- Edit the hydrogens - try using the different methods for editing the atom types.

4'-Pentyl-4-cyanoterphenyl

The first viable room temperature nematic liquid crystal.



- Start with the rings.
- Use the *Sketch Atom* tool to link the rings.
- Remember the CN bond is a triple bond.
- Add the hydrogens last.

This is the end of the tutorial.

Sketching a porphyrin

Purpose: To introduce the manipulation of fragments and use of the Display Style dialog.

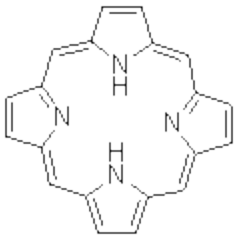
Modules: Materials Visualizer

Time:

Prerequisites: Sketching simple molecules

Background

Porphyrins are macrocyclic compounds that contain four pyrrole rings linked by one-carbon bridges. The molecules are flat and have a conjugated system of 18 π-electrons. Porphyrin derivatives with various side chains on the pyrrole rings are some of the most important life-sustaining compounds in nature. One example is heme, the iron-porphyrin complex responsible for the red color of arterial blood. The molecule that you are going to build in this exercise is porphine, the core from which all porphyrins are derived:



Structure of porphine

Introduction

In this tutorial, you will sketch porphine using the sketching tools in the Materials Visualizer. This will require you to copy, paste, rotate, and translate individual fragments, introducing you to the Materials Visualizer environment.

This tutorial covers:

- Getting started
- To sketch a five-membered ring
- To copy, paste, translate, and rotate fragments
- To connect fragments
- To edit bond types
- To add hydrogen atoms and clean the structure
- To change the display style
- To export an image

1. Getting started

Begin by starting Materials Studio and creating a new project called Porphine. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Porphine** as the name and click the **OK** button.

The new project is created with *Porphine* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

2. To sketch a five-membered ring

Before you can start to sketch, you need to open a new 3D Atomistic document in the project.

Click on the **New** arrow  on the **Standard** toolbar. Select **3D Atomistic Document** from the dropdown list.

A new 3D Atomistic document is created and you are now ready to start sketching.

In the **Project Explorer** right-click on the document name **3D Atomistic.xsd** and select **Rename** from the shortcut menu. Type in the name **porphine.xsd** and press the **ENTER** key.

The first step in building porphine is to construct a pyrrole ring. You will do this by sketching a five-membered carbon ring and replacing one of the carbon atoms with a nitrogen.

Click the **Sketch Ring** button  on the **Sketch** toolbar. With the cursor over the **porphine.xsd** 3D Viewer, press the **5** key.

The number in the ring next to the sketching cursor indicates the size of the ring that will be drawn. The default setting is for a 6-membered ring, but you can specify the size of the ring you require, from 3-membered to 8-membered, by pressing the appropriate number on the keyboard.

Click in **porphine.xsd** to sketch a five-membered ring.

A five-membered ring is placed in the 3D Atomistic document. All the carbon atoms are linked by single bonds. There is no point in adding any double bonds at this stage as you would have to delete them later because of the conjugated nature of the porphine structure. The next step is to change one of the carbon atoms to a nitrogen atom.

Select the atom you wish to change by holding down the **SHIFT** key and clicking on it.

Tip: Holding down the SHIFT key forces the selection mode. This is a shortcut that allows you to select rather than draw when a sketching tool is selected.

Click on the **Modify Element** arrow  on the **Sketch** toolbar and select **Nitrogen** from the dropdown list. Press the **CTRL + D** keys to deselect the atom.

The selected atom changes color to blue, indicating that it is now a nitrogen atom.

3. To copy, paste, translate, and rotate fragments

In this section, you will make three copies of the fragment and translate and rotate them into the positions you require. The first step is to select the fragment.

Choose the **3D Viewer Selection Mode** button  on the **3D Viewer** toolbar. Select one of the atoms in the five-membered ring, right-click and choose **Select Fragment** from the shortcut menu.

The whole ring is selected, yellow squares appear on all the atoms and bonds. The next step is to make a copy of the ring.

Select **Edit | Copy** from the menu bar, then click the **Paste** button  on the **Standard** toolbar.

Tip: You can also use the standard Windows shortcut keys, CTRL + C and CTRL + V, to copy and paste structures.

A new ring is added to `porphine.xsd` and the size of both rings is fitted to the size of the 3D Viewer. It is now necessary to zoom out so that you can translate the fragments.

Select the **3D Viewer Zoom Mode** tool  from the **3D Viewer** toolbar. Click in **porphine.xsd**, hold down the left mouse button, and drag the cursor down.

Tip: If you have a mouse with a wheel, you can use this to zoom in on the structure. You can also translate the structure by holding down the wheel and dragging.

Now you should move one of the fragments to the left of the 3D Viewer.

Click the **3D Viewer Selection Mode** button  . Make sure that one entire 5-membered ring fragment is selected.

Hold down the **SHIFT** and **ALT** keys and right-click and drag the fragment to the left. Release the mouse button when the fragment is in the correct position.

Tip: If you are using a mouse with a wheel or a middle button, you can translate the fragment by holding down the SHIFT key and the middle mouse button or wheel and dragging.

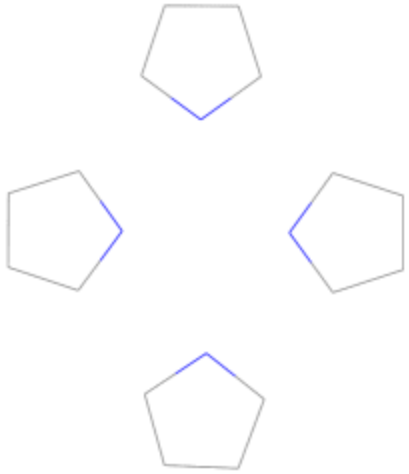
This time, you must rotate the fragment.

Move the cursor to the edge of the 3D Viewer window. Hold down the **SHIFT** key and click and hold the right mouse button. Move the cursor along the edge of the window.

The fragment rotates about the z-axis.

Note: Materials Studio uses a trackball rotation system. This means that the location of the cursor on the screen affects the axis around which you rotate. To rotate in the x and y axes, drag the cursor in the center of the 3D Viewer while holding the SHIFT key and the right mouse button.

Using what you have learned, add two more rings to the document and arrange them as shown below.



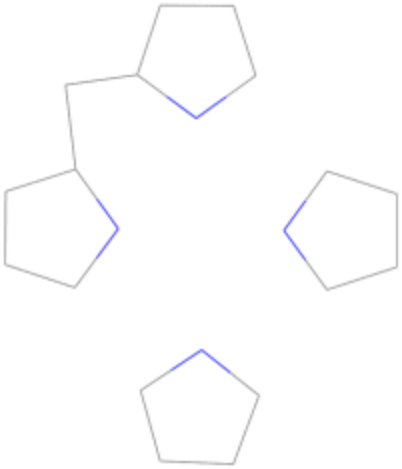
Intermediate structure showing correctly positioned rings

If you make a mistake while rotating, you can easily reset the entire view.

Click the **3D Viewer Reset View** button  on the **3D Viewer** toolbar. Deselect everything by double-clicking in **porphine.xsd**.

4. To connect fragments

The next stage is to link the fragments together with carbon bridges, as shown below.



Intermediate structure with a one-carbon bridge

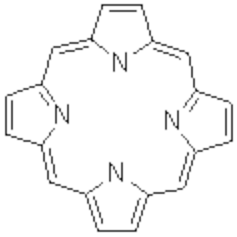
Select the **Sketch Atom** tool .

Place the cursor over one of the carbon atoms next to a nitrogen atom and, when it turns light blue, click on it. Move the cursor halfway between the two rings to sprout a bond and click to place the bridging carbon atom. Position the cursor over the nearest carbon atom that is adjacent to the nitrogen in the next ring. When the carbon atom changes color to orange, click once more to attach the bond.

Repeat these steps until the four rings are connected to form a circular structure.

5. To edit bond types

Now that you have sketched all the non-hydrogen atoms, you should edit the bond types to obtain the correct number of double bonds. There are two methods of doing this. The first is to use the *Sketch Atom* tool, clicking on individual bonds to change their bond order. Look at the structure shown below to see which bonds have to be changed to double bonds.



Intermediate structure with correct bond types

Select the **Sketch Atom** tool , choose a bond and click on it.

The bond type changes from single to double. This method is useful if you need to modify a few bonds as you sketch. However, if you have a lot of bonds to change, as in this case, you should use the *Modify Bond Type* tool.

Click the **3D Viewer Selection Mode** button . Hold down the **SHIFT** key and select all the bonds that you want to change to double bonds.

Click on the **Modify Bond Type** arrow and select **Double Bond** from the dropdown list.

The selected bonds all change from single to double bonds.

6. To add hydrogen atoms and clean the structure

You will now add hydrogen atoms to the structure.

Click anywhere in the 3D Viewer to deselect everything. Click the **Adjust Hydrogen** button .

The *Adjust Hydrogen* tool automatically fills any empty valences in a structure with hydrogen atoms. If all bond types have been set correctly in your structure, a single hydrogen atom should be connected to

each bridging carbon atom and two of the nitrogen atoms. Two hydrogen atoms should be attached to each ring. If your structure does not look like this, go back and check that you constructed it correctly.

The final step in the building process is to set the structure to a reasonable initial geometry using the *Clean* tool.

Click the **Clean** button  .

The *Clean* tool does not perform an energy minimization of the structure, but, instead, uses a look-up table of standard bond lengths and angles to give a first approximation to the correct geometry.

Note: The *Clean* operation should not be a replacement for geometry optimization with a good Hamiltonian or forcefield. However, using the *Clean* tool prior to carrying out an energy minimization is good practice because starting from a chemically reasonable initial geometry will reduce the computation time required to reach the optimized structure.

7. To change the display style

This section gives a brief introduction to the display styles that are available in the Materials Visualizer.

Click the **Display Style** button  on the **3D Viewer** toolbar.

This opens the Display Style dialog. There are 5 basic display styles available for atoms and bonds on the *Atom* tab. The current style is *Line* and the other styles are *Stick*, *Ball and stick*, *CPK*, and *Polyhedron*.

Click the **Stick** display style option.

The structure should now be represented as cylinders rather than lines. If you want to change the radius of these cylinders, you can do so using the *Stick radius* control.

Change the value in the **Stick radius** text box from 0.2 to **0.4** and press the **TAB** key.

The width of the sticks increases. If you do not want to show the bond types, this representation can be removed from the display.

Uncheck the **Bond order** checkbox.

In `porphine.xsd`, all the bonds are represented as cylinders. No distinction is made between single and double bonds.

Change the **Stick radius** back to **0.2** and select the **Ball and stick** option.

The structure should now be displayed as a ball and stick model. You can also view it as set of solid spheres using the *CPK* display style.

Select the **CPK** option. **Close** the Display Style dialog.

Tip: For reports and publications, it is frequently necessary to prepare high quality pictures of molecular structures. For more detailed guidance on high quality graphics, refer to Resolution and graphical quality.

To rotate the model, select the **3D Viewer Rotation Mode** button  and drag the cursor over the **porphine.xsd** document while pressing the left mouse button. To force rotation around the x-, y-, or z-axis, press the **X**, **Y**, or **Z** key, right-click and drag the cursor.

You can also change the background color of your documents.

Select the **Backgrounds** tab on the **Display Options** dialog.

You can choose between a single background color or a range of colors, or you could produce your own bitmap image to use as a background.

Select **Black-LightBlue** from the list of background options.

A color gradient from black to light blue is used as the background for the 3D Atomistic document. If you prefer a plain background, you can select a color of your choice from the palette on the Color dialog.

Select the **Solid color** option, then click on the color chooser  to display the Color dialog. Select a color from the palette and **close** the dialog.

8. To export an image

You can export the image shown in a 3D Atomistic document as a bitmap so that it can be included in other documents or sent to colleagues. Bitmap images are saved with the extension `.bmp` and can be edited using a simple bitmap editor such as Windows Paint.

Select **File | Export...** from the menu bar to display the Export dialog. Click on the **Save as type** arrow and choose **Structure Bitmap (*.bmp)** from the dropdown list.

When the bitmap format is selected, the *Options...* button becomes active.

Click the **Options...** button to open the Bitmap Export Options dialog.

You can use this dialog to adjust the number of pixels in the bitmap image to suit your needs. In this case, you do not need to alter any of the settings.

Click the **OK** button on the Bitmap Export Options dialog.

On the Export dialog, select a folder in the file browser where you want the bitmap to be saved and click the **Save** button.

Now you will save the project.

Select **File | Save Project** from the menu bar.

This completes this tutorial.

If you changed any of the display settings, you should restore the default settings before continuing.

From the menu bar, select **View | Display Options** to display the Display Options dialog. Ensure that the **Quality** slider is below the midpoint of the scale.

This will maintain good client-side performance.

Select **Modify | Default Atom Style** from the shortcut menu to display the Default Atom Style dialog. Ensure that the **Display style** is set to **Line**, which is the most convenient setting for sketching and manipulating molecules.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

The project is saved and the open documents are closed.

This is the end of the tutorial.

Sketching organometallic structures

Purpose: Introduces the Fragment Browser as an aid to sketching complex structures and illustrates one use of the Find Symmetry tool for nonperiodic systems.

Modules: Materials Visualizer

Time:

Prerequisites: Sketching simple molecules

Introduction

The Materials Visualizer contains tools for determining the symmetry of both periodic and nonperiodic structures. The concept and application of symmetry in periodic systems is well known, but the use of symmetry when building nonperiodic systems is less common. However, symmetry can play an important role when you are looking at organometallic structures.

In this tutorial, you will use the symmetry tools in Materials Studio to help you to construct two enantiomers of an organometallic structure. After this, you will use the fragment library to construct and define your own fragments and use these to build a more complex organometallic structure.

This tutorial covers:

- Getting Started
- To sketch the initial structure
- To use the Find Symmetry tool
- To add the rings and clean the structures
- To create user-defined fragments
- To sketch with the fragments

1. Getting started

Begin by starting Materials Studio and creating a new project called Organometallic. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

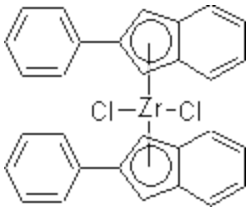
Open the New Project dialog, enter **Organometallic** as the name and click the **OK** button.

The new project is created with *Organometallic* listed in the Project Explorer.

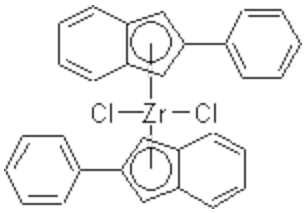
Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

2. To sketch the initial structure

The two structures you are going to draw are enantiomers. The structures are shown below in both meso and rac forms.



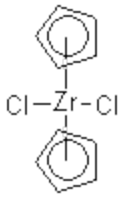
Meso form - the final conformation has Cs symmetry



Rac form with C2 symmetry

C1 symmetry systems have only identity transformations. Cs symmetry systems have identity transformations and a single mirror plane. C2 symmetry systems have identity transformations and a two fold rotation. So Cs and C2 are both based on C1 with the addition of a second operator.

First you will draw the core of this structure which has Cs symmetry, shown below, create the corresponding structure with C2 symmetry, and finally add the rings.



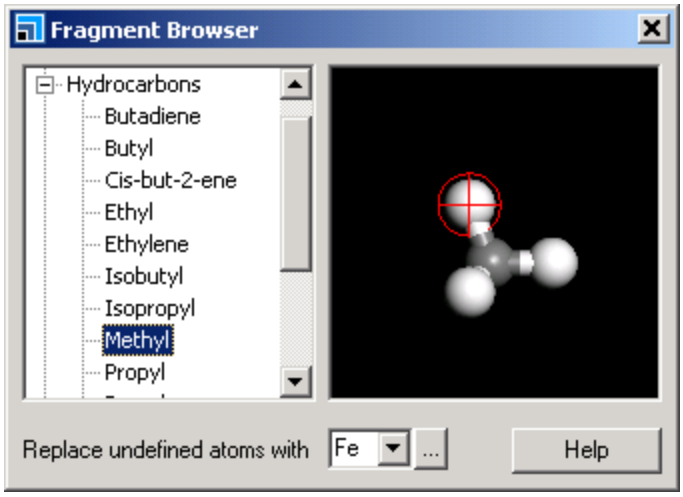
The core structure

You begin by opening a new structure document and sketching the core.

Click on the **New** arrow  on the **Standard** tool bar and select **3D Atomistic Document**.

Click on the **Sketch Fragment** arrow  on the **Sketch** toolbar and choose **Fragment Browser**.

This opens the Fragment Browser dialog.



Fragment Browser dialog

On the left, a list of the fragments available in Materials Studio is displayed, and on the right, a model of the currently selected fragment is shown. This model can be rotated, the red cage around the hydrogen atom indicates that this is the connection point for the fragment. The attachment atom can be changed to any other atom by double-clicking on the desired atom.

Click the **-** to collapse the **Hydrocarbons** node, then click the **+** to expand the **Metal Templates** node.

A list of the different metal center fragments in Materials Studio is displayed. The metallocene you will sketch has a tetrahedral conformation.

Select **4 coordinate Td**.

The default metal center is iron, but you require a zirconium center. Instead of sketching the fragment and then editing the metal atom, you can tell Materials Studio to replace the metal center before sketching.

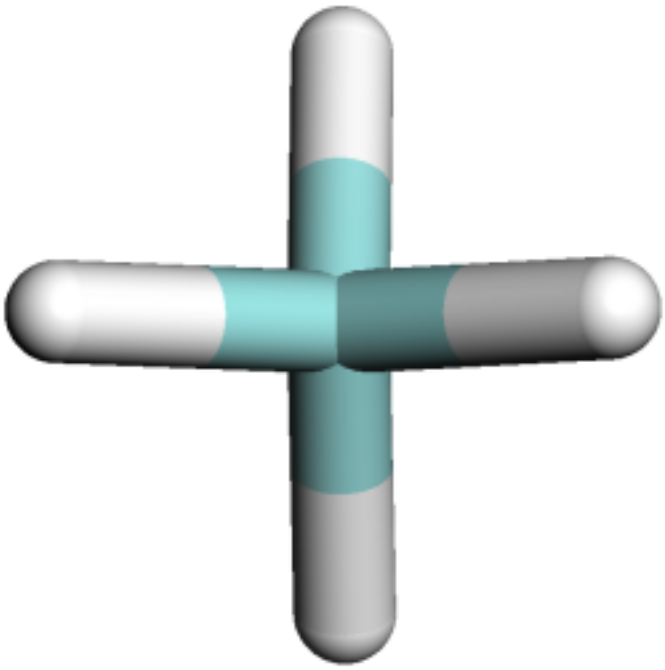
Click the ... button for **Replace undefined atoms with** to open the Periodic Table dialog. Select **Zr** and click the **OK** button.

Click once anywhere in the 3D Viewer to add the tetrahedral structure.

A tetrahedral structure is displayed in the 3D Viewer. Before you add the other substituents to this structure, you should rotate the structure core so that it appears as shown below.

Right-click in the 3D Viewer and select **Display Style** to open the Display Style dialog. Select **Stick** from the list of display styles, and close the dialog.

Right-click and drag in the 3D Viewer to rotate the fragment until it is aligned in the **+** shape illustrated below.



Alignment of metal core

Tip: To ensure that the rest of the tutorial works correctly, the structure must be oriented *exactly* as shown here.

Now you are ready to add the chlorine substituents.

Choose the **Selection** tool  from the **3D Viewer** toolbar.

Hold down the **SHIFT** key and click on the **two hydrogen atoms** to the left and right of the Zr center to select them. Click on the **Modify Element** arrow  and select **Chlorine**. Click anywhere in the 3D Viewer to deselect everything.

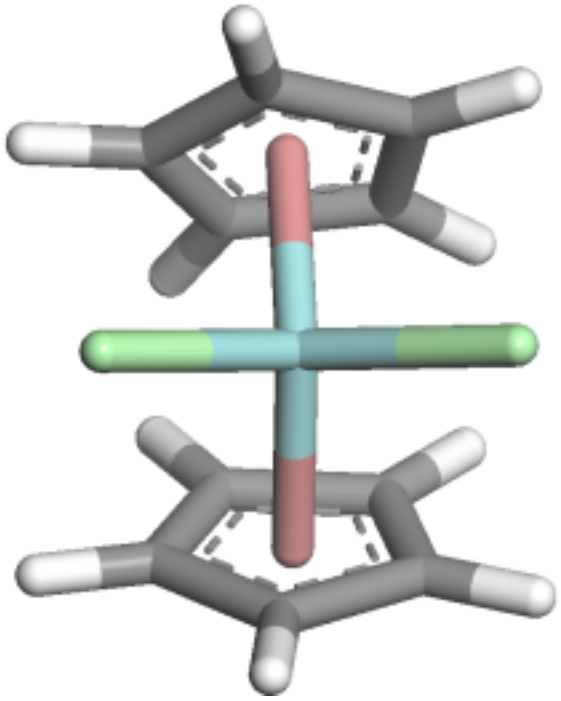
The two hydrogen atoms you selected are now chlorine atoms. The next stage is to add the cyclopentadiene ligands.

On the **Fragment Browser** dialog, collapse the **Metal Templates** node and expand the **Ligands** node. Select the **Cyclopentadienyl** fragment.

The cyclopentadienyl ligand uses a dummy atom to denote its connection point.

In the 3D Viewer, click on the **top** and **bottom hydrogen atoms** to add two cyclopentadienyl rings. **Close** the Fragment Browser dialog and change to **Selection** mode.

The core structure is displayed.



The core model

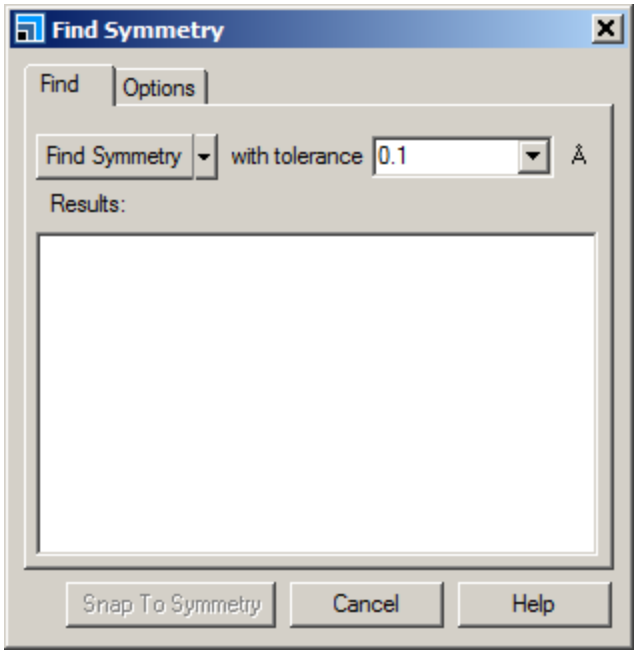
Click the **Clean** button  .

3. To use the Find Symmetry tool

The next step is to determine the symmetry of the system.

Click the **Find Symmetry...** button  on the **Symmetry** toolbar.

This opens the Find Symmetry dialog.



Find Symmetry dialog

On the **Options** tab ensure that **Reorient structure after update** is unchecked. On the **Find** tab click the **Find Symmetry** button.

The *Results* window should report the symmetry group for the structure as Cs. If C1 is displayed, the cleaning operation has distorted the structure so there is no mirror plane within the tolerance used by the Find symmetry tool. In this case you should increase the tolerance and try again to find the symmetry. When the desired Cs symmetry has been found you will snap the atom coordinates to their symmetrical positions.

If the symmetry is reported as C1, choose a larger value for **Tolerance** and click the **Find Symmetry** button again.

When the symmetry is reported as Cs click the **Snap To Symmetry** button.

Now you should make a copy of the core structure and change its symmetry to C2. To alter the symmetry of the core structure you must change the orientation of the cyclopentadienyl ring.

In the **Project Explorer**, right-click on **3D Atomistic.xsd** and select **Rename** from the shortcut menu. Change the filename to **meso** and press the **ENTER** key.

Select **meso.xsd** in the **Project Explorer**, right-click and select **Copy** from the shortcut menu.

Select the **Organometallic** project root, right-click and select **Paste** from the shortcut menu.

A copy of the *meso* 3D Atomistic document is created, named `meso (2).xsd`.

In the Project Explorer, right-click on the new **meso (2).xsd** and select **Rename** from the shortcut menu. Change the filename to **rac**.

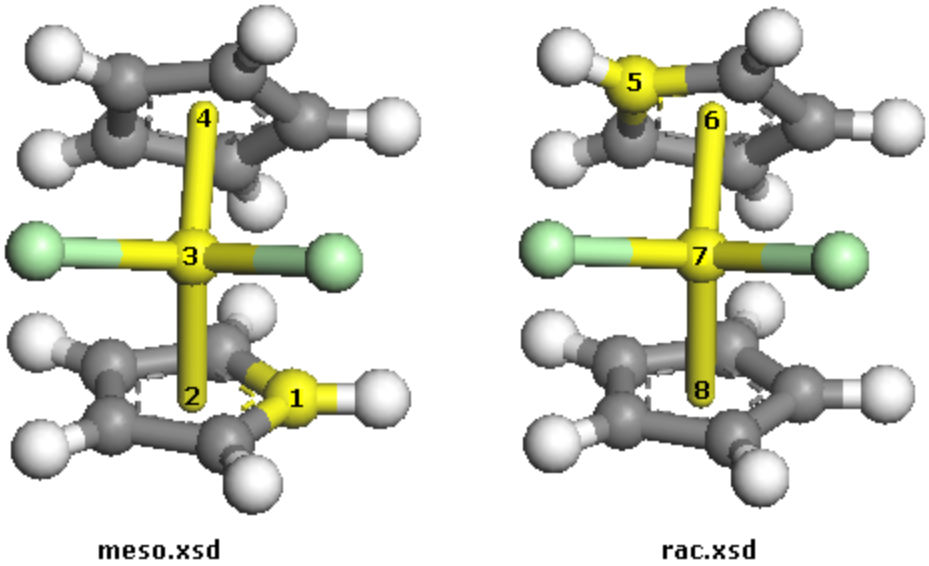
Right-click in the 3D Viewer and drag to rotate the molecule so that it is in the same orientation as the meso structure.

Materials Studio allows you to organize how you view the open documents in the workspace area.

Make sure that **meso.xsd** is the active document. Select **Window | Tile Vertically** from the menu bar.

Right-click in **meso.xsd** and select **Display Style** to open the Display Style dialog. Select **Ball and stick** from the list of display styles. Click once in **rac.xsd** and select **Ball and stick** again, then close the Display Style dialog.

You will now modify the conformation of the structure so that it has C2 symmetry.



Torsions that need to be defined to convert `rac.xsd` to C2 symmetry

Tip: To ensure that the rest of the tutorial works correctly, the meso and rac structures must be oriented *exactly* as displayed. The torsion angle 1234 *must* be close to 90 °, if the angle is close to 60 ° you should rotate your structure through 180 ° so that the cyclopentadienyl ligand swap places.

In the meso structure, illustrated on the left above, the torsion angle 1234 is approximately 90 °. To set the symmetry of `rac.xsd` to C2, you must set the torsion angle in the `rac.xsd` structure, illustrated on the right above, to the same value as that of the meso structure. The Find Symmetry tool has different levels of sensitivity and, at this level, your two structures should be mirror images of each other (ignoring the selection). Therefore, you should measure the torsion angle 1234 in `meso.xsd` and then set torsion angle 5678 in `rac.xsd` to the same value.

Make sure that **meso.xsd** is the active document. Click on the **Measure/Change** arrow  and select **Torsion**. Click on atoms **1**, **2**, **3**, and **4**, indicated in the diagram above, in that order.

A torsion angle is displayed in red. Make a note of this value. Now define the equivalent torsion in `rac.xsd`.

Note: To define a geometry monitor that can be changed, you must choose atoms that are all connected. If you do not do this, you will not be able to change the value of the geometry monitor. In this case, the dummy atom is bonded by π bonds to the carbon atom, but the bonds are not visible in this display style.

Make **rac.xsd** the active document. Click on the **Measure/Change** arrow  and select **Torsion**. Click on atoms **5**, **6**, **7**, and **8** in the diagram above, in that order.

Now change the torsion angle in `rac.xsd` to the same value as the torsion in `meso.xsd`. Since you know exactly what value you want to use, you can use the Properties Explorer to make the change.

If the Properties Explorer is not visible, select **View | Explorers | Properties Explorer** from the menu bar. Change the Properties Explorer **Filter** to **Torsion**.

Angle is the first property in the list.

Double-click on **Angle** to open the Edit Angle dialog. Change the value to the one you recorded for the meso structure. Click the **OK** button.

The 3D Viewer updates with the new geometry.

The next stage is to use the Find Symmetry tool to calculate the symmetry of the new structure.

Click the **Find Symmetry...** button  on the **Symmetry** toolbar to open the Find Symmetry dialog.

Make sure the tolerance is **0.1** and click the **Find Symmetry** button.

This time symmetry group C2 should be found. If it is not, use the Clean functionality again to make small adjustments to the torsion angles and recalculate the symmetry function. Alternatively you could use a larger tolerance for the Find Symmetry tool.

Click the **Snap to Symmetry** button.

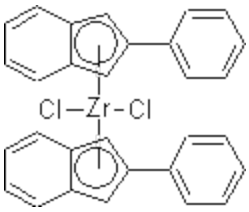
This may change the coordinates of the atoms in the structure slightly so they are exactly consistent with the symmetry found. Before continuing, remove the torsion monitors.

Change to **Selection** mode  . Select the **torsion angle** and press the **DELETE** key. Make **meso.xsd** the active document and repeat the procedure.

4. To add the rings and clean the structures

Now that you have built the core structures and defined their symmetries, it is easy to add the rings required to complete the meso and rac structures.

The meso structure



The meso structure with Cs symmetry

Double-click on **meso.xsd** in the **Project Explorer** to make it the active document.

Now add the phenyl rings that are fused directly to the cyclopentadienyl rings.

Click the **Sketch Ring** button . Hover the cursor over the bond that you want to fuse the ring to and when it changes color to blue, hold down the **ALT** key and click once. Repeat the procedure for the equivalent bond in the other cyclopentadienyl ring.

As the Find Symmetry tool is very sensitive to small changes in geometry, you should adjust the hydrogens and clean the structure before checking the symmetry again.

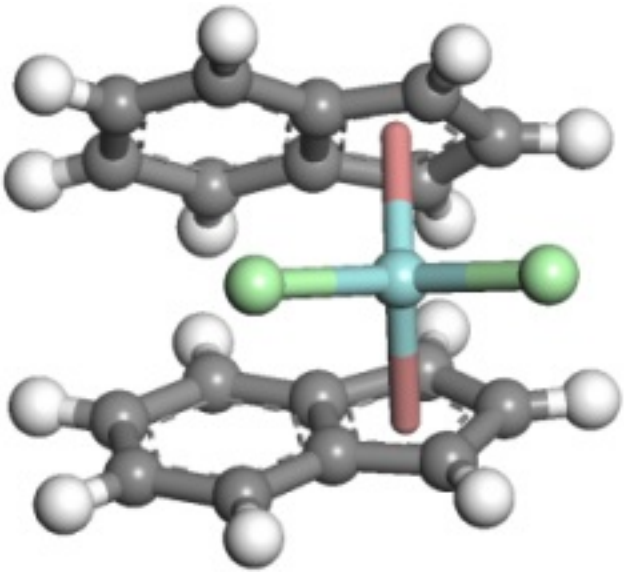
Click the **Adjust Hydrogen** button , followed by the **Clean** button .

Click the **Find Symmetry...** button to open the Find Symmetry dialog. Click the **Find Symmetry** button.

If the symmetry is shown as C1 you should increase the tolerance and click the **Find Symmetry** button again.

Click the **Snap to Symmetry** button.

The structure should now look like the one shown below and should have only Cs symmetry.



The intermediate meso model

The final step is to add the unfused phenyl rings, add hydrogens, and clean the structure.

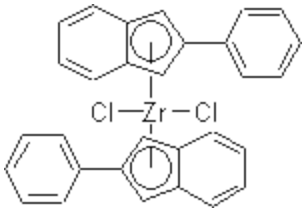
Close the **Find Symmetry** dialog and click the **Sketch Ring** button  . Hold down the **ALT** key and click on the **hydrogen** on the cyclopentadienyl ring that is opposite the fused bond. Repeat this for the second ligand. Click the **Adjust Hydrogen** and **Clean** buttons.

Finally, you should check that the symmetry is still Cs.

On the Find Symmetry dialog click the **Find Symmetry** button.

Click the **Snap to Symmetry** button.

The rac structure



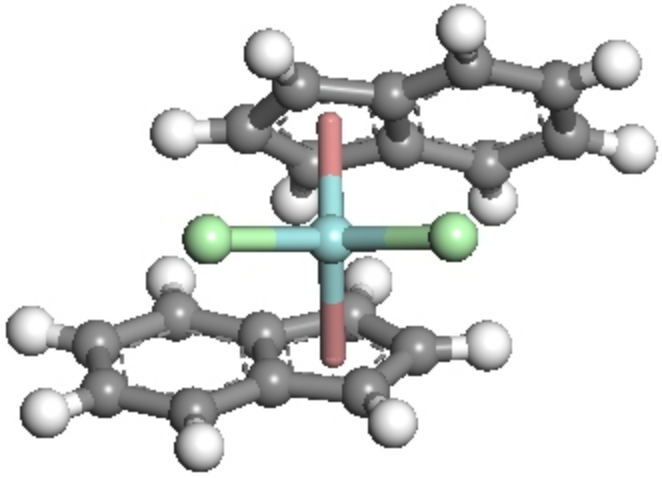
The rac structure with C2 symmetry

Make **rac.xsd** the active document.

This time you should add phenyl rings to opposing sides of the two cyclopentadienyl ligands to maintain the C2 symmetry.

Click the **Sketch Ring** button. Hover the cursor over the bond that you want to fuse the ring to and, when it changes color to blue, hold down the **ALT** key and click once. Repeat the procedure for the opposite bond in the other cyclopentadienyl ring.

As before, add hydrogens and clean the structure after each step.



The intermediate rac model

Finally, add the two unfused phenyl rings.

Add the phenyl rings to the second hydrogen of the cyclopentadienyl ring as described for the meso model. Remember to press the **ALT** key to generate aromatic rings.

Click the **Adjust Hydrogen** and **Clean** buttons.

Now check the symmetry of the system again, it should still have C2 symmetry.

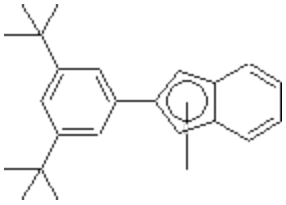
On the Find Symmetry dialog, click the **Find Symmetry** button and then the **Snap to Symmetry** button.

Before you continue, save the project.

Click the **Save Project** button  .

5. To create user-defined fragments

Materials Studio allows you to define your own fragments and save them to the library. In this section, you will build a ligand similar to those constructed in the previous sections and use it to make a more complex metallocene. The ligand you are going to construct is shown below.



The ligand

Open a new 3D Atomistic Document. Click on the **Sketch Fragment** arrow and choose **Fragment Browser** to open the Fragment Browser dialog.

Select the **Cyclopentadienyl** fragment from the **Ligands** section. Click once in the 3D Viewer to place the cyclopentadienyl fragment.

Now you should sketch the two phenyl rings.

Click the **Sketch Ring** button, hold down the **ALT** key and click on one of the C-C bonds in the cyclopentadiene ring.

A 6-membered ring is fused to the cyclopentadienyl ring.

Hold down the **ALT** key and click on the **hydrogen** opposite the bond with the fused 6-membered ring. Click the **Adjust Hydrogens** button.

Now add the tertiary butyl substituents in the meta positions on the unfused ring. Instead of sketching the substituents, they can be obtained from the fragment library.

On the Fragment Browser dialog, select the **Tertiary Butyl** fragment from the **Hydrocarbons** library. Click on the two **hydrogens** in the meta positions on the unfused phenyl ring to add the t-butyl groups. Close the **Fragment Browser**.

Click the **Clean** button.

The next step is to define this new fragment. To maintain consistency in the display styles in the Fragment Browser, you should view this in ball and stick format.

If the document is not already in ball and stick format, right-click in the 3D Viewer and select **Display Style** to open the Display Style dialog.

Select **Ball and stick** and close the dialog.

Now you can define the fragment.

Click on the **Sketch Fragment** arrow and select **Define Fragment**.

This opens the Define Fragment dialog. You have to select a connection point. For this fragment, the connection point is the hydrogen atom that is attached to the dummy atom in the cyclopentadienyl ring.

Click the **Selection** button  . Select the **hydrogen** atom attached to the dummy atom and click the **Define** button on the Define Fragment dialog.

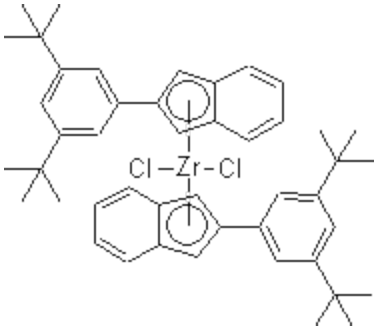
A red cage is displayed around the connecting atom. The final step in this procedure is to choose a fragment library and name for the fragment. In this case, you will put the new fragment in the User library and call it t-but-cp.

Click in the **Fragment Name** text box and type in **t-but-cp**. Click the **Add** button. If a dialog opens asking about the creation of the User library, click the **Yes** button. Close the Define Fragment dialog.

You have successfully added a new fragment to the fragment library.

6. To sketch with the fragments

Now that you have defined a new fragment, you can use it to sketch this molecule.



The target structure

The first step is to sketch the metal center.

Open a new 3D Atomistic Document. Open the **Fragment Browser dialog** and select **4 coordinate Td** from **Metal Templates**. Click once in the 3D Viewer to place the metal atom.

Now you can add on the ligands.

On the Fragment Browser dialog, select the **t-but-cp** ligand from the **User** library. Click on the top **hydrogen** attached to the Zr atom. Click and hold the mouse button on the bottom **hydrogen**.

Holding the mouse button down while sketching a fragment displays a torsion monitor. The fragment can be rotated by moving the mouse.

Move the mouse to rotate the fragment until it is in a similar configuration to the one shown above. Click the **Clean** button.

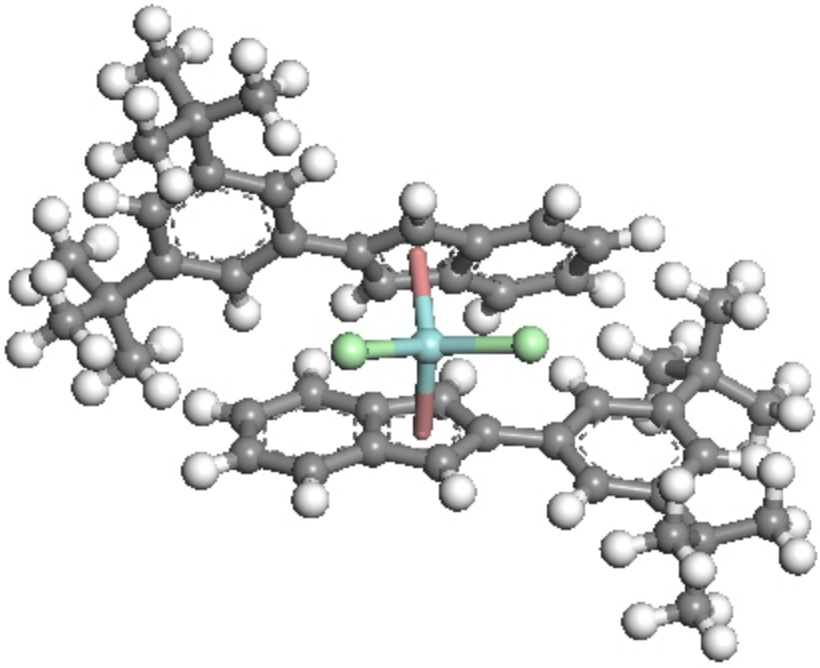
Note: The Clean operation is not an energy minimization, so for an accurate structure, you should optimize the geometry using an appropriate semiempirical or ab initio program.

The final step is to edit the remaining two hydrogens attached to the metal center to make them chlorines.

Click the **Selection Mode** button on the toolbar. Select the **two hydrogens** attached to Zr by clicking on them while holding down the **SHIFT** key. Click the **Modify Element** button and select **Chlorine**.

Click anywhere in the 3D Viewer to deselect the atoms. Click the **Clean** button.

You have now finished sketching the structure. If you wish to experiment further with this structure, try changing the dihedral angle as you did for the meso and rac structures so that it looks similar to the one shown below.



The target model

Using the Project Explorer, rename this 3D Atomistic document t-butyl.

Right-click on the name highlighted in the **Project Explorer** and select **Rename**. Type in **t-butyl** and press the **ENTER** key.

Before finishing the tutorial, change the window view so that you can see all three structures you have drawn.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

In the Project Explorer, double-click to open **meso.xsd**, **rac.xsd**, and **t-butyl.xsd**. Select **Window | Tile Vertically** from the menu bar.

This is the end of the tutorial.

Overlaying and aligning molecules

Purpose: Introduces the collection document and demonstrates how it can be used to overlay and align molecules.

Modules: Materials Visualizer

Time:

Prerequisites: Project management

Introduction

Whether you are comparing two crystal structures from a Polymorph prediction or comparing optimized conformations of molecules, the ability to overlay sets of molecules or crystals for visualization is a vital part of molecular modeling. The 3D Atomistic Collection document in the Materials Visualizer allows you to overlay molecules, slabs, and crystals in the same 3D Cartesian space without any physical interaction between the systems.

This tutorial illustrates how you can use collection documents to overlay molecules and demonstrates how to align multiple structures.

This tutorial covers:

- Getting started
- To insert and select structures in a collection document
- To align structures by their principal moments

1. Getting started

Begin by starting Materials Studio and creating a new project called Collection. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Collection** as the name and click the **OK** button.

The new project is created with *Collection* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

2. To insert and select structures in a collection document

The first step is to load in a series of structures. You will use the corrosion inhibitors from the QSAR tutorial and import them into a study table.

Click **New** arrow  on the **Standard** toolbar and select **Study Table Document** from the dropdown list to create a new study table document.

Click the **Insert From File** button  on the **Standard** toolbar to display the Insert Into Active Document dialog. Navigate to the **Examples\QSAR\Structures** folder and double-click on **Corrosion.sd** to open the file.

The corrosion data are displayed in the study table. You can extract the structures from the study table into a 3D Atomistic Collection document (`.xod` file).

Select the set of structures in rows **1** to **7** of column **A** in the study table. Right-click on any of the selected cells and choose **Extract To Collection** from the shortcut menu.

The selected structures are extracted to a collection document named `Extracted From Study Table.xod`.

Note: You can also insert structures into a collection document from a series of separate 3D Atomistic documents in the current project. To do so, create a new 3D Atomistic Collection document, select the documents that you wish to insert in the Project Explorer, then right-click on one of them and select *Insert Into* from the context menu.

If you wish to view the contents of a 3D Atomistic Trajectory document in a collection document, you must first insert the frames into a study table and then extract the structures as described above.

Collection documents support many of the features that are available in 3D Atomistic documents; the structure viewing and manipulation tools, for example. In addition, molecules imported into a collection document retain certain types of data that may have been calculated for that structure, such as field, surfaces, or habits. The most important difference between `.xsd` and `.xod` documents is that in the latter, molecules are chemically isolated, allowing them to be in close proximity (for example for alignment) without interacting with each other. In contrast, molecules in 3D Atomistic documents are affected by their environment.

You can control the selection of molecules in a collection document using the Physical Systems dialog.

Right-click in the collection document and select **Physical Systems** from the shortcut menu.

This opens the Physical Systems dialog, this can be used to select and change the visibility of the structures in the collection document.

In the Physical Systems dialog, click on **Corrosion - 1** and then **Corrosion - 7**.

As you click on the structure names in the Physical Systems dialog, the structures are selected in the collection document.

Tip: You can select multiple structures by using the SHIFT and CTRL keys to modify selection in the usual way.

You can change the visibility of molecules irrespective of whether they are selected in the Physical Systems dialog.

With **Corrosion - 7** selected, click on the checkbox for **Corrosion - 3** in the Physical Systems dialog.

The Corrosion - 3 structure is removed from view, although it is still present in the collection document.

You can also delete molecules from the collection document.

On the Physical Systems dialog, check the **Corrosion - 3** checkbox to switch its display back on.

Select **Corrosion - 1** and press the **DELETE** key.

The molecule is deleted from the collection document and is no longer shown in the Physical Systems dialog.

3. To align structures by their principal moments

There are two tools available for aligning molecules in the Materials Visualizer. One tool allows you to align a set of molecules in a specific direction and the other, Superpose Structures, allows to align molecules with respect to each other. For this tutorial, you will align the molecules in a specific direction.

In the Physical Systems dialog, select **Corrosion - 2**. Click on the **Create Centroid** arrow  and select **Principal Axes** from the dropdown list.

The principal axes are calculated and displayed in the collection document for the selected molecule.

Tip: You can perform alignment using any of the averaged geometry objects that can be calculated using the *Create Centroid* tool.

Repeat the above steps for molecules **Corrosion - 3** through to **Corrosion - 7**. **Close** the Physical Systems dialog.

Now that the principal axes have been calculated and displayed for each molecule in the collection document, you can align the molecules.

Click in the **Extracted From Study Table.xod** document to deselect all the objects. Hold down the **ALT** key and double-click on one of the principal axes objects. All the principal axes objects are selected.

To align molecules in Materials Visualizer, you first align the view and then align the molecules to fit the view. In this tutorial, you will align the principal moments with the x, y, and z axes, so you must set up the view appropriately.

Click the **3D Viewer Reset View** button  and then click the **Align Onto View** button  .

The molecules are rotated and aligned so that their principal moments are aligned with the x, y, and z axes.

If you wish to continue working on these structures, you can return them to the study table or extract them to separate 3D Atomistic documents.

Right-click in **Extracted From Study Table.xod** and select **Return To Study Table** from the shortcut menu.

The molecules are returned to the study table, overwriting the original structures. You could now proceed by optimizing these structures or calculating properties using the Models dialog.

With the collection document in focus, click in it to deselect the principal axes objects, then right-click and select **Extract To Atomistic Documents** from the context menu.

The structures contained within the collection document are extracted to separate 3D Atomistic documents and are placed within the folder that is currently selected in the Project Explorer.

Tip: If you have particular molecules selected in the Physical Systems dialog when you choose *Extract To Atomistic Documents* from the shortcut menu, only the selected molecules will be extracted into `.xsd` documents.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

This is the end of the tutorial.

Precise positioning and movement of atoms

Purpose: Illustrates the use of Move To mode, the precise movement tools, and the alignment tools in the Materials Visualizer.

Modules: Materials Visualizer

Time:

Prerequisites: Sketching simple molecules

Background

The ability to move and place fragments or atoms in specific positions can be important when setting up initial structures. For example, being able to place a molecule accurately in the center of a zeolite channel or a specific distance from a surface makes it easy to set up complex systems quickly.

The Materials Visualizer has a set of tools, accessible using the *3D Movement* toolbar, designed to help with these tasks. There are tools that translate and rotate selected atoms by specific amounts and others that enable you to move entire fragments to a geometrical center or to align objects. A range of geometric objects are available in the Materials Visualizer, including centroids, best fit lines and planes, and principal axes, enabling you to perform many different types of alignment.

Introduction

In this tutorial, you will use the precise positioning and alignment tools to place a chloromethane molecule in the main channel of a zeolite framework. You will then use the movement tools to move the chloromethane along the zeolite pore.

This tutorial covers:

1. Getting started

Begin by starting Materials Studio and creating a new project called Zeolite. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Zeolite** as the name and click the **OK** button.

The new project is created with *Zeolite* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

2. To import the zeolite and define a centroid

The first step is to import the zeolite framework.

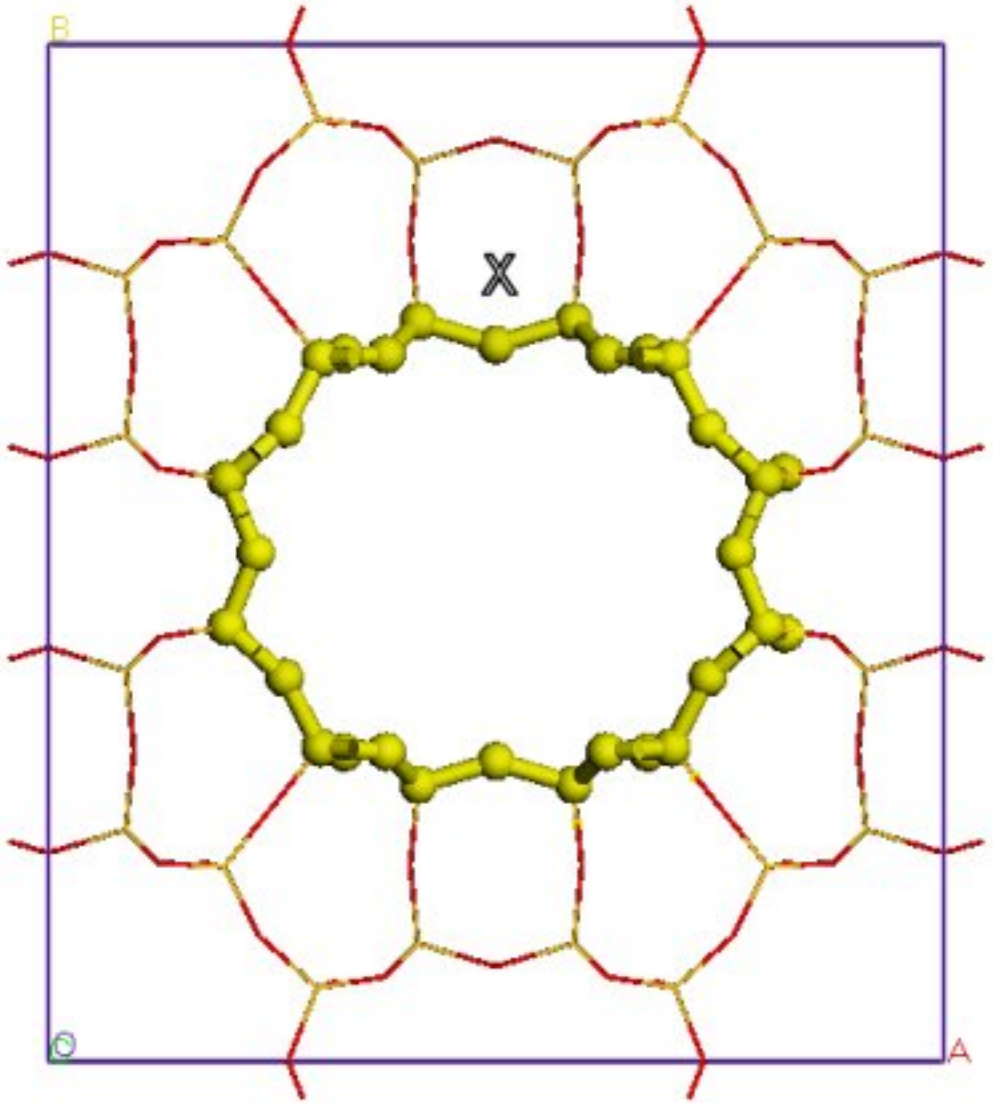
Select **File | Import...** from the menu bar or click the **Import** button  on the **Standard** toolbar to open the Import Document dialog. Navigate to and select **Structures\zeolites\MOR.msi**, then click the **Open** button.

The zeolite framework is imported into the project. Initially, the structure has a high degree of symmetry and this must be reduced before continuing with the tutorial as it would restrict your ability to add atoms and move them around the pores. You will lower the symmetry of the structure by assigning it to the simplest space group, P1.

Select **Build | Symmetry | Make P1** from the menu bar.

To place the chloromethane molecule in the center of the zeolite channel, you must first define a centroid. A centroid is a geometrical object that defines the center of a set of atoms.

In this tutorial, you will place the chloromethane molecule in the middle of the central channel. To do this, you need to select all the atoms that define the channel (shown in ball and stick display style in the figure below).



Zeolite channel atoms selected for centroid definition

The easiest way to do this is to use the lasso selection tool.

Position the cursor in the position indicated by the X in the figure above. Hold down the **SHIFT** and **Q** keys, click and hold the left mouse button and drag the cursor around the atoms that define the channel so that the lasso selects all the atoms.

The next step is to define the centroid for the selected atoms.

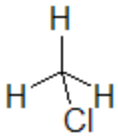
Click on the **Create Centroid** arrow  on the **Sketch** toolbar and select **Centroid** from the dropdown list. Click anywhere away from the structure in **MOR.xsd** to deselect the atoms.

A green centroid object is defined and displayed at the center of the channel.

Tip: You can change the properties of the centroid using the Properties Explorer. For example, you can change whether the centroid is defined by a mass-weighted average of the atom coordinates or a simple geometric average by changing the setting of the *IsWeighted* property. The default setting uses the mass-weighted average.

3. To sketch chloromethane and align it along the channel

Start by sketching chloromethane.



Structure of chloromethane

Click on the **New** arrow  on the **Standard** toolbar and select **3D Atomistic Document** from the dropdown list.

In the Project Explorer, right-click on **3D Atomistic.xsd** and select **Rename** from the shortcut menu. Change the name of the document to **chloromethane.xsd**.

Use the tools on the **Sketch** toolbar to construct a chloromethane molecule.

Click the **Adjust Hydrogen** button  and then the **Clean** button  .

The correct number of hydrogens are added the structure and it is adjusted to a reasonable geometry. Now you need to copy and paste the penetrant chloromethane molecule into the zeolite framework.

Ensure that **chloromethane.xsd** is the active document and press **CTRL + C**. Double-click on **MOR.xsd** in the Project Explorer, then right-click and select **Paste** from the shortcut menu.

The chloromethane molecule should be pasted into the bottom left-hand corner of the cell.

Before you place the molecule in the center of the channel, you can use the alignment tools to orient the carbon-chlorine bond so that it runs parallel to the channel.

Hold the **SHIFT** key and select the carbon and chlorine atoms of the chloromethane molecule. Click on the **Create Centroid** arrow  on the **Sketch** toolbar and select **Best Fit Line** from the dropdown list.

A green dashed line is displayed, showing the best fit line between the two atoms. You can now align this line with the plane of the screen.

Press the **HOME** key to reset the view.

Select the green best fit line object. Click on the **Align Onto View** arrow  on the **3D Movement** toolbar and select **Align In/Out** from the dropdown list.

The carbon-chlorine bond should now be pointing down the channel. You can delete the best fit object you created.

Rotate the structure so that you can see the best fit line. Select the best fit line object and press the **DELETE** key.

4. To move chloromethane to the center of the channel

The next stage is to use the *Move To* tool to position the carbon atom of chloromethane on the centroid.

Rotate the cell so that you can see the central carbon atom, colored gray, of the chloromethane molecule.

Note: You will see three centroids displayed. The two centroids outside the cell are symmetry replicates of the one in the center of the cell.

Click the **Move To** button  on the **3D Movement** toolbar.

Move the cursor over the **carbon** atom of the chloromethane and, when it changes color to blue, click the left mouse button. Move the cursor over the **centroid** and when it changes color to blue, click once more.

The chloromethane molecule moves to the center of the channel and the carbon atom of the chloromethane is positioned over the centroid.

Tip: The default behavior is for the entire fragment containing the selected atom to move. You can move specific atoms by selecting them and then holding down the ALT key while using the *Move To* functionality.

Click the **3D Viewer Selection Mode** button  on the **3D Viewer** toolbar. Right-click in **MOR.xsd** and select **Display Style** from the shortcut menu to display the Display Style dialog.

On the **Lattice** tab change the **Style** to **In-Cell**. Use the arrow keys to rotate the cell to view it from different angles.

Now that the chloromethane molecule is in the center of the zeolite channel, you can remove the centroid object.

Select the centroid object, right-click in **MOR.xsd** and choose **Delete** from the shortcut menu.

5. To position the chlorine atom at the edge of the cell

You can use another property of centroids to help position the chloromethane so that the chlorine atom is at the edge of the cell. As moving a centroid also moves the parent fragment, you can define a centroid on the chlorine atom and then edit the properties of the centroid to move the chlorine atom.

Select the chlorine atom of the chloromethane molecule in **MOR.xsd**. Click on the **Create Centroid** arrow  and select **Centroid** from the dropdown list.

A centroid is defined on the chlorine atom.

If the Properties Explorer is not visible, select **View | Explorers | Properties Explorer** from the menu bar.

The Properties Explorer shows all the properties of the centroid. Properties that are displayed in gray cannot be edited, but those shown in black can be altered.

In the Properties Explorer, select **Centroid** from the **Filter** dropdown list. Double-click on the **CentroidXYZ** property to open the Edit CentroidXYZ dialog.

Change the **Z** value to **0.00** and click the **OK** button.

In the 3D Viewer, rotate the cell by holding down either the **X**, **Y**, or **Z** key and the right mouse button and dragging the cursor across the screen.

The chloromethane will now be oriented so that the chlorine is exactly on the edge of the cell at z = 0.

6. To move the chloromethane molecule by specific amounts

The Materials Visualizer provides a set of tools that enable you to move fragments and objects by specific amounts.

Click the **3D Viewer Reset View** button  and then press the **LEFT** arrow key twice.

This rotates the cell so that the channel runs from left to right across the screen.

Double-click on the chloromethane fragment and click the **Movement** button  on the **3D Movement** toolbar.

This opens the Movement dialog which contains tools that allow you to translate or rotate selected fragments by precise regular displacements, the magnitude of which you can specify.

Select the **Distance** option in the **Translation** section of the Movement dialog. Click the **Move Right** button  and then the **Move Left** button  .

The chloromethane fragment is translated by exactly 0.5 Å in the specified direction each time you click one of the buttons.

Note: The translation and rotation tools act relative to the x, y, and z axes of the screen, not the axis indicators displayed in the bottom right-hand corner of 3D Viewers.

You could explore the potential energy surface of the zeolite pore by moving the chloromethane molecule around inside the channel in increments of 0.5 Å, saving the resulting structures in a study table, and then performing energy calculations on the series.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

This is the end of the tutorial.

Docking molecules onto surfaces

Purpose: Introduces using the Surface Builder to cleave a crystal structure and place a fragment on a new surface.

Modules: Materials Visualizer

Time:

Prerequisites: Project management

Introduction

Surface chemistry, in particular chemisorption and heterogeneous catalysis, plays a vital role in many industrial processes. Valuable insights into the chemistry and physics of these processes can be obtained using molecular modeling and computational methods. This knowledge forms a crucial input into the chemical design process.

This tutorial illustrates how Materials Studio can help with computational research in surface chemistry. It details how to build an atomistic surface model and how to dock a small chemical component to that surface.

This tutorial covers:

- Getting started
- To cleave and align the surface
- To build a supercell
- To build a slab
- To position molecules on a surface

1. Getting started

Begin by starting Materials Studio and creating a new project called Platinum. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Platinum** as the name and click the **OK** button.

The new project is created with *Platinum* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

2. To cleave and align the surface

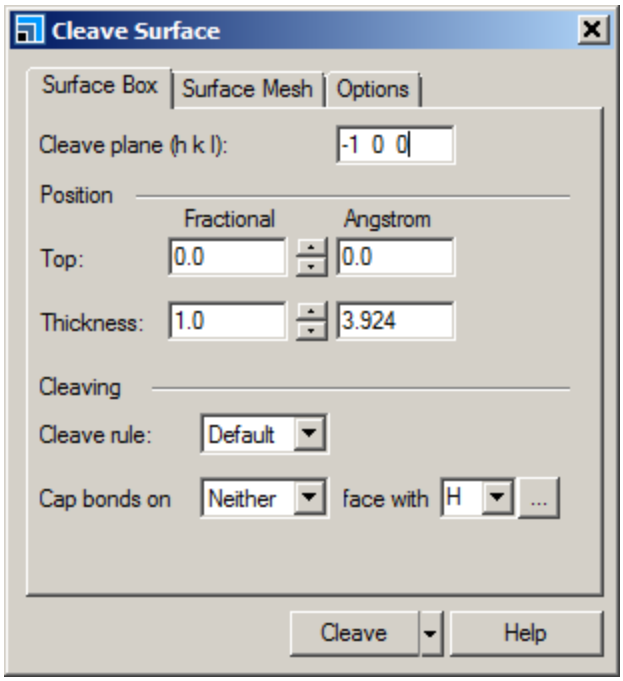
In this tutorial, you are going to work with the crystal structure of platinum metal, which you can import from the extensive library of pre-built molecules, crystals, and materials supplied with your Materials Studio installation.

Select **File | Import...** from the menu bar or click the **Import** button on the **Standard** toolbar to display the Import Document dialog. Navigate to and select **Examples\Documents\3D Model\Pt.xsd**, then click the **Open** button.

The 3D Atomistic document `Pt.xsd`, containing the crystal structure of platinum metal, is imported into the current project and displayed in a 3D Viewer. Next you will cleave the surface.

Select **Build | Surfaces | Cleave Surface** from the menu bar.

This opens the Cleave Surface dialog.



Cleave Surface dialog, Surface Box tab

Blue dashed lines are displayed on the crystal indicating the plane you are cleaving. This information is also given in the *Cleave plane (hkl)* text box at the top of the *Surface Box* tab of the Cleave Surface dialog. The default plane is (-1 0 0). The active surface in platinum that you want to cleave is the (1 1 1) surface.

In the **Cleave plane (hkl)** text box, enter **1 1 1** and press the **TAB** key.

Click the **3D Viewer Reset View** button on the **3D Viewer** toolbar.

The blue box indicating the cleave plane moves to the (1 1 1) crystal plane. You can choose where you want the top of the surface to be and the thickness of the surface using the *Position* controls on the *Surface Box* tab.

On the Cleave Surface dialog, click once on the up spin control to increase the **Top** value in the **Fractional** column to **1.0**.

The cleave plane box moves up to the next set of atoms (note that the equivalent physical distance value increases to 2.265 Å). If you use the spin controls to move the position of the box, each click will make the cleave plane box jump to the next set of atoms. This is particularly useful if you have a cell containing various different types of atoms.

You can also change the thickness of the cell.

Click three times on the up spin control to increase the **Thickness** setting in the **Fractional** column to **4.0**.

The thickness of the cleave plane box increases and the equivalent physical distance increases to 6.796 Å. Now that you have set up the surface parameters, you can cleave the cell.

Click the **Cleave** button.

A new 3D Atomistic document, `Pt(1 1 1).xsd`, is opened and a 2D periodic structure is displayed as a white rhombus alongside the platinum atoms. You can alter the *Top* and *Thickness* settings for the surface again on the Recleave Surface dialog and both 3D Atomistic documents will be updated automatically.

Note: The Cleave Surface dialog is renamed as the Recleave Surface dialog when a surface has been generated and is in scope. You can observe this change by switching the focus between `Pt.xsd` and `Pt(1 1 1).xsd`.

On the Recleave Surface dialog, click twice on the up spin control to increase the **Thickness**, then **close** the dialog.

Click the **Reset View** button 

`Pt(1 1 1).xsd` is updated with the new surface structure.

The cleave plane is at an angle to the Cartesian axes shown by the axis indicator. The molecule can be aligned to the Cartesian axes by selecting either the surface atoms or the 2D lattice.

Select the 2D lattice (represented by the white rhombus).

Aligning the 2D lattice will align all the atoms associated with the surface. Generally, you should align the view first and then align the molecule or object to the view. As you have already reset the view, you can now align the molecule.

The *Align Onto View* tool provides a range of alignment options. You will use the default option first.

Click the **Align Onto View** button  on the **3D Movement** toolbar.

The surface is rotated so that the 2D lattice is aligned along the x-axis and in the xy plane.

Click on the **Align Onto View** arrow  and select **Align With View YZ Plane** from the dropdown list.

Click on the **Align Onto View** arrow again and select **Align Horizontal**.

The platinum surface is now aligned in the xz plane.

3. To build a supercell

You have now built a 2D cell from a 3D crystal. However, for many applications, it is desirable to view the contents of several cells. You can increase the number of cells that are displayed whilst retaining the periodicity of one cell, or you can make a supercell from a number of cells. To illustrate this, you will first increase the number of cells you are visualizing and then make a supercell.

Click anywhere in **Pt(1 1 1).xsd** to deselect the 2D lattice, then click on the **Display Style** button on the **3D Viewer** toolbar to display the Display Style dialog.

On the **Atom** tab, choose the **Ball and stick** display option. Select the **Lattice** tab.

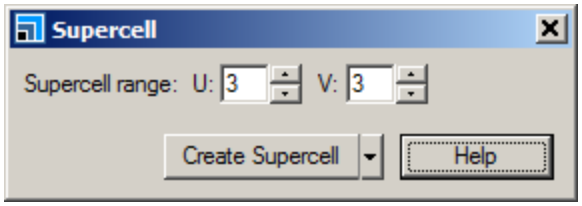
You can change the number of cells viewed by increasing the *U* and *V* display ranges on the *Lattice* tab of the Display Style dialog.

Click twice on the up spin controls for both **Max. U** and **Max V**. **Close** the Display Style dialog.

Each time you click on one of the spin controls, the 3D Atomistic document is updated, the final document now contains a 3 × 3 surface. However, this surface still retains the original periodicity. Although useful for visualization purposes, increasing the display ranges for U and V does not increase the size of the surface unit cell. To do this, you must use the supercell building functionality in Materials Studio.

Select **Build | Symmetry | Supercell** from the menu bar.

This opens the Supercell dialog.



Supercell dialog

The supercell range is read from the currently displayed 3D Atomistic document. You will create a 3 × 3 supercell.

Click the **Create Supercell** button and close the dialog.

A larger surface is built, comprising nine of the original unit cells. This structure is now a reasonable size such that calculations can be performed without molecules on the surface interacting with periodic images of themselves.

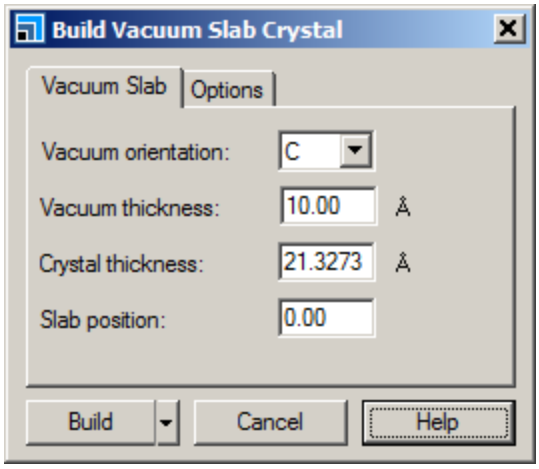
This system has 2D periodicity. In order to use it with a quantum mechanics program, such as CASTEP or DMol^3, you need to convert it to a 3D lattice by creating a slab with a region of vacuum.

4. To build a slab

A slab is a 3D periodic cell with a layer of vacuum separating periodic images of a surface. This enables you to put molecules onto the surface, in the vacuum region, so that the molecule does not interact with a periodic image of the surface above it.

Select **Build | Crystals | Build Vacuum Slab...** from the menu bar.

This opens the Build Vacuum Slab Crystal dialog, which allows you to specify the orientation, thickness, and position of the region of vacuum.



Build Vacuum Slab Crystal dialog, Vacuum Slab tab

Increase the **Vacuum thickness** from 10.00 to **20.00** Å. Click the **Build** button.

`Pt(1 1 1).xsd` is updated to display a cell with the platinum surface at the bottom and a large area of vacuum above. As this system is 3D periodic, there is a layer of atoms at the top of the cell. You can change the display style so that these atoms are not visible.

Select **View | Display Style** from the menu bar to open the Display Style dialog.

On the **Lattice** tab change the **Style** from Default to **Original**. Close the Display Style dialog.

5. To position molecules on a surface

The final stage in this tutorial is to build a small molecule and then position it on the surface. To do this, you will sketch a molecule of methane in a new 3D Atomistic document, copy and paste it into the slab, and dock it with the surface.

Click on the **New** arrow  on the **Standard** toolbar and select **3D Atomistic Document** from the dropdown list.

Click the **Sketch Atom** button  on the **Sketch** toolbar, click once in the new 3D Viewer, and press the **ESC** key to finish sketching.

You have sketched a single carbon atom in the 3D Atomistic document. You will change this into methane by using the *Adjust Hydrogen* and *Clean* tools.

Click the **Adjust Hydrogen** button  on the **Sketch** toolbar, followed by the **Clean** button  .

The next step is to copy and paste the methane molecule into the document containing the slab.

Select **Edit | Copy** from the menu bar. Double-click on **Pt(1 1 1).xsd** in the Project Explorer, then click the **Paste** button  on the **Standard** toolbar.

Tip: You can also use the standard Windows shortcut keys, CTRL + C and CTRL + V, to copy and paste structures.

The methane molecule is pasted into the slab cell. Now you have to select, translate, and rotate the molecule until it is docked with the surface.

Hold down the **SHIFT** and **ALT** keys, plus the right mouse button. Drag the cursor upward.

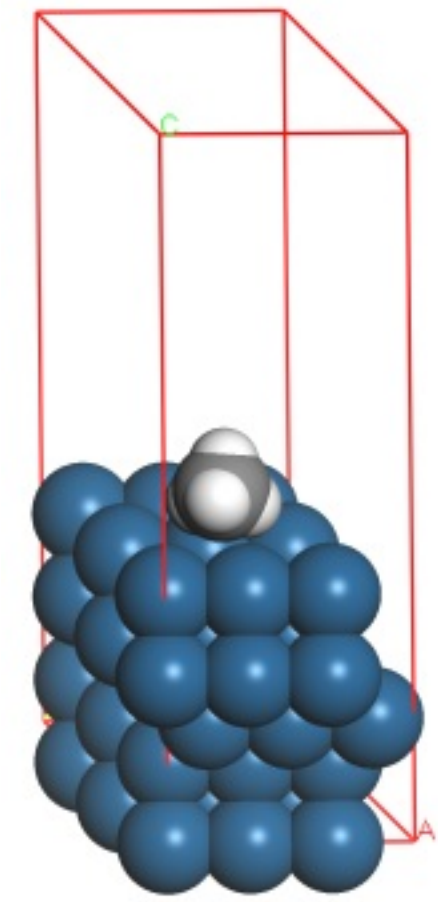
Tip: If you have a three-button mouse or a mouse with a wheel, you can drag while pressing the wheel or middle button along with the SHIFT key to translate without having to hold down the ALT key as well.

The molecule translates up the screen. It is useful to visualize the surface and the methane molecule using the space-filling representation in order to help with the positioning of the methane molecule.

Position the molecule just above the Pt surface.

Click in the 3D Viewer to deselect everything. Click the **Display Style** button  on the **3D Viewer** toolbar to open the Display Style dialog. Select the **CPK** option on the **Atom** tab and **close** the dialog.

The slab should look similar to this.



Pt surface and CH_4 molecule in CPK display style

Double-click on the methane molecule to select it. Translate the molecule to the middle of the surface. You may have to change your view of the entire surface to do this.

To successfully dock your molecule on a surface, you should rotate it so that a hydrogen atom is orientated downward toward the surface. You can rotate a fragment by holding down the SHIFT key and the right mouse button while dragging the cursor. Materials Studio uses a trackball rotation system. This means that the location of the cursor on the screen affects the axis around which you rotate. When the cursor is in the middle of the screen, dragging up and down rotates about the y-axis, while moving left and right rotates about the x-axis. If you wish to rotate in the z plane, move the cursor to the edge of the screen and then drag it along the edge.

Position the cursor in the middle of the 3D Viewer. Hold down the **SHIFT** key and the right mouse button. Drag the cursor left and right, then up and down.

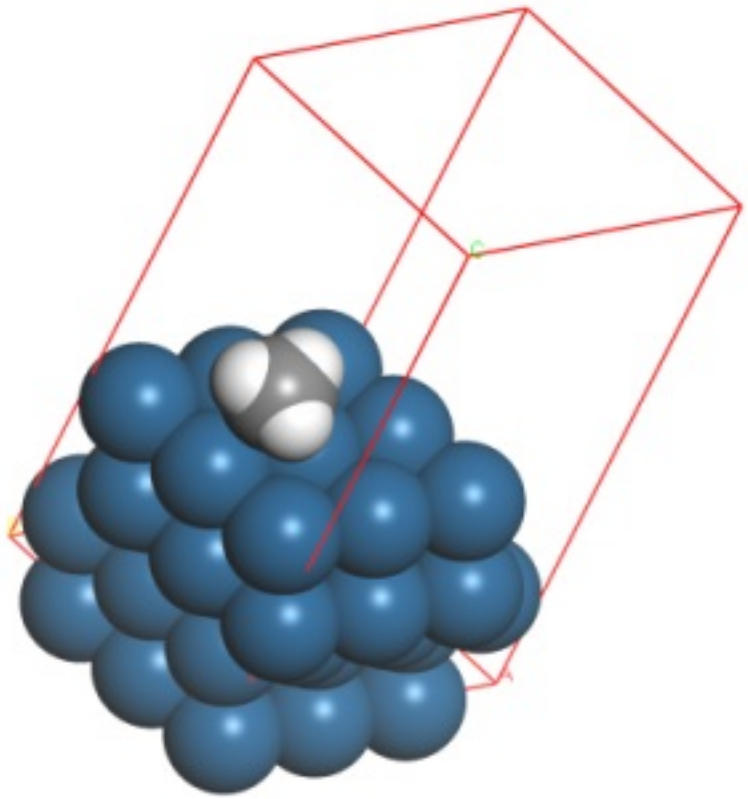
The fragment rotates about the x and y axes, respectively.

Move the cursor to the edge of the 3D Viewer. Hold down the **SHIFT** key and the right mouse button. Drag the cursor along the edge of the document.

The fragment rotates in the z plane.

Use these rotation and translation functions to position your methane molecule. When you have finished, deselect the methane molecule by double-clicking in an empty part of the 3D Viewer.

Your system should look similar to this.



Pt surface with CH_4 molecule docked

You have successfully docked a methane molecule onto your platinum surface. You can now perform energy or dynamics calculations on this structure using tools such as CASTEP, DMol^3, or Forcite.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

This is the end of the tutorial.

Using the polymer builder

Purpose: Introduces the polymer builder, which can be used to build homopolymers, block copolymers, random copolymers, and dendrimers.

Modules: Materials Visualizer

Time:

Prerequisites: Project management

Introduction

The Build Polymers tool in the Materials Visualizer makes constructing complex polymers easy. The polymer builder includes an extensive library of common monomer units, but it can also be used with custom repeat units. You can build homopolymers, block polymers, and random copolymers, adjusting a range of properties such as the tacticity and reactivity of the monomers. Materials Studio also allows you to construct dendrimers.

This tutorial covers:

- Getting started
- Building a homopolymer
- Building a block copolymer
- Building a random copolymer
- Building a dendrimer

Getting started

Begin by starting Materials Studio and creating a new project called Polymer. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Polymer** as the name and click the **OK** button.

The new project is created with *Polymer* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

Building a homopolymer

All of the polymer building tools allow you to construct polymers from custom repeat units that you have defined; alternatively, you can use repeat units from the extensive library provided with your Materials Studio installation. The first example below demonstrates how to build and define your own repeat unit. Later examples use pre-built repeat units.

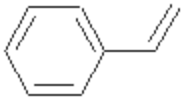
1. To build the repeat unit

Open a new 3D Atomistic document.

Click on the **New** arrow  on the **Standard** toolbar and select **3D Atomistic Document** from the dropdown list.

The structure you are going to sketch is called styrene, which is the repeat unit in an aromatic polymer called poly(*p*-phenylene vinylene) (PPV). PPV has been shown to be a conductor when doped with various electron-accepting or electron-donating compounds. In addition, PPV derivatives are extensively used in the construction of polymer light-emitting diodes for flat panel displays.

Note: Although polymerization of styrene produces the well-known material polystyrene, the repeat unit in polystyrene is actually ethylbenzene.



Structure of styrene

You will start by sketching a phenyl ring.

Click the **Sketch Ring** button  on the **Sketch** toolbar. Hold down the **ALT** key and click in the 3D Atomistic document.

A phenyl ring, without the hydrogen atoms, is sketched in the 3D Atomistic document, with the aromatic partial double bonds represented by dotted lines. The next step is to draw the carbon chain.

Click the **Sketch Atom** button  on the **Sketch** toolbar. Check that **C** is the **Element used to sketch**.

If it is not, click the **Element used to sketch** arrow  and choose **Carbon** from the dropdown list.

Move the cursor over one of the carbon atoms in the ring. When the atom changes color to light blue, click on it and move the cursor away to sprout a bond. Click again to place the first carbon atom in the side chain. Move the cursor away and then click once more to add the second carbon atom. Press the **ESC** key to stop sketching.

Now you should add the double bond between the two carbon atoms in the side chain.

Hover the cursor over the middle of the bond connecting the two carbon atoms in the side chain. When it changes color to light blue, click on it once.

The bond changes from a single to a double bond.

The final step is to add hydrogens to the structure and clean up the geometry.

Click the **Adjust Hydrogen**  and **Clean**  buttons on the **Sketch** toolbar.

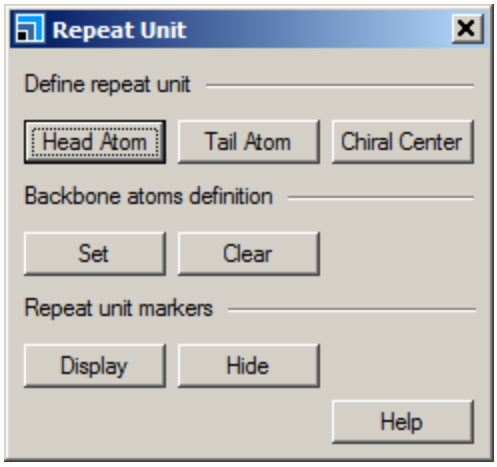
2. Setting the head and tail atoms

Click the **3D Viewer Selection Mode** button  on the **3D Viewer** toolbar.

Now specify the head atom.

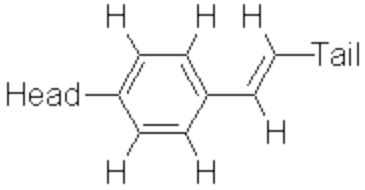
Select **Build | Build Polymers | Repeat Unit** from the menu bar.

This opens the Repeat Unit dialog.



Repeat Unit dialog

In the 3D Atomistic document, select the hydrogen atom labeled 'Head'. Click the **Head Atom** button on the Repeat Unit dialog.

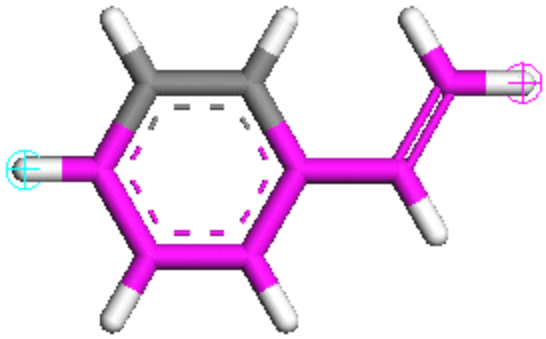


Head and tail atoms

A blue cage appears around the hydrogen atom, indicating it has been defined as the head atom.

In the 3D Atomistic document, select the hydrogen atom labeled 'Tail'. Click the **Tail Atom** button on the Repeat Unit dialog and **close** the dialog.

A magenta cage appears around the hydrogen atom and the backbone of the polymer is highlighted.



Styrene repeat unit

Before building the polymer, rename the repeat unit so that it is easy to find later when you have several documents open.

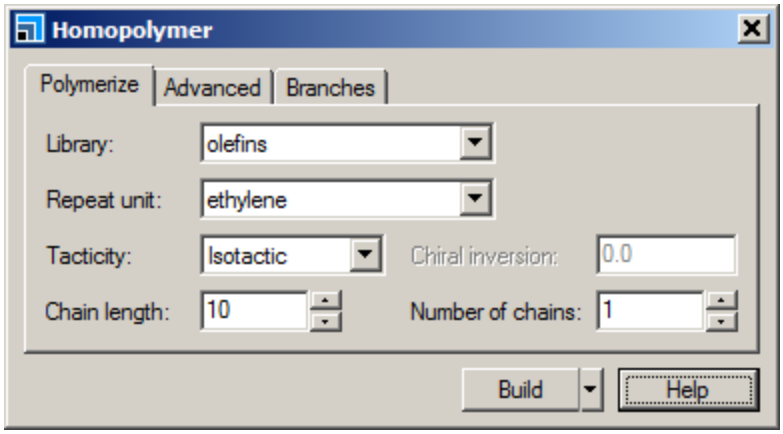
Click on **3D Atomistic.xsd** in the Project Explorer. Right-click and select **Rename** from the shortcut menu. Change the name of the file to **p-phenylene vinylene.xsd**.

3. Building the polymer

You have now built and defined your repeat unit. Next, you will build a homopolymer.

Select **Build | Build Polymers | Homopolymer** from the menu bar.

This opens the Homopolymer dialog.



Homopolymer dialog, Polymerize tab

The *Polymerize* tab displays a list of libraries that contain pre-defined repeat units.

To use the repeat unit you have just created, select **Current project** from the **Library** dropdown list.

Now that you have defined a library, you can select the repeat unit to be used. If more than one repeat unit is defined in the current project, they will all be listed.

Select **p-phenylene vinylene** from the **Repeat unit** dropdown list.

You will construct a polymer with a chain length of 20 units; the default setting is 10.

Click in the **Chain length** text box and change the value from 10 to **20**. Click the **Build** button and close the Homopolymer dialog.

The new polymer is displayed in a new 3D Atomistic document called `Polyp-phenylene vinylene.xsd`. Save this polymer and the project.

Click the **Save Project** button on the **Project** toolbar. Select **Window | Close All** from the menu bar.

Building a block copolymer

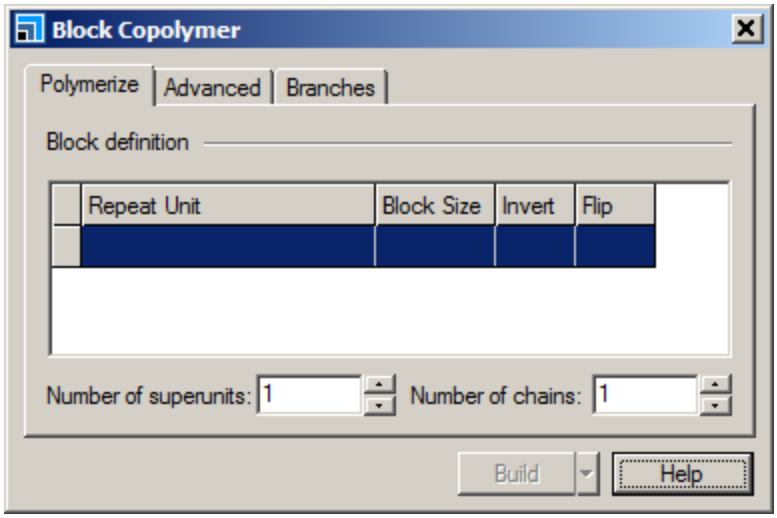
Block copolymers are made up of blocks of different polymerized monomers. Polymerization of monomer A, followed by monomer B will form a diblock copolymer AB; triblocks, tetrablocks, multiblocks, and so on can also be prepared. Block copolymers are made using living polymerization techniques, such as atom transfer free radical polymerization (ATRP), reversible addition fragmentation chain transfer (RAFT), ring-opening metathesis polymerization (ROMP), and living cationic or living anionic polymerizations.

Ethylene oxide/propylene oxide copolymers have applications as low foam, nonionic surfactants in detergents, agrochemicals, and paints.

1. To use the Block Copolymer dialog

Select **Build | Build Polymers | Block Copolymer** from the menu bar.

This opens the Block Copolymer dialog.



Block Copolymer dialog, Polymerize tab

The Block Copolymer dialog consists of three tabs:

- *Polymerize* tab contains the initial block definition section
- *Advanced* tab allows you to specify initiators and terminators and the torsion angle between the repeat units
- *Branches* tab enables you to attach branches to the polymer

Select the **Advanced** and **Branches** tabs to view the options available. When you are finished, select the **Polymerize** tab again.

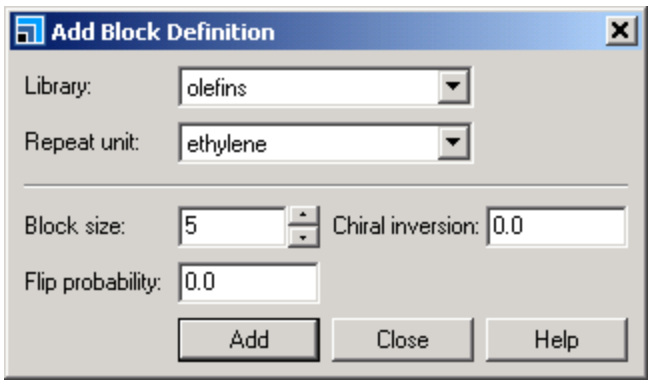
Now that you are familiar with the Block Copolymer dialog, you can start to construct the polymer.

2. To specify the repeat units

First you will select the repeat units and specify the block sizes. You are going to build a block copolymer constructed of 5 units of polyethylene oxide, 10 units of polypropylene oxide and a further 5 units of polyethylene oxide.

Click in the empty **Repeat Unit** cell in the **Block definition** grid on the **Polymerize** tab.

This opens the Add Block Definition dialog.



Add Block Definition dialog

Move the Add Block Definition dialog on the screen so that you can view both the Block Copolymer and the Add Block Definition dialogs at the same time.

The next you will select the monomers you are going to use. The pre-defined oxypropylene and oxyethylene monomers you are going to use are located in the oxides library supplied with your Materials Studio installation.

Select **oxides** from the **Library** dropdown list on the Add Block Definition dialog. Select **oxyethylene** from the **Repeat unit** dropdown list.

As the *Block size* is set to 5 by default, there is no need to change this value. The *Flip probability* is the probability of head-to-head or tail-to-tail interactions occurring in the polymer. As you only want head-to-tail interactions, you should leave this set to zero. You can now add this block of monomers to the block definition.

Click the **Add** button on the Add Block Definition dialog.

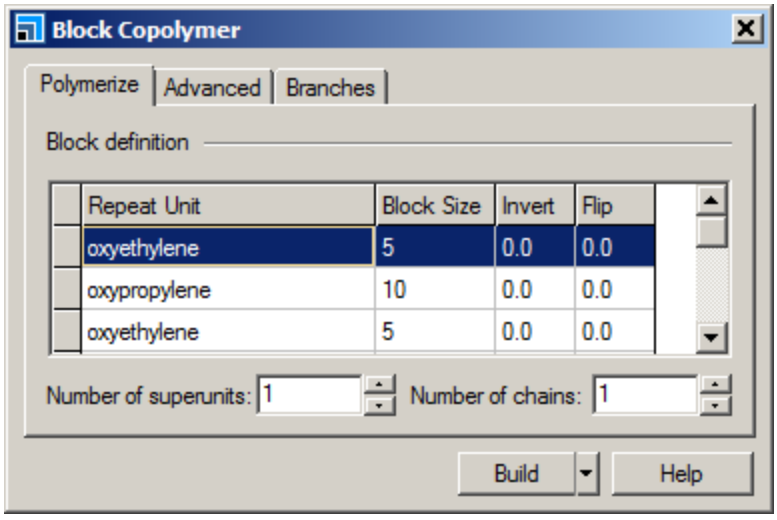
The oxyethylene block you have defined appears in the *Block definition* grid on the *Polymerize* tab of the Block Copolymer dialog. You should now add the next block, which consists of 10 units of oxypropylene.

Select **oxypropylene** from the **Repeat unit** dropdown list on the Add Block Definition dialog. Set the **Block size** to **10** and click the **Add** button.

The second block appears in the second row of the *Block definition* grid. Now add a further block of 5 oxyethylene units.

Change the **Repeat unit** back to **oxyethylene** and the **Block size** back to **5** on the Add Block Definition dialog, then click the **Add** button and close the dialog.

You have now defined the block copolymer fully and the Block Copolymer dialog should look like this:



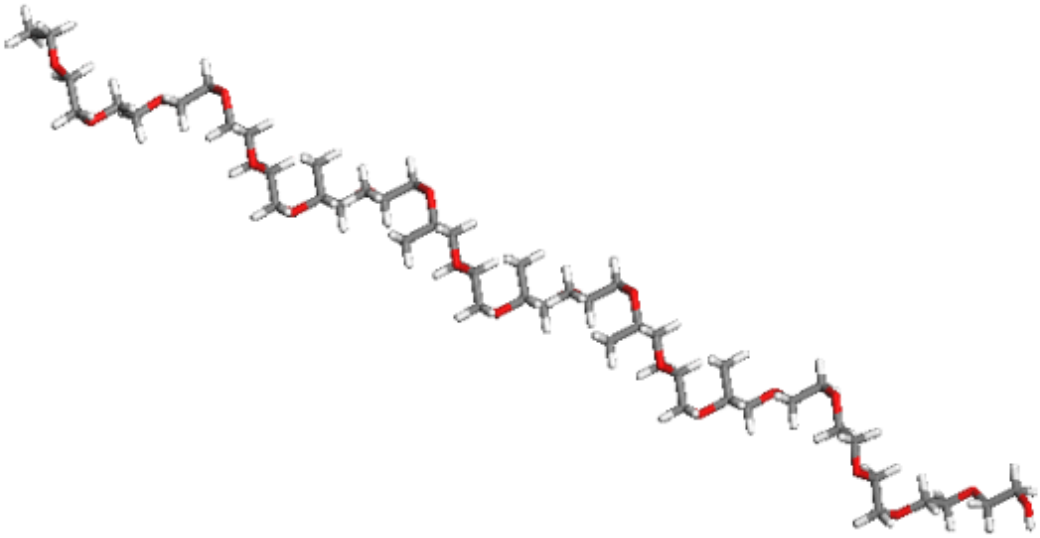
Block Copolymer dialog with polymer definition parameters added

3. To build and manipulate the polymer

The final step is to build the block copolymer.

Click the **Build** button on the Block Copolymer dialog.

A new 3D Atomistic document called `Blockoxyethyleneoxypropyleneoxyethylene.xsd` containing the new block copolymer is created. The structure should look similar to this.



The block copolymer

This structure represents a single unit of the block copolymer. If you want to build multiple units, you need to specify how many before building the polymer.

Enter a value of **2** in the **Number of superunits** text box on the **Polymerize** tab of the Block Copolymer dialog. Click the **Build** button.

A new document is produced containing two copies of the block copolymer linked together.

The Block Copolymer dialog also gives you the option to build two separate chains.

Change the **Number of chains** setting from 1 to **3**, click the **Build** button and close the Block Copolymer dialog.

A system is produced containing three polymer chains each composed of two block copolymer units. These chains can be separated using the SHIFT and ALT keys.

Click on one of the **atoms** in one of the chains. Right-click and choose **Select Repeat Unit** from the shortcut menu.

A single polymer repeat unit is selected.

Double-click on the selected repeat unit.

The whole polymer chain is selected.

Hold down the **SHIFT** and **ALT** keys, then right-click and drag the cursor across the screen.

As you move the mouse, the chain moves with it. Use this technique to move the polymer chains apart to check that you have three separate fragments.

Try rotating the selected chain by pressing the SHIFT key, then right-clicking and dragging the mouse. When you have finished, save the project and close the new 3D Atomistic documents.

Select **File | Save Project** from the menu bar and then **Window | Close All**.

This is a quick way to clear a large number of documents from the workspace. If you save the project and the documents as you proceed, you can still use *Close All* to clear the workspace whilst keeping the documents accessible from the Project Explorer.

Building a random copolymer

The Random Copolymer dialog allows you to construct copolymers of any number of species, controlling the connectivity and composition independently. In this example, a random mixture of butadiene and acrylonitrile will be constructed. The acrylonitrile content of a commercial polymer can be anywhere between 18 and 48%. As the acrylonitrile content is increased, the temperature flexibility decreases, but the resistance to petroleum-based compounds increases. The polymer has many applications in the sealant industry.

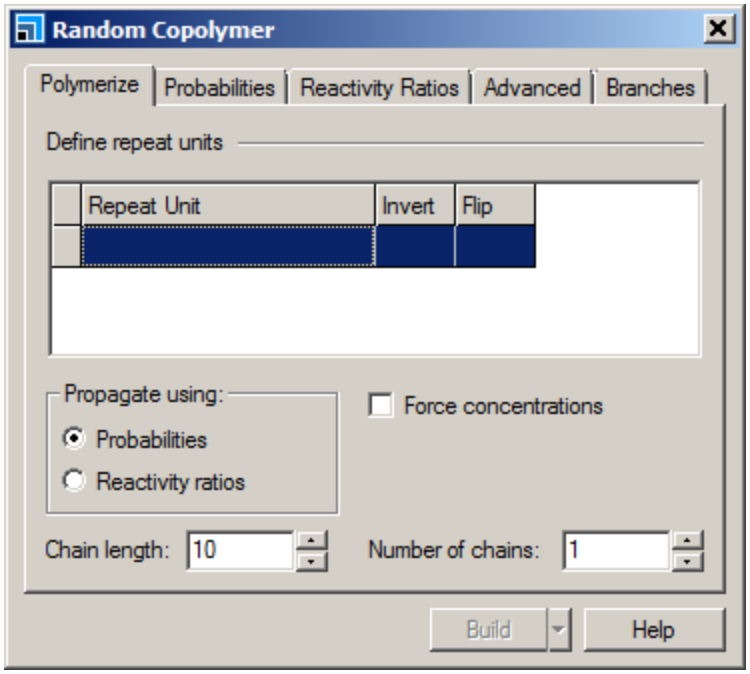
You are going to build two copolymers: the first will use the default values and will be a 1:1 mix of the two monomers; the second will be 1:4 mix of acrylonitrile and butadiene.

1. To specify the repeat units

The Random Copolymer dialog is accessed from the *Build Polymers* options on the *Build* menu. It looks similar to the Block Copolymer dialog.

Select **Build | Build Polymers | Random Copolymer** from the menu bar.

This opens the Random Copolymer dialog.



Random Copolymer dialog, Polymerize tab

The first step is to tell the copolymer builder which units you want to build with and what size of polymer you want.

Click in the empty **Repeat Unit** cell in the **Define repeat units** grid on the **Polymerize** tab to open the Add Repeat Unit dialog.

Select **dienes** from the **Library** dropdown list on the Add Repeat Unit dialog. Select **c_butadiene** from the **Repeat unit** dropdown list. Click the **Add** button.

The *cis*-butadiene monomer is added to the *Define Repeat Units* grid on the Random Copolymer dialog.

On the Add Repeat Unit dialog, select **acrylates** from the **Library** dropdown list and **acrylonitrile** from the **Repeat unit** dropdown list. Click the **Add** button and close the Add Repeat Unit dialog.

Now you should increase the chain length from 10 to 20.

Use the spin control on the **Chain length** text box on the Random Copolymer dialog to change the value from 10 to **20**.

There are two different ways you can propagate the polymer, using either probabilities or reactivity ratios:

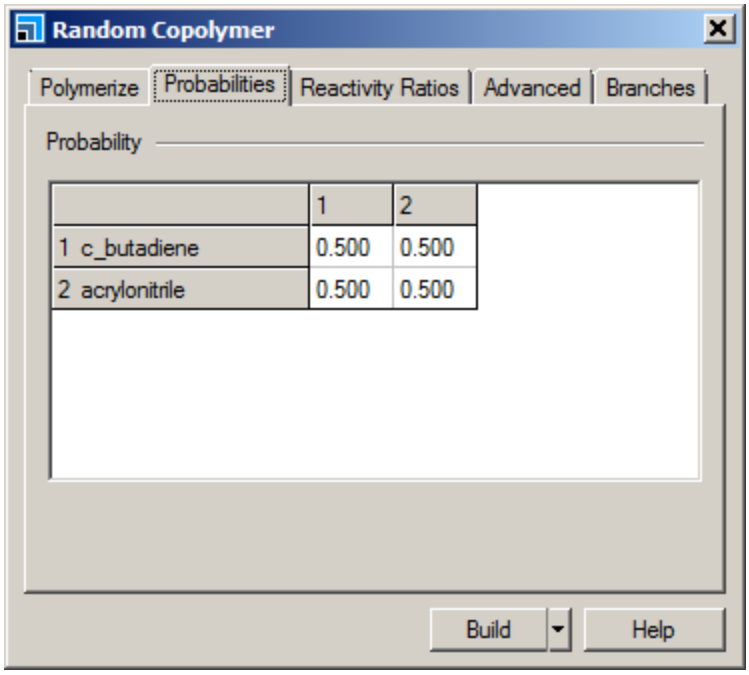
- Probabilities give the relative likelihood of each monomer being attached to the chain at the next step of the reaction and can be used to mimic the concentrations.
- Reactivity ratios determine the copolymer composition in an analogous way to experimental synthesis. The inputs required are concentrations of reactants and rate constants for the various attachment alternatives.

In this section, you will build a polymer from a 1:1 mix of the monomers, initially, and then a 1:4 mix of acrylonitrile and butadiene using probabilities to set the composition.

2. To use probabilities to set composition

Probabilities are specified as a matrix on the *Probabilities* tab.

Select the **Probabilities** tab.



Random Copolymer dialog, Probabilities tab

This tab contains the probability matrix. The numbers in the matrix are read by row. So, in the example shown above, the first row specifies that there is a 50% probability of *cis*-butadiene attaching to a chain that ends in a *cis*-butadiene unit and a 50% chance that acrylonitrile will be added next if the previous unit is a *cis*-butadiene. The total of the values in each row must be 1. The second row displays similar information for a growing chain ending with acrylonitrile. The default values are 0.500 in each cell. Since a 1:1 mixture of the two repeat units is required, the default values can be left unchanged.

As you do not need to specify any initiator or terminator settings, you can ignore the *Advanced* tab. Now you can build the random copolymer.

Select the **Polymerize** tab of the Random Copolymer dialog and click the **Build** button.

A new 3D Atomistic document containing the random copolymer is created. Move the Random Copolymer dialog so that you can see the new structure, but do not close it.

As there is a 50% chance of either of the monomer units adding to the previous one, the numbers of the different repeat units in each polymer can change. If you build some more polymers without changing the settings, you should be able to see differences in the number of monomers of each type in the structures.

Click the **Build** button on the Random Copolymer dialog several more times to build new polymers.

There should be small differences in the composition of each polymer chain built.

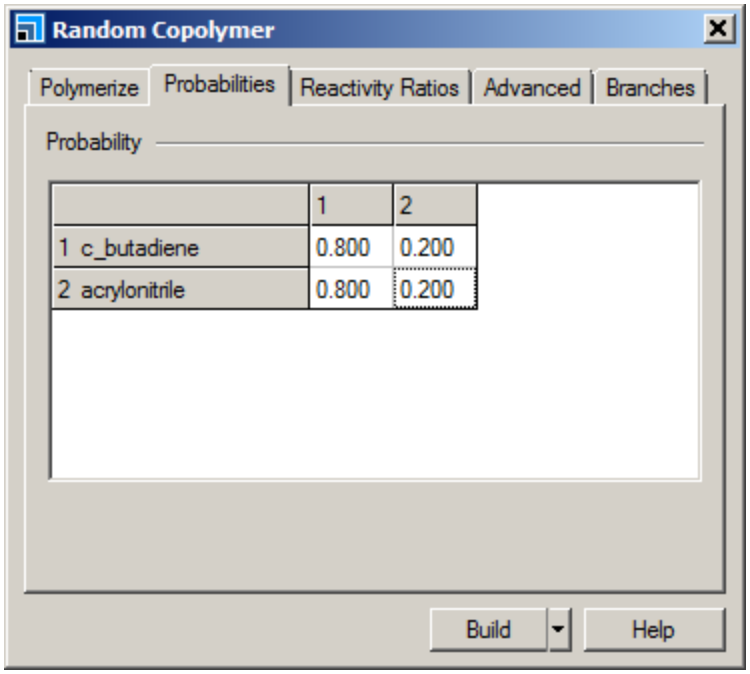
Now you are going to construct a polymer composed of a 1:4 mixture of the monomers. This entails changing the probabilities in the probability matrix. As you want less acrylonitrile than butadiene, you should adjust the probabilities so that they favor the diene repeat unit.

Select the **Probabilities** tab on the Random Copolymer dialog. Click in the 1,1 matrix cell (the cell in row **1** and column **1**). Change the probability in the cell from 0.500 to **0.800** and press the **TAB** key.

You have set the probability of a further unit of butadiene being added to a terminal butadiene group to 0.8. As the probabilities in each row must add up to 1, you need to set the probability of a unit of acrylonitrile adding to terminal butadiene (the 1,2 matrix element) to 0.2.

Click in the 1,2 matrix cell and change the probability from 0.500 to **0.200**. Press the **TAB** key.

Repeat this procedure for the second row of the matrix so that it looks like this.



Random Copolymer dialog showing probability settings

These settings will produce a ratio of acrylonitrile to butadiene of approximately 1:4 in the resulting polymer.

Click the **Build** button.

A new document containing the polymer is produced, as before.

Click the **Build** button a few more times and check the ratio of repeat units in each case.

3. To force the concentrations

In the limit of infinitely long chains, these probabilities become exact, but for finite chains, there are often small deviations. To guarantee a 1:4 ratio of acrylonitrile to butadiene in the polymer, you can use the *Force concentrations* option on the *Polymerize* tab.

Select the **Polymerize** tab. Check the **Force concentrations** checkbox and click the **Build** button.

If you repeat the build several times, you will see that the ratio of repeat units is exactly 1:4 acrylonitrile to butadiene each time because the specified ratio is imposed, regardless of the probability. This is useful if you are only interested in polymers that contain a specific ratio of monomer repeat units.

Select **File | Save Project** from the menu bar and then **Window | Close All**.

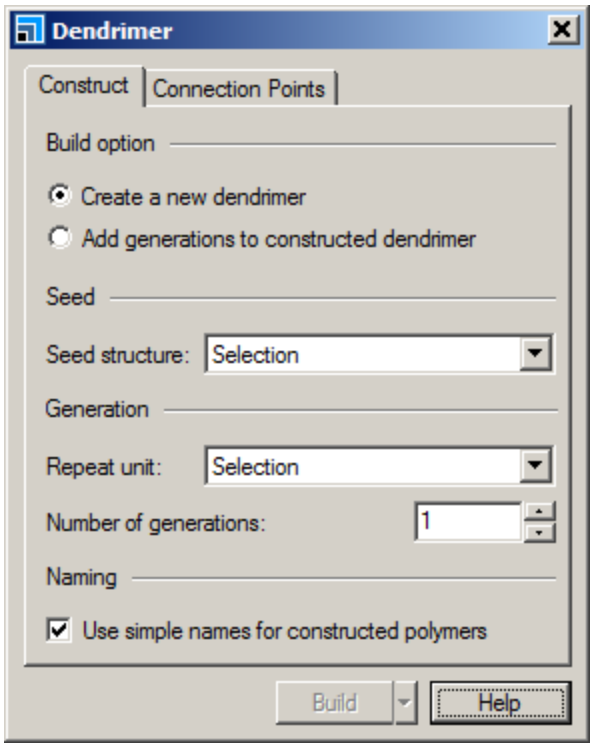
Building a dendrimer

Dendrimers are branched compounds that grow from a central core. In this section, you will build up a dendrimer layer-by-layer using the Dendrimer dialog. This dialog also gives you the option of building up multiple layers in a single step, but the first approach will help you to visualize the construction process.

1. To build the dendrimer

Select **Build | Build Polymers | Dendrimer** from the menu bar.

This opens the Dendrimer dialog.



Dendrimer dialog, Construct tab

You will start by specifying the dendrimer seed and repeat unit. The seed is the initial unit from which the dendrimer grows.

Select **ammonia** from the **Seed structure** dropdown list.

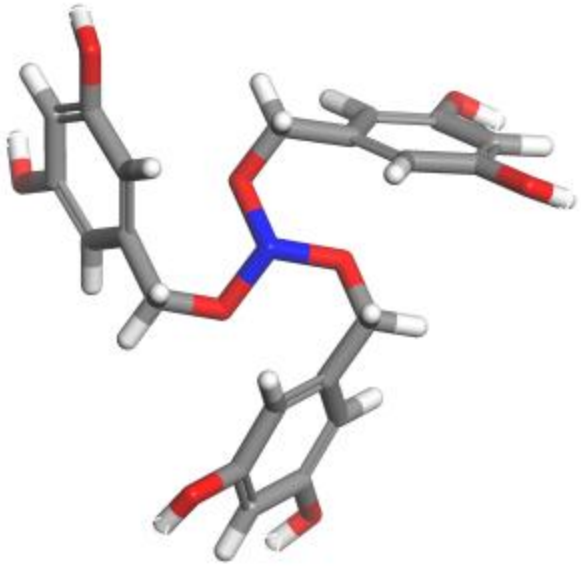
Now define the repeat unit that is to be added to the connection points on the seed.

Select **35dihydroxy_benzyl_alcohol** from the **Repeat unit** dropdown list.

For the time being, you can leave the *Number of generations* set to 1.

Click the **Build** button.

A new 3D Atomistic document called `Dendrimer.xsd` containing the dendrimer is created. It consists of an ammonia core with three 3,5-dihydroxybenzyl alcohol repeat units attached. The connection points for the next layer are indicated by white cages.



The initial dendrimer

Before adding a second layer to your dendrimer, you should clean up the geometry of the initial structure.

Click the **Clean** button  on the **Sketch** toolbar.

Note that when you built the initial dendrimer, the build option on the *Construct* tab changed from *Create a new dendrimer* to *Add generations to constructed dendrimer*, making it easy for you to add a second layer of dihydroxybenzyl alcohol units.

Click the **Build** button on the Dendrimer dialog, followed by the **Clean** button on the toolbar.

A second layer of repeat units is added to the dendrimer. You can change the repeat unit you are adding so that you have different repeat units in some of the layers.

On the Dendrimer dialog, change the **Repeat unit** to **propylene_oxide** and click the **Build** button and close the dialog.

A third layer of repeat units is added to the dendrimer, but this time, they are propylene oxide units instead of dihydroxybenzyl alcohol.

2. To color the dendrimer

At this stage, the display can get confusing and it helps to color the dendrimer by repeat unit. You can do this by selecting connected atoms and working down through the layers.

The first step is to color the whole dendrimer.

Right-click in the 3D Atomistic document and select **Display Style** from the shortcut menu to open the Display Style dialog. In the **Coloring** section on the **Atom** tab, select **Repeat Unit** from the **Color by** dropdown list. Keep the Display Style dialog open.

Each repeat unit of the dendrimer is colored differently. The next step is to select the dihydroxybenzyl alcohol units comprising the second generation of the dendrimer.

Click the **3D Viewer Selection Mode** button  . Select one atom in each of the six dihydroxybenzyl alcohol units comprising the second generation of the dendrimer. Right-click on one of the selected atoms and choose **Select Parent** from the shortcut menu.

Click on the color chooser on the **Atom** tab of the Display Style dialog and choose magenta from the palette on the Color dialog. Click the **OK** button.

All the dihydroxybenzyl alcohol units comprising the second generation of the dendrimer are colored magenta.

You can use the Connected option on the Atom Selection dialog to select atoms that are linked to the nitrogen.

Click on the central nitrogen atom in the dendrimer. Select **Edit | Atom Selection** from the menu bar to open the Atom Selection dialog.

Change the **Select by Property** setting to **Connected**. Set the **Selection mode** to **Add to the existing selection**. Click the **Select** button and close the dialog.

The three atoms closest to the central nitrogen atom are selected, in addition to the nitrogen itself.

Right-click on one of the selected atoms and choose **Select Parent** from the shortcut menu.

Now the three dihydroxybenzyl alcohol units attached to the central nitrogen atom, plus the nitrogen itself, are selected.

On the **Atom** tab of the Display Style dialog, click on the color chooser to display the Color dialog. Select pale blue from the palette and click the **OK** button.

While holding down the **Q** key, click and drag the mouse around the central nitrogen atom and the 3 oxygen atoms attached to it.

Pressing Q while clicking and dragging the mouse enables lasso selection, regardless of the current cursor mode.

With the central NO_3 fragment at the center of the dendrimer selected, click on the color chooser on the **Atom** tab of the Display Style dialog and choose red from the palette on the Color dialog. Click the **OK** button.

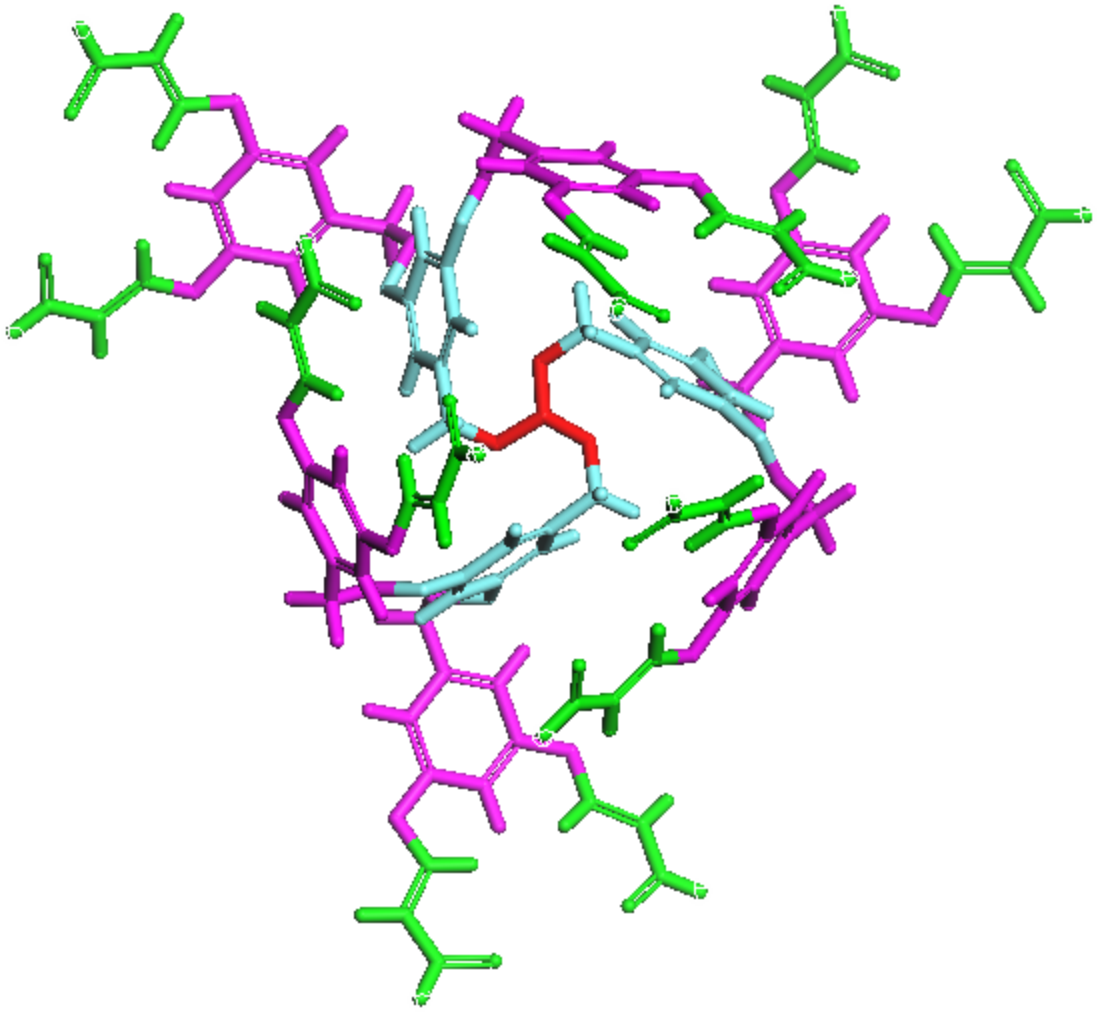
Lastly, you will color the propylene oxide repeat units all the same color.

Select one atom in each of the terminal propylene oxide repeat units, right-click in the 3D Viewer and choose **Select Parent** from the shortcut menu.

Color the selected atoms green, using the color chooser on the Display Style dialog. Click anywhere in the 3D Viewer to deselect everything.

Select the **Stick** option from the **Display style** section on the **Atom** tab and close the Display Style dialog.

You should end up with a dendrimer that looks similar to that shown below.



The dendrimer colored by generation

An alternative method for generating a colored dendrimer is to save each layer with a different color. For dendrimers head atoms and connection points can be defined using the *Connection Point* tab of the Dendrimer dialog.

If you have administrator privileges, once you have colored and saved all of the layers, the repeat units that have been defined (and colored) can be saved to the location used by the Polymer Builder as its source of seeds and repeat units. These are `Structures\repeat-units\dendrimers\structures\` for repeat units and `Structures\repeat-units\dendrimers\seeds\` for the seed structures.

Note: This will not work if the file is saved to a different folder.

With the correct folder structure, you can simply add the files together when you build a dendrimer. This method is much faster, so it is appropriate for the generation of large dendrimers.

Finally, you should save the project.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

This is the end of the tutorial.

Using the layer builder

Purpose: Uses the layer builder to construct an interface between two surfaces and a metal-polymer-metal layered structure.

Modules: Materials Visualizer, Amorphous Cell

Time:

Prerequisites: Project management, Using the polymer builder

Background

There are many different situations in modeling where you need to look at interactions at interfaces. Examples of these are the interaction between a polymer and a metal surface and the interface between two surface layers. Materials Studio contains a layer building tool that allows you to generate different layered structures or interfaces with ease.

Introduction

Build Layers provides a simple yet powerful solution to building systems where different materials types are used. This tutorial shows two examples of the use of the layer builder, building a metal-polymer-metal system and twinning in silicon.

This tutorial covers:

- Getting started
- Twinning in silicon
- Building a metal-polymer-metal system

Note: The second part of this tutorial requires the use of the Amorphous Cell module.

Getting started

Begin by starting Materials Studio and creating a new project called Layer. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Layer** as the name and click the **OK** button.

The new project is created with *Layer* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

Twinning in silicon

Crystal twinning occurs when two separate crystals share some of the same crystal lattice points in a symmetrical manner. The result is an intergrowth of two separate crystals in a variety of specific configurations. A twin boundary or composition surface separates the two crystals. Pure silicon is used to produce ultra-pure silicon wafers used in the semiconductor industry, in electronics and in photovoltaic applications. It is important to study and understand the formation of defects, such as twinning, in pure silicon crystals. This part of the tutorial covers generation of a twin boundary in silicon using the surface builder and the layer builder.

1. To cleave the two surfaces

First you must create a new folder to work in.

Click on the Layer project root  in the Project Explorer. Right-click and select **New | Folder** from the shortcut menu. Rename the folder **silicon**.

Now, you must import the silicon structure into the `silicon` folder.

Select the **silicon** folder. Click the **Import** button  on the **Standard** toolbar to open the Import Document dialog. Navigate to **Examples\Documents\3D Model** and import **Si.xsd**.

The crystal structure of silicon is displayed in a 3D Viewer. Now, you must cleave the (3 1 0) surface of the silicon.

Select **Build | Surfaces | Cleave Surface** to open the Cleave Surface dialog. Change the **Cleave plane (hkl)** to **3 1 0** and increase the **Fractional Thickness** to **9.0**. Click the **Cleave** button.

A new 3D Atomistic document is displayed containing the cleaved surface. Now, you need to cleave the second surface to match this.

Make the original Si crystal structure the active document. On the Cleave Surface dialog, change the **Cleave plane (h k l)** to **-3 1 0**. Click the **Cleave** button and **close** the dialog.

You now have two new documents, `Si (3 1 0)` and `Si (-3 1 0)`. Before you build your layered structure, you need to reorient the layers, as this will make the later alignment stages easier.

With the cursor over one of the new 3D Viewers, right-click and select **Lattice Parameters** from the shortcut menu to open the Lattice Parameters dialog.

On the **Advanced** tab click the **Reorient to standard** button. Make the other document active and click the **Reorient to standard** button again. **Close** the dialog.

You are ready to build your layered structure of the twinned silicon.

2. To build the layered structure

Build Layers is used to build your twinned silicon.

Select **Build | Build Layers** from the menu bar to open the Build Layers dialog.

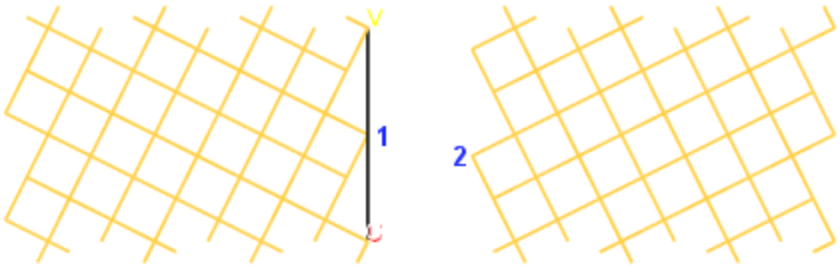
On the **Define Layers** tab, specify **Si (3 1 0).xsd** as **Layer 1** and **Si (-3 1 0)** as **Layer 2**. Click the **Build layered structure as a surface** radio button.

You have defined your two layers and specified that you wish to build them as a surface instead of a crystal.

Select the **Matching** tab and check that your lattice parameters match. Click the **Build** button.

The layered structure is displayed in the document `Layer.xsd`.

Rotate the structure using the right arrow key so that it appears as in the diagram below.



Silicon layer

You should see that the two layers are not aligned properly, as indicated above by the numbers 1 and 2, which mark atoms that should be equivalent. You need to adjust the alignment of the two layers.

3. To change the layer alignment

You will change the alignment of the layers by looking at the difference between the fractional coordinate values for the two atoms highlighted above. The easiest way to do this is by using the Properties Explorer.

Choose **View | Explorers | Properties Explorer** from the menu bar. Click on atom 1 indicated above. You may have to rotate the structure to do this.

In the **Properties Explorer**, double-click on **FractionalXYZ**. Note down the **X**, **Y**, and **Z** values. Repeat this for atom 2.

Tip: If you cannot easily select the atoms, set the *Display Style* to Ball and Stick.

Looking at the axes in the bottom corner of the screen, you should see that X and Y correspond to U and V. As you want to offset one surface in the V direction, you need to compare the two Y fractional coordinates. These should have values of 0.5 for atom 1 and 0.4 for atom 2. Therefore, you need to offset the second layer by 0.1 and you can do this from the Layer Builder.

Select the **Layer Details** tab on the Build Layers dialog. Change the **Origin offset** in direction **v** for **Layer 2** to **0.1**. Click the **Build** button and close the dialog.

Rotate the structure using the left arrow key.

A new layered structure is displayed and in this structure, the atoms are aligned correctly.

4. To generate the final structure

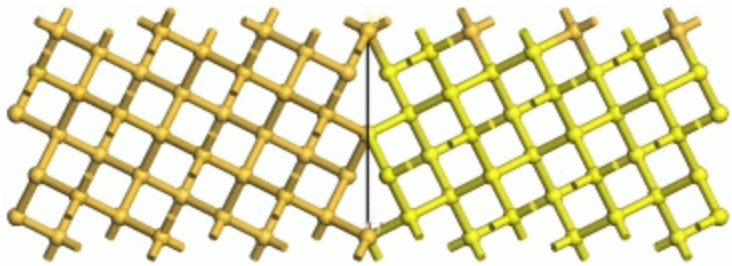
The final stage is to translate the right-hand layer so that the two layers overlap and then to remove the coincident atoms. When a layered structure is built, each layer is automatically defined as a set.

Choose **Edit | Edit Sets** from the menu bar to open the Edit Sets dialog. Select **Layer 2**. Click the **Select** button and close the dialog.

The layer that is separated from the surface lattice is selected. You have to translate this so that the atoms in the first layer are coincident. You can force the translation of fragments in a set direction by holding down the X, Y, or Z keys. However, this does not translate the fragment relative to the axis indicator, but relative to the screen, where X is left to right, Y is up and down, and Z is in and out. Therefore, you need to translate in the X direction.

Hold down the **SHIFT** + **ALT** keys and the right mouse button. Hold down the **X** key. Move your mouse so that the atoms in first layer are coincident, as shown below.

Tip: If you have a three-button mouse, or one with a wheel, you can translate by using the middle mouse button or wheel and the SHIFT key. You still have to hold down the direction key as well if you want to force translation in a particular direction.

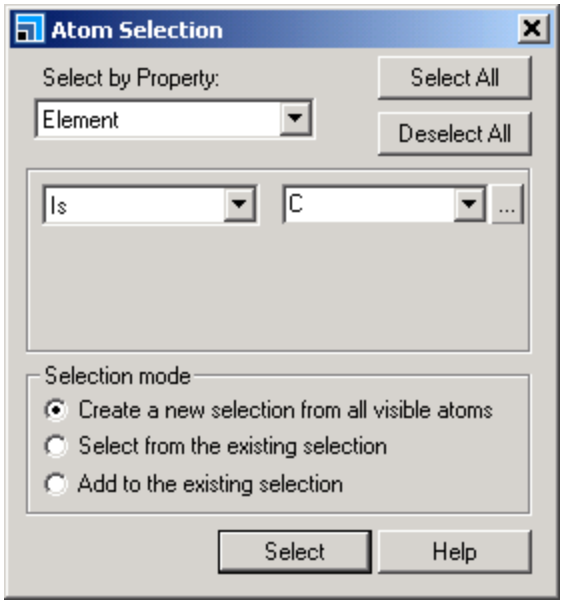


Silicon layer overlap

You should remove the coincident atoms using the advanced selection tools to select them.

Select **Edit | Atom Selection** from the menu bar.

This opens the Atom Selection dialog.



Atom Selection dialog

Select **Z Coordinate** from the **Select by Property** dropdown list. Change the **Equal to** setting to **Inclusive Range** and set the range to **-0.1 to 0.1**.

This selects all the atoms in a Z coordinate range of -0.1 to +0.1.

Change the **Selection mode** to **Select from the existing selection**. Click the **Select** button and close the dialog.

Only the coincident atoms are selected.

Press the **DELETE** key.

The coincident atoms are deleted, leaving the correct structure.

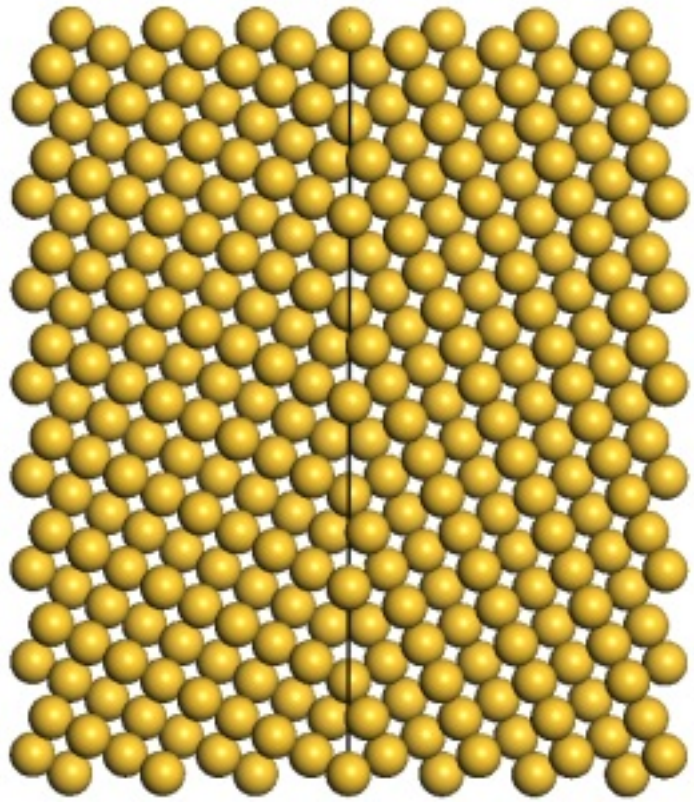
Click on the **Calculate Bonds** arrow  on the **Atoms and Bonds** toolbar and select **Delete Bonds**.

All the bonds are removed from the twinned structure.

Right-click in the 3D Atomistic document and select **Display Style** from the shortcut menu to open the Display Style dialog.

On the **Atom** tab, select the **CPK** display style and change the **CPK scale** to **0.5**. On the **Lattice** tab increase the **Max. V** value to **3.00** in the **Range** section. **Close** the Display Style dialog.

You have generated a twinned structure of silicon.



The twinned structure of silicon

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

Building a metal-polymer-metal system

This part of the tutorial covers generation of an organic-inorganic interface using the surface builder, the polymer builder, and the layer builder.

- To import the metal surfaces
- To create the waxy polymer
- To build the layered structure

1. To import the metal surfaces

In this example, you are going to build a system containing waxy carbon chains with iron surfaces. To do this, you need to import the iron crystals and create a supercell of them.

Click the **Layer** project root in the Project Explorer. Right-click and select **New | Folder**. Rename the folder **polymer-metal**.

Click the **Import** button and import the **Fe.xsd** file.

Before you start, you need to change the display style to ball and stick.

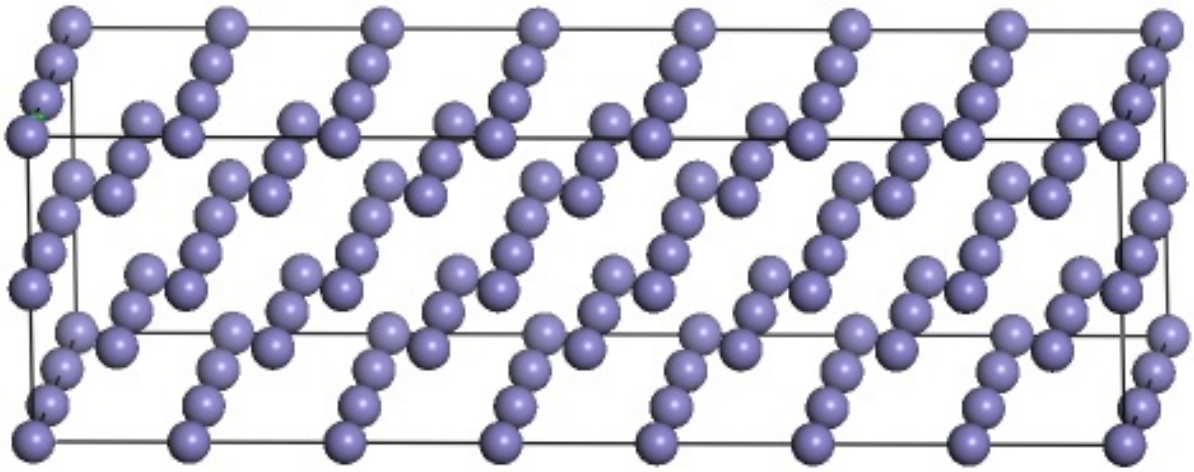
Open the **Display Style** dialog. On the **Atom** tab, select the **Ball and stick** option and close the dialog.

The dimensions of the crystal cell are too small to pack a polymer on to and calculate realistic interactions. Therefore, you need to use the Supercell tool to increase the size of your cell.

Choose **Build | Symmetry | Supercell** from the menu bar to open the Supercell dialog.

Change **A** to **7**, **B** to **3**, and **C** to **2**. Click the **Create Supercell** button.

A supercell is displayed.



Supercell of Fe crystal

Before continuing, you need to note the new lattice parameters, as you will use these when creating your waxy polymer.

In the 3D Atomistic document, right-click and select **Lattice Parameters** from the shortcut menu to open the Lattice Parameters dialog. Note down the values of the lengths **a** and **b** and close the dialog.

2. To create the waxy polymer

Creation of the waxy polymer requires you to build a polymer and then build an amorphous cell containing the polymer.

Choose **Build | Build Polymers | Homopolymer** from the menu bar.

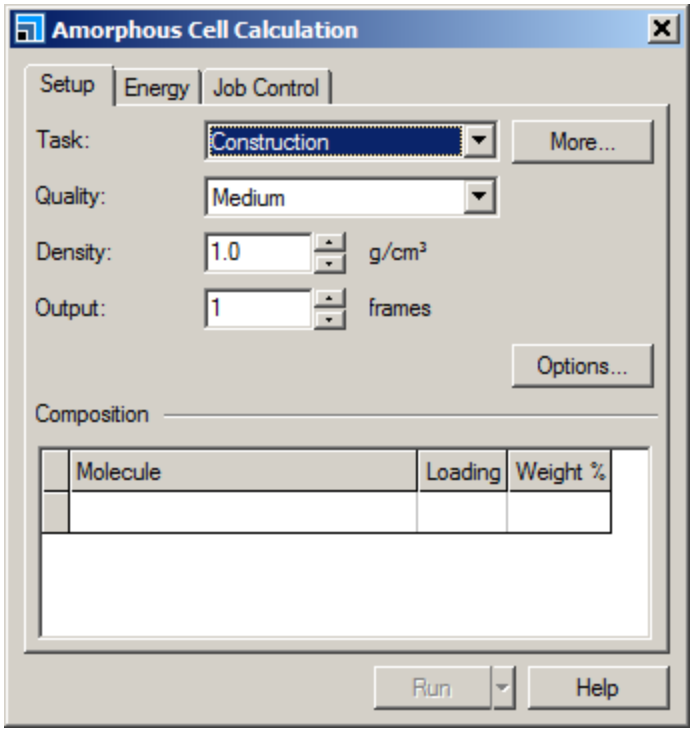
This opens the Homopolymer dialog. You are going to build a homopolymer of ethylene containing 4 repeat units. As ethylene is the default repeat unit, you just need to change the number of repeat units.

Change the **Chain length** to **4**. Click the **Build** button and close the dialog.

A short 8-carbon polymer chain is displayed. However, this is an idealized description of a polymer and is not realistic. You can change this by building an amorphous cell containing the polymer. Amorphous Cell uses a modified Markov process (Allen and Tildesley, 1987) with bond conformational probabilities chosen to account for both intramolecular and intermolecular non-bonded interactions

Select **Amorphous Cell**  from the **Modules** toolbar and choose **Calculation** or select **Modules | Amorphous Cell | Calculation** from the menu bar.

This opens the Amorphous Cell Calculation dialog.



Amorphous Cell Calculation dialog, Setup tab

Select **Confined layer** from the **Task** dropdown list. Choose **Polyethylene.xsd** from the first row in the **Molecule** column in the **Composition** table and set the **Loading** to **5**.

When you change the number of molecules in the cell, the cell parameters change to keep the density constant.

The density of waxy polymers is about 0.7 g/cm^3, so you should change the target density to reflect this.

Change the **Density** from 1 to **0.7**.

The default cell type is 3D periodic, however, if you are going to build a structure consisting of three layers, the middle layer must be a confined layer. When you change the density, the cell parameters in the next section change again. However, you want the a and b cell parameters to match those of the Fe supercell you created previously.

Click the **More...** button to open the Amorphous Cell Confined Layer dialog. Select **Orthorhombic** from the **Lattice type** dropdown list and set **a** and **b** to the values you noted for the Fe supercell. Close the dialog.

You are now ready to build your amorphous polymer.

Click the **Run** button and close the dialog.

When you click the *Run* button, a new folder is displayed in the Project Explorer, entitled `Polyethylene AC Layer`. After a few seconds, the Job Explorer displays the status of your job. This contains the different job steps, setup, starting, running, and complete. When the job has completed, your resulting amorphous cell containing 5 polymers is displayed in the `Polyethylene.xtd` document in the `Polyethylene AC Layer` folder.

Make **Polyethylene.xtd** the active document. Rotate the cell.

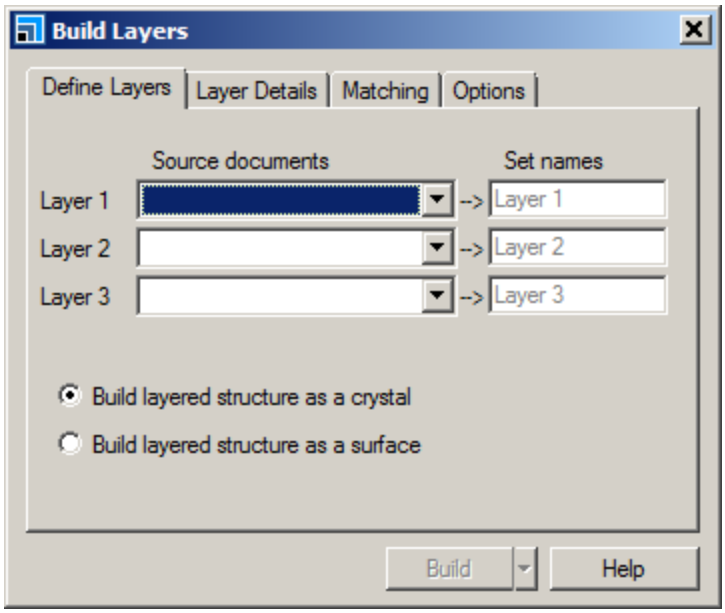
You should see that the polymers are confined in a layer in the box.

3. To build the layered structure

You are going to build a structure consisting of a metal layer, the wax layer and then a second metal layer.

Choose **Build | Build Layers** from the menu bar.

This opens the Build Layers dialog.



Build Layers dialog, Define Layers tab

Select **Fe.xsd** from the **Layer 1** dropdown list, choose **Polyethylene.xtd** for **Layer 2**, and **Fe.xsd** for **Layer 3**.

You have defined the content of your layers.

Select the **Layer Details** tab.

This contains information about the various layers, such as whether there is a vacuum present. Note that there is no vacuum assigned.

Select the **Matching** tab.

This tab allows you to set up the lattice parameters for your layer. As you have already built your wax layer so that it matches the metal layers, you do not need to do anything here.

Select the **Options** tab and check **Configure for confined shear use** checkbox.

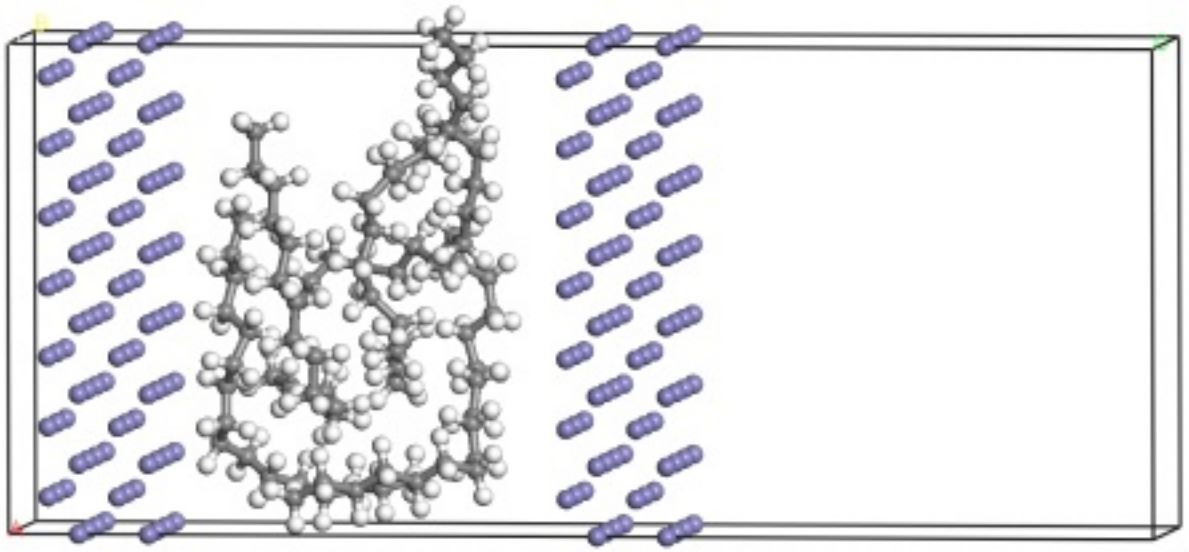
When you use a layered structure with the confined shear in Amorphous Cell or Forcite, the layers need special names and checking this box sets the layered structure correctly.

Select the **Layer Details** tab.

There is now a vacuum of 20.0 Å defined on the third layer. This is to stop any interaction with the first layer as a result of periodic boundary conditions.

Click the **Build** button and close the dialog.

The new layered structure is displayed in a document entitled `Layer.xsd`.



Fe-Polymer-Fe layer

This structure could now be used in conjunction with Amorphous Cell or Forcite to calculate the shearing properties of the wax.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

This is the end of the tutorial.

References

Allen, M. P.; Tildesley, D. J. *Computer Simulation of Liquids*, Oxford University Press: London (1987).

Using the crystal builder

Purpose: Introduces the powerful crystal building and visualization tools, including hydrogen bond visualization.

Modules: Materials Visualizer

Time:

Prerequisites: Project management

Introduction

Crystal structures can be imported into 3D Atomistic documents, but Materials Studio features a powerful crystal building tool which allows you to build your own crystals. In this tutorial you will import a prebuilt crystal and use the visualization techniques available in Materials Studio to create a high quality graphical image of the crystal, that could be easily pasted into other Windows-based software programs or saved as a bitmap. You will also build a new crystal structure by adding atoms to a pre-defined unit cell, and then calculate the bonds and hydrogen bonds between the atoms and molecules in the crystal.

This tutorial covers:

- Getting started
- Importing and visualizing a crystal of histidine
- Building a crystal of urea

Getting started

Begin by starting Materials Studio and creating a new project called Crystal. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Crystal** as the name and click the **OK** button.

The new project is created with *Crystal* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

Importing and visualizing a crystal of histidine

1. To import a prebuilt crystal structure into Materials Studio

Included in Materials Studio is a structure library that contains many different types of structures from ceramic materials to organic compounds. The structure that you should import is a molecular crystal called histidine.

Click the **Import** button  on the **Standard** toolbar.

This opens the Import Document dialog.

Navigate to **Examples\Documents\3D Model** and select the file **histidine_resolved.xsd**. Click the **Open** button.

The 3D Atomistic document `histidine_resolved.xsd` opens in a 3D Viewer and the filename is listed in the Project Explorer. The structure can be rotated using the *Rotation* tool  , by clicking and moving the mouse in the 3D Viewer. If you wish to force rotation in a single direction, that is x, y, or z, you can do this by holding down the relevant key on the keyboard, plus the right mouse button, and then moving the mouse.

Hold down the **Z** key and the right mouse button. Move the mouse to the left and right.

The structure rotates in the z direction. If you wish to set the view back to the original viewpoint, you can use the *Reset View* button.

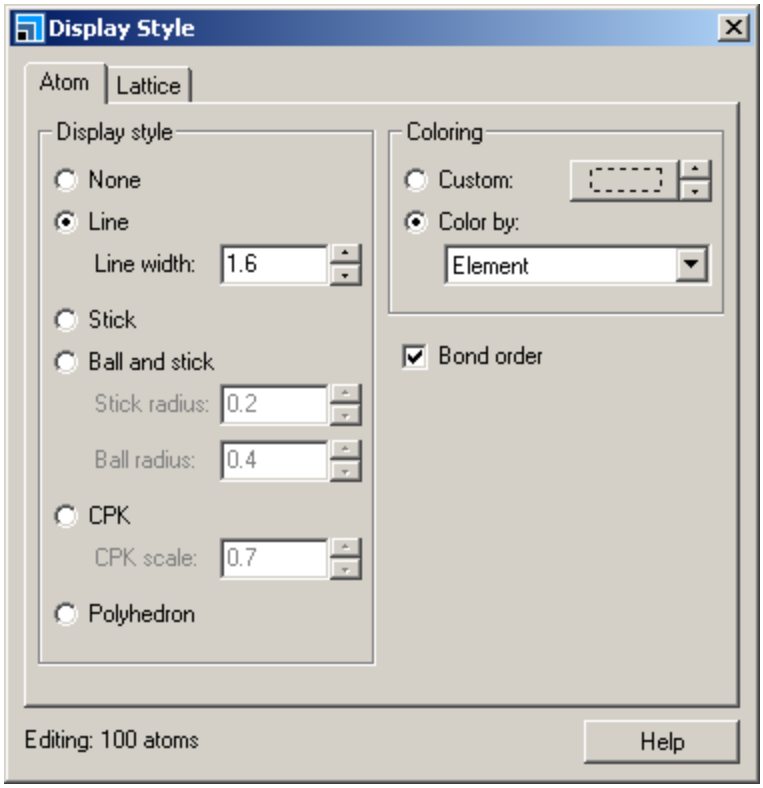
Click the **Reset View** button  on the **3D Viewer** toolbar.

2. To change the display styles

Materials Studio has a range of powerful display options and you will be introduced to some of these in the course of this tutorial. You will start off with the basic display settings, such as ball and stick.

Right-click anywhere in the 3D Viewer and select **Display Style** from the shortcut menu.

This opens the Display Style dialog.



Display Style dialog, Atom tab

This dialog has several tabs that deal with changing the display of atoms or surfaces, adding thermal ellipsoids, and lattice display options for periodic structures.

Select the **Stick** option on the **Atom** tab.

The model changes from being a simple line structure to a stick model constructed from cylinders. If the 3D Viewer window is not occupying all of the workspace area, you can resize it by clicking on the *Maximize* button.

Click the **Maximize** button on the 3D Viewer.

The 3D Atomistic document now occupies the full workspace area. You can see that the double bonds in the system are displayed as two cylinders running parallel to each other. If you do not want the display to differentiate between the bond orders, you can remove this using the Display Style controls.

Uncheck the **Bond order** checkbox.

The display styles for different bond orders are now the same. Change the display style to *Ball and stick*.

Click the **Ball and stick** radio button.

Next, you will change the display style of groups of atoms. To demonstrate this, you will display the chlorine atoms in *CPK* style. You must first select all the chlorine atoms.

Hold down the **ALT** key and double-click on one of the green chlorine atoms.

All four of the chlorine atoms change color to yellow, indicating that they are selected. This is a shortcut key that allows you to select all examples of a particular element on the screen. Now, you simply change the display style.

Click the **CPK** radio button.

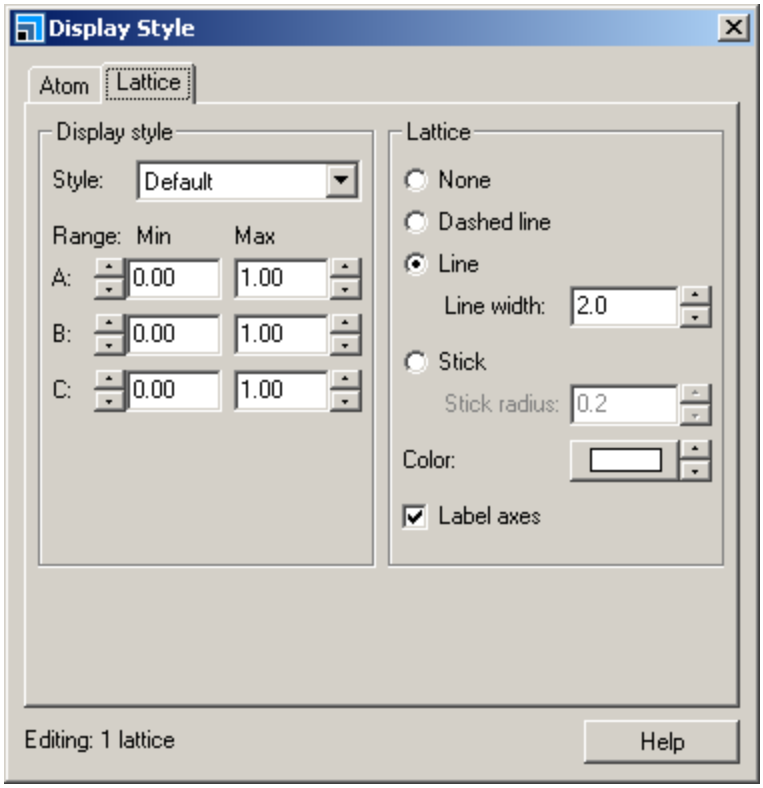
The display style of the chlorine atoms changes to large CPK (Corey-Pauling-Koltun) spheres with their radii dependent on the van der Waals radius of the element they represent. However, most structures look better with a slightly smaller CPK size, so that the spheres do not dominate the structure too much. The overall CPK size can be scaled down.

Click in the **CPK scale** text box and change the value from 0.7 to **0.5**.

Reset the **CPK scale** to **0.7** again by clicking the up arrow. Click anywhere in the 3D Viewer to deselect the chlorine atoms .

The cell display can also be changed.

Select the **Lattice** tab on the Display Style dialog.



Display Style dialog, Lattice tab

The *Lattice* tab contains two distinct areas. The *Display style* area contains information about the style of the cell representation and the range of cells viewed. The *Lattice* area allows you to change the style of the cell lattice box representation. You will change the cell display style. The *Style* dropdown list contains four options:

- Default - Molecules are translated so that their centers of geometry lie within the cell.
- In-Cell - All atoms are translated into the unit cell. Exactly one cell's worth of atoms are displayed.
- Original - Atoms are shown where their symmetry defines them. No extra translations are made.
- None - Neither the atoms nor the lattice are shown.

Select **In-Cell** from the **Style** dropdown list. Observe the change in the 3D Viewer. Repeat this for the **Original** option. Finally, return the **Style** setting to **Default**.

Now, change the *Range* values so that more than one cell is displayed.

In the **Range** section, click in the **Max** box for the **A** parameter and change the value from 1.00 to **3.00**. Press the **TAB** key.

Three cells are displayed in the x direction. Now increase the B and C values similarly.

Change the **Max** value for **B** from 1.00 to **3.00** and that for **C** from 1.00 to **5.00**. Press the **TAB** key after each change to apply the new settings.

The cells are extended in all three dimensions. Do not rotate the structure yet. When you have this number of cells, you may want to remove the lattice in order to improve visualization of the bulk material.

Click the **None** radio button in the **Lattice** section. Close the Display Style dialog.

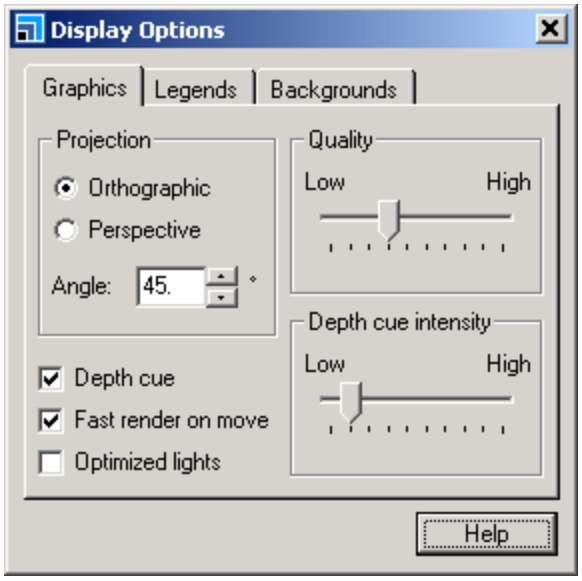
The lattice is removed from the display.

Now that you have a good representation of the structure, you can increase the quality for a final output image. It is best to leave this stage until last, as otherwise, the calculation times required for manipulation of the image can become excessive.

Select **View | Display Options** from the menu bar.

This opens the Display Options dialog.

Note: The Display Options dialog can also be accessed by right-clicking in the 3D Atomistic document and selecting *Display Options* from the shortcut menu.



Display Options dialog

The projection commands on the *Graphics* tab allow you to choose either orthographic or perspective projection. For large structures such as the one you are visualizing, perspective projection is useful.

Select the **Perspective** radio button.

The display changes to a perspective view and the structure is zoomed in. To return to a view where the structure fits to the screen, click on the *Fit to View* button.

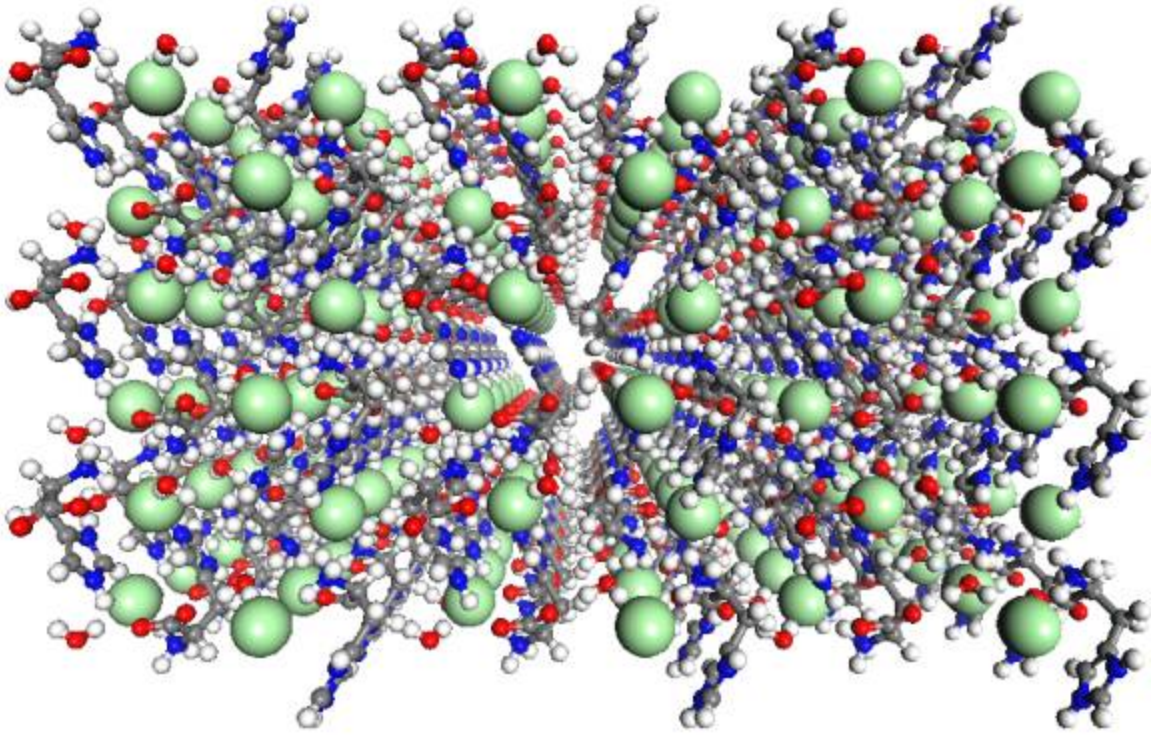
Click the **Fit to View** button  on the **3D Viewer** toolbar.

Tip: The *Quality* setting is used for both on-screen and printed output, which should be similar in appearance. The influence of this setting depends on the available graphics support on your computer. For more detailed guidance on high quality graphics, refer to the Resolution and graphical quality topic.

Note: If you plan to print the structure, you should change the background color to white.

Select the **Backgrounds** tab. On the color control palette, select the background color you require and click the **OK** button.

This structure should look similar to this.



Extended structure of histidine

You can now export this structure as a bitmap that can be inserted into any document.

Select **File | Export...** from the menu bar to open the Export dialog. Select **Structure Bitmap (*.bmp)** from the **Save as type** dropdown list. Enter a filename and click the **Save** button.

If you need a larger version of a structure, for example for a poster, you can increase the output resolution using the *Options...* button on the Export dialog.

Before you move to the next section, change the projection back to orthographic, then remove `histidine_resolved.xsd` from the project.

On the Display Options dialog, change the **Projection** back to **Orthographic**.

Close the Options dialog and then **histidine_resolved.xsd**. Click the **No** button on the dialog asking if you want to save the document as part of the project.

Building a crystal of urea

Now that you have been introduced to the visualization functions, you are going to build a crystal of urea. You will do this by building a crystal cell and placing the atoms into the cell.

1. To construct the cell

The first step is to open a new 3D Atomistic document to construct your cell in.

Click the **New** button  and select **3D Atomistic Document** from the dropdown list.

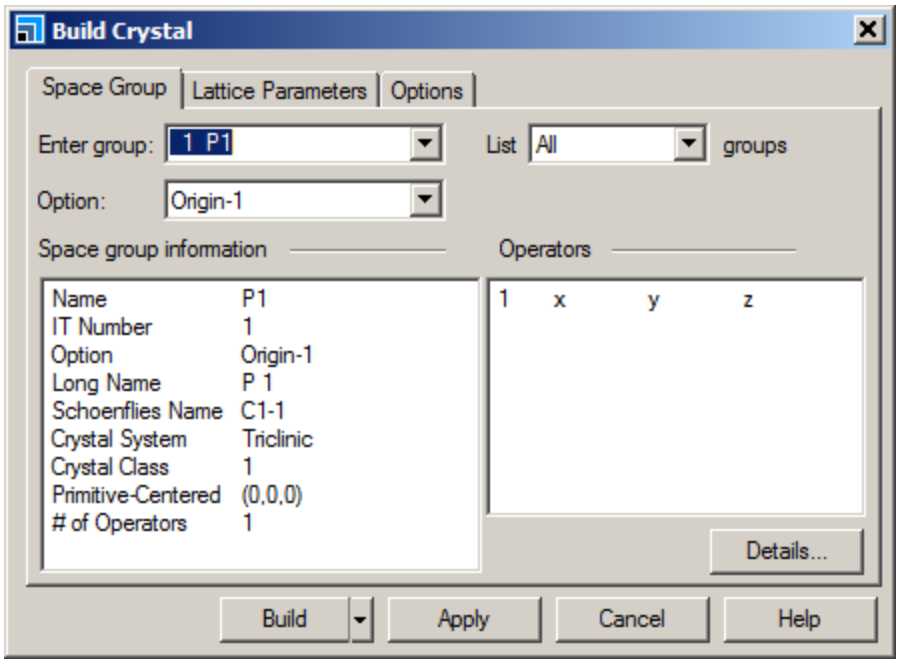
Now that you have an empty 3D Atomistic document, you can construct your cell. In this section, you will just construct a cell, but not add any atoms into it.

Select **Build | Crystals | Build Crystal...** from the menu bar.

This opens the Build Crystal dialog which has three tabs, entitled *Space Group*, *Lattice Parameters*, and *Options*. You should build a cell which has a space group of P-42$_1$m and whose lattice parameters are:

a =	5.576	α =	90.0
b =	5.576	β =	90.0
c =	4.686	γ =	90.0

You can enter the space group information as either the name or the number of the space group or you can choose one from the dropdown list.



Build Crystal dialog

Click in the **Enter group** text box and type in **P-421m**. Press the **TAB** key.

This sets the space group at 113 P-421M and the *Space group information* box changes to display details of the space group. The *Operators* box also updates with the symmetry operations that are related to that space group.

The next step is to set up the lattice parameters.

Select the **Lattice Parameters** tab.

This displays the lattice parameters. Due to the symmetry of the selected space group, only certain parameters can be set. Under the *Lengths* fields, the constraints implied by the symmetry are stated. In this case, parameter *a* must be equal to *b*.

Click in the **Length a** text box and change the value to **5.576**.

The *b* value changes to reflect the value that you have entered for *a*.

Click in the **c** text box. Type in the value **4.686**.

You are now ready to build your cell.

Click the **Build** button on the Build Crystal dialog.

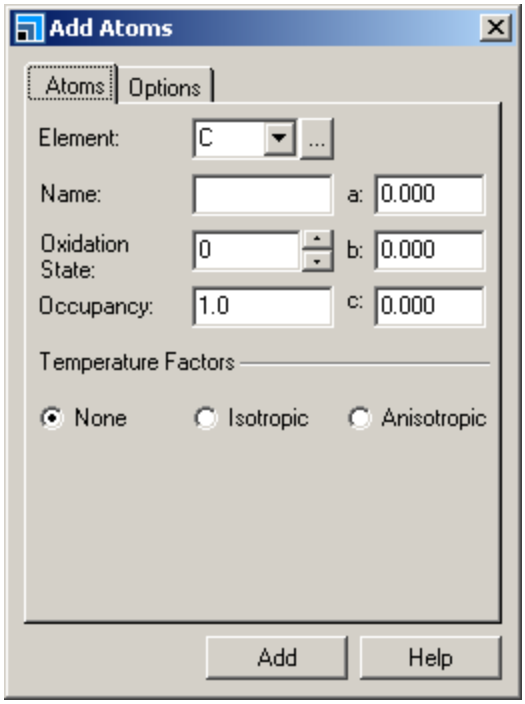
The dialog is closed automatically and an empty cell is displayed in the 3D Viewer. Before you begin to introduce atoms into your cell, it is a good idea to change the display settings from *CPK* back to *Ball and stick*.

Select **Modify | Default Atom Style** from the menu bar to open the Default Atom Style dialog. Select the **Ball and stick** option and close the dialog.

Now you can start to add atoms into your cell.

Select **Build | Add Atoms** from the menu bar.

This opens the Add Atoms dialog.



Add Atoms dialog

The Add Atoms dialog allows you to specify the atoms you want to add, the name you want to give that atom and the a, b, and c fractional coordinates. The *Options* tab contains extra bond settings and the choice of either fractional or Cartesian coordinates. You will enter the coordinates in fractional form. As the symmetry of the space group is so high, you have only to enter the coordinates for three of the heavy atoms and two hydrogens. In some cases, where the symmetry requirements are lower, you can use the *Adjust Hydrogen* tool to add the hydrogens after you have constructed the initial model.

Tip: Hydrogens can only be adjusted on non-metal atoms for which there are no symmetry images.

The coordinates of the atoms that you want to add are:

Atom	a	b	c
C1	0.0000	0.5000	0.3284
O2	0.0000	0.5000	0.5966
N3	0.1480	0.6448	0.1787
H4	0.2620	0.7620	0.2910
H5	0.1290	0.6290	-0.0420

Before you start to add the atoms, make sure that the *Test for bonds as atoms are created* option is enabled.

Select the **Options** tab on the Add Atoms dialog. Check the **Test for bonds as atoms are created** checkbox. Select the **Atoms** tab again.

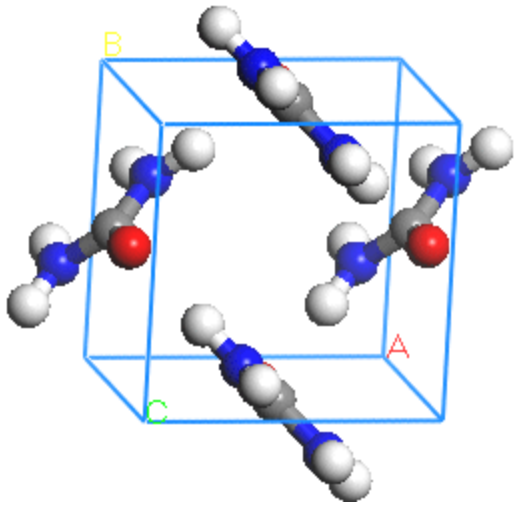
Carbon is the default atom type and so you just need to add a name for it.

In the **Name** text box, enter **C1**. Enter **0.500** in the **b** field and set the value of **c** to **0.3284**. Click the **Add** button.

The atom appears in the crystal cell and a further three atoms are also displayed, due to the symmetry of the cell.

Repeat this for the other atoms, remembering to set the coordinates each time and to change the name of the atom as well as the element type. When you have finished, close the Add Atoms dialog.

When you have added all the atoms into the cell, it will look like this:



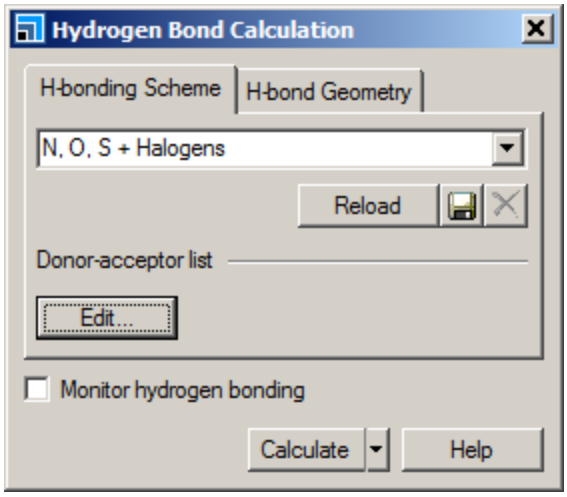
Intermediate crystal model of urea

2. To calculate hydrogen bonds

The tool for calculating and displaying hydrogen bonds in Materials Studio is very flexible and is located in the *Build* menu.

Select **Build | Hydrogen Bonds** from the menu bar.

This opens the Hydrogen Bond Calculation dialog.



Hydrogen Bond Calculation dialog

There are different hydrogen bonding schemes available in the dialog, you can change the atoms that are allowed to hydrogen bond using the dropdown list at the top of the *H-bonding Scheme* tab. If you wish to add in extra atoms, you can edit the *Donor-acceptor list*. There are also two sliders that relate to the hydrogen bond length and angle. These values can range from 1 to 4 Å and from 0 to 180 °, respectively.

Click the **Calculate** button.

The hydrogen bonds are displayed as cyan dashed lines. If you increase the maximum distance to 4 Å, more hydrogen bonds are displayed.

Select the **H-bond Geometry** tab. Drag the **Maximum hydrogen-acceptor distance** slider to **4**. Click the **Calculate** button and close the dialog.

Hydrogen bonds are now displayed between more atoms as the acceptance distance has been increased.

Select **File | Save Project** from the menu bar.

The project is now saved.

This is the end of the tutorial.

Library enumeration using the analog builder

Purpose: Illustrates the use of the analog builder to enumerate libraries of molecules.

Modules: Materials Visualizer

Time:

Prerequisites: Sketching simple molecules

Background

The development of high throughput laboratory techniques has been mirrored by advances in computational methods aimed at the design and combinatorial testing of libraries comprising many thousands of molecules. The two main methods that are employed for the enumeration of such combinatorial libraries are reaction enumeration, where a generic reaction and lists of reagents are defined, and Markush enumeration, which involves the definition of a core scaffold and a range of possible substituents.

The Analog Builder employs a Markush enumeration methodology to construct libraries from multiple cores and fragments defined by 3D coordinates. Once you have defined a scaffold and its connection points, you can design the collections of substituents to be attached. The Analog Builder then enumerates out the different possible combinations, generating a suite of similar structures that can number in the thousands.

Introduction

In this tutorial, you will use the Analog Builder to enumerate a series of organometallic molecules. You will use three different metal cores to generate a library of 240 analogs.

This tutorial covers:

- Getting started
- To define the cores
- To define the R-groups
- To choose the output options
- To define new fragments

1. Getting started

Begin by starting Materials Studio and creating a new project called Enumerate. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Enumerate** as the name and click the **OK** button.

The new project is created with *Enumerate* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

2. To define the cores

In a Markush schema a core is the molecular scaffold onto which the substituents, or R-groups, are attached. In this tutorial, you will use manganese, chromium, and titanium as core scaffold structures.

In the Project Explorer, right-click on the **Enumerate** project root and select **New | 3D Atomistic Document** from the shortcut menu. Click on the **Sketch Fragment** arrow  on the **Sketch** toolbar and select **Fragment Browser** from the dropdown list.

This opens the Fragment Browser dialog, you will use this to define the metal templates that will be employed as core structures in your Markush schema.

On the Fragment Browser dialog expand the **Metal Templates** node. Select **4 coordinate Td** from the expanded list of template metals and select **Mn** from the **Replace undefined atoms with** dropdown list. Click once in the new document.

The selected fragment is sketched in the 3D Atomistic document.

In the Project Explorer, right-click on **3D Atomistic.xsd** and select **Rename** from the shortcut menu. Change the name of the document to **Mn.xsd**.

You have created a core structure for manganese.

Repeat the above steps to create new 3D Atomistic documents called **Cr.xsd** and **Ti.xsd** containing tetrahedral chromium and titanium cores, respectively.

Note: Cores do not have to be obtained from the fragment library. They could be imported from the folder of pre-built structures supplied with your Materials Studio installation or, alternatively, you could opt to sketch a structure that you wish to use as a core.

Now that you have your cores, you are ready to define the connection points where the R-groups will be attached.

Select **Build | Build Analogs** from the menu bar.

This opens the Build Analogs dialog. You can define connections points by selecting an atom and clicking on the *Set* button on the *Cores* tab.

Click the **3D Viewer Selection Mode** button  on the **Sketch** toolbar and select one of the terminal hydrogen atoms in the **Ti.xsd** document. Click the **Set** button on the Build Analogs dialog. Repeat this process for two of the other hydrogen atoms.

You have defined three connection points on your scaffold structure, labeled R1, R2, and R3. Notice that as you click the *Set* button, the R-group number increases automatically.

Note: Only singly bonded terminal atoms can be used as connection points.

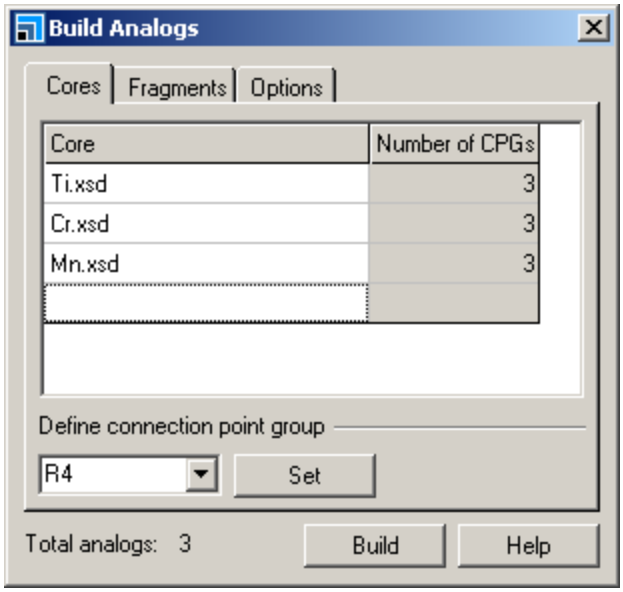
Tip: If you wish, you can assign several atoms to the same connection point group. Select all of the atoms that you wish to define as a connection point group before you click the *Set* button.

The final step in defining the cores for the Analog Builder is to specify which cores will used to build the analog library.

On the **Cores** tab, click in the empty cell in the **Core** column of the grid and select **Ti.xsd** from the dropdown list.

Repeat the above steps to define 3 connection points named **R1**, **R2**, and **R3** on the Cr and Mn cores before adding them to the list of cores on the Build Analogs dialog.

You should finish with three cores defined on the *Cores* tab of the Build Analogs dialog, each containing the same three connection point groups (CPGs), as shown below.



Build Analogs dialog, Cores tab, with metal cores defined

The total number of analogs that will be built is shown in the *Total analogs* field at the bottom left corner of the dialog. This value is continually updated as the inputs and parameters for the enumeration are defined. Notice that this value is currently 3, as you have not yet defined any R-groups.

3. To define the R-groups

Select the **Fragments** tab of the Build Analogs dialog.

This tab allows you to define R-groups for the building process. There are three enumeration options:

All groups separate - All R-groups are treated independently. In this case, you would define a list of fragments for each R-group in each core; therefore, the three R-groups and three cores that you have defined would require you to set up nine R-group lists.

Match groups across cores - R-groups with the same designation share the same lists of fragments. In this case, you would define a list of fragments for each R-group; therefore, the three different R-groups defined in your three cores would require you to set up three R-group lists.

Match all groups - All R-groups are considered to be identical. In this case, you would only need to define a single list of fragments.

Select the **All groups separate** option.

Nine different connection point groups are displayed in the *Connection point groups* list, comprising R1-R3 for Ti, Cr, and Mn.

Select the **Match groups across cores** option.

All the cores are now grouped together, with entries in the list for each of the three R-groups.

Note: If you have selected either the *All groups separate* or *Match groups across cores* options and assigned fragments to the various connection point groups, you should be aware that if you then choose one of the other options, then the fragments will be automatically assigned across the connection point groups to comply with the new setting. However, if you then reselect the original option, the fragment assignment will not change - the original settings will not be reinstated. Therefore, it is advisable that you decide what attachment scheme to use before you start selecting fragments to be attached to the connection point groups.

Since you have defined multiple cores, you will use *Match groups across cores* option. Now you can define the fragments that will be added to each connection point.

Double-click on the row containing **R1** in the **Connection point groups** list.

This opens the Choose Fragments dialog which contains the same fragments that are available in the Fragment Browser, so if you need to define custom fragments, you must add them to the fragment library first. For details on creating custom fragments, see the defining new fragments section.

For the R1 CPG, you will define some organometallic ligands.

Expand the **Ligands** node on the Choose Fragments dialog. Hold down the **CTRL** key and select **Allyl**, **Ammonia**, **Butadienyl**, and **Carbon Monoxide**, then click the  button.

The fragments are transferred to the *Selected fragments* list.

Click the **OK** button.

The fragments are now associated with the R1 connection point group.

Tip: Connection point groups which have not had fragments associated with them are shown in bold in the *Connection point groups* list. When fragments have been defined for the R-groups, the bold text changes to standard text.

You can also add fragments from multiple libraries at the same time.

Double-click on the row containing **R2** in the **Connection point groups** list to display the Choose Fragments dialog.

Expand the **Ligands** node in the **Available fragments** list and select **Ethenyl**, **Ethylenediamine**, and **Ethylenediaminetetraacetate**. Transfer these to the **Selected fragments** list by clicking the  button.

Expand the **Functional Groups** node, select **Thiol** and transfer it to the **Selected fragments** list. Click the **OK** button.

For R3, you will define all the halogens in the fragment library.

Double-click on the row containing **R3** in the **Connection point groups** list to display the Choose Fragments dialog. Select the **Halogens** node and click the  button.

All the fragments in the *Halogens* category in the fragment library are transferred to the *Selected fragments* list.

Click the **OK** button on the Choose Fragments dialog.

The *Total analogs* field at the bottom of the Build Analogs dialog should now indicate that a total of 192 potential analogs will be constructed using the current enumeration parameters. You can review the different fragment groups by clicking on the rows in the *Connection point groups* list.

On the **Fragments** tab of the Build Analogs dialog, select the row containing **R1** in the **Connection point groups** list, followed by those containing the **R2** and **R3** connection point groups.

The fragments contained in each connection point group are displayed. You can remove fragments from the enumeration by selecting them in the *Selected fragments* list and pressing the DELETE key or by double-clicking on the fragment to display the Choose Fragments dialog and using  .

Select the row containing **R2** in the **Connection point groups** list. Select **Ethylenediaminetetraacetate** from the **Selected fragments** list and press the **DELETE** key.

Double-click on the row containing the **R2** connection point group to display the Choose Fragments dialog. Add **Methyl** from the **Hydrocarbons** library and **Phosphine** from the **Ligands** library to the **Selected fragments** list, then click the **OK** button.

A number of potential analogs should now have risen to 240, reported as *Total analogs* on the Build Analogs dialog.

4. To choose the output options

The *Options* tab of the Build Analogs dialog allows you to define the output options for the Analog Builder. You can choose to output the results in a study table, a trajectory file, or both. For this tutorial, you will output the analogs to a study table.

Note: The study table and trajectory documents referred to here store the analogs in the project as a hidden `.sd` file. The `.std` and `.xtd` files that may be produced by an Analog Builder run provide different views onto the data contained in the `.sd` file. If you wish to use this file with another application, you can find the native `.sd` file with the other Materials Studio project files on your hard drive.

Select the **Options** tab of the Build Analogs dialog. Ensure that **Study table only** is selected from the **Return results as** dropdown list.

Now you need to specify the naming convention to be used for the analogs.

Select **Core and fragment numbers** from the **Name structures by** dropdown list.

Note: It is not possible to specify the name of a structure file embedded within a study table document. The naming options specified are used to populate the *Structure Name* column in the study table.

You can also choose to apply post-processing to the analogs that are built by the Analog Builder.

Checking the *Clean structures* checkbox indicates that the *Clean* functionality of the Materials Visualizer will be used. This tool employs a lookup table of common bond lengths and angles to generate an approximate starting geometry for each analog structure. Using this option can significantly increase the calculation time for analog building.

Note: The *Clean* operation should not be a replacement for geometry optimization with a good Hamiltonian or forcefield. If your fragments and cores have already been optimized, it may be better to use a classical, semiempirical, or quantum mechanical method to optimize them instead of using the *Clean* option.

Checking the *Add hydrogens* checkbox indicates that the *Adjust Hydrogen* functionality of the Materials Visualizer will be used to fill empty valences with hydrogens and to recalculate the positions of current hydrogen atoms for each analog structure.

You will clean the structures of your analogs in this tutorial.

Check the **Clean structures** checkbox and click the **Build** button.

The status bar at the bottom of the Materials Studio window indicates the progress of the Analog Builder job. The various stages of building, cleaning, and inserting the analogs into the study table are reported in the status bar. In this case, the entire procedure should only take a few seconds.

When the process is complete, a study table will be returned containing the analog structures, their names (according to the naming scheme you specified), and the core and fragments comprising each analog.

Close the Build Analogs dialog and double-click on one of the analog structures in **Ti.std**.

The structure is displayed in a Study Table Detail View.

Close the **Study Table Detail View**.

Select column **D** in the study table. Click the **Sort Ascending** button on the **Study Table Viewer** toolbar.

The rows are ordered by the fragment attached to R1.

Tip: There are many other actions you can perform on the analogs in the study table, including optimizing their structures with Forcite, VAMP, or DMol^3, or aligning them.

Select **File | Save Project** from the menu bar and then **Window | Close All**.

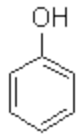
The project is saved and all of the open documents are closed.

5. To define new fragments

The *Sketch Fragment* tool of the Materials Visualizer has a feature that allows you to define your own custom fragments and add them to the fragment library for subsequent use with the Analog Builder or for sketching.

In this example, you will sketch phenol and add it to the fragment library.

Start by sketching phenol, the structure of which is shown below.



Structure of phenol

Create a new **3D Atomistic Document** and rename it **phenol.xsd**.

Use the tools on the **Sketch** toolbar to construct phenol. Add the correct number of hydrogen atoms to the structure by clicking the **Adjust Hydrogen** button and then give the structure a reasonable initial geometry by clicking the **Clean** button.

Note: In order for a structure to be valid for addition to the fragment library, it must be contiguously bonded and nonperiodic. The fragment may be constructed by sketching or can be imported from a pre-existing file.

Click on the **Sketch Fragment** arrow on the **Sketch** toolbar and select **Define Fragment** from the dropdown list.

This opens the Define Fragment dialog. The first step in adding a custom fragment to the fragment library is to define the connection point, this is the point at which it will be attached to other atoms during sketching and analog building operations. For phenol, the connection point is the hydroxyl hydrogen.

Note: Only singly bonded terminal atoms can be used as connection points. Multiple connection points are not allowed; you cannot add a fragment with multiple connection points to the fragment library.

Click the **3D Viewer Selection Mode** button  and select the hydroxyl hydrogen atom in **phenol.xsd**. Click the **Define** button on the Define Fragment dialog.

A connection point, indicated by a red cage around the atom, is defined on the phenol molecule.

Select **Rings** from the **Fragment Library** dropdown list and enter the name **Phenol** in the **Fragment Name** box. Click the **Add** button and then close the dialog.

The phenol fragment is added to the *Rings* section of the fragment library, as confirmed by the message Fragment Phenol created in library Rings in the status bar.

Tip: If you wish, you can also create a new library for the fragment you are adding by entering a name directly into the *Fragment Library* field.

You will now be able to use the phenol fragment for sketching or as an R-group for the Analog Builder.

Select **File | Save Project** from the menu bar or click the **Save Project** button  on the **Project** toolbar.

This is the end of the tutorial.

Building mesoscale molecules

Purpose: Illustrates how to use the mesomolecule builder to build bead representations of molecules.

Modules: Materials Visualizer

Time:

Prerequisites: Project management

Introduction

Mesomolecules can be used to define the molecular topology of molecules such as polymers and surfactants as beads for use in Mesocite calculations. A simple but powerful builder enables the building of a wide variety of bead structures including random copolymers and dendrimers, structures that were previously very hard to generate in mesoscale calculations. This tutorial covers the building of block copolymers, random copolymers, and branched structures.

This tutorial covers:

- Getting started
- To add bead types to the project
- To build block copolymers
- To build random copolymers
- To build branched structures

1. Getting started

Begin by starting Materials Studio and creating a new project called Mesomolecule. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Mesomolecule** as the name and click the **OK** button.

The new project is created with *Mesomolecule* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

2. To add bead types to the project

Before building a mesoscale molecule, you must first define the bead types that will be used to construct the molecules. Bead types are stored in the project so should be defined for each system you are working with.

Select **Build | Build Mesostructure | Bead Types** from the menu bar or click the **Bead Type** button on the **Mesostructure** toolbar.

This opens the Bead Types dialog. Bead types have two main properties that are used in every simulation, the name and color. You can also specify the bead type radius which is used when visualizing beads using the CPK style.

Click in the **Bead Type** text box and type **ethyleneoxide**. Press the **TAB** key.

You have created a bead type called ethyleneoxide. Repeat this creating a new bead type called ethylene.

Click in the empty **Bead Type** text box and type **ethylene**. Press the **TAB** key.

When you add another bead type to the project, the bead types are ordered alphabetically. You can change the color of the bead type.

Select the **ethyleneoxide** bead type and click the **Properties...** button to open the Bead Type Properties dialog.

Change the color of the bead type. Click on the **ethylene** field on the **Bead Type** dialog.

You can swap between the bead types and see the properties.

Tip: Importing a document with undefined bead types into a project will automatically create the bead types in the projects. If you use the same bead types regularly, you can build them into a document and simply re-import the document rather than defining them for each project.

Close the **Bead Types** and **Bead Type Properties** dialogs.

3. To build block copolymers

Now that you have defined bead types in the project, you can use them to build mesoscale molecules. Initially, you will build a block copolymer consisting of 5 beads of ethylene and 5 beads of ethyleneoxide.

Select **Build | Build Mesostructure | Mesomolecule** from the menu bar or click the **Mesomolecule** button  on the **Mesostructure** toolbar.

This opens the Build Mesomolecule dialog. First you should add 5 beads of ethylene.

Select **ethylene** from the **Component Name** dropdown list. Increase the **Number** to **5**.

Now do the same for ethyleneoxide.

Select **ethyleneoxide** from the **Component Name** dropdown list. Increase the **Number** to **5**. Click the **Build** button.

A new document called `Mesomolecule.xsd` is created. It contains a diblock copolymer of 5 beads each representing ethylene and ethyleneoxide. You can change the display style of the mesomolecules using the Display Style dialog.

Right-click in the 3D Viewer and select **Display Style** to open the Display Style dialog. On the **Bead** tab change the style of the beads to **Ball and stick** and close the dialog.

If you want to build a repeating block copolymer, you can do this by specifying the *Number of repeat units*.

On the **Build Mesomolecule** dialog, change the **Number of repeat units** to **4**. Click the **Build** button.

A new document called `Mesomolecule (2).xsd` is created containing the repeated block copolymer.

4. To build random copolymers

Building random copolymers using a string representation can be difficult, but it is simple using the mesomolecule builder. There are two different types of random copolymer that you can construct. The first one you will build is randomized in each repeat unit.

On the **Build Mesomolecule** dialog, change the **Number** of **ethylene** and **ethyleneoxide** components to **2**. Check the **Randomize order within repeat unit** checkbox. Click the **Build** button.

The new document contains a structure with four repeat units and the beads are randomized in each repeat unit. If you examine the structure you will see that each consecutive set of four beads contains two ethylene and two ethyleneoxide.

In the **Project Explorer**, rename the model document to **RandomRepeatUnit.xsd**.

If you want to create a truly random copolymer, you should change the number of components to mimic the ratio of beads in the copolymer. To reproduce the above case, you will need to build a single repeat unit containing eight beads of ethylene and eight beads of ethyleneoxide.

Increase the **Number** of the **ethylene** and **ethyleneoxide** components to **8**. Decrease the **Number of repeat units** to **1**. Click the **Build** button.

In the newly created model document, you have a random copolymer of sixteen beads with eight beads of each component.

5. To build branched structures

Branched structures are very important for the modeling of polymers. There are two ways to add branches to a structure using the Mesomolecule Builder tools. You can add branches to either selected beads or to terminal beads. Initially, you will build a dendrimer by adding to the terminal beads. First, you should build the seed of the dendrimer, three beads of ethylene.

On the Build Mesomolecule dialog select the **ethyleneoxide** row and press the **DELETE** key.

Change the **Number** of **ethylene** components to **3**. Uncheck the **Randomize order within repeat unit** checkbox and click the **Build** button.

This will create a seed containing three beads of ethylene. Now you can add two generations of ethyleneoxide.

Click on the **ethylene** component and select **ethyleneoxide** from the dropdown list and increase the **Number** to **4**. Check the **Add to branch points** checkbox and click the **More...** button.

This opens the Mesomolecule Branches dialog. Here you can specify the number of branches and how you want to add them.

Select **Branch from terminal** beads. Change the **Number of generations** to **2**. On the **Build Mesomolecule** dialog, click the **Build** button.

Rotate the view to see the dendrimer.

A bead representation of a dendrimer is created with two generations. You can add a third generation by simply adding again to the same document.

On the **Build Mesomolecule** dialog, click on the **ethyleneoxide** component and select **ethylene**.

On the **Mesomolecule Branches** dialog, change the **Number of generations** to **1**.

On the **Build Mesomolecule** dialog, click the **Build** button.

Note: Currently, there is no clean functionality for the Mesomolecule builder tool so you will sometimes have intersecting connectors between beads. However, when the molecules are built into the mesostructure, the mesoscale modeling tools will remove any intersections.

You can also add branches to selected beads. For example, you can add a branch to the ethylene beads in the `RandomRepeatUnit.xsd` document.

Make **RandomRepeatUnit.xsd** the active document. Press and hold the **ALT** key and double-click on a green **ethylene** bead.

All the ethylene beads are selected. This time you will build a branch containing 1 bead of ethyleneoxide and 2 beads of ethylene. The order of the beads define the order in the branch with the bead at the top being the bead that connects to the branch point. The branch will connect with the ethyleneoxide.

On the **Build Mesomolecule** dialog, delete the existing components. Define the branch as consisting of **1** bead of **ethyleneoxide** and then **2** beads of **ethylene**. On the **Mesomolecule Branches** dialog, select **Branch from selected beads**. Set the **Number of branches to attach** to **1**. **Build** the mesomolecule.

You should have single branches from each ethylene with the ethyleneoxide as the branch connection point.

If you want to build a polymer where the branch repeats regularly but the backbone is all the same polymer, you can do this by using a temporary bead and then redefining it. In this example, you will build a backbone which consists of twenty ethylene beads and you will add a branch of three ethylene beads every fourth ethylene bead in the backbone.

On the **Build Mesomolecule** dialog, uncheck the **Add to branch points** option. Build a new mesomolecule composed of **5 repeat units** of **3 ethylene** beads and **1 ethyleneoxide** bead.

Although you cannot sketch a bead or connector, you can delete them.

Select the terminating **ethyleneoxide** bead on the chain. Press the **DELETE** key.

You can now select the ethyleneoxide beads and add your branches to the beads.

In the model document, hold down the **ALT** key and double-click on an **ethyleneoxide** bead.

On the **Build Mesomolecule** dialog, define a molecule which consists of **1 repeat unit** of **3 beads of ethylene**. Check the **Add to branch points** checkbox.

On the **Mesomolecule Branches** dialog, select **Branch from selected beads**. **Build** the mesomolecule and close the Build Mesomolecule and Mesomolecule Branches dialogs.

This adds the branches to the ethyleneoxide beads. Finally, you can edit the bead types of the ethyleneoxide beads.

With the **ethyleneoxide** beads still selected, in the **Properties Explorer**, double-click on the **BeadTypeName** in the Properties Explorer to open the **Modify Bead Type** dialog. Select **ethylene**, click the **OK** button and close the dialog.

You have now built a bead representation of a regularly branched polymer of ethylene.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

This is the end of this tutorial.

Building bulk mesostructures

Purpose: Introduces the functionality of the mesostructure template builder and mesostructure builder

Modules: Materials Visualizer

Time:

Prerequisites: Building mesoscale molecules

Introduction

The mesoscale template builder allows you to build a complex input structure for a Mesocite calculation. It enables you to pack mesoscale molecules into 3D periodic structures with a variety of shapes. It allows you to add slabs, droplets, rods, shells, and tubes and fill these shapes with mixtures of mesoscale molecules.

In this tutorial, you are going to use the mesostructure template builder to build a system containing a droplet on an adsorbent slab embedded in a solvent. You will also build a second system with the droplet penetrating into the slab, as well as mesostructures containing a surface packed droplet which enables you to add order to your system.

This tutorial covers:

- Getting started
- To build the mesomolecules
- To create the formers
- To assign fillers to the formers
- To build a packed mesostructure
- To create the droplet on the surface
- To create a surface packed droplet

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

1. Getting started

Begin by starting Materials Studio and creating a new project called bulk_mesostructures. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **bulk_mesostructures** as the name and click the **OK** button.

The new project is created with *bulk_mesostructures* listed in the Project Explorer.

2. To build the mesomolecules

You need to create both mesostructure templates and the mesomolecules to fill them, and this can be done in either order. In this tutorial, you will create the mesomolecules first. This is a two step process: first defining the bead types and then building the mesomolecules themselves.

Select **Build | Build Mesostructure | Bead Types** from the menu bar to open the Bead Types dialog. Define bead types for **Oil**, **Solvent**, **SurfHead**, and **SurfTail** and close the dialog.

Tip: You can create bead type names with an unlimited number of characters. However, forcefield types are limited to 5 characters in the name. In the above example, SurfHead would be given a forcefield type of SurfH. If you are going to use the typing tool for the DPD task in Mesocite, it is better to use shorter bead type names so that the forcefield type is identical to the bead type.

Now you can build the mesomolecules. You will build the following:

Name	Topology
Surfactant	SurfHead 1 SurfTail 4
Octene	Oil 1
Water	Solvent 1

Select **Build | Build Mesostructure | Mesomolecule** from the menu bar to open the Mesomolecule Builder dialog. Select **Solvent** as the **Component Name**, set the **Number** to **1**, and click the **Build** button to build a mesomolecule consisting of 1 bead of Solvent.

In the Project Explorer, rename the document **Water.xsd**.

Build a mesomolecule consisting of **1** bead of **Oil** and rename the document **Octene.xsd**.

Build a mesomolecule consisting of **1** bead of **SurfHead** and **4** beads of **SurfTail**. Rename the document **Surfactant.xsd** and close the Build Mesomolecule dialog.

Tip: If you are going to use these structures with the DPD task in Mesocite, you should assign the forcefield types before building the mesostructure. You can do this by selecting *Modules | Mesocite | Forcefield Manager* to open the *Mesocite Forcefield Manager* dialog, then click the *DPD...* button to open the *Create DPD Forcefield* dialog. For each of the mesomolecule documents, click the *Type* button to create new forcefield types for the beads.

3. To create the formers

A template consists of a set of mesoscale objects, or Formers, to which you will assign different materials, or Fillers. The first step when creating a template is to build the System former.

Select **Build | Build Mesostructure | Mesostructure Template** from the menu bar to open the Build Mesostructure Template dialog.

The system former is a rectangular box that will contain all other formers. The extent of the system former defines the overall size of the box. You will build a cubic box that is 60 units in each direction.

Note: Mesostructure templates do not have units defined but for use in Mesocite, you should assume that 1 unit = 1 Å.

In this tutorial the system former is the solvent box in which the droplet and the slab will be embedded. You can fill the system former at this point with solvent using the Filler dropdown list. Later in this tutorial you will use alternative methods for assigning fillers.

Set all the values for the **Extent (X Y Z)** dimensions to **60**. Type **Solvent** in the **Filler** field and click the **Build** button.

A new mesostructure document, `Mesostructure Template.msd`, opens. This contains a box, the System former, of extension 60 × 60 × 60. The box is colored blue, which is the color of the Solvent filler assigned to it.

To simplify document reference later, you should rename the mesostructure template.

In the Project Explorer, select **Mesostructure Template.msd**. Rename the document to **DropletInSurfaceTemplate.msd**.

The next step is to add the other formers to the system. A former represents the type, shape, and position of the mesoscale phases. Formers can have a diverse range of shapes.

There are several different Former types available; Droplet, Rod, Slab, Shell, and Tube. In this case, you are going to add a slab and a droplet. First add a slab to the system.

Select **Slab** from the **Former type** dropdown list.

You can specify the depth, orientation, position, and other characteristics of the slab. The slab you are going to add should take up about a third of the box. As the size of the box in each direction is 60 units, the depth of the slab should be 20.

Change the **Depth** to **20.0**.

In this case you want to align the slab in the x-z plane, that is normal to the y-direction.

Change the **Orientation** to **AlongY**.

The Position property sets the position of the center point of the former. It can be set in Cartesian or fractional coordinates. So, in order to add the slab along the edge of the box, you should set the y-position to the Cartesian coordinate of 10.0.

Change the **Coordinates** to **Cartesian**. Change the second field of **Position (x y z)** to **10.0**. Leave the **Filler** field blank and click the **Add** button.

A slab former is added along the bottom of the cell. The slab former is colored gray, indicating that no filler has been assigned to it yet.

Tip: You can move formers using the standard translation tools on the 3D Movement dialog or by using the mouse buttons.

Finally you will add the droplet former to the system. The droplet will be of radius 15 and will be positioned in the middle of the box, with the center on the upper surface of the slab.

Change the **Former type** to **Droplet**. Change the **Radius** to **15.0** and change the second field of **Position (x y z)** to **20.0**. Leave the **Filler** field blank and click the **Add** button.

A droplet former is added with its center on the upper surface of the slab. The former is still colored gray, indicating that no filler has been assigned to it yet.

4. To assign fillers to the formers

The next stage is to create and assign the fillers. A filler represents the material that a former consists of and relates to one or more mesomolecule types. This allows much flexibility in working with the templates as, once you have set up a template, you can re-use it for multiple simulation runs with different molecule types.

Each former can be assigned one filler. This is done on the *Fillers* tab.

Select the **Fillers** tab on the Build Mesostructure Template dialog.

This tab shows a list of fillers defined in the document. At this point the list should already have one entry, Solvent, which is the filler you assigned to the system former on starting the template. You will extend the list with the materials for the droplet and the slab formers.

First add a filler material for the droplet.

Click the **Add** button.

A new filler is created called Filler 1. You will change this name.

Type in the name **Soap**.

Once you have defined the filler, you can associate it with a former. The easiest way to do this is to select the former in the `DropletInSurfaceTemplate.msd` document. The number of formers selected is displayed next to the *Assign* button.

Select the **Droplet** former in **DropletInSurfaceTemplate.msd**. On the **Fillers** tab, click the **Assign** button.

The droplet former should change color to green, the color of the Soap filler.

Tip: You can also create and assign fillers as you add the formers to the template. To do this you should select or define the material using the *Fillers* dropdown list on the *Add Formers* tab before adding the former using the *Add* button.

The final filler that you will add to this simple system is the oil filler for the slab.

Add a new Filler and rename it **Oil**. In **DropletInSurfaceTemplate.msd**, select the **Slab Former**. On the **Fillers** tab, click the **Assign** button.

The slab former is now displayed in the red color of Oil.

Tip: You can assign a filler to more than one former by selecting multiple formers.

Now all formers have been assigned a filler, you can match the mesoscale molecules to the fillers. Before proceeding, you should look at the *Formers* tab.

Select the **Formers** tab.

The *Formers* tab shows the formers that are in the template. The former name contains the filler assigned to it. In this case you should have System of Solvent, Slab of Oil, and Droplet of Soap. You can change the visibility of the formers using the checkboxes. The *Formers* tab also provides a way of selecting the formers if you have many formers in a template.

Select the **Droplet of Soap** former.

This selects the droplet former in the document.

The *Former* tab lists the formers in the order in which they were added to the system. This order is important in the assignment of fillers to the formers. The template builder will fill the formers one-by-one, starting with the former lowest in the tree, and working its way up. So when two formers overlap, the one lowest in the list claims the overlapping space.

You should note that the formers can be moved up and down in the list. You will use the move controls later on in this tutorial.

Close the **Build Mesostructure Template** dialog.

5. To create a packed mesostructure

Once you have built your mesoscale template, you can then map the fillers onto the mesomolecules you built in the first section.

On the **Mesostructure** toolbar, click the **Mesostructure** button  or select **Build | Build Mesostructure | Mesostructure** from the menu bar.

This opens the Build Mesostructure dialog, containing a list of filler materials present in the active document. In the first column you should see the fillers you have already defined: Solvent, Oil, and Soap. In the second column you can specify one or more mesoscale molecules to be associated with each filler. If you specify more than one molecule per filler you can set the composition in the third column. For this simple case, you are going to add one mesoscale molecule to each filler.

Click in the **Mesoscale Molecule** column for the **Solvent** filler.

A dropdown list will open, with the mesomolecules that you built previously: Surfactant, Octene, and Water.

Select **Water.xsd** for the filler **Solvent**. Repeat this for the filler **Soap** and select **Surfactant.xsd**. Repeat again for the **Oil** filler and select **Octene.xsd**. Click the **Build** button and close the dialog.

A new document, `DropletInSurfaceTemplate Packed.xsd`, is created. It contains the water, octene, and surfactant molecules packed in the formers of the associated fillers.

You should see that the droplet goes right through the adsorbent layer. Save this project and close all the documents before continuing.

Select **File | Save Project** followed by **Window | Close All** from the menu bar.

6. To create the droplet on the surface

The droplet that you created in the above section interpenetrated into the surface. You can also create a droplet that sits on the surface of the slab by using the *Formers* tab.

Re-open **DropletInSurfaceTemplate.msd** and open the **Build Mesostructure Template** dialog.

Any point in the simulation cell can only be owned by one former. If two formers are overlapping, the former that is lower in the tree list will take ownership of the overlapping space. As you can see on the *Formers* tab, Droplet is lower in the list than Slab. Therefore, the droplet owns the intersecting space and interpenetrates into the Slab. By changing the hierarchy, you can significantly change the mesostructure.

On the **Formers** tab select **Slab of Oil**. Click the **Move to bottom of tree** button  and close the dialog.

The Slab former moves to the bottom of the tree. Now you can build another packed mesostructure template document but you should save it as a different template before you do this.

Select **File | Save As...** from the menu bar. Change the **File name** to **DropletOnSurfaceTemplate.msd** and click the **Save** button.

You are now ready to build another mesostructure.

Open the **Build Mesostructure** dialog.

The molecule types and fillers should still be set.

Click the **Build** button and close the dialog.

A new file named `DropletOnSurfaceTemplate Packed.xsd` is created. The droplet should now be a hemisphere rather than the full sphere shown before.

Select **File | Save Project** from the menu bar, followed by **Window | Close All** from the menu bar.

7. To create a surface packed droplet

In the previous examples all formers were packed randomly with molecules. To build initial structures containing micelles, bilayers, or coatings requires more controlled packing. This control is provided by the surface packing functionality of the template builder. In this final part of the tutorial you will use this to build a droplet with a micellar substructure.

You are going to replace the droplet former by a droplet former that is surface packing enabled. First delete the droplet former in the template document `DropletOnSurfaceTemplate.msd`.

Re-open **DropletOnSurfaceTemplate.msd**. Select the **Droplet** former and press the **DELETE** key.

Now add a new droplet former to the template that is enabled for surface packing.

Open the **Build Mesostructure Template** dialog. Change **Former Type** to **Droplet**. Leave the **Radius** and **Position (x y z)** settings unchanged. Check the **Enable surface packing** checkbox. Select **Soap** from the **Filler** dropdown list and click the **Add** button.

This will create a droplet former as in the previous example. However, this time the former is enabled for surface packing, indicated by the dots on the surface of the droplet.

Tip: You can also change the surface packing status of a former directly by editing the SurfacePackingEnabled property of a selected former in the Property Explorer.

As before, since the droplet former is added last, it will be packed first, resulting in a penetrating droplet. To create a droplet on the surface, first move the droplet former to the top of the former list.

On the **Formers** tab, select **Droplet of Soap** and click the **Move to top of tree** button  . Close the dialog.

Before defining the packing rules for the molecule, you should save the template as a new name.

Select **File | Save As...** from the menu bar. Change the **File name** to **DropletOnSurfaceSPTemplate.msd** and click the **Save** button.

By enabling a former surface for surface packing, you can stick and align mesomolecules to it. You will first have to specify which bead in the mesomolecule is to be packed on the surface ("head"). You can also specify which bead in the molecule is used to orient the molecule normal to the surface ("tail"). This specification is achieved using sets of beads in the original mesomolecule documents that you created. The sets can be automatically created using the Build Mesostructure dialog.

Open the **Build Mesostructure** dialog, on the **Options** tab click the **More...** button.

This opens the Bead Packing Options dialog which enables you to create, select, and delete tags for beads for special packing options.

Open **Surfactant.xsd** and select the **SurfHead** bead. On the **Bead Packing Options** dialog, click the **Create** button.

A set is created, labeled BeadTag_Head which identifies the bead as the head bead for packing. You should do the same for the tail.

Select the terminating **SurfTail** bead. On the **Bead Packing Options** dialog, change the **Bead tag** to **Tail** and click the **Create** button and close the dialog.

You have now marked the appropriate beads so that the heads should be on the surface of the micelle and the tail beads packed inside.

Change focus back to **DropletOnSurfaceSPTemplate.msd**. On the Build Mesostructure dialog, click the **Build** button.

A new bead structure document is returned with the head of the surfactant molecules packed onto the surface of the droplet.

Tip: By default, the chain orientations are randomized leading to some chains being on the surface of the micelle. You can control this using the Randomize conformations checkbox on the Options tab.

The molecules are oriented such that the end-to-end vector is normal to the droplet surface, pointing inside the former volume.

This is the end of this tutorial.

Coarse graining atoms to beads

Purpose: Demonstrates how to use the coarse graining tools

Modules: Materials Visualizer

Time:

Prerequisites: Using the polymer builder

Introduction

Building coarse grained, or bead, representations of molecules requires mapping from the atomistic to bead representation. The user could build a model of the system of interest using the Mesomolecule building tools, using their knowledge of the system. Alternatively, it is also useful to generate a bead model directly from an atomistic representation. In this tutorial, you will use the coarse graining tools to generate bead representations of atomistic models. You will do this using simple repeat units to coarse grain polymers according to their monomer units and use patterns to generate bead models of structures with no subunit information.

This tutorial covers:

- Getting started
- Coarse graining a polymer using repeat units
- Coarse graining a nanotube using patterns
- Coarse graining a mixed system of polymer and drug

1. Getting started

Begin by starting Materials Studio and creating a new project called CoarseGrain. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **CoarseGrain** as the name and click the **OK** button.

The new project is created with *CoarseGrain* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

2. Coarse graining a polymer using repeat units

If a molecule has subunit information such as repeat units or protein data contained in a PDB file, you can automatically convert each type of subunit to a bead type. When converting from an atomistic to bead representation, there are two steps - finding the different beads in the molecules and then generating the bead model. You will perform both of these steps in this first section, although they can also be performed in a single step.

Build a **block copolymer** of **5** monomers of **ethylene** and **5** monomers of **oxyethylene** using the polymer building tools.

This structure has two main monomers, ethylene and oxyethylene, giving two different bead types. However, in order to preserve the atomistic structure, the coarse grainer is sensitive to the presence of hydrogens, so the terminating monomer units will have different types to non-terminating monomer units.

Select **Build | Build Mesostructure | Coarse Grain** from the menu bar or click the **Coarse Grain** button  on the **Mesostructure** toolbar to open the Coarse Grain dialog.

The coarse grainer works by looking for substructures and matching them to the existing structures. There are three main ways to perform a coarse graining:

- Patterns - Use a study table containing existing marked up structures that can be matched against your current structure
- Motion groups - Use motion groups defined on your existing structure as beads
- Subunits - Use subunit or repeat unit information

One or a combination of the above methods can be used on a single structure.

In this first example, you will coarse grain using repeat unit data so that each repeat unit is a bead. As Subunits is the default setting for this dialog, you do not need to make any changes.

By default, identifying bead types and creating a mesoscale structure is carried out in one step, however this does not allow precise control of the bead names. You can disable the automatic creation or update of the typing document Study Table.

Uncheck the **Automatically update typing document** checkbox.

The next step is to identify unique subunits in the molecule. These will be stored in a study table so that you can view and edit their names before coarse graining.

In the **Bead typing** section, click the **Create** button.

A study table is created called `Bead Typing.std` with the atomistic structure for typing in column A and the Bead Type Names in column B. The Bead Type Name is the name that will be given to identical beads when the coarse graining calculation is performed.

In the **Structure** column, double-click on **ethylene**.

A detail view opens, this is the terminating ethylene repeat unit. You can change the name of this structure so that when the beads are generated they have a more descriptive name.

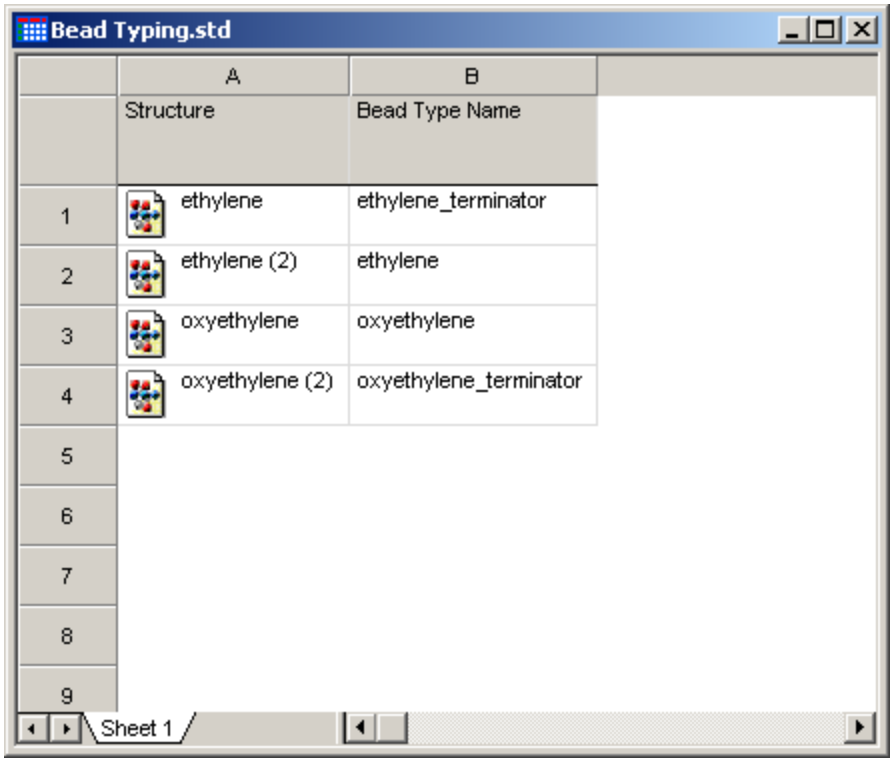
In the **Bead Type Name** column, change the **ethylene** text to **ethylene_terminator**. Close the detail view for **ethylene**. Double-click to open the detail view for **ethylene (2)**.

The second type of ethylene repeat unit is the mid-chain repeat unit, you should change the name for this structure.

In the **Bead Type Name** column, change the **ethylene (2)** text to **ethylene**. Close the detail view for this structure.

You should repeat this for the oxyethylene units so that, when you create the beads, more descriptive names are used.

Open the detail views for the oxyethylene structures. Change the names so that you have **oxyethylene** and **oxyethylene_terminator**.

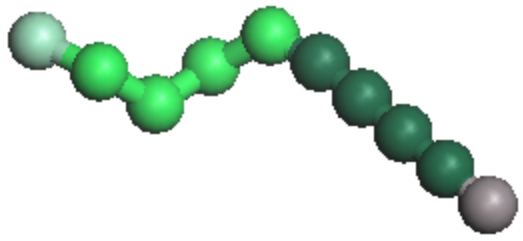


Bead Typing Study Table with modified Bead Type Names

Now that you have assigned descriptive names to the structures for typing, you can generate the bead representation of the polymer.

Make **Blockethyleneoxyethylene.xsd** the active document and click the **Build** button on the Coarse Grain dialog.

A new document, `Blockethyleneoxyethylene CG.xsd`, is generated. This contains the bead representation of the polymer with the terminating monomer units in different colors to the monomer units in the main chain.



Ball and stick representation of Blockethyleneoxyethylene_CG.xsd

When the bead model is generated, new bead types, with the names you specified, are automatically added to the project.

Select **Build | Build Mesostructure | Bead Types** from the menu bar or click the **Bead Types** button on the **Mesostructure** toolbar. On the **Bead Types** dialog, select **ethylene_terminator** and click the **Properties...** button.

The *Mass* property of the bead type is defined from the sum of the elements in the structure. The *Radius* is defined as a radius of a best fit sphere to the atoms in the structure.

On the **Bead Types** dialog, change to **oxyethylene**.

The *Mass* and *Radius* reported on the Bead Type Properties dialog are updated for the oxyethylene bead type.

Tip: You can also use the Bead Type Properties dialog to change the default color of beads.

Close the **Bead Type Properties** dialog and **Bead Types** dialog.

This short example has demonstrated how to coarse grain a system which has repeat units. If you have no repeat unit data, you can assign motion groups. However, if you have a repeating pattern, you can use the *Patterns* method to automatically coarse grain a repeating system.

Select **File | Save Project** from the menu bar followed by **Window | Close All**.

3. Coarse graining a nanotube using patterns

A carbon nanotube consists of multiple benzene rings. You could coarse grain it using the phenyl rings as the subunit, or you could use a larger repeat unit. In this example, you will coarse grain a nanotube using a pattern consisting of a phenyl ring with six attached phenyl rings. This level of coarse graining was recently used by Liba et al. to perform simulations of nanotube interactions. The first step is to build a carbon nanotube.

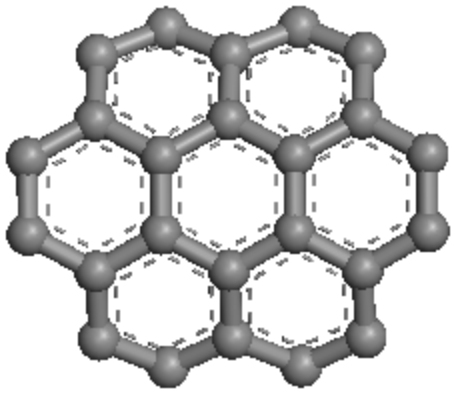
Select **Build | Build Nanostructure | Single-Wall Nanotube** to open the Build Single-Wall Nanotube dialog.

You will build a similar nanotube to that used by Hanein et al. In this case, you will build two identical copies of the nanotube, one to coarse grain and the other to generate a template.

Uncheck the **Periodic nanotube** checkbox. Set **Repeat Units** to **41**. Click the **Build** button then click the **Build** button a second time. Close the dialog.

This will generate two separate `.xsd` documents, each containing a nanotube about 100 Å in length. You will edit `SWNT (2).xsd` and remove most of the atoms to create a pattern. The fastest way to do this is to use the 3D Viewer Selection tool to remove the unnecessary atoms.

With the default view on the nanotube, select half of the tube and press the **DELETE** key. Rotate the nanotube until the long axis is across the screen. Use the **3D Viewer Selection** tool to select and remove the other atoms until you have the group of atoms for the pattern structure shown below.



Pattern defined for coarse graining the nanotube, displayed in ball and stick style

You should give this a more descriptive name.

Rename the document to **C24_rings.xsd**.

There may be cases where you have multiple patterns for coarse graining. So that you can apply multiple patterns they should be stored in a study table.

Tip: You can use the study table to build up a library of patterns.

Create a new study table document and rename it **patterns.std**. In the **Project Explorer**, right-click on **C24_rings.xsd** and select **Insert Into** from the shortcut menu.

In your pattern study table a new column is created called Structures, with C24_rings as the structure in row 1. You can now coarse grain the nanotube using this pattern.

Open the **Coarse Grain** dialog. In the **Method** section, check the **Patterns** checkbox and select **patterns.std** from the dropdown list. Uncheck the **Subunits** checkbox.

You can preview the match between your atomistic and bead structure.

Change focus to **SWNT.xsd**. Rotate the nanotube so that you can see the whole structure. On the **Coarse Grain** dialog, click the **Preview** button.

You will see that motion groups are defined on most of the atoms. However, the whole nanotube cannot be matched using the C24_rings pattern. A warning is displayed reporting that some atoms cannot be matched to beads. The unmatched atoms can be selected by the coarse grainer. In this case there is no pattern that matches all atoms so the atoms that cannot be matched should be deleted.

On the warning dialog, click the **OK** button. Click on the title bar of **SWNT.xsd** and press the **DELETE** key.

The excess atoms are deleted from the nanotube and you have motion groups defined for each group of atoms which matches the pattern. In the previous example, you explicitly created the study table containing the typing document so that you could edit the names of the beads. In this case you have already set the name of the pattern so the bead type names do not need to be defined in a typing document. A typing document study table can be automatically updated.

On the **Coarse Grain** dialog, check the **Automatically update typing document** checkbox and click the **Build** button.

The study table containing the atom grouping and bead type names is automatically updated and the new structure SWNT CG.xsd is created containing the coarse grained single walled nanotube.

Select **File | Save Project** from the menu bar followed by **Window | Close All**.

4. Coarse graining a mixed system of polymer and drug

Coarse graining is not restricted to patterns or subunits but can use a combination where appropriate. To demonstrate this, you will coarse grain a mixed system containing a drug and polymer. You will define a pattern to coarse grain the drug, cinnamide, and use the repeat units of the polymer to coarse grain the polymer. A 3D periodic structure containing cinnamide and polyoxyethylene has been provided.

Import **Examples\Documents\3D Model\polyoxyethylene_cinnamide.xsd**.

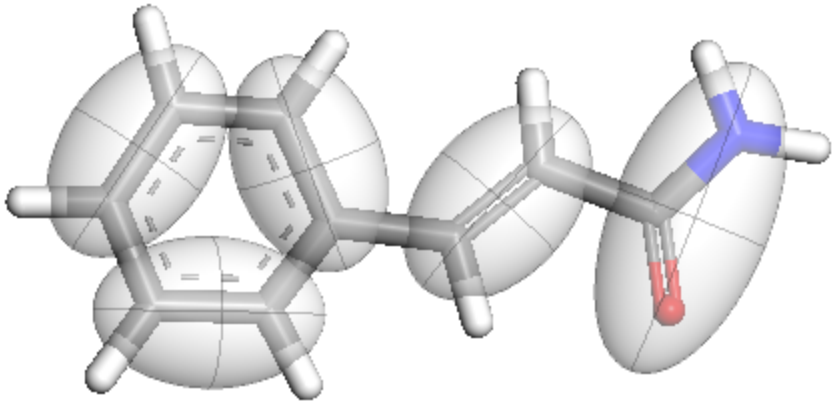
This structure consists of 3 molecules of cinnamide and 10 molecules of polyoxyethylene. This first step is to create a template of cinnamide.

Create a new **3D Atomistic Document** and rename it **cinnamide.xsd**. Change focus to **polyoxyethylene_cinnamide.xsd** and locate one of the cinnamide molecules in the cell. Copy this molecule and paste into **cinnamide.xsd**.

You can use the entire molecule as a new pattern which, on coarse graining, will replace each molecule by a single bead. In this case you will use a more fine-grained representation, where each molecule is replaced by a mesoscale molecule with 5 beads, each containing about 2 non-hydrogen atoms.

You can specify the desired grouping of atoms using motion groups in the pattern document. On coarse-graining this grouping will be carried over to each match in the structure. This way each molecule is coarse grained in the same way without having to assign motion groups in the input to all molecules individually.

In the document into cinnamide.xsd create motion groups on the atoms in the amide group, the ethylene group in the side chain, and 3 groups of atoms in the ring to define them as groups of atoms corresponding to beads.



Suggested motion group definitions for the coarse graining of cinnamide

As with the case of the nanotube, you need to insert this structure document into a study table so that you can use it as a pattern.

Make **patterns.std** the active document. In the **Project Explorer**, right-click on **cinnamide.xsd** and select **Insert Into** from the shortcut menu.

Now you are ready to perform the coarse graining. For this example, you will generate the typing document and then perform the build in two steps.

Change focus back to **polyoxyethylene_cinnamide.xsd**. On the **Coarse Grain** dialog, check **Subunits** and **Patterns**. Click the **Update** button.

The bead typing study table is updated with the unique groups in the template and the subunits from the structure. You should see that the previous oxyethylene structures for typing are left intact but 4 new bead types are added.

The bead type structures CH_2NO, C_2H_2, C_2H correspond to the groups in the template. The C_2H_2 in the side chain and the group in the ring correspond to the same bead type, since they have the same topology.

The remaining new bead type structure corresponds to the oxyethylene group terminated by a hydroxyl group. You can change the name to something more descriptive.

In **Bead Typing.std**, change the **Bead Type Name** of OXYE_2 to **oxyethylene_terminator_2**.

You can now coarse grain the periodic structure

Change focus back to **polyoxyethylene_cinnamide.xsd** and click the **Build** button.

A new document is opened called `polyoxyethylene_cinnamide CG.xsd`. This contains coarse grained representations of the polymer and the automatically coarse-grained cinnamide from the pattern structure.

This is the end of the tutorial.

References

Orly Liba, David Kauzlari, Zeév R. Abrams, Yael Hanein, Andreas Greiner, and Jan G. Korvink, "A dissipative particle dynamics model of carbon nanotubes", Molecular Simulation, Vol. 34, No. 8, July 2008, 737-748

Working with isosurfaces and slices

Purpose: Introduces the isosurfaces and slices tools available in the Materials Visualizer.

Modules: Materials Visualizer

Time:

Prerequisites: Project management

Background

The Materials Visualizer provides a range of powerful tools for viewing and analyzing volumetric data, such as fields, isosurfaces, and slices. Many Materials Studio applications generate fields, such as

particle densities, potentials, and so forth, and you can generate isosurfaces and slices to view and analyze particular aspects of a field. You can also view and analyze fields and surfaces generated by other modeling packages, for example, surfaces can be imported through the `.msi` file format.

Introduction

This tutorial shows how to manipulate isosurfaces and slices for a benzene molecule. The benzene structure has been optimized and the electron density and electrostatic potential for this molecule have been calculated using DMol^3.

This tutorial covers:

- Getting started
- To add an isosurface
- To change the display style of an isosurface
- To use color maps
- To add and color slices
- To manipulate slices

1. Getting started

Begin by starting Materials Studio and creating a new project called Isosurface. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the New Project dialog, enter **Isosurface** as the name and click the **OK** button.

The new project is created with *Isosurface* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

2. To add an isosurface

An example document has been provided containing the data for the electron density and electrostatic potential of benzene.

Click the **Import** button on the **Standard** toolbar to open the Import Document dialog. Navigate to **Examples/Documents/3D Model/benzene.xsd** and click the **Open** button.

The volumetric rendering tools are available from the Volume Visualization toolbar.

Select **View | Toolbars | Volume Visualization** from the menu bar. Select the **Create Isosurfaces** tool .

This opens the Choose fields to Isosurface dialog. You need to choose a field for which to create an isosurface.

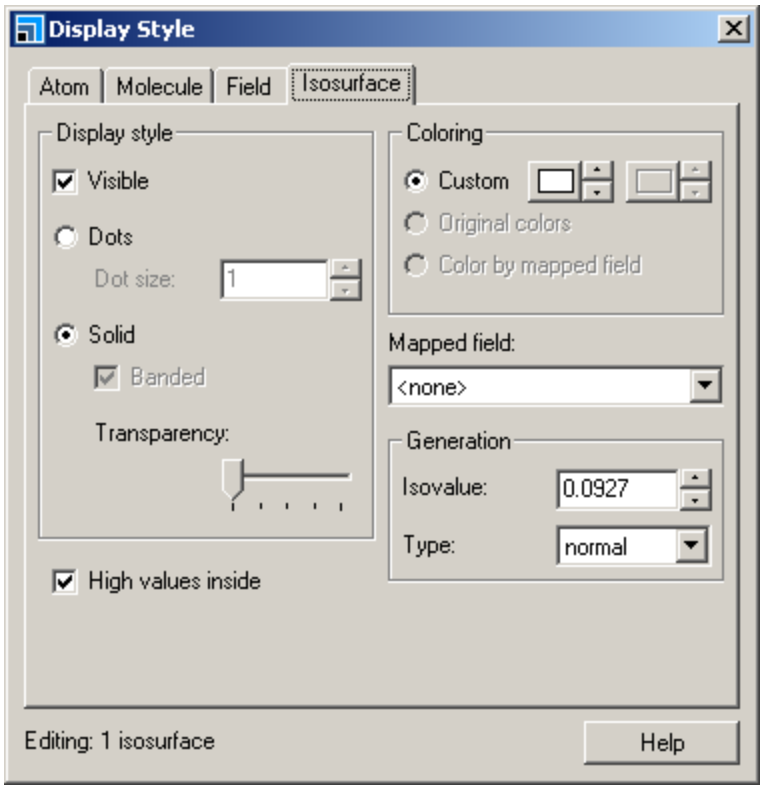
Select **DMol3 total electron density** and click the **OK** button.

A white isosurface, indicating the electron density, is displayed.

3. To change the display style of an isosurface

You can change how an isosurface is displayed using the Display Style dialog.

Right-click in the 3D Viewer and select **Display Style** from the shortcut menu to open the Display Style dialog. Choose the **Isosurface** tab.



Display Style dialog, Isosurface tab

You can change the display style of the isosurface from solid to dots.

In the **Display style** section, click the **Dots** radio button. Increase the **Dot size** to **3**.

This can be useful if you are looking at a complex system, as it speeds up the redraw time. For the rest of this tutorial, you will use the solid display style.

In the **Display style** section, click the **Solid** radio button.

You can change the transparency of a surface to make it less opaque. Before you do this, you should set the atom display style to *Ball and stick* so that you can see the effect of the transparency.

Choose the **Atom** tab and select **Ball and stick**. Return to the **Isosurface** tab and drag the **Transparency** slider to the middle mark.

The surface becomes more transparent.

Rotate the molecule. Change the transparency back to fully opaque.

As you rotate the model, the isosurface automatically changes to a dot representation. This is the volumetric equivalent of the fast render on move functionality that can be seen when rotating atoms and bonds in the higher quality display modes.

You may notice a slight "halo" displayed on the edges of the isosurface where it meets a dark background. This is an artifact of the rendering process and can usually be removed using the Properties Explorer.

In the **Properties Explorer**, select **Isosurface** from the **Filter** dropdown list. Double-click on **IsInsideVisible** to open the Edit IsInsideVisible dialog. Select the **No** option and click the **OK** button.

The "halo" should disappear.

The isosurface is a surface formed by points whose field values are identical. Therefore, you can increase or decrease the size of the isosurface by changing the isovalue.

Use the **Isovalue** up spin control on the **Isosurface** tab of the Display Style dialog to increase the isovalue.

As you increase the isovalue, the isosurface decreases in size and vice versa.

Note: If the specified isovalue falls outside the range for which the field of the isosurface is defined, then no isosurface will be displayed.

You can control how much of the isosurface is displayed by modifying the range of the underlying field.

Choose the **Field** tab. Use the **Display range 1st Max** spin control to change the **Max** value to **0.49**.

Changing the display range of the field also affects the display range of the isosurface.

Note: For periodic systems you can extend the display range above 1.0 and below 0.0.

Use the **Display Range 1st Max** spin control to change the **Max** value back to **1.0**.

You can change the color of the isosurface in various ways. The most simple of these is to use the color chooser to change the color of the entire isosurface.

Change back to the **Isosurface** tab. Click on the color selector next to the **Custom** option. Select a new color from the Color dialog and click the **OK** button.

The whole of the isosurface changes color.

Note: If more than one isosurface is present, you should select the one that you want to modify before selecting a new color. Otherwise, all the isosurfaces will change color.

You can also color by mapped field. This allows you to, for example, map the electrostatic potential onto the electron density.

Select **DMol3 electrostatic potential** from the **Mapped field** dropdown list. **Close** the Display Style dialog.

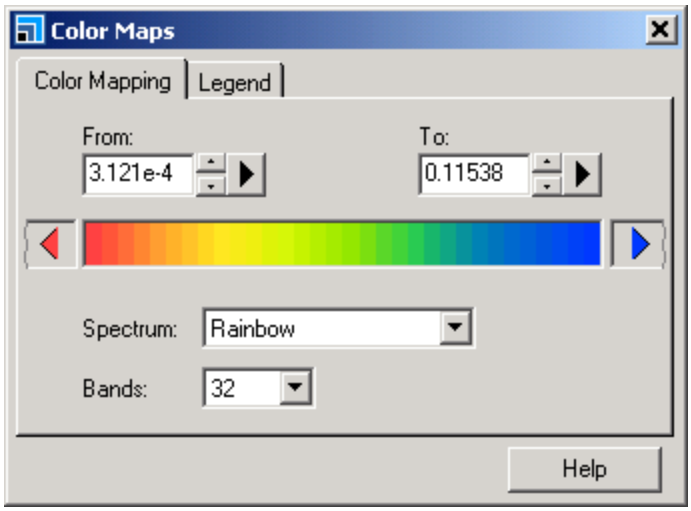
The color of the isosurface changes to reflect the mapped electrostatic potential. In the *Display style* section, the *Banded* checkbox becomes active. This subdivides the isosurface into uniformly colored regions, each of which corresponds to a range of values for the mapped field.

4. To use color maps

You can also change the coloring of the isosurface using the Color Maps dialog.

Right-click in the 3D Viewer and select **Color Maps** from the shortcut menu.

This opens the Color Maps dialog.



Color Maps dialog

The *From* and *To* boxes indicate the range of values covered by the spectrum of colors. There are numerous spectrum color ranges defined.

Select **Blue-White-Red** from the **Spectrum** dropdown list.

The color of the isosurface changes so that any section of the isosurface with a value equal or lower than that of the *From* box is colored blue. These colors change with the increasing values until any part of the isosurface that has a value equal to or higher than that in the *To* box is colored red. You can see which color refers to which value of isosurface by hovering over that color in the color chooser.

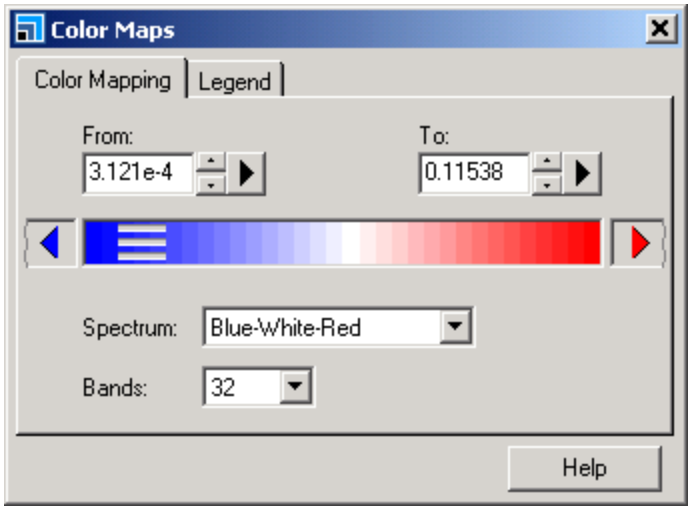
Hover the mouse pointer over any of the colors in the color chooser bar on the **Color Maps** dialog.

A number is displayed as a tooltip: This indicates the value of the isosurface assigned to that color.

You can make certain colors transparent by selecting them in the color chooser.

In the color chooser bar, left click to select any three sections.

The sections of the isosurface with the colors that you selected are now transparent in the 3D Viewer.



Color Maps dialog with 3 sections transparent

Tip: You can make individual sections transparent by clicking on the section or you can drag the mouse to make many contiguous sections transparent.

Click on the first of the three sections you made transparent and drag your mouse to the third one.

You can also change the number of bands into which the sections are cut.

Change the number of **Bands** to **128**.

The isosurface appears smoother as the bands are now much smaller.

As stated earlier, the values in the *From* and *To* boxes define the color ranges and these can be changed. You can either simply enter a new value or use pre-calculated values. The pre-calculated values are available by clicking on the right arrow button associated with the *From* and *To* boxes.

Click the right arrow button for the **From** box.

You should see field minimum, mean, and maximum values and mapped minimum, mean, and maximum values. The field values correspond to the values in the whole field of data, that is, the electron density. The mapped values correspond only to the values contained in the mapped field, that is, the specific electron density at the specified isovalue.

To see this in action, you can change the isovalue.

Open the **Display Style** dialog and, on the **Isosurface** tab, change the **Isovalue**. Close the dialog.

The coloring on the isosurface changes.

On the **Color Maps** dialog, click on the right arrow for the **From** box.

The mapped field ranges will have changed to indicate the new range of mapped field data in the isosurface.

Select **Mapped Minimum** for the **From** box. Click on the right arrow for the **To** box and select **Mapped Maximum**. Close the Color Maps dialog.

The isosurface should now have the same coloring as it did previously.

The mean value is provided for occasions when the maximum value is very high due to presence of large outlying values. In these cases, coloring to those large values is not relevant and using the mean value gives a much better spread of colors. You will use these values again in the section on coloring slices.

5. To add and color slices

Slices can be added to your model allowing you to see field value distributions through a plane rather than on a surface. You can add slices in several ways depending on how you want them to be oriented. There are several preset orientations such as best fit and parallel to different axes. You will initially add a slice using the *Best Fit* method.

Click on the **Create Slices** arrow  and select **Best Fit**.

This opens the Choose Fields to Slice dialog.

Select **DMol3 electrostatic potential** and click the **OK** button.

A red slice is displayed in the plane of the benzene ring. No color shading is displayed as it is using the full field range. To add colors, you need to use the Color Maps dialog once more.

Click on the slice to select it.

When a slice is selected, the border changes color to yellow and a yellow cross-hair is displayed at its center of rotation.

Right-click in the 3D Viewer and select **Color Maps**. Change the **From** value to **Mapped Minimum** and the **To** value to **Mapped Mean**.

In this case, the mapped maximum value is very high due to the presence of outlying values and you should therefore use the mapped mean, as this gives a more accurate representation of the spread of values.

The isosurface is obstructing the view of the slice, therefore, you will remove it from view.

Select the **Volumetric Selection** tool  to open the Volumetric Selection dialog. Expand both the nodes.

Under the DMol^3 electron density node is your isosurface and under the DMol^3 electrostatic potential is your slice. You can either delete your isosurface or make it transparent.

Uncheck the **Isosurface1** checkbox and close the dialog.

This removes the isosurface from view but does not delete it. As with the isosurface, you can use the Color Maps dialog to make certain values transparent.

On the **Color Maps** dialog, click on the red left arrow and the first two red bars on the color chooser and close the dialog.

When the colors are removed, you can see a box that represents the edge of the slice. This can be removed using the Display Style dialog.

Open the **Display Style** dialog, on the **Slice** tab, uncheck the **Show frame** checkbox. Close the dialog.

You can add multiple slices to the model.

Click the **Reset View** button  . Click on the **Create Slices** arrow  , select **Parallel to 1st & 3rd Axis** to open the Choose Fields to Slice dialog.

Select **DMol3 electrostatic potential** and click the **OK** button.

A second slice is displayed along the x-z plane. It uses the same color map settings as the first slice.

Note: Any slice can have custom color settings, regardless of the number of slices on screen.

You can also add slices through bonds or atoms by selecting the objects and adding the slice.

Select a C-C bond and click the **Create Slices** button to open the Choose Fields to Slice dialog. Choose **DMol3 electrostatic potential** and click the **OK** button.

A slice is displayed perpendicular to the bond. The cross-hair is displayed on the selected object.

Tip: You can also generate slices through selected atoms.

6. To manipulate slices

Slices can be rotated and translated using the normal methods for selected objects.

From the menu bar, select **View | Display Options** from the menu bar to open the Display Options dialog.

Uncheck **Fast render on move** and close the dialog.

Select the last slice you generated by clicking on the frame. Hold down the **SHIFT** and **ALT** keys and click and drag with the right mouse button.

The slice is translated normal to its axis and the slice information is updated as the slice moves through the field.

Hold down the **SHIFT** key and click and drag with the right mouse button.

The slice rotates with the center of rotation indicated by the cross-hair.

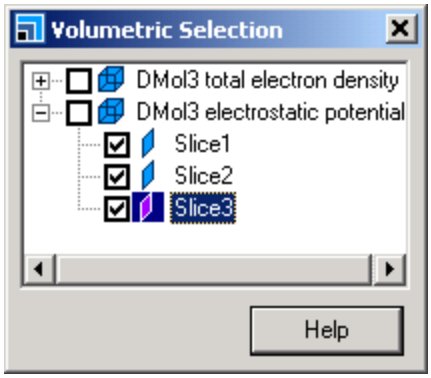
Tip: If you have a three-button mouse or wheel mouse, you can translate and rotate using SHIFT and the middle mouse button/wheel and SHIFT and the right mouse button, respectively.

Note: If you wish to align the slice along a precisely known crystallographic direction, you can use the Properties Explorer to specify slice position and slice normal.

You can use the Volumetric Selection dialog to remove slices.

With the slice still selected, click the **Volumetric Selection** button to open the Volumetric Selection dialog. Expand the **DMol3 electrostatic potential** node.

The Volumetric Selection dialog is displayed.



Volumetric Selection dialog

Press the **DELETE** key.

The slice is removed from the model.

In the **Volumetric Selection** dialog, click on **Slice2**. Press the **DELETE** key.

The second slice is removed from the model.

In the **Volumetric Selection** dialog, expand the **DMol3 total electron density** node and check **Isosurface1**.

The isosurface overlays on the slice.

Select **File | Save Project** from the menu bar or click the **Save Project** button  on the **Project** toolbar.

This is the end of the tutorial.

Field segregation and analysis

Purpose: Demonstrates how to perform field segregation on an Atom Volumes Field.

Modules: Materials Visualizer

Time:

Prerequisites: Working with isosurfaces and slices

Introduction

The volumetric visualization tools in Materials Visualizer provide a powerful way of visualizing field data generated by mesoscale, Sorption and quantum methods and also by the atom volumes and surfaces tool. Isosurfaces are used to aid the visualization of field data by linking field points at a specific isovalue. If an isosurface which contains isolated segments is generated, it is not possible to select these individual segments without selecting all segments for an isosurface.

One approach to solve this is to allow the underlying field to be segregated into many subfields. Each subfield, or segregate, represents a unique segment of the original field. A segregate field can be selected, and various useful properties such as the field volume and geometric center can be obtained, allowing improved analysis of field data.

Field segregation can be used on any field in Materials Visualizer, providing access to free volume distributions from an amorphous cell, micelle size distributions from mesoscale calculations, and allowing you to perform Sorption calculations on restricted pores in a zeolite.

In this tutorial, you will calculate a Connolly surface for a zeolite. Using the underlying Atom Volumes Field, you will segregate the field at a specific isovalue and then analyze the segregates.

This tutorial covers:

- Getting Started
- To calculate a Connolly surface
- To segregate an Atom Volumes Field
- To analyze the segregates

1. Getting started

Begin by starting Materials Studio and creating a new project called Segregates. For more detailed guidance on creating a new project, see the Project management tutorial.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.
Open the New Project dialog, enter **Segregates** as the name and click the **OK** button.

The new project is created with *Segregates* listed in the Project Explorer.

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

2. To calculate a Connolly surface

The first step is to generate field data to segregate. You will generate a Connolly surface which is based on an underlying Atom Volumes Field. You can generate an Atom Volumes Field for any structure, but in this example you will use a zeolite.

Click the **Import** button  on the **Standard** toolbar to open the Import Document dialog, navigate to and open **Examples\Documents\3D Model\TON.msi**.

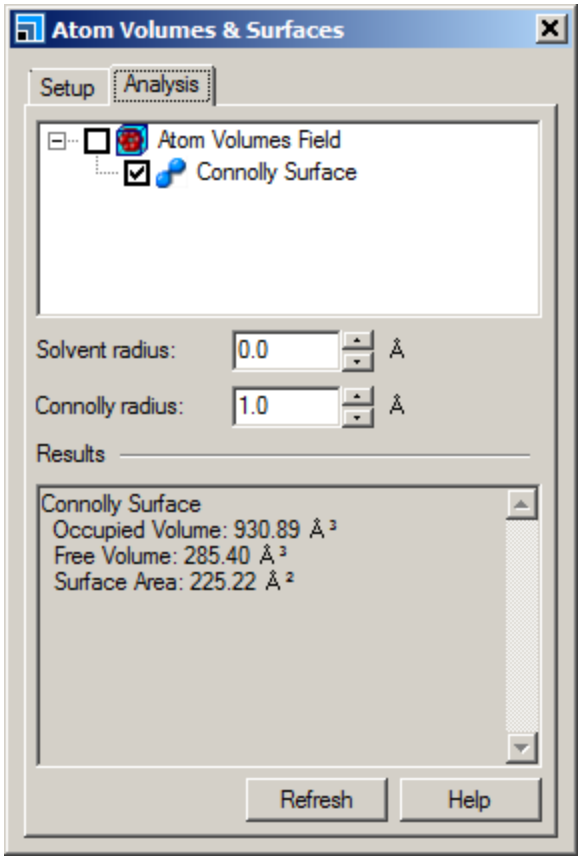
Now you can calculate a Connolly surface using the *Atom Volumes & Surfaces* tool.

Select **Tools | Atom Volumes & Surfaces** from the menu bar.

This opens the Atoms Volumes & Surfaces dialog. The default task is to calculate a Connolly surface. You can also calculate Solvent surfaces by changing the task, but you will use a Connolly surface for this tutorial.

Click the **Create** button.

Isosurfaces are generated in the atomistic document and the dialog changes to the Analysis tab.



Analysis tab on Atom Volumes & Surfaces dialog

The tree view on the dialog shows the presence of an Atom Volumes Field even though it is not displayed at the moment. The checkbox shows that the Connolly surface is visible. You can display the field by checking the *Atom Volumes Field* checkbox.

Check the **Atom Volumes Field** checkbox.

The field is displayed with low values in red and high values in blue. You can make the field invisible for now.

Uncheck the **Atom Volumes Field** checkbox.

You can change the radius of the Connolly probe to see the effect of probe size on free volume in the structure.

Click on the **Connolly radius** spin down control.

As you decrease the size of the Connolly probe, the free volume in the structure increases as the isosurfaces increase in size and form connected structures. For the rest of this tutorial, you need to have some isolated segregates so you should increase the probe radius.

Set the **Connolly radius** to **0.90**. Close the Atom Volumes & Surfaces dialog.

3. To segregate the Atom Volumes Field

If you try to select one of the sections of the isosurface, you will see that the entire isosurface is selected. This is a limitation if you want to find the volume of an isolated section of isosurface.

Click on one of the sections of isosurface.

The segregation splits the underlying field into separate field segregates. Each of these can be selected to examine properties like the volume and the center of the segregate. The tools for creating, managing, and manipulating segregates are on the Volume Visualization toolbar.

Click anywhere in the 3D Viewer to deselect everything. Select **View | Toolbars | Volume Visualization** from the menu bar. Click the **Create Segregates** button  .

Segregated fields are displayed as smaller field boxes within the structure with the fields in different colors. You can select individual field segregates to see the volumes.

With the **Properties Explorer** open, click on one of the small field segregates.

The Properties Explorer Filter changes to *Segregate*. Here you can see the different properties such as the *FieldVolume* indicating the volume of the field and the *SegregateXYZ* which displays the center of the segregate.

Click in the model document to deselect the segregate.

You can select segregates using the Volumetric Selection tool on the Volume Visualization toolbar.

Click the **Volumetric Selection** button  on the Volume Visualization toolbar.

This opens the Volumetric Selection dialog which displays a tree view of the volumetric data. You can hide the Connolly surface.

Uncheck the **Connolly Surface** checkbox.

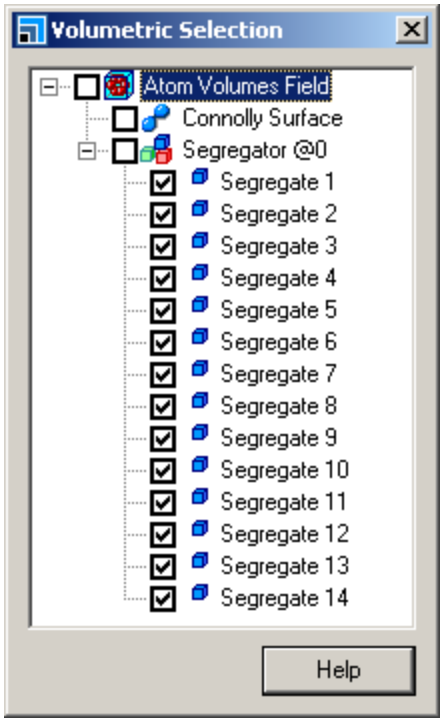
The segregates are represented by the *Segregator* branch indicated by the + Segregator @0 line. The @0 shows that the field was segregated at an isovalue of 0. You can expand the branch to see the segregates by clicking on +.

Click on **+** to expand the **Segregator @0** branch.

There are several segregates in the structure. You can increase the size of the Volumetric Selection dialog to see all the segregates.

Move your cursor to the bottom-right of the dialog. When the cursor changes to a double-headed arrow, click and drag right and down.

You should see there are 14 segregates.



Expanded Volumetric Selection dialog.

You can control which areas of field are segregated using either the Properties Explorer or the Display Style dialog.

Right-click in the 3D Viewer and select **Display Style** from the dropdown list to open the Display Style dialog, change to the **Segregate** tab.

You can use the *Display style* and *Coloring* sections to control how the segregates appear. The *Constraints* section allows you to control which type of segregates are displayed. The isovalue controls the threshold in the field for the segregation, similar to the isovalue property of an isosurface.

Increase and decrease the **Isovalue**. Set the value back to **0.0**.

Changing the isovalue dynamically recalculates the segregates.

Tip: When changing the isovalue, the field display updates can be quite time consuming if you have a large, heavily segregated field. In this case, it is better to set the value explicitly rather than use the spin controls.

You can also specify whether you want the segregates to be field values that are higher or lower than the isovalue or you can choose both.

Change **Values** to **Low**.

Choosing *Low* selects the field points that are the inverse of the default *High* settings. In this example, the low values are the field values where there are atoms. Changing the *Value* to *All* includes both higher and lower values in separate segregates.

Change **Values** back to **High**.

The final constraints are the *Connectivities*. This controls whether the segregates are accessible or isolated. Isolated segregates are self-contained in the cell, while accessible segregates are infinitely connected.

Change **Connectivities** to **Isolated**.

Only the twelve segregates which are not infinitely connected are displayed.

Change **Connectivities** to **Accessible**.

Only the two segregates which are infinitely connected are displayed.

Tip: Using only the accessible, connected segregates would allow you to limit the search space for a Sorption calculation to only the accessible pores in a zeolite.

Change **Connectivities** back to **All**.

Note: The above properties are also available through the Properties Explorer and through the MaterialsScript API. If you wish to perform the same calculation on numerous structures, it may be more efficient to use MaterialsScript.

In their initial state, the field segregates are only displayed as fields. You can add isosurfaces to them using the standard isosurface tool.

On the **Volumetric Selection** dialog, hold down the **SHIFT** key and select all the segregates. Click the **Create Isosurfaces** button  .

Isosurfaces are created on all the segregates. They use the isovalue which was used for the segregation and are colored the same as their segregate fields.

4. To analyze the segregates

You can analyze properties such as the size and separation distributions of the segregates using the *Create Segregates* tool.

Click on the **Create Segregates** arrow and select **Analyze Segregated Field**.

This opens the Segregate Analysis dialog. The default option is to analyze the segregate size.

Click the **Analyze** button.

A chart is generated showing you the distribution of the segregate sizes. You should see a large peak near zero indicating the smaller isolated segregates and two small peaks above 140 which correspond to the two accessible segregates.

Tip: You can get the actual volumes for each segregate automatically by using MaterialsScript to iterate through all the segregates in the collection.

Change focus back to **TON.xsd**. In the **Segregate Analysis** dialog, select **Segregate major axis** and click the **Analyze** button.

This analysis fits an ellipsoid to the segregate and then plots the major axis of the ellipsoid.

Change focus back to **TON.xsd**. In the **Segregate Analysis** dialog, select **Segregate radius (best-fit sphere)** and click the **Analyze** button.

This analysis fits a best fit sphere to the segregate and then plots the radius of the sphere.

Change focus back to **TON.xsd**. In the **Segregate Analysis** dialog, select **Segregate separation** and click the **Analyze** button.

This analysis plots the distribution of the distances between the segregates.

Tip: You can perform analysis on a subset of the visible segregates by selecting the segregates first before analyzing them.

Select **File | Save Project** from the menu bar or click the **Save Project** button  on the **Project** toolbar.

This is the end of the tutorial.

Building transport devices for electron transport calculations

Purpose: Introduces the building of electrodes and transport devices.

Modules: Materials Visualizer, DFTB+

Time:

Prerequisites: Using the polymer builder, Precise positioning and movement of atoms

Background

Electron transport calculations require two or more electrodes for a calculation to proceed. An electrode is a semi-periodic object that is semi-infinite into the electrode and away from the device.

An electrode consists of a wire and tip. The wire is the part of the electrode that supplies or receives the current to or from the central device. The tip of the electrode is optional and is treated as part of the device.

A Transport Device consists of the electrode and the device. The device is the material on which you are simulating the effect of transport.

Introduction

In this tutorial you will use the Transport Device tools in Materials Visualizer to build a simple molecular transport device, cleave an electrode from a crystal, and create a periodic transport device. You will learn about the concepts involved in defining electrodes and best practice for building transport devices.

This tutorial covers:

- Getting started
- To build a simple molecular transport device
- To extend the simple transport device
- To cleave electrodes from a crystal
- To insert a device between cleaved electrodes

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

1. Getting started

Begin by starting Materials Studio and creating a new project.

If Materials Studio is not already open, double-click on the **Materials Studio** icon on your desktop to start the program or, alternatively, select **Accelrys | Materials Studio 8.0** from the list of programs on the Windows **Start** menu.

Open the **New Project** dialog and enter **DFTB_electrode** as the project name, click the **OK** button.

The new project is created with *DFTB_electrode* listed in the Project Explorer.

2. To build a simple molecular transport device

In this first example, you will import a polyacetylene oligomer to act as your electrode. This example will demonstrate some of the requirements for an electrode and transport device.

Select **File | Import...** from the menu bar or click the **Import** button on the **Standard** toolbar to open the Import Document dialog. Navigate to and select **Examples\Documents\3D Model\PA_10mer.xsd**, then click the **Open** button.

A 3D atomistic document containing a 10-mer of polyacetylene is opened. To define the electrodes, and hence create the transport device, you will use the Build Electrode tool.

Select **Build | Build Transport Device | Build Electrode** to open the **Build Electrode** dialog.

The Build Electrode dialog works on a molecular structure and allows you to define electrodes. The electrodes direction must be aligned along the X, Y or Z direction. The *Build* button is disabled because the molecule is not aligned correctly and because it does not have a periodic repeat. You will align the long molecular axis of the molecule along the x-axis.

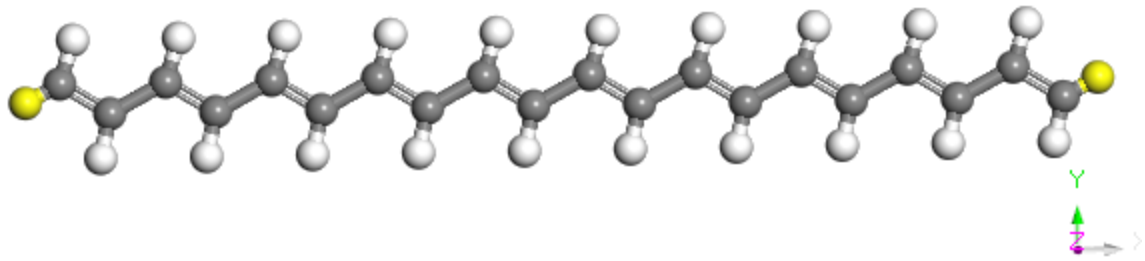
Click the **Home** button on the 3D Viewer toolbar. Press **CTRL + A** to select the entire structure.

Click the **Align Onto View** arrow on the 3D Movement toolbar and select **Align Left/Right** from the dropdown list.

You should also set the electrode direction on the Build Electrode dialog. For this example, you will build two electrodes: one in the +X and one in the -X direction.

On the **Build Electrode** dialog, change the **Electrode direction** to **+X**.

The *Build* button is still disabled as the structure is not periodic. To make it periodic, you must delete the hydrogens that would have been head and tail atoms on the repeat unit. These atoms are highlighted in yellow in the image below.



Atoms highlighted for deletion

Select the highlighted atoms and delete them.

The *Build* button on the Build Electrode dialog is now enabled.

Click the **Build** button.

You will see a warning dialog about removing molecule or polymeric hierarchy.

Click the **OK** button. Right-click in the 3D Atomistic document and select **Remove Molecule Hierarchy**. Click the **Build** button.

You will see that a pink box and arrow are created. The pink box defines which atoms are included in the wire part of the electrode and the arrow displays the direction of the infinite periodic repeat.

Change the **Electrode direction** to **-X** and click the **Build** button.

Another electrode is created at the opposite end of the chain, pointing in the -X direction. You now have two electrodes defined on your molecule and have created a basic transport device that can be used in an electron transport calculation.

Structures containing electrodes can only be used as input to the Electron Transport tasks in DFTB+ and DMol^3. Before performing an electron transport calculation, you should optimize the structure first. You will do this, and create a more complex device in the next section. Before doing this, you need to remove the electrodes that you have just created.

Select **Build | Build Transport Device | Unbuild Electrode**.

This will remove both of the electrodes from the document.

Note: There are other restrictions based on structures containing electrodes. All modules will have their Run buttons disabled apart from DFTB+ and DMol^3 if the focus is on a document containing electrodes. Many of the building tools will also be disabled once an electrode object is defined.

3. To extend the simple transport device

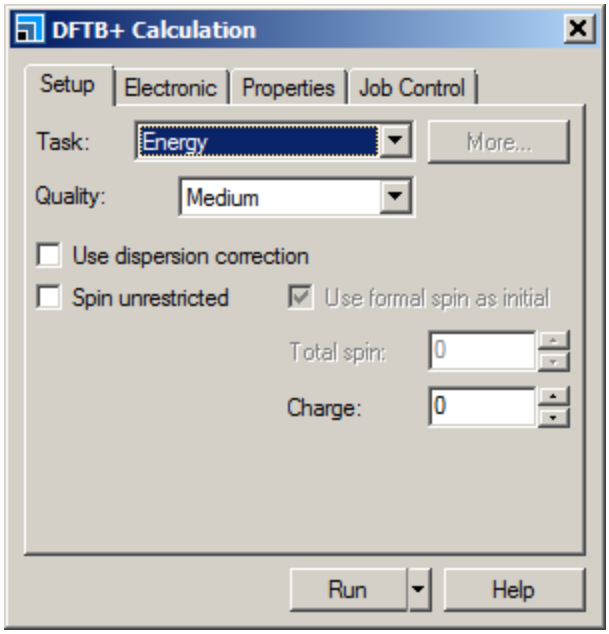
Before re-building the transport device and extending it to include tips, you should optimize the structure of the existing polymer chain. You should also add the hydrogens back onto the chain prior to optimization.

Click the **Adjust Hydrogen** button.

You are ready to optimize the structure.

Click the **DFTB+**  button on the **Modules** toolbar and select **Calculation** or choose **Modules | DFTB+ | Calculation** from the menu bar.

This opens the DFTB+ Calculation dialog.



DFTB+ Calculation dialog, Setup tab

Select **Geometry Optimization** from the **Task** dropdown list. On the **Electronic** tab change the **Slater-Koster library** to **mio**. Click the **Run** button and close the DFTB+ Calculation dialog.

The geometry optimization will take a few seconds to complete and a new folder will be created with the results of the calculation.

Change focus to the optimized structure. Select and delete the terminal hydrogen atoms that you deleted previously.

You are now ready to define the electrodes. In this section, you will define both the wire and the tip of the electrode.

Select the first six carbon atoms and attached hydrogen atoms from the left side of the chain. On the **Build Electrode** dialog, ensure that the **Electrode direction** is set to **-X** and check the **Add selection to tip** checkbox. Click the **Build** button.

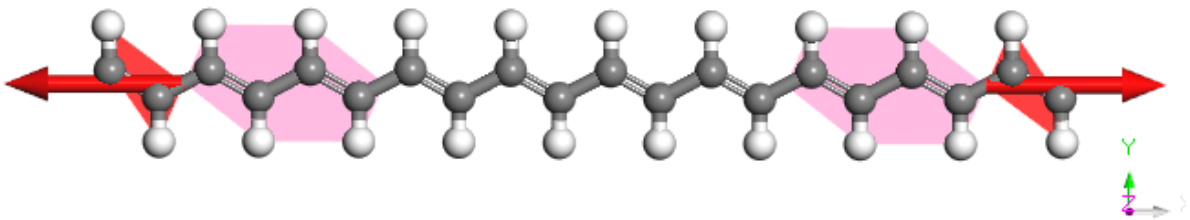
The electrode is created with two parts, the wire has the electrode arrow and the tip is displayed in a more transparent pink box.

Select the last six carbon atoms and attached hydrogen atoms from the right side of the chain. On the **Build Electrode** dialog, change the **Electrode direction** to **+X**. Click the **Build** button and close the dialog.

You now have an optimized transport device with two electrodes, both of which consist of a wire and tip. You can change the display style of the electrode objects using the Display Style dialog.

With the optimized structure in focus click anywhere to discard the selection. Right-click and choose **Display Style** from the shortcut menu. On the **Electrode** tab increase the **Arrow scale** to **1.8**. Change the **Wire color** to **red** and close the dialog.

The transport device should look similar to the image below.



Polyacetylene transport device

Tip: The electrode allows for several levels of selection. By clicking on the wire part all wire atoms will be selected, similar if you click on the tip part all tip atoms will be selected. By double clicking on the electrode, all electrode atoms will be selected.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

4. To cleave electrodes from a crystal

Building a transport device from a single molecule is quite straightforward. However, you may want to study the electron transport properties of a molecule between two metallic electrodes or a periodic system between two periodic electrodes. For these systems, you need to use a combination of the Cleave Electrode and Build Transport Device tools.

The first step is to import a crystal structure from which to cleave an electrode. In this example, you will cleave a surface from titania.

Select **File | Import...** from the menu bar to open the Import Document dialog. Navigate to **Structures\metal-oxides** and select the **TiO2_rutile.xsd** file, click the **Open** button.

The TiO2_rutile model is a crystal structure. To create an electrode from this structure, you need to cleave the electrode.

Note: When building an actual transport device, you should perform a geometry optimization before creating the electrode. For this system, you could use the *tiorg* Slater-Koster library.

Select **Build | Build Transport Device | Cleave Electrode** from the menu bar.

The Cleave Electrode dialog enables you to cleave a surface which is specifically used as an electrode. Electrodes that are cleaved need to have orthogonal surface vectors and be periodic along the cleave direction hence not all cleave planes are allowed.

Change the **Cleave plane (h k l)** to **1 0 0**.

You can fine-tune the electrode by modifying the position of the cleave plane and changing the width of the tip.

Increase the **Tip width** to **2.0**.

You can also choose whether to build two electrodes or just a single electrode. If the surface of the electrode is symmetric with the atoms at the back of the electrode, then there will be no difference between building two electrodes or building a single electrode. For this example, whether you build one or two electrodes does have consequences for the structure. To see the difference, you can cleave both two electrodes and a single electrode.

Click the **Cleave** button.

A new document, TiO2_rutile Electrode, containing a 2D periodic structure and two electrodes is created.

Rename the document **TiO2_2Electrodes**. Change the focus back to **TiO2_rutile.xsd**. On the **Cleave Electrode** dialog, uncheck **Build two electrodes** and click the **Cleave** button. Close the dialog.

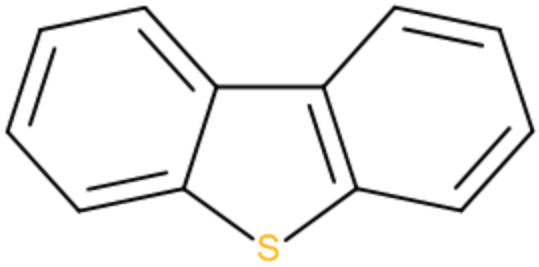
A new document containing a 2D periodic structure and a single electrode is created.

Rename the new document to **TiO2_1Electrode**.

You are now ready to create a transport device.

5. To insert a device between cleaved electrodes

You need to sketch a dibenzothiophene molecule to insert between the two electrodes.



Dibenzothiophene molecule

In a new **3D Atomistic** document, sketch the molecule displayed above. Rename it to **dibenzothiophene**. Align the molecule using **Align Left/Right** from the 3D Movement toolbar.

You will use the Build Transport Device tool to create your transport device. This tool allows you to build devices that are molecular or periodic.

The Transport Device builder requires a document containing an electrode in focus and a material to be inserted.

Change focus to **TiO2_1Electrode**.

Select **Build | Build Transport Device | Transport Device** to open the Transport Device dialog. Select **dibenzothiophene.xsd** from the **Insert** dropdown list.

You can choose whether to align the molecule along the X, Y, or Z axis. As you have aligned the long molecular axis along the X-axis, leave this at X. When you create a transport device it will be 2D periodic so you will have self-interactions between the molecule you are inserting and the periodic image. You can change the minimum supercell size to control the degree of self-interaction. If you increase this, you will have less self-interaction but it will increase the calculation time. For this structure, you can leave this as default.

Click the **Build** button.

A device is built with two electrodes and the molecule inserted between them. The molecule is aligned along the X axis.

Tip: The Transport Device builder will try to estimate the space needed to insert the molecule. If you need to adjust this, you can move the electrodes by selecting them and using the 3D Movement toolbar.

You can now build the transport device with two electrodes.

Change the focus to **TiO2_2Electrodes.xsd**. On the **Transport Device** dialog, change the **Direction** to **Y**. Click the **Build** button.

The long molecular axis of the molecule is aligned along the Y-axis.

Look at the surfaces nearest to the device for **TiO2_2Electrodes** and **TiO2_1Electrode**.

You should see that with the device built from one electrode, the surfaces are mirror images. With the device built from two electrodes, the surfaces are not the same.

Note: You can build more sophisticated transport devices using other tools, such as the Layer Builder in Materials Studio.

Finally, you should save the project.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

This is the end of the tutorial.

Pipeline Pilot Protocols tutorials

The following tutorial illustrates how to utilize Materials Studio to run Pipeline Pilot protocols.

Launching Pipeline Pilot Protocols from Materials Studio

Purpose: Demonstrates how to create a simple Pipeline Pilot protocol and launch it from Materials Studio

Modules: Materials Visualizer

Time: ⏰⏰

Prerequisites: Project management Visualizer Tutorial

Background

The Pipeline Pilot Protocols tool provides a way to launch Pipeline Pilot protocols from Materials Studio. This enables you to take full advantage of many of the features of Pipeline Pilot, including construction of complex workflows using a graphical interface, mixing coarse and fine-grained parallelization, and integrating with third party tools.

Protocols can be developed in the Pipeline Pilot Professional Client which must be connected to an Accelrys Enterprise Platform (AEP) server which has the Materials Studio Collection (MSC) installed. When a protocol is run from the Pipeline Pilot Protocols tool in Materials Studio the calculation is performed on an AEP server.

Introduction

This tutorial demonstrates how to create a simple Pipeline Pilot protocol to calculate molecular weights and molecular formulae for a series of structures in a study table. Once you have created the protocol, you will launch it from Materials Studio and execute it against a study table of structures. Finally, the protocol is edited to improve the usability and to create a HTML report of the structures and properties.

This tutorial covers:

- Getting started
- To build a simple protocol
- To connect and explore the Pipeline Pilot server from Materials Studio
- To expose protocol parameters in Materials Studio
- To run the protocol on the server
- To extend the protocol

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

1. Getting started

Begin by starting Materials Studio and creating a new project called Protocol.

Open the New Project dialog and enter **Protocol** as the name, click the **OK** button.

The new project is created with *Protocol* listed in the Project Explorer.

As you will also be using Pipeline Pilot to create the protocol, you should launch the Pipeline Pilot Professional Client and connect to an AEP server.

If the Pipeline Pilot Professional Client is not already open, double-click on the **Pipeline Pilot Client** icon on your desktop or select **Accelrys | Pipeline Pilot Client** from the list of programs on the Windows **Start** menu to start the program.

Select **Tools | Change Active Server...** from the menu bar to open the Pipeline Pilot Server Location dialog. Enter the **Server name**, including the port of an AEP server where the Materials Studio Collection is installed. For example: `MyServer:9943`

Click the **OK** button.

Note: Pipeline Pilot Client is installed separately from Materials Studio. If you do not have a Pipeline Pilot Client icon on your desktop, please contact your system administrator and request an installation.

2. To build a simple protocol

In this section, you will build a simple protocol in the Pipeline Pilot Professional Client. Initially, you will explore the Pipeline Pilot interface to look at the protocols that are currently available and then build a simple protocol using the components.

Note: This tutorial is not intended to give an in-depth overview of the many features of Pipeline Pilot and so it will cover the minimum required to explore the existing protocols and build a simple protocol.

On the left side of the Pipeline Pilot Professional Client is a tabbed explorer which shows the available protocols and components, the tabs are:

- A tab named by your user name contains all the protocols owned by you
- A Protocols tab contains all the example protocols that are provided with Pipeline Pilot
- A Components tab contains all the components that you can use to create protocols
- A Network tab provides access to shared protocols available on your local network

Tip: Refer to the Pipeline Pilot Help Center for a complete description of the Pipeline Pilot Professional Client and extensive information and guidance on building protocols.

A search bar at the top of the explorer gives an interactive search on the protocols or components in the tab currently in focus.

Select the **Protocols** tab and expand the **Examples** node, then expand the **Materials** node.

Here you will see there are several categories, each of these has different protocols.

Expand the **Advanced** node.

The protocols in the Advanced folder are reasonably complex and generally use some element of scripting in combination with components. You can explore the protocols by clicking to open them. For now, you will change to the Components tab and start to build a protocol.

Select the **Components** tab and expand the **Materials** node.

There are many different types of components available, ranging from simple analysis tools to classical simulation, crystallization, and quantum mechanics components. The first step in this process is to add the components that you need to the protocol. The first action you need to take is to add a component to read in a study table. You can find this component using the Search tool.

In the **Search** text box, enter **Study Table**. From the options returned, double-click to select **Study Table Reader**.

A red component called *Study Table Reader* is added to a new protocol. This component is colored red because it requires a parameter to be set. All the parameters for each component are displayed in the Parameters window.

Examine the **Parameters** window.

You should see that the *Source* parameter is displayed in red, this parameter is used to specify the path and filename of the study table you want to read. As you will be using Materials Studio to choose the document, the value that you enter here will be overwritten but, for now, this requires a value.

Set the *Source* parameter to **data/StudyTables/Drugs.std**.

Tip: Pipeline Pilot includes many example documents and the Materials Studio structure library. Generally, it is useful to point to an existing document so that you can debug the protocol in the Pipeline Pilot Professional client before launching it from Materials Studio.

Now that the parameter is set, the component has turned blue indicating that it is ready to be used. The next component to add is a property calculator, in this case you will calculate the molecular weight of the molecules.

In the Components explorer, expand the **Property Calculators** node in the Materials directory. Double-click on the **Molecular Properties (Materials)** component.

The new component is connected to the *Study Table Reader* by a pipe - this indicates that data read from the study table will be passed into this component. As the study table contains multiple structures, each structure will be a new data record flowing down the pipeline. If you examine the Parameters window, you will see that there is a single parameter named *Output* on the *Molecular Properties (Materials)* component. This controls the properties that will be calculated and added to each data record.

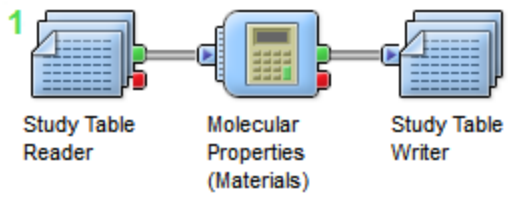
The final component to add is the *Study Table Writer*.

In the **Search** text box on the Components tab, enter **Study Table**. Double-click to add the **Study Table Writer** component to the protocol.

Again, this component is red because you need to specify the location and filename to which the study table will be written. Pipeline Pilot can write files to anywhere that you have access, but for Materials Studio to load the file back into the client, you must write the files into the Job Directory.

Set the **Destination** parameter to **$(jobdir)/results.std**.

This will create a study table called `results.std` which will be downloaded to the Materials Studio client when the protocol completes.



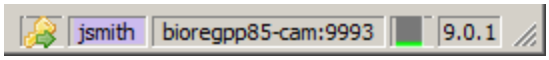
Initial protocol

You will now save this protocol into your protocols folder on the AEP server.

Select **File | Save Protocol** from the menu bar. Enter the **Molecular Properties** as the **Name** and click the **OK** button. Change to the **<user name>** tab on the explorer.

You will see a new protocol called *Molecular Properties*.

Before you connect to the Accelrys Enterprise Platform server from Materials Studio, you will need to know its connection details. In the Pipeline Pilot Professional Client, the user name and the server name and port of the active AEP server are displayed in the lower-right of the program window. Additionally, a bar shows the load on the server and finally the number indicates the version of your AEP server.



Server information

Note down the **server name** and **port number** (if the port number is displayed).

3. To connect and explore the AEP server from Materials Studio

Now that you have explored the components and protocols in Pipeline Pilot Client, you will do the same from Materials Studio.

Change the active application to **Materials Studio**. Select **Tools | Pipeline Pilot Protocols** from the menu bar.

The first time you use this, you will be asked for the location of the AEP server. This requires the server name and port information that you noted down earlier. If you didn't have a port number, you can just enter the server name.

If required, modify the **Server location** to be the **<server name>:<port number>** and click the **OK** button.

Pipeline Pilot can require user authentication and so you may need to add your user login information. This is generally the same as your Windows username and password.

Enter your **username** and **password** and click the **OK** button.

Materials Studio will connect to your Pipeline Pilot server and this may take a few seconds. When it is connected, the Pipeline Pilot Protocols dialog will be displayed. This dialog has three panels, the Protocols explorer, Parameters explorer, and a panel for displaying the details of the protocol or parameter currently selected. At the bottom of this dialog the *Server location* and *Materials Studio Version* on that server are reported and the server can be changed.

In the **Protocols** explorer, expand the **Examples** node then the **Materials** node.

This echoes the Examples section in the Protocols explorer in Pipeline Pilot.

Expand the **Forcite** node and double-click on the **Geometry Optimization with Different Forcefields** node.

The protocol opens and the parameters associated with the protocol are displayed in the top panel, help is displayed in the bottom panel. The initial help provides a description of what the protocol will do.

Click on the **Charging method** parameter name.

The help updates to give you a brief description of what the parameter controls.

You will notice that the *Source* parameter is red. As with the Pipeline Pilot client, this means that a parameter setting or value is missing. You will also notice that the existing value of the *Source* parameter is "Active Document", followed by the name of the active document in brackets if there is a document currently open in Materials Studio. This means that if you open a structure, the *Source* will be set to the current document in focus.

Select **File | New...** from the menu bar, select **Study Table** and click the **OK** button. Rename the study table to **corrosion.std**.

Now that you have a document in focus, the *Source* parameter value changes to "Active Document (corrosion.std)" indicating the protocol will run on the study table.

Note: Unlike other functions in Materials Studio protocols will accept any document type as input. If you provide the wrong document as input the calculation will fail. You should ensure that the parameter help states what type of input document or documents are required.

Now you can open the protocol you created earlier.

On the Pipeline Pilot Protocols dialog, expand the **<username>** node and double-click on the **Molecular Properties** protocol.

You will see that, unlike the previous protocol, the new protocol does not have any parameters exposed. There are many parameters on each component in the protocol, but you need to promote parameters from the component level to the protocol level so that they can be set from Materials Studio.

4. To expose protocol parameters in Materials Studio

To expose the protocol parameters in Materials Studio, you need to edit the protocol again in the Pipeline Pilot Client.

Change to the **Pipeline Pilot Client**.

The Pipeline Pilot Client enables you to edit the general properties of a protocol. From here, you can modify how the protocol will appear in Materials Studio. The first task here is to promote parameters from the components to the protocol - these are the parameters that you will see exposed in the Pipeline Pilot Protocols dialog in Materials Studio.

Right-click in the background of the protocol and select **Edit Protocol...** from the shortcut menu.

The Edit dialog enables you to edit the help text and parameters, control files, and promote parameters.

Select the **Promote** tab.

You will see that the *Study Table Reader* component in the protocol is highlighted in yellow. The only parameter that you need to promote from here is the *Source* parameter.

Select the **Source** parameter and click the **Promote** button.

You have the option to link to a new parameter or link to an existing parameter. As there are no parameters at the moment, the first option is the best. You can also choose to promote any parameters grouped by the selected parameter, in this case you only want to promote the *Source* parameter.

Tip: If you are creating protocols with classical simulations components, you can use the option to link parameters to an existing parameter on the parent so that you only choose the forcefield once and this is used by all the components.

Uncheck the **Promote entire group** checkbox and click the **OK** button.

You can also promote what properties are calculated.

Move to the next component by clicking the **Next>>** button. Select the **Output** parameter and click the **Promote** button. Edit the name of the new parameter to **Properties** and click the **OK** button.

On the **Edit** dialog, click the **OK** button.

You have added the properties to the protocol and changed the name from *Output* to a more meaningful *Properties*.

Select the **Molecular Properties (Materials)** component and then click in the background of the protocol.

You should see that the *Output* parameter for the *Molecular Properties (Materials)* component is now set to "Properties (Promoted)" and the protocol has two parameters, *Source* and *Properties*.

Select **File | Save Protocol** from the menu bar.

The protocol has been saved on the server and you can now see the changes in Materials Studio.

Change back to the **Materials Studio** client. On the **Pipeline Pilot Protocols** dialog, select **Tools | Refresh Protocol List** from the menu bar.

The protocols will be refreshed from the server. You should see that the protocol now has two parameters, *Source* and *Properties*.

5. To run the protocol on the server

The protocol is now ready to be run on the AEP server. You need to add some structures to your study table before you run the protocol.

Select **Edit | Insert From...** on the menu bar. Navigate to **Examples\QSAR\Structures** and open **Corrosion.sd**.

A series of molecules for corrosion inhibition are inserted in the study table.

On the Pipeline Pilot Protocols dialog, click the **Run** button.

In the Project Explorer, a folder is created called `corrosion Molecular Properties`. The job status is displayed in the Jobs Explorer. When the calculation completes, the results folder contains a study table called `results.std` and a text document called `summary.txt`.

Open **results.std**.

You should see that new columns, StructureColumn, Name, Molecular_Weight_Materials, and Molecular_Formula_Materials, have been added to the study table. You will also see that the job information is kept in the Jobs Explorer. This is kept because if you generate non-native Materials Studio documents you might want to access these after the calculation has completed and you can do this through the Jobs Explorer.

6. To extend the protocol

In this last section of the tutorial, you will improve the usability of the protocol by editing the help text, and add another set of properties. You will do this in the Pipeline Pilot Client.

Change to use **Pipeline Pilot Client**. Right-click in the background of the **Protocol** and select **Edit Protocol...** from the shortcut menu.

This time, you will edit the Protocol help to give a more useful description of what the protocol does.

Select the **Help Text** tab.

You can edit both the Summary and the Description text. In this case you will clarify what the protocol does.

In the **Description** box, delete the existing text and enter **Calculates a variety of molecular properties for molecules in a study table. Use the Properties parameter to specify which properties to calculate.**.

You can also edit the displayed help for the parameters you promoted.

Change to the **Parameters** tab. Select the **Source** parameter and click the **Edit Parameter** button. In the **Parameter help** text box, add **Requires a study table as input.** after the existing statement. Click the **OK** button to close the Edit Parameter dialog, then click the **OK** button to close the Edit dialog.

The protocol help and parameter help has been updated. You can also extend the protocol by adding a new component. In this case, you will add the *Molecular Property Counts (Materials)* component.

In the **Search** text box, enter **Molecular** and double-click to add **Molecular Property Counts (Materials)**. Drag and drop the new component between the **Molecular Properties (Materials)** and **Study Table Writer** components.

For this component you will not expose the parameters, so that the user always has to calculate them.

AEP provides the capability to create lots of different document types, such as PDFs, Word documents, and HTML reports, that can be shared. In this example, you will create a simple PDF report. To do this, you will add reporting components for a *Table* and a *PDF Report Viewer*.

In the **Search** text box, enter **Table**, and add the green **Table** component to your protocol. Click on the **green Pass port** of the **Molecular Property Counts (Materials)** component and drag a connection to the **Input port** on the **Table** component.

In the **Search** text box, enter **PDF Report**, and add the green **PDF Report Viewer** component to your protocol. Drag the **PDF Report Viewer** onto the **Table** component.

The Materials data flowing down the pipeline needs to be converted to an image before it can be displayed in the report.

In the **Components tab**, expand the **Materials | Converters** nodes and add a **Material To JPEG** component to your protocol.

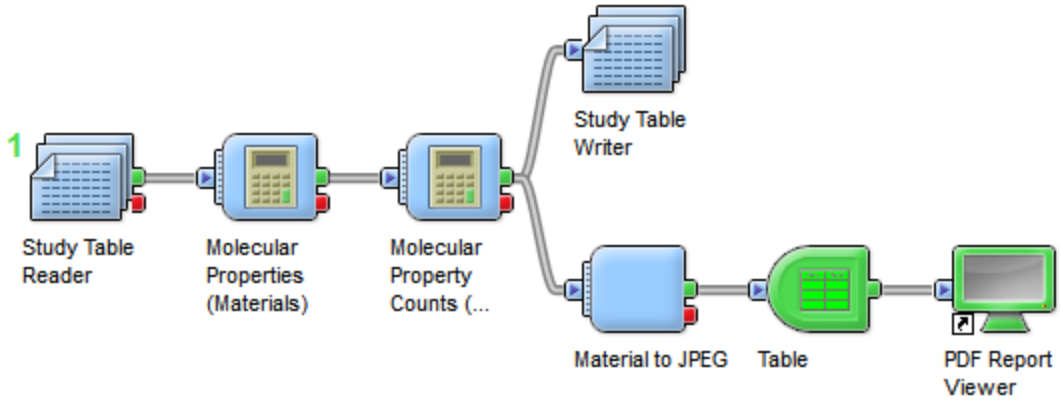
Drag the **Material to JPEG** component over the pipe connecting the **Molecular Property Counts (Materials)** and **Table** components. When the pipe changes color to blue, drop the component.

This will add a new property to the data record containing an image of the molecule. You can modify the name of the data record holding the image of the molecule.

On the **Material to JPEG** component, modify the **JPEG Property Name** parameter to **Material**.

On the Table component, you can remove the column StructureColumn from the table and ensure that the Material image is the first column in the report.

On the **Table** component, in the Parameters window expand the **Data Options** node and set the **Exclude Properties** parameter to **StructureColumn**. Modify the **Column Order** to **Material**.



Final protocol

You can save the protocol and go back to Materials Studio.

Select **File | Save Protocol** from the menu bar.

Change to **Materials Studio**. On the Pipeline Pilot Protocols dialog select **Tools | Refresh Protocol List** from the menu bar.

The protocol and component help has now updated to include clearer descriptions of what the protocol does and the input documents it requires. You can run this protocol on the original study table.

Change focus back to the original **corrosion.std** and click the **Run** button on the Pipeline Pilot Protocols dialog.

When the job completes, the results are returned to a new study table and a PDF document is included in the results folder. You cannot open this inside Materials Studio, but you can open the containing folder in a Windows Explorer.

In the Project Explorer, right-click on the **.pdf** document and select **Open**.

This opens the PDF report if you have Acrobat Reader installed. Note that you can generate far more interesting reports using the components in the Reporting collection but that is outside the scope of this tutorial.

This is the end of the tutorial.

QSAR tutorials

The following tutorial illustrates how to utilize QSAR's capabilities.

Designing new corrosion inhibitors

Purpose: Illustrates the use of descriptor calculations and statistical modeling to design new molecules.

Modules: Materials Visualizer, QSAR, Forcite (optional)

Time: ⏰⏰⏰

Prerequisites: None

Background

Corrosion is a real challenge to many chemical businesses, as well as being a difficult problem to study scientifically (Gråfen et al., 1985). Corrosion is found in circulating water systems, oil wells, building materials, reaction vessels, pipelines, and countless other areas where materials such as fuels, lubricants, detergents, and metalworking fluids are used.

Corrosion occurs when a chemical reaction takes place between a material and the surrounding medium. This requires cathodic and anodic regions on the material surface with a chemical potential difference between them as well as a mechanism for charge transfer. The reactions and regions can depend on the conditions of the medium, for example on pH and the existence of activating anions.

Corrosion inhibitors have been designed to work in several ways, for example blocking either the cathodic or anodic sites, or scavenging activating ions. Before they can act, they must be transported to the material surface, which places restrictions on their solubility. They must then successfully adsorb onto the surface if that is their mode of action. This involves such processes as physisorption and chemisorption. Often, inhibitors must build up thick layers of material, which places restrictions on their bulk properties.

The processes involved are too complex to model from first principles. The best way of using molecular modeling to help with the design of new and better corrosion inhibitors is to encapsulate knowledge about how existing inhibitors perform into a structure-activity relationship (SAR) and use this to predict the behavior of new structures. The structures with the best predicted activity can then be investigated in the lab.

Introduction

In this tutorial, you will perform some of the basic steps involved in designing a new corrosion inhibitor.

This tutorial covers:

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

1. Getting started

Begin by starting Materials Studio and creating a new project.

Open the **New Project** dialog and enter **Corrosion inhibitor** as the project name, click the **OK** button.

The new project is created with *Corrosion inhibitor* listed in the Project Explorer.

Now create a new study table document.

Select **File | New...** from the menu bar to open the New Document dialog. Select **Study Table** and click the **OK** button.

Rename the new study table **CI.std**.

A study table can be thought of as the primary view onto the multiple structures and models which will be created and managed in this tutorial.

You will import an SD file which contains both the structural and experimental data required for this tutorial.

Select **Edit | Insert From...** from the menu bar. Browse to the **Examples\QSAR\Structures** folder and double-click on the **Corrosion.sd** file.

The `Corrosion.sd` file contains the structures and experimental data for 19 different corrosion inhibitor molecules. The structures are inserted into the first column of the study table. Additional columns contain the structure name and corrosion inhibition data for the imported molecules. In this example, the higher the corrosion inhibition value, the better the inhibitor performs.

2. To import and validate the structures and experimental data

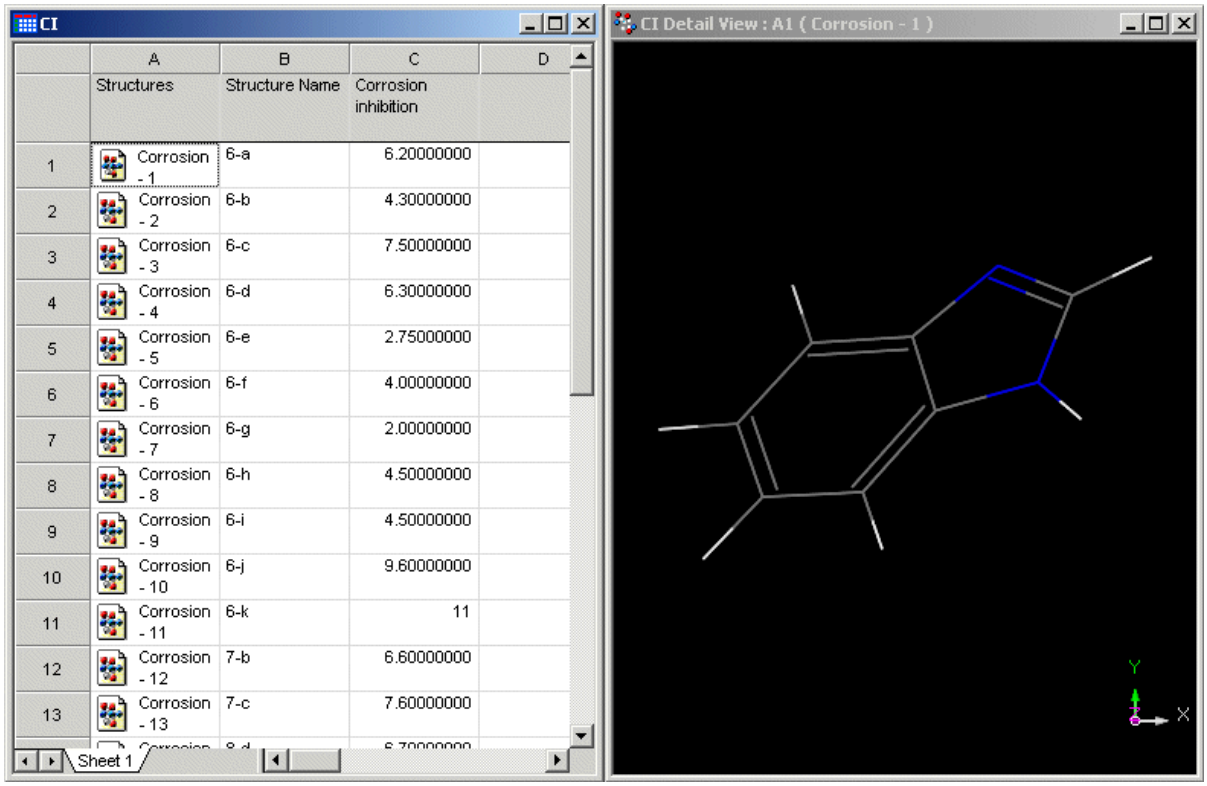
The first step in validating the structures contained in the study table is to visually inspect them and to try to correlate the structural features present with the corrosion inhibition values provided.

Double-click on the structure **Corrosion - 1** in the **CI.std** study table.

This opens a Study Table Document Detail View.

Select **Window | Tile Vertically** from the menu bar.

This arranges the open documents in a way that enables you to see both the structure and the *Corrosion inhibition* column of the study table.



	A Structures	B Structure Name	C Corrosion inhibition	D
1	Corrosion - 1	6-a	6.20000000	
2	Corrosion - 2	6-b	4.30000000	
3	Corrosion - 3	6-c	7.50000000	
4	Corrosion - 4	6-d	6.30000000	
5	Corrosion - 5	6-e	2.75000000	
6	Corrosion - 6	6-f	4.00000000	
7	Corrosion - 7	6-g	2.00000000	
8	Corrosion - 8	6-h	4.50000000	
9	Corrosion - 9	6-i	4.50000000	
10	Corrosion - 10	6-j	9.60000000	
11	Corrosion - 11	6-k	11	
12	Corrosion - 12	7-b	6.60000000	
13	Corrosion - 13	7-c	7.60000000	

Study table and detail view

On the **Study Table Viewer** toolbar, click the **Step Detail View Forward** button  to step through the inhibitor structures listed in the **CI.std** study table.

If you examine the data, you will see that there is a homologous series in this set of compounds, with a linear hydrocarbon chain of increasing length attached to a tri-substituted nitrogen atom. Significantly, the corrosion inhibition of this series is a nonlinear function of the hydrocarbon chain length.

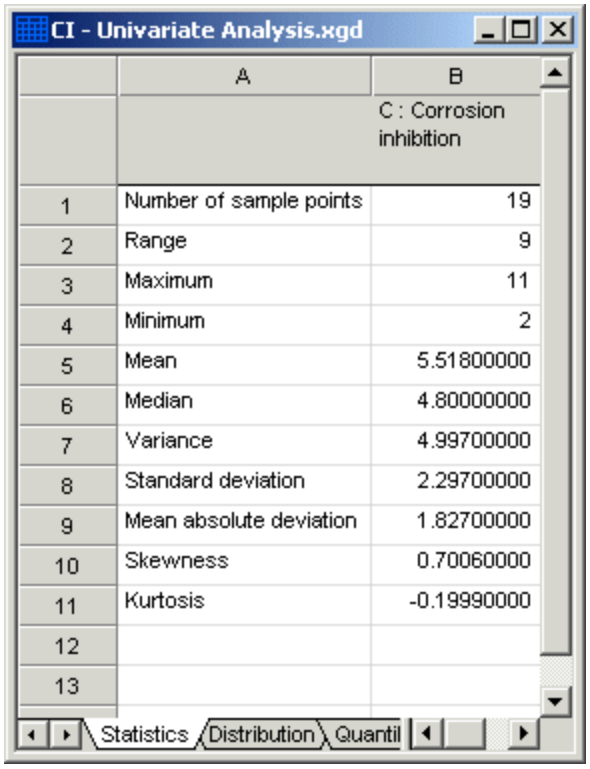
Tip: If the structures do not look geometrically accurate, you can use the Forcite or VAMP models to optimize all the structures in the study table.

Close the **CI Detail View**.

To validate the inhibition data, you should investigate the distribution of the data. Most regression algorithms rely on the data that is being investigated being normally distributed, so if your data are not normally distributed, you should consider applying a numerical transformation to achieve a normal distribution. Materials Studio enables you to analyze your data to determine whether it can be considered to conform to a normal distribution.

Select **CI.std** and click the **Corrosion inhibition** column header, labeled **C** to select the entire column. Select **Statistics | Initial Analysis | Univariate Analysis** from the menu bar.

A new document called `CI - Univariate Analysis.xgd` is displayed. It contains several statistical measures that describe the data in the *Corrosion inhibition* column of the CI study table.



Part of a univariate analysis of the inhibition data

Select the **Distribution** tab in **CI - Univariate Analysis.xgd**.

The *Distribution* tab shows the percentage of data in each decile. If you compare these values with the percentages that would be found in a normal distribution, you can see that, with the exception of Bin 8, the corrosion inhibition data are close to being normally distributed. As such, there is no real need to perform a numerical transformation.

Tip: If you do need to perform a transformation, you can use one of two methods. The *Initial Analysis | Transform Data* capability allows interactive comparison of the Skewness, Kurtosis, and Distribution data for a variety of basic transformations including log, square root, etc. Alternatively, a function model could be created, transforming the column using a wider variety of mathematical functions.

You can plot the data to perform a graphic comparison of your data with a perfect normal distribution.

Hold down the **CTRL** key and click the column headers for **B** and **C**, to select both columns in **CI - Univariate Analysis.xgd**. Select **Tools | Plot Graph** from the menu bar to open the Plot Graph dialog. Change the **Graph type** to **1D**, click the **Plot** button and close the dialog.

A line graph, `CI - Univariate Analysis graph.xcd` is displayed.

Close **CI - Univariate Analysis graph.xcd** and **CI - Univariate Analysis.xgd**. When prompted, click the **Yes** button to save the documents as part of the project.

3. To align the structures

Some of the descriptors that you might use, such as the dipole moment components, depend on having all the molecules in the same alignment. The Materials Visualizer contains tools that allow you to align molecules to a specific axis and then superpose multiple structures so that they all have the same

alignment. As all the molecules in the corrosion inhibition dataset have the same core, you will align this core to a specific axis, and then superpose all the molecules over the core.

The first step is to extract the core from the study table.

Double-click on the structure **Corrosion - 1** in the **CI.std** study table. Press **CTRL + C** to copy the structure.

Click the **New** arrow  on the toolbar and select **3D Atomistic Document** from the dropdown list. Click in the new 3D Atomistic document and press the **CTRL + V** keys.

The core structure will be pasted into the new 3D atomistic document. This will become the pattern for the alignment.

Rename the new document **core.xsd**.

You will align the molecule so that the long molecular axis is aligned with the x axis. You can align molecules by selecting all of the atoms that comprise the molecule and using the *Align Onto View* button. The molecules are then aligned onto the current view.

Tip: You can also align molecules with their principal axis, a best fit line, or a best fit plane. Use the *Create Centroid* button  to generate these other objects.

Click the **Reset View** button  . Double-click on one of the atoms in **core.xsd** and click the **Align Onto View** button  .

The molecule is aligned so that the long axis is aligned with the x axis in the current view. Before you can align the other molecules with the defined core structure, you should remove all the hydrogen atoms to sure there are no conflicts between the core and aligned molecules.

Hold down the **ALT** key and double-click on a white hydrogen atom in **core.xsd** to select all of the hydrogen atoms in the molecule. Press the **DELETE** key.

The hydrogen atoms are discarded from the molecule. You are now ready to superpose the structures. You will use a collection document to view the structures from the study table whilst you are performing the superposition. A collection document allows you to view multiple molecules or physical systems without them physically interacting.

Make **CI.std** the active document and click column header **A** to select the entire column. Right-click on the selected structures and select **Extract To Collection** from the shortcut menu.

A collection document, `Extracted From CI.xod`, is displayed, which contains all the structures from the study table.

Select **Tools | Superpose Structures** from the menu bar.

This opens the Superpose Structures dialog. Materials Studio provides two main types of fit that you can perform with several different methods of fitting. You will use a Target fit using the Field method. The Field algorithm can fit to either a steric or electrostatic field or a combination of the two. These options are defined on the *Fit Method* tab of the Superpose Structures dialog.

On the **Alignment** tab of the Superpose Structures dialog, set the **Target document** to **core.xsd**.

As the molecules all share a common core, you can use the Find pattern functionality to match any common substructures. As you have already removed the hydrogen atoms, you can use `core.xsd` as the core substructure.

On the **Options** tab check the **Find pattern** checkbox and select **core.xsd** from the dropdown list. Click the **Superpose** button. If you see a warning dialog, click the **OK** button. Close the **Superpose Structures** dialog.

The collection document, `Extracted From CI.xod`, is updated with the overlaid structures and a new study table, `Similarity.std` is displayed. This new study table contains all the aligned structures and the similarity of each to the specified core structure. As the core structure was the same in each case, the similarity measure should be practically identical.

In **Extracted From CI.xod** rotate the structures and look at the alignment.

The structures are all aligned around the core structure which is highlighted by green wireframes surrounding each atom that is found in the pattern. You should delete these wireframes before continuing.

Hold down the **ALT** key and double-click on one of the green wireframes in **Extracted From CI.xod**, press the **DELETE** key.

The final step in this process is to return the structures back to the study table.

Right-click in **Extracted From CI.xod** and select **Return To Study Table** from the shortcut menu. If a dialog appears, click the **Yes** button.

The dialogs refer to the fact that you had open views on the structures and ask if you wish to refresh those views with the newly aligned structures.

Select **File | Save Project** from the menu bar followed by **Window | Close All**.

4. To calculate molecular descriptors

You are now going to calculate possible descriptor variables. These are also referred to as independent variables.

Double-click on **CI.std** in the **Project Explorer** and select column **A**.

Clicking on the column heading cell provides an easy way to select all of the data in the column.

Click the **Models** button  on the **QSAR Models** toolbar to open the Models dialog.

The Models dialog is the key component for managing models. A model in QSAR is a process that takes a set of inputs and provides a set of outputs. For example, an energy minimization is a model which takes a structure as input and provides an optimized structure as output.

At this point in a typical QSAR study, you calculate descriptors. These are models which take a single structure as an input and provide a single number or group of closely related numbers as outputs. QSAR simplifies this task by providing a variety of models which calculate a diverse set of descriptors. These can be browsed using the Models dialog.

Click the header of the **Class** column in the Models dialog.

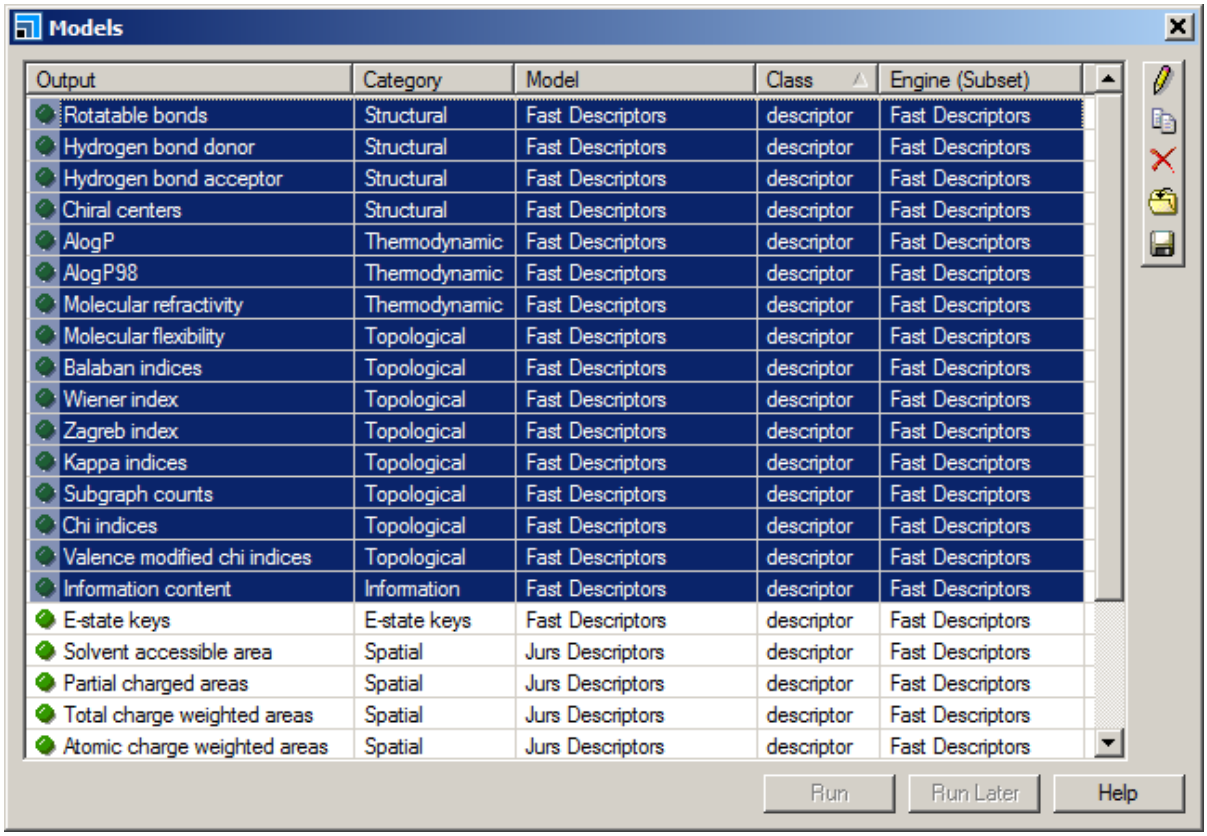
The list of models is sorted by class, displaying the *descriptor* models at the top of the list.

Right-click on an entry in the **Engine** column of the Models dialog, and select **Filter...** from the shortcut menu to open the Filter engine column dialog. Choose **Fast Descriptors** from the dropdown list and click the **OK** button.

Now, both Jurs and Fast Descriptors models are displayed.

Select **Information content** in the **Output** column. Hold down the **SHIFT** key and select **Rotatable bonds**.

The Models dialog should now look like the one shown below.



Models dialog

Click the **Run** button on the Models dialog.

This launches a job to calculate the selected Fast Descriptors and add the results to the study table. The *Job Explorer* will also open, allowing you to monitor the status of the QSAR Models job. Once the job is complete, a Job Completed dialog is displayed.

The Fast Descriptors should be the first descriptors that you calculate for any single-molecule systems. They contain a broad range of descriptors which have been shown to exhibit consistently good correlation with many properties of interest in the pharmaceutical and chemical discovery realms. However, the Fast Descriptors do not directly access the chemistry data model and simulation engines of Materials Studio, which provide significant additional sources of chemical information. To illustrate

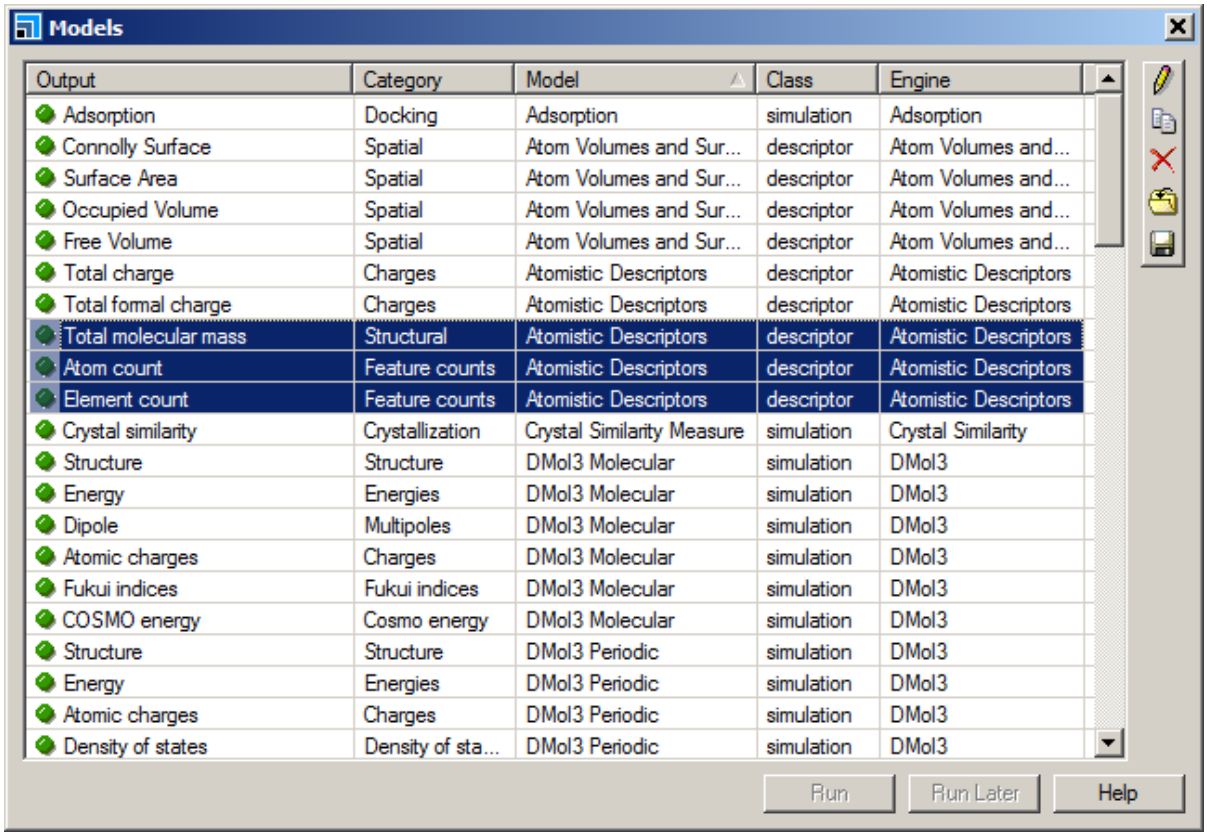
the value of these additional information sources, you should now add Atomistic Descriptors, which access the chemistry data model.

Right-click in the **Engine** column on the Models dialog and select **Remove Filter** from the shortcut menu, to display all of the entries.

Tip: You can have filters on multiple columns active at the same time.

Click the **Model** header in the Models dialog. Select **Element count** in the **Output** column. Hold down the **SHIFT** key and select **Total molecular mass**.

The Models dialog should now look like the one shown below.



Models dialog

Click the **Run** button and close the dialog.

As before, you will see the job displayed in the Job Explorer, and a confirmation dialog will open when the job is complete.

Tip: When calculating descriptors, you should start with the simplest descriptors first. The Fast Descriptors and the basic element descriptors are either 1D or 2D descriptors, meaning they are not geometry-dependent. If you can build a good model with these simple descriptors, you do not have to be concerned with the accuracy of the structures you use (for example the exact bond angles).

The `CI.std` study table now contains values for each of the model outputs, displayed in blue.

Click and drag the scroll bar at the bottom of the study table to the right, to scroll through the study table, and inspect some of the model outputs.

Note: There are constant columns; for example, the *Chiral centers* are all 0. There is no need to explicitly remove these columns. The regression engines will filter them out automatically.

You can also lock columns so that when you scroll across the table, some of the columns remain visible at all times.

Scroll to the left of the study table. Select column **C** and click the **Lock** columns button  in the toolbar. Now scroll to the right in the study table.

You will see that only the columns to the right of the locked column will scroll.

5. To perform initial data analysis

Before building a correlation model, you should perform some elementary statistical analyses.

Inspecting the study table suggests some descriptors appear to correlate very well with the corrosion inhibition of the larger members of the homologous series contained in the collection document; for example, the number of rotatable bonds as calculated by Fast Descriptors. This sort of analysis can be made quantitative by generating a correlation matrix.

Press the **ESC** key to deselect all the cells in the study table.

Hold down the **CTRL** key and click on the following headers in the study table: **C**, **D**, **E**, **F**, **H**, **I**, and **J**.

Select **Statistics | Initial Analysis | Correlation Matrix** from the menu bar.

This creates and displays the correlation matrix, `CI - Correlation Matrix.xgd`, of the data in the selected columns.

CI - Correlation Matrix.xgd *

	A	B	C	D	E	
		C : Corrosion inhibition	D : Rotatable bonds (Fast Descriptors)	E : Hydrogen bond donor (Fast	F : Hydrogen bond acceptor (Fast	H : A Des
1	C : Corrosion inhibition	1	0.40731800	-0.21470500	0.01305690	
2	D : Rotatable bonds (Fast Descriptors)	0.40731800	1	0.36171400	0.44101600	
3	E : Hydrogen bond donor (Fast Descriptors)	-0.21470500	0.36171400	1	0.32749700	
4	F : Hydrogen bond acceptor (Fast Descriptors)	0.01305690	0.44101600	0.32749700	1	
5	H : AlogP (Fast Descriptors)	0.43750100	0.97329000	0.28170700	0.39876500	
6	I : AlogP98 (Fast Descriptors)	0.44860600	0.94617200	0.25553300	0.30362700	
7	J : Molecular refractivity (Fast Descriptors)	0.34287700	0.97562600	0.36024100	0.48645100	

Correlation | Input summary

Correlation matrix of seven variables

Inspection reveals that the descriptors most highly correlated with corrosion inhibition include the AlogP models and the molecular refractivity. This is physically reasonable as these describe the solubility requirements of a good inhibitor (one with high AlogP and molecular refractivity values).

Highly correlated descriptors, those with correlation values above 0.9 are colored orange, values between 0.7 and 0.9 are colored yellow. The color scheme also applies for correlation values between -0.7 and -0.9 and below -0.9. All other correlation values are colored white.

Tip: You can also use the correlation matrix to remove descriptors that are highly correlated. If a QSAR model is generated that contains two descriptors that are highly correlated, you should remove one and re-build your QSAR model.

6. To build and validate a structure-activity relationship or model

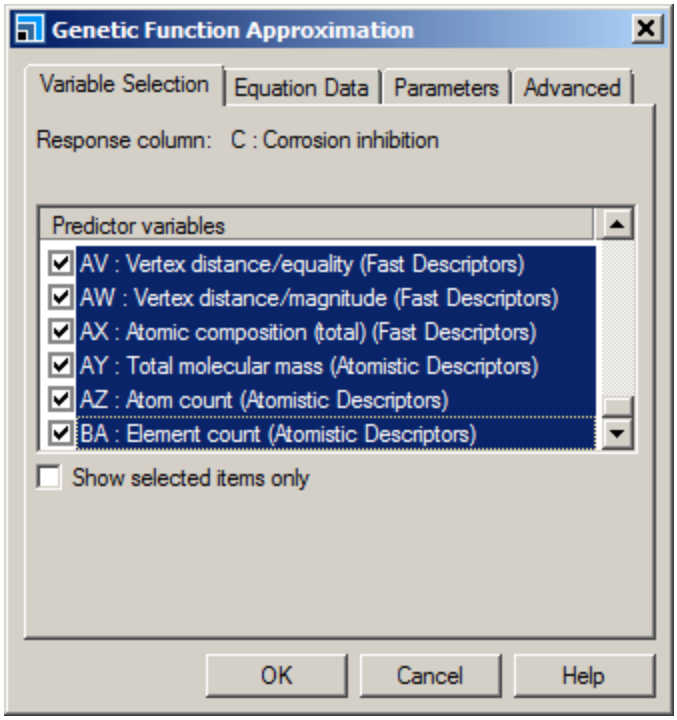
You are now ready to perform a regression analysis of the descriptor variables compared against the measured corrosion inhibition values. There are two separate issues to consider. First, there are many more descriptor variables than measured inhibition values, so you should reduce the number of descriptors. Typically, a ratio between two and five measured values for every descriptor should be sought in order to prevent overfitting. Secondly, you are aiming to obtain a parametric representation of the regression, producing a simple equation which can be validated against your scientific knowledge.

The desire to meet both needs simultaneously helps to guide the choice of statistical data reduction and regression methods from the many options that are available. A genetic function approximation can carry out both data reduction and parametric regression simultaneously. Other methods, such as partial least squares and neural networks, can also perform data reduction, but are typically much more difficult to interpret.

Select the **CI.std** study document and press the **ESC** key to deselect everything. Select the **Corrosion inhibition** column **C**, in the study table. Choose **Statistics | Model Building | Genetic Function Approximation...** from the menu bar.

This opens the Genetic Function Approximation dialog.

Select the first row in the **Predictor variables** list, scroll to the bottom of the list, hold down the **SHIFT** key, and click on the text for the last row. Check any of the checkboxes to enable the entire list.



Genetic Function Approximation dialog, Variable Selection tab

Now all of the columns in the study table are selected for use as input descriptors to the genetic function approximation (GFA) calculation. Columns with constant or non-numerical values have been filtered out. These do not appear in the *Predictor Variables* list.

For now, you should also change the population size to be commensurate with the large number of predictor columns, but you will leave the rest of the GFA parameters at their default values and build an initial model.

Select the **Parameters** tab on the Genetic Function Approximation dialog, change the **Population** to **100**. Click the **OK** button.

The GFA method returns a grid document, `CI-Genetic Function Approximation.xgd`, which contains a report on the regression analysis and a chart document detailing the variable usage vs. generation number. The chart document contains the top five descriptor variables that appear in the model population and gives useful insights into the importance of the descriptors.

Tip: Besides giving information about descriptor usage, this chart can also be used to see if the GFA calculation has converged. If you select a specific number of generations and the calculation has completed all of these, it has not converged and you should re-run the calculation with a higher number of *Maximum generations*.

The grid document contains several tabs relating to the setup and final model.

Make **CI - Genetic Function Approximation.xgd** the active document and select the **Validation** tab.

Tip: If the *Validation* tab is not visible at the bottom of the grid viewer, use the arrow buttons or click and drag the on the divider between the tab display and the scroll bar to reveal additional tabs.

CI - Genetic Function Approximation.xgd

	A	B
		Equation 1
1	Friedman LOF	1.46996100
2	R-squared	0.88610800
3	Adjusted R-squared	0.84230300
4	Cross validated R-squared	0.81310000
5	Significant Regression	Yes
6	Significance-of-regression F-value	20.22861400
7	Critical SOR F-value (95%)	3.04462900
8	Replicate points	0
9	Computed experimental error	0.00000000
10	Lack-of-fit points	13
11	Min expt. error for non-significant LOF (95%)	0.69434900

Summary | Equations | Definitions | Data | Valid

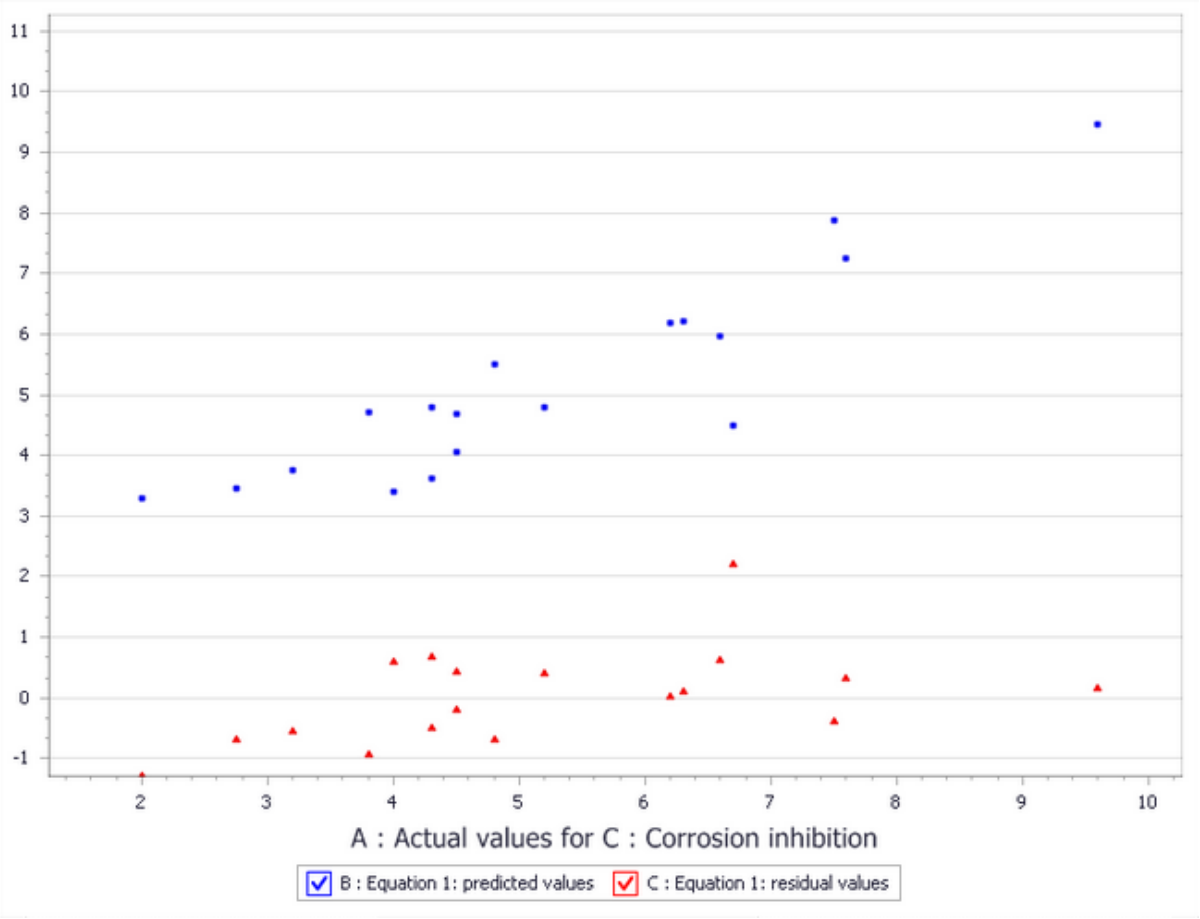
Validation sheet of the Genetic Function Approximation grid document

Note: The values you obtain may be slightly different from those shown in the figure due to randomness in the GFA algorithm. However, the broad features described below should be present.

You can see that although the accuracy of the model, indicated by the R-squared value, is reasonably high, the predictive power, as indicated by the adjusted R-squared and cross validated R-squared values, is rather low, even though the regression is significant according to the F-test.

Select the **Data** tab of the **Genetic Function Approximation.xgd** grid document.

Select the header for column **A**, hold down the **SHIFT** key and select the header for column **C**. Right-click in any of the selected headers (**A**, **B**, or **C**) and choose **Quick Plot** from the shortcut menu.



Plot of predicted inhibition, shown by blue symbols, and residuals, shown by red symbols, versus measured corrosion inhibition

A plot similar to the one shown above is displayed.

The key feature of the graph is the distribution of the residual values against the measured corrosion inhibition values.

> **Tip:** A residual can be defined as the difference between the predicted value in the generated model and the measured value for corrosion inhibition.

A systematic variation is observed which should not be present in a valid model. The model you have built underestimates the corrosion inhibition of the worst inhibitor molecules. Clearly, there are additional sources of performance variation which the model does not capture.

Close the chart document and click the **Yes** button to save the document as part of the project.

You can use the analysis methods available in Materials Studio to identify potential outliers in your dataset. An outlier can be defined as a data point whose residual value is not within two standard deviations of the mean of the residual values. Although the number of outliers can vary depending on the quality of the dataset (for example incorrect measurements of physical properties or errors in molecular structures will reduce the dataset quality), a good test of your QSAR model is to identify potential outliers.

To perform an outlier analysis, you should add your model to the CI study table.

Select the **CI-Genetic Function Approximation.xgd** grid document. Select **Statistics | Apply Results...** from the menu bar to open the Apply Genetic Function Approximated Results dialog. Select **Equation1: prediction** from the **Type of data to apply** list, and click the **OK** button.

The model is added to the study table in a new column labeled, *GFA equation 1: prediction for C: Corrosion inhibition*. You are now ready to perform an outlier analysis.

Select column **C** in **CI.std** and choose **Statistics | Model Building | Outlier Analysis...** from the menu bar to open the Outlier Analysis dialog.

You can perform outlier analysis on any of the columns in the study table generated by regression models.

Tip: You can perform outlier analysis on more than one model. Visualization of several models can be useful to see if the same outliers are appearing in all the models.

Ensure that **GFA equation 1** is selected in the **Prediction models** list and click the **Plot** button.

Two charts are displayed in the `CI Outlier analysis.xcd` document. One contains the residual values plotted against the corrosion inhibition measurements and the other displays the residual values plotted against study table row number. Each chart contains a dotted line that indicates the critical threshold of two standard deviations beyond which a value may be considered to be an outlier. You can look at these to see if there is any systematic pattern of the residual values with the property or with study table row number.

You should see there is one statistical outlier that is above the two standard deviations threshold.

Select the outlier on the chart.

You could remove this point or try to add more descriptors and build a better model. For this tutorial you will add more descriptors, but you should bear in mind that the value could be a genuine outlier.

7. To add atom-based descriptors

It is possible to build an improved model by adjusting the GFA parameters; for example, by increasing the population size or including spline terms. However, there are only minimal incremental returns on this if you do not first extend the number of descriptors available.

You can achieve this by adding descriptors that depend on the geometry of the structure or that account for electronic properties. You will add the charge on specific nitrogen atoms in the structures to your model.

Atom-based descriptors are easily generated by marking the atoms on the current structures and then calculating the properties for those atoms. To mark the atoms, you first need to create a template. As you have already created a template for the alignment, you can re-use this.

Make **core.xsd** the active document. Hold down the **ALT** key and double-click on one of the green wireframes to select them. Press the **DELETE** key.

The wireframes are discarded. You should now define sets that specify the atoms which will be used as descriptors.

Choose **Edit | Edit Sets** from the menu bar to open the Edit Sets dialog. Select the nitrogen atom with two single bonds and click the **New...** button. Enter the name **N(H)** and click the **OK** button.

Select the other nitrogen atom in the ring and add a new set called **N(Ring)**, close the Edit Sets dialog.

You have now defined the two atoms for which you want to calculate the property.

Make **CI.std** the active document and press the **ESC** key. Select column **A** and open the Models dialog. Double-click on the **Mark Structures** model to open the Model Editor - Mark Structures dialog. Select the **Inputs** tab.

The mark structures model creates a series of marked structures on which you will perform a set of VAMP calculations. The input for this model is the pattern fragment, `core.xsd`, which you defined in the step 3 above.

For **Template Fragment** select **core.xsd** from **Value** the dropdown list. Click the **Save** button and close the Model Editor - Mark Structures dialog. On the Models dialog, click the **Run** button and close the dialog.

A job is launched and upon completion the results are returned to the CI study table.

Scroll across to the right-hand side of the study table.

Two new columns have been added, *Marked structure (Mark Structures)* and *Fragments found (Mark Structures)*. All the rows for *Fragments found* should contain 1.

Double-click on the cell containing **Corrosion - 1** in the **Marked structure** column to open a 3D detail view of the structure. Click the **Step Detail View Forward** button  , to check the appropriate atoms are marked for each structure in the series. Close the 3D detail view.

Note: If you have marked any spurious atoms, you can edit these manually.

You are now ready to calculate the VAMP properties for the marked atoms. As you are going to calculate the charges on the marked atoms, you will select the *Marked structure* column as your input column instead of column *A*.

Select the header for column **BC - Marked structure (Marked Structures)**, to select the entire column and open the Models dialog. Right-click in the **Engine** column and select **VAMP** from the dropdown list in the Filter engine column dialog. Click the **OK** button.

Select the **Atomic charges** model and click the **Run** button. Close the Models dialog.

This job will take a few minutes to complete as it is performing a semiempirical quantum mechanics calculation for each structure in the study table.

Note: You can calculate multiple properties on marked structures as well as specific atom-based properties.

Scroll to the right-hand side of the CI study table.

Three new columns have been added, *ESP charge (VAMP Electrostatics)*, *Coulson charge (VAMP Electrostatics)*, and *Mulliken charge (VAMP Electrostatics)*. These contain multiple values in each cell, which must be split before they can be used as descriptors.

Select the columns **ESP charge**, **Coulson charge**, and **Mulliken charge**. Right-click on one of the column titles and select **Split Arrays** from the shortcut menu.

The arrays are split into a *N(H)* and *N(Ring)* column for each of the three charges. You are now ready to build new models.

8. To build and validate a new model

In order to build a new model you can repeat the steps described in the section Building a structure-activity relation or model above. However, it can also be useful to change the GFA parameters as well.

In **CI.std** select the **Corrosion inhibition** column (**C**). Choose **Statistics | Model Building | Genetic Function Approximation...** from the menu bar to open the Genetic Function Approximation dialog.

Select all the rows in the **Predictor variables** list and check any one of the checkboxes in the selected rows to enable all the variables.

Note: Only the split array columns are displayed in the *Predictor variables* list - the original array columns are not included.

You now need to remove from the selection the column containing the prediction from the initial GFA calculation.

Select the **BB: GFA equation 1: prediction for C: Corrosion inhibition** variable and uncheck the checkbox to remove this item from the predictor variables.

The number of terms in a QSAR model can indicate whether your model is overfitting. Too many terms may mean that the R^2 value is high but the cross-validated R^2 value is low, as the model is strongly affected by changes in the training set. Therefore, you should try to build the best model with the lowest number of terms. The GFA automatically tries to do this but you can save some time by setting lower values for the initial and maximum equation length.

On the **Equation Data** tab set the **Initial equation length** to **4** and the **Maximum equation length** to **6**.

You should also change the population size and maximum number of generations.

On the **Parameters** tab change the **Population** to **200**, the **Maximum generations** to **5000**, and the **Number of top equations returned** to **10**. Click the **OK** button.

These changes in the GFA parameters attempt to address several problems which can occur when building a model.

The first problem relates to the set of initial equations chosen for the model. This set should aim to give a dense, uniform coverage of the equation space, meaning that it includes all possible variables, pairs of variables, triplets and so on. This ensures that there is a nonzero probability of having one or more equations in the regions of equation space that are in the same basin of attraction as the final top equations. Increasing the population size parameter can help ensure that the coverage of equation space is adequate.

Unfortunately, the choice of initial equations is random, so some nonuniformity will always occur. This can manifest itself within the model that is generated as a dependency on the order of the columns in the source study table. You can think of this as getting trapped in a local minimum. The behavior is exacerbated by a well-known dynamic effect of the GFA method, whereby equations with important descriptors are killed off early in the evolution because they exhibit only moderate performance (as measured by the Friedman LOF value in the default GFA case). The way to counter this problem is to increase the mutation rate parameter, thereby allowing these terms to return to high-performance equations and be in a position to survive. In general, it is a good idea to consider as large a population as you can afford computationally, and to explore the sensitivity to the mutation rate by performing several different runs. Your goal in model building is to have a set of top equations which has no dependency on the details of the GFA initialization or dynamics.

Select the **Equations** tab of the **CI-Genetic Function Approximation(2).xgd** grid document.

The ten final equations are displayed on the *Equations* tab. Column *A* contains abbreviations for the descriptors and column *B* contains the full descriptors.

Select the **Validation** tab of the **CI-Genetic Function Approximation(2).xgd** grid document.

CI - Genetic Function Approximation (2).xgd

	A	B	C	D	E	F
		Equation 1	Equation 2	Equation 3	Equation 4	Equation 5
1	Friedman LOF	1.77120900	1.78953300	1.79641600	1.82914900	1.86867200
2	R-squared	0.92589800	0.92513200	0.92484400	0.92347400	0.88029300
3	Adjusted R-squared	0.89739700	0.89633600	0.89593700	0.89404100	0.84609100
4	Cross validated R-squared	0.87047700	0.86757300	0.86731600	0.86277600	0.71940000
5	Significant Regression	Yes	Yes	Yes	Yes	Yes
6	Significance-of-regression F-value	32.48685100	32.12757700	31.99452000	31.37544100	25.73806000
7	Critical SOR F-value (95%)	3.04462900	3.04462900	3.04462900	3.04462900	3.16016300
8	Replicate points	0	0	0	0	0
9	Computed experimental error	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
10	Lack-of-fit points	13	13	13	13	14
11	Min expt. error for non-significant LOF (95%)	0.56007400	0.56296400	0.56404500	0.56916100	0.69177500

Summary | Equations | Definitions | Data | Validation | Input summary

Validation sheet of the GFA analysis report for the second set of models

The models returned are all much more accurate, in part, because of the addition of the new VAMP descriptors. The adjusted R^2 and cross validated R^2 values indicate that the models are also more robust. However, the GFA does not perform a full cross-validation procedure as it does not refit the model form for each row that is omitted, but simply refits the parameters. Thus, these indicators of robustness should be treated with caution.

In some cases, the top models may be very similar, or even identical, to the displayed precision. You could try increasing the number of models returned to investigate which different functional forms can be used to fit the data. For the present system, the inclusion of the charge on the nitrogen atoms, as calculated by VAMP, is physically sensible because this contributes to the strength of the electrostatic interactions that play a key part in the adsorption mechanism, which is necessary for successful corrosion inhibition.

Select **Statistics | Apply Results...** from the menu bar to open the Apply Results dialog. Select **Equation 1: prediction** and **Equation 1: residual values**, click the **OK** button.

The new GFA model and residuals are inserted into the study table.

Select the **Corrosion inhibition** column, **C**. Scroll to the right-hand side of the study table. Hold down the **CTRL** key and select the **GFA (2) equation 1: prediction for C: Corrosion inhibition** and **GFA (2) equation 1: residual values for C: Corrosion inhibition** columns. Click the **Quick Plot** button on the toolbar.

The accuracy of the model is very high, and the residuals appear to have no systematic dependence on the measured inhibition. This indicates that the residual variation is random.

Close the plot and click the **Yes** button to save it to the project.

9. To create a new candidate corrosion inhibitor

Now that you have a candidate equation you can use it to extrapolate the behavior of new molecular structures. This is best done in small steps; for example, starting from a structure with measured values and making small changes to it. As you make these changes, you will have to re-optimize the structure.

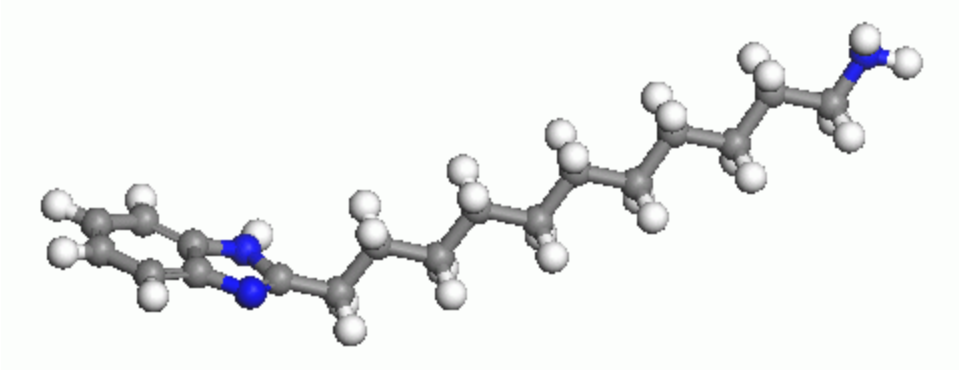
Start by sorting the experimental data.

Select the **Corrosion inhibition** header and click the **Sort Ascending** button on the **Study Table Viewer** toolbar.

The structure with the highest corrosion inhibition value, Corrosion - 11, is now at the bottom of the study table.

Scroll to the bottom of the study table and double-click on **Corrosion - 11** in the **Structure** column. Copy the structure.

Create a new 3D Atomistic document and paste the structure. Click once in the new 3D Atomistic document to deselect everything and rotate the structure until the two hydrogens on the terminal amine group are visible.



Trial inhibitor structure prepared for editing

Select one of the two amine hydrogens and click the **Modify Element** arrow  on the **Sketch** toolbar, choose **Carbon** from the dropdown list. **Adjust hydrogens** and **Clean** the structure.

Rename the new document **Trial Inhibitor.xsd**.

The difference between Corrosion - 11 and the new trial inhibitor, the capping of the amine with a methyl, is structurally similar to the difference between the structures Corrosion - 4 and Corrosion - 12. This resulted in a small increase in the measured inhibition, so similar results might be expected in this case.

Note: The next section of the tutorial requires a Forcite license. If you do not have Forcite, proceed to section 10.

As the new structure is not optimized and all the other structures were optimized using the COMPASS forcefield, for the sake of consistency, you should optimize the geometry of the trial inhibitor before inserting it into the study table.

Select **Modules | Forcite | Calculation** from the menu bar to open the Forcite Calculation dialog. On the **Setup** tab select **Geometry Optimization** from the **Task** dropdown list. On the **Energy** tab select **COMPASS** from the **Forcefield** dropdown list. Click the **Run** button and close the dialog.

A new folder is created, `Trial Inhibitor Forcite GeomOpt`, and, when the calculation is complete, the results are downloaded into this folder. This should only take a few seconds.

Tip: If you are starting off with a new set of structures to build a QSAR model, you can optimize them in the study table using the Forcite model.

10. To predict inhibition of the candidate

The candidate can be added to the study table by using the *Insert From...* option on the *Edit* menu, by copying and pasting the candidate structure, or by using the *Project Explorer*. If you wish to add a small number of molecules, the *Project Explorer* is the easiest option.

Make **CI.std** the active document. In the **Project Explorer**, right-click on **Trial Inhibitor.xsd** in the **Trial Inhibitor Forcite GeomOpt** folder and select **Insert Into** from the shortcut menu.

A link is made to the new inhibitor in the *Structures* column at row *20*.

Right-click on the row heading cell for **20** and select **Calculate** from the shortcut menu.

This calculates all of the descriptor and statistical models for the new inhibitor structure.

Scroll to the right-hand side of the CI study table.

The predicted inhibition of the new trial structure is displayed. This should have a higher inhibition value of around 15.

Note: The residual column contains an *#N/A* error as there is no experimental activity from which to calculate the residual.

Tip: You can try to improve the QSAR model by altering more variables in the GFA settings. For example, try to build a model with linear splines.

This is the end of the tutorial.

References

Gråfen, H., Kuron, D., Botta, A., "Investigations Into The Determination of the Influence of Functional Groups In N-containing Inhibitors on the Corrosion Protection Efficiency", *Werkstoff Korros.*, **36**, 407 (1985).

Scripting tutorials

The following tutorials illustrate how to utilize Materials Studio's scripting capabilities.

- Using scripting to calculate the interaction energy between two layers
- Executing scripts from the User menu

Using scripting to calculate the interaction energy between two layers

Purpose: Introduces scripting for the Properties Explorer and running Forcite calculations.

Modules: Materials Visualizer, Forcite, COMPASS

Time: ⏰⏰

Prerequisites: None

Introduction

Calculating the interaction energy between two surfaces is a standard task when using classical simulations. The interaction energy is defined as:

$E_{Int} = E_{total} - (E_{layer1} + E_{layer2})$

This tutorial illustrates how you can use scripting to read in a trajectory and frame by frame calculate the energy for the cell and for individual layers using Forcite. The energy and structures are written to the study table so it is easy to analyze.

The input trajectory for this script must already have the layers defined as sets of atoms called Layer1 and Layer2.

Note: The intention of this tutorial is to provide an overview of writing and testing scripts in Materials Studio. Any Perl-specific commands will not be explained in detail.

This tutorial covers:

- Getting started
- To define the input document and create the study table
- To initialize the Forcite energy calculation
- To calculate the surface area of the cell
- To create the loop over the trajectory
- To create temporary documents to hold the layers
- To calculate the single point energies and interaction energy

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

1. Getting started

Begin by starting Materials Studio and creating a new project.

Open the **New Project** dialog and enter **MS_API** as the project name, click the **OK** button.

The new project is created with *MS_API* listed in the Project Explorer. The next step is to load the trajectory for which you are going to calculate energies.

Click the **Import** button  to open the Import Document dialog. Navigate to the **Examples\Documents\3D Model** folder and double-click on **Layer.xtd**.

The trajectory is displayed in a new 3D Viewer.

2. To define the input document and create the study table

The first step when creating a script is to open a new script document.

The Perl Script Document allows you to edit Perl scripts in Materials Studio. It has some basic editor features such as line numbering, syntax coloring, and brace matching. All of these can be customized using the view settings.

Click the **New** arrow  and select **Perl Script Document** from the dropdown list. Select **View | Viewer Options...** from the menu bar.

This opens the Script Viewer Options dialog, you can edit the fonts, tab sizes, script coloring and print formatting.

Close the **Script Viewer Options** dialog.

The new document contains the following lines:

`#!perl` - defines it as a Perl script

`use strict;` - forces the user to define any variable they will use

`use Getopt::Long;` - Perl's standard method for passing arguments into scripts

`use MaterialsScript qw(:all);` - tells the script to expect commands to access the MaterialsScript module. This is essential for all scripts using Materials Studio scripting functionality.

The Perl Script Document contains two panes in the window. The top pane is the editor pane where you create your scripts. The lower pane contains tabs for Syntax Check and Output. These tabs can contain messages from syntax checking and debugging, these are valuable as you generate and test your scripts.

Now that you have a Perl script document, you can start creating your script. The first task is to specify the document you are going to load. Unless otherwise instructed, you should always type on the next blank line at the bottom of the document.

Type in the Perl script document

```
my $doc = $Documents{"Layer.xtd"};
```

This defines the variable `$doc` as the trajectory document `Layer.xtd` in the `$Documents` collection. The `$Documents` collection refers to all the atomistic, trajectory, collection, study table, and forcefield documents in the current folder. The first time you specify a new variable you need to use `my` to define the variable as you have specified `use strict;` above.

Tip: When you are writing a script, it is good practice to comment what you are doing. This makes it easier for other people to read your scripts. Perl reads a line starting with a # as a comment. You could add `# Specifies the input trajectory file` here.

Note: When loading or creating documents, you do not need to specify their type as this is determined automatically by the extension specified. For example, `.xtd` is recognized as a trajectory document.

Now you will create a new study table document to hold your results.

```
my $newStudyTable = Documents->New("InteractionEnergy.std");
my $calcSheet = $newStudyTable->ActiveSheet;
```

The first of these two lines creates a new study table called `InteractionEnergy.std` and assigns it to a reference called `$newStudyTable`. As the study table document can contain multiple tabs or sheets, you need to choose which sheet you are working on. You can do this using the collection API, where you would specify `$newStudyTable->Sheets(0)`, or by specifying the `ActiveSheet`. In this example, you will use the ActiveSheet of the study table.

Note: By default, when you type an opening bracket or brace a closing one is not automatically added. This can be enabled on the **Script Viewer Options** dialog.

The next step is to create the column headings in the study table. You are going to create a study table with eight columns - one for each structure and associated energy and one for the final interaction energy.

```
$calcSheet->ColumnHeading(0) = "Cell";
$calcSheet->ColumnHeading(1) = "Total Energy of Cell";
```

This line uses the ColumnHeading property of the study table to define the text that will go at the top of each column heading. A zero-based index refers to each column numerically with ColumnHeading(0) being Column A in the study table.

Use **Copy** and **Paste** to create the other lines for the column headings: `"Layer1"`, `"Energy of Layer1"`, `"Layer2"`, `"Energy of Layer2"`, `"Interaction Energy"`, and `"Interaction Energy per angstrom^2"`. Remember to increment the ColumnHeading property index as you create the new columns.

You should have eight lines with the last one being `$calcSheet->ColumnHeading(7) = "Interaction Energy per angstrom^2";`.

The help for MaterialsScript commands is available by putting the cursor in the command and pressing the F1 key or by searching through the online help.

Click on or move the cursor over the `ColumnHeading` property and press the **F1** key.

The Materials Studio Help opens the "ColumnHeading Property" topic giving a brief description of what it does and an example of its use. It also includes links to related commands.

Click on the **Study Table Documents** link.

This topic explains the collection API and how it relates to study tables. It also gives an overview of other commands related to study tables.

At this point, you should check the syntax of the script and start to debug it.

On the **Scripting** toolbar, click the **Check Syntax**  button.

In the *Syntax Check* tab, you should get the message `'-e syntax OK'`. The *Check Syntax* tool goes through the script looking for any Perl syntax issues. For example, if you have missed the semi-colon from the end of a line or not closed open brackets, the *Check Syntax* tool will report an error. If you have correctly followed the instructions above, you should not get any errors at this point.

As Perl is loosely bound, the *Check Syntax* tool will not find mistakes in the MaterialsScript function names until runtime. To find these, you can run the script on the client. This will enable you to debug the script as any errors are reported on the *Output* tab.

On the **Scripting** toolbar, click the **Debug**  button.

Any errors are reported on the *Output* tab. Again, you should have no errors. As the *Debug* tool runs the script on the client, you should have generated an empty study table with the column headings set.

Tip: . Perl is case sensitive so always check the names of documents to ensure that they are consistent with the name in the script.

3. To initialize the Forcite energy calculation

So far you have used the `$Documents` API to access documents in the project and create new documents. You can also access numerous modules with all the functionality being called using `Modules-><MODULE_NAME>`. You can run a Forcite single point energy task with all the default parameters by using:

```
Modules->Forcite->Energy->Run($doc);
```

To allow more control, you can use the ChangeSettings command to change individual settings in a module.

In the **Script Viewer** enter:

```
my $forcite = Modules->Forcite;
$forcite->ChangeSettings(Settings(CurrentForcefield => "COMPASS"));
```

By specifying `my $forcite = Modules->Forcite`, this allows you to shorten the call to Forcite later on in the script and you will use the shorter version of `$forcite->Energy->Run($doc);`

Tip: You could also use `LoadSettings` to load in the state module describing the settings of the calculation.

```
Modules->Forcite->LoadSettings("MySettings");
```

This enables you to rapidly develop scripts and experiment with settings before committing the changes using the `ChangeSettings` command.

4. To calculate the surface area of the cell

This simple calculation assumes that the surface is parallel to the AB plane, that is, the long axis of the box is in the C direction. The lattice information that you need is stored in the Lattice3D filter on the Properties Explorer.

Change focus to **Layer.xtd**. Select **Lattice 3D** from the **Filter** dropdown list on the **Properties Explorer**.

You can see the properties LengthA and LengthB. You can access these properties by mimicking the properties explorer.

Make **Perl Script.pl** the active document and enter :

```
my $lengthA = $doc->Lattice3D->LengthA;
my $lengthB = $doc->Lattice3D->LengthB;
```

You can see that the API maps onto the Properties Explorer very closely with the only change being the removal of the whitespace between Lattice and 3D.

Notes:

There are two main rules you have to remember when filtering using the Properties Explorer.

1. If there can be more than one object, you should pluralize the filter name and use the collection API. For example, if you want to get the number of atoms in a molecule, you could filter by the index:
   `my $moleculeSize = $doc->Molecules(0)->NumAtoms;`
   This will give you the number of atoms on the first molecule. Alternatively, you can filter by the name on the molecule:
   `my $moleculeSize = $doc->Molecules("benzene")->NumAtoms;`
   This is the name as displayed in the Properties Explorer.
2. If there are spaces in the name of the property you are filtering on, you need to remove those spaces. For example, Lattice 3D in the Properties Explorer becomes Lattice3D in the MaterialsScript API.

To get the surface area, you simply multiply lengthA by lengthB.

```
my $surfaceArea = $lengthA * $lengthB;
```

You can also add a print statement here. Print statements will print out to the *Output* tab when running through the *Debug* tool and create a `.out` text file when running on the server. They can be useful when debugging scripts to find properties at a certain time.

```
print "The surface area is $surfaceArea angstrom^2\n";
```

5. To create the loop over the trajectory

There are several different types of loop structure available in Perl and, for this example, you will use the **for** loop. This will enable you to loop over each frame in the trajectory. To use this, you will need the total number of frames in the trajectory. This data is stored on the Trajectory filter in the Properties Explorer.

Change focus to **Layer.xtd**. Select **Trajectory** from the **Filter** dropdown list on the **Properties Explorer**.

The number of frames in the trajectory is stored in the read-only NumFrames property.

Make **Perl Script.pl** the active document and enter

```
my $numFrames = $doc->Trajectory->NumFrames;
```

The Trajectory filter is another special case where there can only be one object in the document so you do not need to pluralize the property name. You can add a print statement here to print the number of frames.

```
print "Number of frames being analyzed is $numFrames\n";
```

In the **for** loop, you will use a counter variable to count the frames. As you are only going to use the counter variable inside the loop, you can initialize it locally, within the **for** statement.

```
for (my $counter = 1; $counter <= $numFrames; ++$counter) {

}
```

It is good scripting practice to tab indent the commands in loops. This makes it easier for others to read the script and also helps with debugging. As you are iterating over the frames in the trajectory and want to perform the same tasks on each frame, you will type the rest of the commands between the curly braces as these are the commands that are repeated in the loop.

You will use the **for** loop to loop over the frames in the trajectory and you will use the value of `$counter` to define the frame you want to work on.

```
$doc->Trajectory->CurrentFrame = $counter;
```

This sets the current frame to the value of counter.

Note: Trajectories are 1-based, so that the first frame is always numbered 1 whereas study tables are 0-based with the first row or column starting at 0. This means when you write into the study table, you should write $counter-1 as you will see later in the tutorial.

6. To create temporary documents to hold the layers

The next steps are to create new documents in which you will copy the cell, and the layers for the current frame. You will do this in the same way you used to create a new study table. You should continue to type these between the curly braces in the **for** loop.

```
my $allDoc = Documents->New("all.xsd");
my $layer1Doc = Documents->New("layer1.xsd");
my $layer2Doc = Documents->New("layer2.xsd");
```

This creates three empty documents and you can now copy the cell into each document and then delete the atoms you do not want.

```
$allDoc->CopyFrom($doc);
```

This command copies everything from `$doc` into `$allDoc`. You can now repeat this for the layers and delete the atoms that are defined in the sets.

```
$layer1Doc->CopyFrom($doc);
$layer1Doc->UnitCell->Sets("Layer 2")->Atoms->Delete;

Repeat the above two lines for $layer2Doc, changing the set to "Layer 1".
```

Note: When you refer to atoms in a periodic structure, you need to access them through the `UnitCell`, `AsymmetricUnit`, or `DisplayRange` filters. There are subtle differences between the three but, for most cases, UnitCell will give the desired results. For more information, please see the online help.

You can then place the structures into the study table using the `$calcSheet` variable you assigned earlier in the script.

```
$calcSheet->Cell($counter-1,0) = $allDoc;
```

The cell command uses the syntax Cell(row, column).

Repeat the above line twice, placing `$layer1Doc` into column index 2 and `$layer2Doc` into column index 4.

At this point, you can test the script that you have written.

Click the **Check syntax** button  .

Before using the debug tool, you should temporarily change the **for** loop so that it only reads in the first few structures and not the whole trajectory whilst you are debugging the script.

In the **for** loop, change the `$numFrames` entry in `$counter<=$numFrames` to 3, to give `$counter<=3`. Click the **Debug** button  .

You should have generated a study table containing the structures. You will have also generated all the extra structure documents and later in the script you will add in some lines to delete these.

Double-click on some of the structures to check the layers are correct.

Delete all the documents except **Layer.xtd** and your **Perl script** document.

7. To calculate the single point energies and interaction energy

The final step in the tutorial is to calculate single point energies for the structures and then calculate the interaction energy. You will run a Forcite single point energy calculation which will add the energy as a property called PotentialEnergy to the document. Then you want to put the energy into the study table.

```
$forcite->Energy->Run($allDoc);
$calcSheet->Cell($counter-1, 1) = $allDoc->PotentialEnergy;
```

Repeat this for `$layer1Doc` using column index 3 and `$layer2Doc` using column index 5.

Tip: You don't necessarily have to calculate the energy for the total cell as this will already be on the document if the trajectory was written by Forcite Plus. You can tell this by interrogating the TrajectoryType property on the Trajectory filter of the Properties Explorer. If this has a value of trj, it has been written by Forcite Plus. You could add an **if** statement into the script to conditionally calculate the energy depending on the trajectory type.

Now you can retrieve the energies from the study table so that you can calculate the interaction energy.

```
my $totalEnergy = $calcSheet->Cell($counter-1, 1);
my $layer1Energy = $calcSheet->Cell($counter-1, 3);
my $layer2Energy = $calcSheet->Cell($counter-1, 5);
```

The final step is to calculate the interaction energy. This is just a simple statement:

```
my $interactionEnergy = $totalEnergy - ($layer1Energy + $layer2Energy);
$calcSheet->Cell($counter-1, 6) = $interactionEnergy;
```

You can also calculate the interaction energy per Å^2.

```
my $interactionEnergyArea = $interactionEnergy / $surfaceArea;
$calcSheet->Cell($count-1, 7) = $interactionEnergyArea;
```

As this is a **for** loop, you should discard the temporary documents you have created:

```
$allDoc->Discard;
```

Repeat this for `$layer1Doc` and `$layer2Doc`.

You should now test this again on your client.

Perform a **syntax check**.

You should get an error and this will be displayed on the Syntax Check tab. This should say "`Global symbol "$count" requires explicit package name at -e line 74.`" Your line number may be different. This means that `$count` has been used but not declared using the **my** function. This is a deliberate typo and `$count` should be replaced by `$counter`.

Change `$count` to `$counter` on the line:

```
$calcSheet->Cell($count-1, 7) = $interactionEnergyArea;
```

Perform another **syntax check** and run a **debug**.

If the calculation completes successfully, you can run the job on the server. Before doing so, you should now change the **for** loop back so that it iterates over the entire trajectory. You can also change the number of documents that Forcite writes for each calculation using WriteLevel => "Silent". This enables you to remove the text documents that are written out for each calculation.

Locate the `$forcite->ChangeSettings(Settings(CurrentForcefield => "COMPASS"));` line. Modify this to `$forcite->ChangeSettings(Settings(CurrentForcefield => "COMPASS", WriteLevel => "Silent"));`

In the **for** loop, change `$counter<=3` back to `$counter<=$numFrames`. Click the **Run on server** button  .

The script and all the files in the folder are submitted to the calculation. This is deliberate so that if you want to run on multiple files, all you need do is put them in the same folder as the script. However, if you are just intending to run on one structure, it may be best to create a new folder for the script and structure.

Note: This is just one way to complete this tutorial. You could also insert the trajectory into the study table using the InsertInto command and then read the structure from the cells in the study table. The average interaction energy could be calculated and printed to the output window.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

This is the end of the tutorial.

Executing scripts from the User menu

Purpose: Demonstrates how to use the Script Library to add scripts to the User menu in Materials Visualizer.

Modules: Materials Visualizer

Time: ⏰⏰

Prerequisites: Using scripting to calculate the interaction energy between two layers

Introduction

Scripts can be executed from an existing project either on the client or on a server. This is very useful when you are developing and debugging a script. When a script is complete, you can modify it and execute it as a command from the User menu. This has the advantage that you can execute the script on the active document and without having to change the input document each time you want to run it on a new structure or study table document. Where required, you can also create customized interfaces so that arguments can be passed into the script for fine control of the calculation settings. If you are working in a group, this enables you to deploy scripts quickly and easily within the group.

This tutorial focuses on using the Script Library tools to add scripts to a library and associate them with a menu command. You will also edit the script to enable customized parameters to be passed into the script.

This tutorial covers:

- Getting started
- To modify a script and add it to the scripting library
- To create a new User Menu command and execute the script
- To add custom arguments and execute the script
- Adding existing commands and scripts to the scripting library

Note: In order to ensure that you can follow this tutorial exactly as intended, you should use the Settings Organizer dialog to ensure that all your project settings are set to their Accelrys default values. See the Creating a project tutorial for instructions on how to restore default project settings.

1. Getting started

Begin by starting Materials Studio and creating a new project.

Open the New Project dialog and enter **ScriptingLibrary** as the name, click the **OK** button.

The new project is created with *ScriptingLibrary* listed in the Project Explorer.

In this tutorial, you will modify an existing script to demonstrate how a script can be exposed through the User menu.

Click the **Import** button  to open the Import Document dialog. Navigate to the **Examples\Scripting** folder and open **SubstitutionalDisorder.pl** and **TON.xsd**. Select **File | Save Project** from the menu bar.

This imports a script which allows you to add substitutional disorder by replacing a percentage of elements with a new element. The structure `TON.xsd` can be used as an example input structure.

2. To modify a script and add it to the scripting library

Before a script can be added to the script library, the script must be modified so that it will accept the active document. To do this, you need to edit the script and locate the section where the document is opened and replace this with the `ActiveDocument` command.

Make **SubstitutionalDisorder.pl** the active document and scroll to the bottom of the script document.

The document is opened using:

```
my $xsd = $Documents{"TON.xsd"};
```

Locate the line containing:

```
my $xsd = $Documents{"TON.xsd"};
```

Replace this with:

```
my $xsd = Documents->ActiveDocument;
```

Note: The `ActiveDocument` command will only work when the script is running using the User menu. It will not work when run using Debug or Run on Server.

As you are going to make further changes to the script later in the tutorial, you should modify the name of the script to reflect the version number.

Change the name of the script to **SubstitutionalDisorderV1.pl**.

Before adding a script to the library, you should run a syntax check against the script to ensure that you have not made any simple errors

On the **Scripting** toolbar, click the **Check Syntax**  button.

If you find any errors, you should correct these before adding the script to the script library.

The next step is to add the script to the script library.

Select **Tools | Scripting | Library...** from the menu bar.

The Script Library dialog contains two tabs - the Library tab provides a view onto all your scripts organized in folder locations. The User Menu tab enables you to define how the scripts are displayed in Materials Studio and control how the calculations are setup. You will initially focus on the Library tab.

The main purpose of the Library tab is to manage scripts in a single or multiple locations. When you add a script to the script library, a copy of the script is made in the script library location and you should

have write access to that location. The default location is My Favorites which is created in the Materials Studio Project location. For this tutorial, you will just use the default My Favorites location.

Tip: You can add new locations such as network paths to shared folders, this allows you to share scripts with a group of Materials Studio users.

You can add a script to the library from the existing project using the *Add...* button in the File section.

On the Script Library dialog, click the **Add...** button in the File section. In the Add From Project dialog select **SubstitutionalDisorderV1.pl** from the dropdown list and click the **OK** button.

The SubstitutionalDisorderV1 script is added into the scripting library. You are now ready to create a User menu entry so that you can run the script. As the script is going to run from the script library location, you can delete the script in the project.

In the Project Explorer, select **SubstitutionalDisorderV1.pl** and press the **DELETE** key.

Tip: If you want to edit any scripts that are in the Script Library, you can select the script and click the *Import* button. This will import the script into the current Materials Studio Project.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

3. To create a new User Menu command and execute the script

Once you have a script in the Script Library, you can now create a User Menu entry so that you can run that script from the User menu.

On the Script Library dialog, select the **User Menu** tab.

The User Menu tab enables you to define the command which will launch the script and how it is configured to run. You will begin by defining a new command.

Click the **Command** button to add a new command. Change the **Title** from **My Command** to **Substitutional Disorder**.

You can enter a description of the Command in the Description text box.

Change the **Description** to **Changes a percentage of elements from Silicon to Aluminum**.

The next step is to associate a script with the Command.

Click the  button for the **Script** text box.

This opens the Choose Document dialog, allowing you to select the script from your Script Library.

In the **Choose Document** dialog, expand the **My Favorites** tree and select **SubstitutionalDisorderV1.pl**. Click the **OK** button.

You can choose whether to run the script on the Client or on the Server. If you choose to run on the Client, you are limited to running on the active document. If you decide to run on the server, you can choose between active document, current folder, or current folder and subfolders. For this example, you will run on the Client.

Note: If you set the script to execute on a server, the choice of which server the script is executed on is defined from the *Script Job...* command on the User menu.

Most scripts will require a certain type of document as input. You can choose whether to restrict the document to a specific type or choose any document.

Set **Requires** to **3D Atomistic document**. Close the **Script Library** dialog.

The User menu is now displayed on the menu bar.

Tip: You can use Groups on the Script Library dialog to group commands together on the User menu and you can drag and drop the commands in the list on the User Menu tab to organize their appearance on the User menu.

Make **TON.xsd** the active document and select **User | Substitutional Disorder** from the menu bar.

When the command is executed, four silicon atoms in the zeolite are modified to aluminum (more than four atoms may appear to be substituted because of periodic boundary conditions).

When you first run the command, there are no messages returned when the command finishes executing. If messages are returned from the script, the script will be displayed when the command finishes executing.

Change focus to **TON.xsd** and select **User | Substitutional Disorder** from the menu bar repeatedly until no more Si atoms are available for substitution and the script is displayed. Close **TON.xsd** but do not save changes.

As there are no more atom positions that can be substituted because of Lowenstein's rule, an error is returned from the script and the whole script, including an error, is displayed. This is a read-only view on the script in the scripting library and is provided for information only. To edit the script, you can either edit the version in the project or import the version from the Script Library.

Select **File | Save Project** from the menu bar, followed by **Window |Close All**.

4. To add custom arguments and execute the script

You have successfully modified a script and made it executable from the User menu. However, in many cases, it is useful to pass arguments into the script to control certain parts of the calculation. In this example, you want to allow the user to control the percentage of atoms that are going to be changed, the element type of the atom you want to change and the new element you want to change it to. Finally, you might want to set whether to force Lowenstein's rule onto the substitution.

To do this, you will modify the script again to enable arguments to be passed into the script. You can use the Scripting library to import the original script back into the project.

Select **User | Library...** from the menu bar. Select **SubstitutionalDisorderV1.pl** on the Library tab and click the **Import** button in the File section.

The last version of the script is imported into Materials Visualizer so that you can edit it.

With the script in focus, try to select **User | Substitutional Disorder** from the menu bar.

As you have specified that a 3D atomistic document is required to execute the Substitutional Disorder command, the command is grayed out because you have the script document in focus.

Perl provides a standard way to pass arguments into scripts by using the `Getopt::Long` module. This is required for processing the arguments so you must add this to the "use" statements at the top of your script.

Scroll to the top of **SubstitutionalDisorderV1.pl** and locate
```
use MaterialsScript qw(:all);
```
On the next line, add
```
use Getopt::Long;
```

Now you can modify the arguments that get passed into the script. It is easiest to do this where you define the variables at the bottom of the script. `GetOptions` requires a hash list containing the argument names. Arguments can take different inputs such as strings, floating point numbers, integers, and boolean values. In this example, you will modify the percentage number of atoms you wish to change (an integer), the elements you want to modify (strings), and whether to use Lowenstein's rule (a boolean).

Scroll to the bottom of the script. In the line above:
```
my $xsd = Documents->ActiveDocument;
```
add the following:
```
my %Args;
```

This defines the hash list that will contain the arguments.

On the next line type:
```
GetOptions(\%Args, "Percent_Atoms=i", "Original_Element=s", "New_
Element=s", "Obey_Lowenstein=s");
```

You have now defined the input arguments and their types where `i` is an integer and `s` is a string. The last edit you need to make to the script is to associate the arguments with the script variables. As these are contained in a hash list, you just have to set the variables to the hash values.

At the bottom of the script, modify:

```
my $percentChange = 15;
```

to

```
my $percentChange = $Args{Percent_Atoms};
```

Modify:

```
my $originalElement = "Si";
```

to

```
my $originalElement = $Args{Original_Element};
```

Modify:

```
my $newElement = "Al";
```

to

```
my $newElement = $Args{New_Element};
```

Modify:

```
my $obeyLowenstein = "Yes";
```

to

```
my $obeyLowenstein = $Args{Obey_Lowenstein};
```

Note: This example uses capitalized argument names. However, by default argument name comparison is performed case-insensitively by the Perl `GetOptions()` function and for Perl hash key lookups.

You should save this script as `SubstitutionalDisorderV2.pl`.

Save the script as **SubstitutionalDisorderV2.pl**.

Before adding the script to the library, you should again run a syntax check.

On the **Scripting** toolbar, click the **Check Syntax**  button.

If you find any errors, you should correct these before adding the script to the script library.

The next step is to add the new version of the script into the script library and create a command to execute it.

On the **Library** tab of the Script Library dialog, click the **Add...** button for File. Select **SubstitutionalDisorderV2.pl** from the dropdown list and click the **OK** button.

Next you should edit the previous Substitutional Disorder command and configure it to use the new script.

Select the **User Menu** tab and select the **Substitutional Disorder** command. Set the **Script** to **SubstitutionalDisorderV2.pl**.

The final step is to define the arguments that will be requested when you execute the command. The argument names that you create in this step should match the argument names that you entered into

the GetOptions line in the script so it is useful to have the script visible when defining the arguments for the command.

Click the **Arguments** button.

On the Define Arguments dialog click in the **<click to add argument>** text to create an **Untitled** argument. Change the **Name** to **Percent_Atoms**, the **Data type** to **Integer**, and set the **Default value** to **10**.

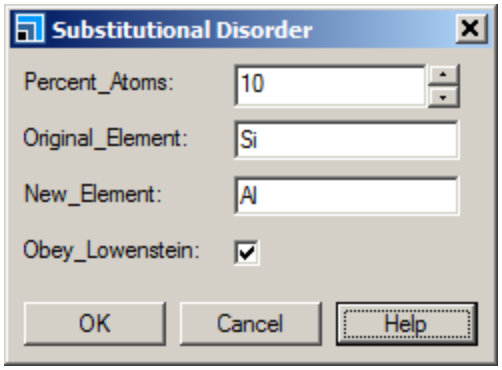
Repeat this to create **Original_Element** (using **String** and **Si** as data type and default value), **New_Element** (using **String** and **Al** as data type and default value), and **Obey_Lowenstein** (using **Boolean** and **Yes**).

Close this dialog and the **Script Library** dialog.

You have now defined the arguments in the script and mapped them to arguments that will be displayed when you execute the command.

Open **TON.xsd**. Select **User | Substitutional Disorder** from the menu bar.

You will be presented with a dialog showing the arguments that you defined previously.



The new arguments dialog

Modify the arguments in any way you prefer and click the **OK** button.

Any arguments that you defined are now passed to the script when it is executed.

5. Adding existing commands and scripts to the scripting library

Tip: If you want to share *Commands* from the *User* menu with colleagues, you can do this by exporting the command or group of commands. A colleague can then import the command into their *User* menu. If the commands point to scripts that are not in a shared folder, you should also send the scripts with the *User* menu.

As a useful example of how to share commands and scripts, the stress-strain script and associated command can be imported into the scripting library. The stress-strain script executes a sequence of molecular dynamics runs in order to determine the stress-strain relationship of a material in the linear elastic region.

Open the **Script Library** dialog and, on the **Library** tab, click **Add** button for **Location**.

A new folder is created, named Untitled.

Change the name of the new folder to **Examples**.

The stress-strain script is stored in the \share\Examples\Scripting folder.

For a default installation of Materials Studio this is:
C:\Program Files (x86)\Accelrys\Materials Studio 8.0\share\Examples\Scripting.

In the bottom panel of the **Library** tab, click the **<click to add path>** item.
In the **type path here** field, enter the full path to your \share\Examples\Scripting folder.

The *Examples* folder of the scripting library tree now displays all the files in the \share\Examples\Scripting directory.

On the **User Menu** tab, click the **Import...** button. Navigate to the **Examples\Scripting** folder and open **StressStrain User Menu.xml**.

A new command, named *StressStrain*, is added to the list of commands.

Select the **StressStrain** command.

The details of the new command are displayed including title and description. The script which the command relates to is shown in red.

Click the  button for the **Script**.

A tree view of the library is displayed.

Expand the **Examples** folder and select **StressStrain.pl**, click the **OK** button and then close the Script Library dialog.

The script name is now displayed in black. The command is now available for use.

Select **File | Save Project** from the menu bar, followed by **Window | Close All**.

This is the end of the tutorial.