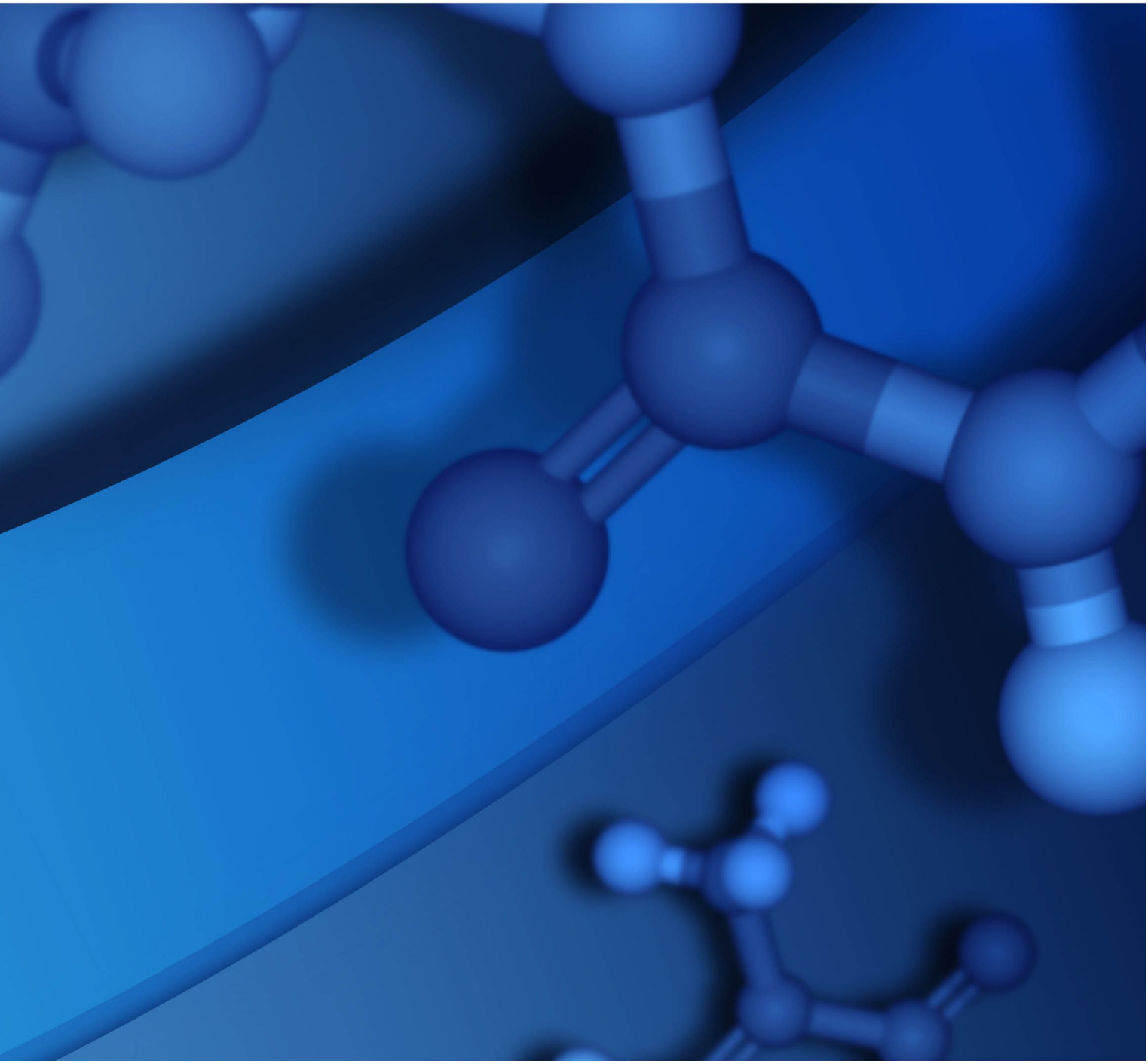
DASSAULT SYSTEMES

BIOVIA

USER GUIDE

MATERIALS VISUALIZER

8.0



Acknowledgments and References

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Contents

Materials Visualizer

Introduction

The Materials Visualizer presents a rich array of functionality through menus, toolbars, explorers, and viewers.

The following topics and their subtopics describe how to work with the basic elements of the Materials Visualizer:

Further Information

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

Managing projects

Materials Studio projects are directory-based, which means that the project is defined by the documents in the project directory structure on your hard disk. For example:

- Adding a document or folder to the project adds it to the project folder on your hard disk.
- Moving a document or folder within the project moves it on your hard disk.
- Renaming a document or folder in the project renames it on your hard disk.
- Removing a document or folder from the project deletes it from your hard disk.

Projects are self-contained, i.e., a project cannot contain references to documents outside of the project folder. This insures that projects can be copied easily and moved and shared between users across a network or via e-mail.

By default, Materials Studio creates projects in a folder that is used by the operating system as a common repository for documents. The location of this folder depends on the version of the operating system you are using. The default location for Materials Studio projects is displayed in *New Projects* on the Locations tab of the Options dialog.

Projects in Materials Studio

A Materials Studio project consists of a project file and a project folder.

Project file

A Materials Studio project file has an `.stp` extension. Its name is identical to the name of the project.

Project folder

A project folder resides at the same location on the hard disk as its project file. It is named by adding the word Files to the name of the project. The project folder includes two subfolders, `Modules` and `Documents`, as well as the project log. The `Modules` folder contains information internal to the Materials Studio modules. The `Documents` folder contains project documents and folders. You can browse and modify its content using the Project Explorer.

A project can be moved outside of Materials Studio by moving the project file together with the root project folder.

Project log

Materials Studio creates a project log for each project. The project log contains information recorded by the Materials Visualizer and the Materials Studio application modules.

> **Note:** In this version of Materials Studio, the project log is restarted for each session.

To view the project log, select *View | Project Log* from the menu bar. The log is displayed in a viewer but it is not a project document. Some applications may also provide direct access to the log when information has been written to it which might be of immediate interest to the user.

The log consists of a list of stored messages and information associated with each message, detailing:

- Time the log entry was written
- Source of the log entry
- Type of log entry
- Text of the message

Log entries may be any of the following types, INFO, WARN, or ERROR, depending on the nature of the message.

Project operations

The File menu contains a variety of commands that you can use to create, open, and save projects.

Creating a new project

When you create a project in Materials Studio, a project folder and a project file are generated. Any document that you create later on will reside within the project folder.

To create a new project

1. Select *File | New Project* from the menu bar to display the New Project dialog.
2. Locate the directory in which you want to create the new project, enter a name for the project, and click the *OK* button.

Opening an existing project

Only a single project can be open in Materials Studio at any one time. If you open a second project while another project is still open, Materials Studio will prompt you to save the open project.

To open an existing project

1. Select *File | Open Project* from the menu bar to display the Open Project dialog.
2. Navigate to and select the project (`.stp` file) you wish to open, then click the *Open* button.

When you open a project, it will be added to the list of recently accessed documents that is displayed when you select *Documents* from the Windows *Start* menu.

Saving a project

You should periodically save the changes that you have made to the current project. Select *File | Save Project* from the menu bar to save your modifications.

Renaming a project

You cannot rename a project in Materials Studio, but you can use Windows Explorer to do it.

To rename an existing project

1. Browse to the location of the project file using the Windows Explorer. Project files have an `.stp` extension.
2. Rename the project file. For example, `OldProjectName.stp` to `NewProjectName.stp`.
3. In the same folder you will see a project folder called `OldProjectName Files`. Rename it `NewProjectName Files`.

Copying a project

You can also use Windows Explorer to copy projects.

To copy an existing project

1. Browse to the location of the project file (`.stp`) using the Windows Explorer.
2. In the same folder you will see the project folder. It has the same name as the project file with a `Files` suffix.
3. Copy the project file and the project folder to a new location.

Dialogs for managing projects

The following topics describe dialogs relevant to managing projects.

File Associations dialog

You can use the *File Associations* dialog to associate document file formats with Materials Studio, and view them from Materials Studio by double-clicking them in Windows Explorer and other applications.

The dialog lists the document formats that are available for loading or saving in Materials Studio. You should review the formats that do not contain a checkmark in either the *Claim* or *Never Claim* columns. For each format, you should consider whether you want to retain ownership by Materials Studio, or leave it with the current owner. The table explains the content of each column and suggests guidelines for use.

Column	Content
Extension	Displays the Windows file extension
Claim	Check this option to assign ownership to Materials Studio.
Never Claim	Check this option if you don't want Materials Studio to claim ownership over the document format. Materials Studio will not list this format again.
Current Owner	The application that owns the document format. You should generally **not** transfer formats owned by major applications such as Microsoft Windows, Microsoft Office, Internet Explorer, or another application that you use more frequently than Materials Studio.
Materials Studio Document	The document type Materials Studio can load from or save to the file format.

Click the *Cancel* button to defer a decision until the next time Materials Studio is started.

Check the *Don't show this window again* option when you have decided on all the file associations.

To update file associations

If you have previously set up file associations and chosen not to display the File Associations dialog, but need to update which file types are claimed by Materials Studio, follow these steps:

1. Select *Tools | Options...* from the menu bar to open the Options dialog.
2. On the General tab check the *Display File Associations dialog if there are any association conflicts* checkbox and click the *OK* button.
3. Close Materials Studio and then restart the application.
4. The *File Associations* dialog is displays when Materials Studio starts, check the file types that you want Materials Studio to claim, or uncheck those it should not claim.
5. Click the *OK* button and continue to use Materials Studio.

Access methods

Displayed when Materials Studio is started if there are conflicts and the *Display File Associations dialog if there are any association conflicts* checkbox is checked on the General tab of the Options dialog.

New Document dialog

You can use the New Document dialog to create a new empty document.

The icons in the *Document* pane represent all the types of document that you can create in Materials Studio. Select a document icon and click the *OK* button to create a new document.

Tip: Materials Studio automatically saves new documents under a default document type name which you can change using *File | Save As...*.

Access methods

Menu	*File	New...*
Toolbar	

New Project dialog

You can use the New Project dialog to create a new Materials Studio project.

File name: Specifies the name of the project that you want to create.

Save as type: Selects the file type from among all the project file formats that Materials Studio can open. Materials Studio projects have the filename extension `.stp`.

Browse to a location where you want to create a new project, give it a name and click the *OK* button.

Note: If a project with the same name already exists in the selected location, you will be asked if you want to overwrite it. If you choose to do so, Materials Studio will ask you if you want to remove all the documents created in the prior project. Normally, you will select *Yes* to start working with an empty project. If you choose to keep all the documents, the new project will be populated with the documents from the previous project.

OK: Closes the dialog and opens a new project with the specified name.

Cancel: Closes the dialog without creating a project.

Access methods

Menu	*File	New Project...*

Open Project dialog

You can use the Open Project dialog to locate and open a Materials Studio project.

File name: Specifies the name of the project that you want to open. Select the file formats that will be displayed in the file list area. In this case, you have a single option, Project Files (*.stp).

Tip: Choose *File | Recent Projects* from the menu bar to see a list of the last nine most recently used projects.

Open: Closes the dialog and opens the specified project.

Cancel: Closes the dialog without opening a project.

Access methods

Menu	*File	Open Project...*
Toolbar	

Save As dialog

You can use the *Save As* dialog to save the active document with a new name as part of the project.

File name: Specifies the new name for the document you are saving.

Save as type: Specifies file format to save as. The dropdown list shows the file formats.

Options...: Provides access to settings that control how some file formats are exported from Materials Studio. *Options* is enabled when the *Save as type* option is set to a file format that has export options.

Note: Materials Studio does not prompt for a filename for a new document when you choose *File | Save*. Rather, it automatically saves new documents under a default document type name which you can change using *File | Save As...* .

Save: Closes the dialog and saves the current file to the specified location.

Cancel: Closes the dialog without saving the file.

Access methods

Menu	*File	Save As...*

Options dialog

The Options dialog has the following tabs:

- General tab
- Locations tab
- Graphics tab
- Jobs

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

Cancel: Closes the dialog without updating any settings.

Help: Displays the Help topic for the current tab.

Access methods

Menu	*Tools	Options...*

General tab

The *General* tab of the Options dialog allows you to change default settings for the Materials Studio environment.

Display File Associations dialog if there are any association conflicts: When checked, indicates that Materials Studio will display the File Associations dialog when it is started the next time if any file association conflicts are detected. In Windows, 'file association' means that a file of a certain type can be associated with a particular program, for example, HTML files are usually associated with a browser program, such as Internet Explorer. This means that if you double-click on an HTML file, the associated program, for example, Internet Explorer, will be launched.

When you install Materials Studio, the installation program will automatically register new file types and associate them with Materials Studio. Some file types may have been registered with other programs already - this is a conflict which cannot be resolved by the installation program. If such conflicts exist, the File Associations dialog will be displayed and you can decide if you want to associate certain file types with Materials Studio.

Open the most recently used project: When checked, indicates that Materials Studio will automatically open the most recently used project when it starts without displaying the Welcome to Materials Studio dialog. If unchecked, Materials Studio will prompt you to open a project or create a new one.

Disable Undo/Redo: When checked, indicates that Materials Studio will respond faster, but at the same time, you will not be able to undo operations.

Enable Autosave every: When checked, indicates that all of the documents in the current project will be saved automatically at the interval specified in the associated text box. Default = checked.

Note: Autosave only saves any 3D model, study table, grid, chart, text or HTML documents that are present in the current project. Other files, such as settings and project files, are not saved automatically.

Autosaved files are placed in the directory specified under *Autosave* on the Locations tab.

Note: Clicking the *OK* button accepts all changes made on the Options dialog. Clicking the *Cancel* button cancels all of the changes made on the dialog. If you made changes on more than one tab of the Options dialog, none of the changes will be saved.

Access methods

Menu	*Tools	Options...	General*

Locations tab

The *Locations* tab of the Options dialog allows you to change the location of folders and files used by Materials Studio.

You can modify the location of the following folders shown in the field:

- *New Projects* - Used as the default folder for new projects created on startup using the New Project dialog.
- *Workspace* - Used to store short-lived data files outside of the current project for some Materials Studio applications. It is recommended that this folder is located on a local hard disk, in an existing temporary files folder.
- *Structures* - Used to store sample structure data located outside of the current project. By default, this address points to the structure folder location that you specified during the Materials Studio setup process. If you have your own library of structures that you would like to use, you can change the address to point to your structure folder.
- *Autosave* - Used to store autosaved files. The *Autosave* function is enabled via the General tab of the Options dialog.

Modify...: Opens the *Browse For Folder* dialog, allowing you to choose a new location for the selected folder.

When creating a new project, load settings from: Specify the location of the template project from which initial settings are taken when new projects are created. Click the ... button to display the Open Project dialog and browse to the new location. The default location for the template project is in your Windows user profile, for example, `C:\Users\[user name]\AppData\Roaming\Accelrys\Materials Studio\[version]\Templates\Normal.stp` on Windows.

Tip: To transfer settings to and from the template project, use the Settings Organizer dialog.

Note: Clicking the *OK* button accepts all changes made on the Options dialog. Clicking the *Cancel* button cancels all of the changes made on the dialog. If you made changes on more than one tab of the Options dialog, none of the changes will be saved.

Access methods

Menu	*Tools	Options...	Locations*

Graphics tab

The *Graphics* tab of the Options dialog allows you to change default graphics settings for the Materials Studio environment.

Disable hardware acceleration: When checked, indicates that Materials Studio will avoid using the installed client video driver. This option is provided for special cases where the installed client video driver does not support the OpenGL specification.

Disable OpenGL shaders: When checked, indicates that Materials Studio will avoid using OpenGL shaders when using hardware acceleration. OpenGL shaders allow for faster high quality rendering, but may not be supported on some older graphics cards. You should only disable this option if you experience problems with 3D graphics.

Disable antialias: When checked, indicates that Materials Studio will avoid using advanced antialias features. Antialiasing allows for smooth-edged high quality rendering, but may not be supported on some older graphics cards. You need only consider disabling this option if you experience problems with 3D graphics stability or speed.

Note: Clicking the *OK* button accepts all changes made on the Options dialog. Clicking the *Cancel* button cancels all of the changes made on the dialog. If you made changes on more than one tab of the Options dialog, none of the changes will be saved.

Tip: After clicking *OK*, close and reopen any active 3D Viewer windows to see the effects of the change.

Access methods

Menu	*Tools	Options...	Graphics*

Jobs tab

The *Jobs* tab of the Options dialog allows you to change default settings for the Materials Studio job submission.

Download results automatically on job completion: When checked, indicates that on completion of every job the necessary files will be automatically downloaded to the results folder. When unchecked, the output files can be downloaded manually on job completion using the Job Explorer. Default = checked.

Always use compression for file transfers: When checked, files exchanged between client and server will use compression. When unchecked, compression will only be used if enabled on the server. Default = unchecked.

Tip: For jobs whose output contains many flat text files efficiency of downloading the results can be increased by checking the *Always use compression for file transfers* checkbox. This is often most beneficial for jobs transferring large study tables.
You can employ this setting for all jobs on a specific gateway using the Server Console. Uncheck the *Always use compression for file transfers* checkbox on the Connection tab of the Gateway Properties dialog.

Note: File compression will not be used when submitting jobs to a Materials Studio gateway that has a version lower than 7.0, regardless of the job compression setting. Such gateways do not support compression and decompression in file transfers.

Note: Clicking the *OK* button accepts all changes made on the Options dialog. Clicking the *Cancel* button cancels all of the changes made on the dialog. If you made changes on more than one tab of the Options dialog, none of the changes will be saved.

Access methods

Menu	*Tools	Options...	Jobs*

Export dialogs

Export dialog

You can use the *Export* dialog to save the active document outside of the project using any export file format supported by Materials Studio.

File name: Specifies the new name for the document you are saving.

Save as type: Contains all the file formats available for the file.

Options...: Provides access to settings that control how some file formats are exported from Materials Studio. This is enabled when the *Save as type* option is set to a file format that has export options.

Save: Closes the dialog and saves the current file to the specified location.

Cancel: Closes the dialog without saving the file.

Note: The chosen export options specific to each file type are retained and applied every time the Export dialog is used.

Access methods

Menu	*File	Export...*

AVI Export Options dialog

Materials Studio can export trajectory files and Kinetix Configuration documents in AVI format. Select *File | Export...* from the main menu and set *Save as type* to Movie Clip (AVI). Click the *Export* button to generate an AVI using the start frame, end frame and step size from the trajectory. By default, a pixel dimension which matches the current size of the 3D Viewer or the image in the Configuration Viewer window is used. To generate an AVI with values other than the defaults, click the *Options...* button to open the AVI Export Options dialog.

Start frame: Specify the start position within the frame sequence. This will be the first frame of the resulting AVI file.

End frame: Specify the end position within the frame sequence. This may be the last frame of the resulting AVI file. However, if the step size increment used is such that the specified frame is overstepped, the resulting AVI will not contain the frame.

Step size: Specify the increment size of the frame sequence. The AVI will step through the trajectory using this value.

Playback speed (fps): Specify the desired playback speed for the AVI, in frames per second. Whether or not this playback speed is attained depends on the capabilities of the machine used.

Use current window size: When checked, indicated that the pixel dimension of the 3D Viewer window will be used for the AVI. Uncheck this option to specify a different size. Default = checked.

Size: Specify the dimensions of the AVI in pixels. Materials Studio can export AVI images with dimensions up to 1024 by 1024 pixels.

Changing the value of one of the pixel dimensions will cause the other value to be adjusted automatically, so that the aspect ratio of the new AVI frames is the same as that in the 3D Viewer.

Note: The controls governing the dimensions of the AVI image are not available for export of Kinetix Configuration documents. For these the dimensions of the image in the Configuration Viewer will always be used.

Quality: Specify the compression of AVI. The visual quality of the AVI file is directly related to the file size and playback performance. This control allows the you to select the amount of compression performed on the images as they are assembled into the AVI. The following options are available:

- Low (fast playback)
- Medium
- High (slow playback)

The *Low* setting produces an 8-bit RLE compressed AVI file. This option generates the smallest AVI files which are the most likely to play at the specified *playback speed*. The image quality will be acceptable for the *Line* Display style, but will show severe banding with all other display styles.

The *Medium* setting will produce a 16-bit AVI file. This is the default quality setting. 16-bit AVI files are larger and may play slowly on some machines.

The *High* setting will produce a 24-bit AVI file. 24-bit AVI files are very large and may play extremely slowly on many machines.

Tip: Unchecking the *Fast render on move* option on the Display Options dialog will produce high visual quality AVI files.

Note: By default, the values for the start frame, end frame and step size are not retained between export operations. Instead, they are always derived from the trajectory. All other AVI export options are retained between export operations.

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

Cancel: Closes the dialog without updating any settings.

Help: Displays the Help topic in a browser.

Note: The chosen export options specific to each file type are retained and applied every time the Export dialog is used.

Access methods

Menu	*File* | *Export...*, set *Save as type* to Movie Clip (*.avi) and click *Options...*

Bitmap Export Options dialog

Materials Studio can export files in BMP format. Select *File* | *Export...* from the main menu and set *Save as type* to Structure Bitmap (*.bmp). Click the *Export* button to generate an image with pixel dimensions which match the current size of the 3D Viewer window. To specify a different image size click the *Options...* button to open the Bitmap Export Options dialog.

Use current window size: When checked, indicates the pixel dimensions of the current 3D Viewer window will be used. Uncheck this option to specify a different image size. Default = checked.

Size: Specify the dimensions of the bitmap in pixels. Materials Studio can export bitmap images with dimensions of up to 10000 by 10000 pixels.

Maintain aspect ratio: When checked, indicates that the proportionality of the dimensions will be maintained. Default = checked.

Changing the value of one of the pixel dimensions will cause the other value to be adjusted automatically, so that the aspect ratio of the new bitmap is the same as that in the 3D Viewer.

If this option is unchecked, changing the value of one or both of the pixel dimensions is likely to cause distortion of the output image relative to the original.

Tip: Setting the *Quality* on the Display Options dialog to High will produce a high quality bitmap image.

Note: If bitmap options are changed, these changes are retained and will be used by default during the next BMP file export.

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

Cancel: Closes the dialog without updating any settings.

Help: Displays the Help topic in a browser.

Note: The chosen export options specific to each file type are retained and applied every time the Export dialog is used.

Access methods

Menu	*File* | *Export...*, set *Save as type* to Structure Bitmap (*.bmp) and click *Options...*

CAR Export Options dialog

Materials Studio can export files in the CAR format. Select *File* | *Export...* from the main menu.

By default, CAR and MDF files are exported with Win32 EOL characters. To specify export using UNIX EOL characters, set *Save as type* to InsightII Molecular Files (*.car, *.cor) and click the *Options...* button.

UNIX format: Specifies that UNIX EOL characters are generated on export.

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

Cancel: Closes the dialog without updating any settings.

Help: Displays the Help topic in a browser.

Note: The chosen export options specific to each file type are retained and applied every time the Export dialog is used.

Access methods

Menu	*File	Export...*, set *Save as type* to InsightII Molecular Files (*.car,*.cor) and click *Options...*

MSD/MTD Export Options dialog

Materials Studio can convert mesoscale structure documents (MSD) to atomistic 3D structure documents (XSD), and vice versa. It can also convert mesoscale trajectory documents (MTD) to atomistic 3D trajectory documents (XTD). Open the XSD, MSD, or MTD file to be converted, then select *File | Export...* from the menu bar.

On conversion, mesoscale molecule sets will be replaced by beads and bead connectors, or vice versa, preserving the molecular topology. The length scale converts between the unit of length in the mesoscale document to Å in the atomistic document. The frame times in the mesoscale document are converted to picoseconds in the atomistic document.

Length scale: Specifies the number of Å in one mesoscale length unit.

Mass scale: Specifies the number of amu in one mesoscale mass unit.

Energy scale: Specifies the number of kcal/mol in one mesoscale energy unit.

Time scale: Reports the number of ps in one mesoscale time unit. The time scale is derived from the length, mass and energy scales, and updates automatically.

Note: Certain mesoscale objects are not transferred to the atomistic document. These include formers and fillers. If present, fields are transferred and rescaled in size.

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

Cancel: Closes the dialog without updating any settings.

Help: Displays the Help topic in a browser.

Note: The chosen export options specific to each file type are retained and applied every time the Export dialog is used.

Access methods

Menu	*File	Export...*, set *Save as type* to 3D Mesoscale Files (*.msd) and click *Options...*
Menu	*File	Export...*, set *Save as type* to 3D Atomistic Files (*.xsd) and click *Options...*
Menu	*File	Export...*, set *Save as type* to 3D Atomistic Trajectory Files (*.xtd) and click *Options...*

MSI Export Options dialog

Materials Studio can export files in the MSI format. Select *File | Export...* from the menu bar.

By default, MSI files are exported with Win32 EOL characters. To specify export using UNIX EOL characters, set *Save as type* to Cerius2 Structure Files (*.msi) and click the *Options...* button.

UNIX format: Specifies that UNIX EOL characters are generated on export.

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

Cancel: Closes the dialog without updating any settings.

Help: Displays the Help topic in a browser.

Note: The chosen export options specific to each file type are retained and applied every time the Export dialog is used.

Access methods

Menu	*File	Export...*, set *Save as type* to Cerius2 Structure Files (*.msi) and click *Options...*

STD Export Options dialog

Materials Studio can export STD files in formats compatible with earlier versions of Materials Studio. Select *File | Export...* from the menu bar.

Saving files in formats from earlier versions of Materials Studio is particularly useful to transfer data to Pipeline Pilot.

To specify which Materials Studio version format to use, set *Save as type* to Materials Studio Study Table Files (*.std) and click the *Options...* button.

Export version: Specifies version format to use for the export, options are:

- 8.0
- 7.0
- 6.1
- 6.0
- 5.5
- 5.0

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

Cancel: Closes the dialog without updating any settings.

Help: Displays the Help topic in a browser.

Tip: If the document you are exporting contains objects that were not supported in the *Export version* selected, the generated file will not contain those objects and a warning will be displayed.

Note: The chosen export options specific to each file type are retained and applied every time the Export dialog is used.

Access methods

Menu	*File	Export...*, set *Save as type* to Materials Studio Study Table Files (*.std) and click *Options...*

XSD/XTD/XOD Export Options dialog

Materials Studio can export XSD, XTD, and XOD files in formats compatible with earlier versions of Materials Studio. Select *File | Export...* from the menu bar.

Saving files in formats from earlier versions of Materials Studio is particularly useful to transfer data to Pipeline Pilot.

To specify which Materials Studio version format to use, set *Save as type* to one of the native Materials Studio file types and click the *Options...* button.

Export version: Specifies version format to use for the export, options are:

- 8.0
- 7.0
- 6.1
- 6.0
- 5.5
- 5.0

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

Cancel: Closes the dialog without updating any settings.

Help: Displays the Help topic in a browser.

Tip: If the document you are exporting contains objects that were not supported in the *Export version* selected, the generated file will not contain those objects and a warning will be displayed.

Note: The chosen export options specific to each file type are retained and applied every time the Export dialog is used.

Access methods

Menu	*File	Export...*, set *Save as type* to Materials Studio 3D Atomistic Files (*.xsd) and click *Options...*
Menu	*File	Export...*, set *Save as type* to Materials Studio 3D Atomistic Trajectory Files (*.xtd) and click *Options...*
Menu	*File	Export...*, set *Save as type* to Materials Studio 3D Atomistic Collection Files (*.xod) and click *Options...*

Import and Insert dialogs

Insert Into Active Document dialog

You can use the Insert Into Active Document dialog to locate and import a document into the currently active document. The contents of the selected document are inserted into the active document without replacing the current contents. This facility is only available for certain specific combinations of source and target document types.

File name: Specifies the name of the file you want to import. If you select a file in the file list area, this filename is automatically entered for you. You can also type in the name of a file. Select the file formats that will be displayed in the file list area. You can set options for some types of file format using the *Options...* button at the bottom of the dialog.

Options...: Provides access to settings that control how some file formats are imported into Materials Studio. The *Options...* button is enabled when the file type dropdown list for the *File name* option is set to a file format that has import options.

Open: Closes the dialog and inserts the contents of the selected file into the current document.

Cancel: Closes the dialog without inserting the file.

Note: The chosen import options specific to each file type are retained and applied every time the Insert Into Active Document dialog is used.

Access methods

Menu	*Edit	Insert From...*
Toolbar	

Import Document dialog

You can use the Import Document dialog to locate and import a document into a project.

It allows navigation to a location on your computer or network. You can select multiple documents by pressing CTRL and clicking on the documents you want to open or by pressing SHIFT and clicking on the first and last files in the range.

File name: Specifies the name of the file you want to import. If you select a file in the file list area, this filename is automatically entered for you. You can also type in the name of a file. Select the file formats that will be displayed in the file list area. You can set options for some types of file format using the *Options...* button at the bottom of the dialog.

Options...: Provides access to settings that control how some file formats are imported into Materials Studio. The *Options...* button is enabled when the file type dropdown list for the *File name* option is set to a file format that has import options.

Tip: Choose *File | Recent Projects* from the menu bar to see a list of the last nine most recently used projects.

Open: Closes the dialog and imports the selected document.

Cancel: Closes the dialog without importing the document.

Note: The chosen import options specific to each file type are retained and applied every time the Import Document dialog is used.

Access methods

Menu	*File	Import...*
Toolbar	

Import URL dialog

You can use the Import URL dialog to locate and import a document using its URL (uniform resource locator), for example:

```
http://www.Accelrys.com/materials/urea.xsd
```

Note: The URL above is fictitious.

Enter the *URL* for the document you want to import into the text box, or choose from the list of up to ten previously entered URLs.

Press *ENTER* or click the *OK* button to import the document.

OK: Closes the dialog and imports the selected document.

Cancel: Closes the dialog without importing the document.

Help: Displays the Help topic in a browser.

Access methods

Menu	*File	Import URL...*
Toolbar	

Import/Insert Failed or Invalid dialog

Materials Studio was unable to import or insert the document or object. The reason for this should be displayed within the error message box.

Invalid Insertion

If the error message box displayed described the error as an invalid insertion, Materials Studio may not support the insertion of the file that you are requesting into the active document.

Only files of specific formats can be inserted into the active document, depending on its type. Use the file type dropdown list for the *File name* in the Insert Into Active Document dialog as an indicator of the valid formats that may be inserted into the document that is currently active.

Contact BIOVIA Support if you require further assistance.

Conversion of Materials Studio projects

Materials Studio must convert projects that were created in older versions of Materials Studio to the new format before they can be loaded. Newer versions of Materials Studio save additional settings which cannot be understood by older versions of Materials Studio. Projects saved in the newer format cannot be opened by older versions of Materials Studio.

WARNING! This conversion cannot be undone even if you exit Materials Studio without saving the project settings. To create a backup copy of the project's files, click the *No* button and exit Materials Studio. Make copies of all of the project's files (the `.stp` file and the project's Files folder and subfolders).

User settings of Materials Studio projects persist in the project's Modules folder.

Yes: Materials Studio converts the project settings.

No: Cancels loading of the project.

Working with the Project Explorer

The following topics discuss how to use the Project Explorer to manage documents in Materials Studio.

Opening project documents

You can use the Project Explorer to open project documents. Each type of document is opened with a particular viewer.

To open a document that is part of the project

Double-click on the document you want to open in the Project Explorer.

or

1. Select the document(s) you want to open in the Project Explorer.
2. Right-click on one of the selected documents.
3. Select *Open* from the shortcut menu.

or

1. Select the document(s) you want to open in the Project Explorer.
2. Click the *Open* button  on the Project Explorer toolbar.

Documents containing saved module settings can be viewed using any tool associated with that module.

To view saved module settings

Double-click on the document you want to open in the Project Explorer. The default tool for the document is opened and the saved module settings are displayed.

or

1. Right-click on the document you want to open in the Project Explorer.
2. Select a tool to use to view the module settings from the shortcut menu.

or

1. Select the document you want to open in the Project Explorer.
2. Click the *Open* button  on the Project Explorer toolbar. The default tool for the document is opened and the saved module settings are displayed.

Creating new folders

You can use the Project Explorer to create new folders in a project.

To create a new folder

1. Right-click on the folder in the Project Explorer in which you want the new folder to be created.
2. Select *New | Folder* from the shortcut menu.

or

1. Select the folder in the Project Explorer in which you want the new folder to be created.
2. Click the *New Folder* button  on the Project Explorer toolbar.

A new folder named `New Folder` appears below the selected folder. Enter a new name for the folder and press ENTER, or press ESC to cancel editing.

> **Note:** The *New Folder* button and *New | Folder* menu command are enabled only if a folder is selected in the Project Explorer.

Importing documents

The *File* menu contains a variety of commands that you can use to create, import, open, and save documents and projects.

> **Note:** If a document with the same name already exists in the current project, the document name will be incremented with a number in parentheses.

To import a document into the project

1. Select *File | Import...* from the main menu. A file browser dialog will appear and enable you to locate the document you want to import.
2. When you have located the document, select it by clicking on it, and then click the *Import* button. A file will be created in the currently selected project folder and the document will open in a new viewer window.

To import a document into the project using the document URL

1. Select *File | Import URL...* from the main menu. The *Import URL* dialog will appear and enable you to specify the URL (Uniform Resource Locator) of the document you want to import.
2. Enter the *URL* for the document you want to import into the text box, or choose from the list of up to ten previously entered URLs. A file will be created in the currently selected project folder and the document will open in a new viewer window.

To copy a file into the project

1. Locate the file in Windows Explorer and copy it to the clipboard, either:
   - Press *CTRL + C*
   - Right-click and choose *Copy* from the shortcut menu
   - Press *F10* and choose *Edit | Copy* from the menu

   Note: When Trajectories and Study Tables are copied in this way any associated hidden documents are also copied.
2. In the Materials Studio Project Explorer select the target folder or the project root, right-click, and chose *Paste* from the shortcut menu.

Moving documents and folders

You can use the Project Explorer to reorganize documents and folders in your project. You can move any folder or document visible in the Project Explorer to any project folder.

When you move project documents and folders using the Project Explorer, the corresponding items on the hard disk are also moved.

To drag and drop to move a file or folder

1. Locate the file or folder in the *Project Explorer*.
2. Click on the item(s) you want to move to select them.
3. Hold the *left mouse button* down and drag the item(s) onto the target folder.
4. Release the *left mouse button*.
5. If you are moving multiple items, on the dialog checking if you want to move them, click *Yes*.

Copying and pasting documents

The *Project Explorer* shortcut menu contains a variety of commands that you can use to copy, paste, and move documents.

Note: When Trajectories and Study Tables are copied in this way any associated hidden documents are also copied.

To copy and paste a file or folder

1. Locate the file or folder in the *Project Explorer* and copy it to the clipboard, right-click and choose *Copy* from the shortcut menu.
2. Select the target folder or the project root and paste the item(s), right-click and choose *Paste* from the shortcut menu.

Tip: The standard Windows shortcuts to copy (*CTRL + C*) and paste (*CTRL + V*) are not currently available in the *Project Explorer*.

To drag and drop to copy a file or folder

1. Locate the file or folder in the *Project Explorer*.
2. Click on the item(s) you want to copy to select them.
3. Hold the *left mouse button* down and drag the item(s) onto the target folder.
4. Press the CTRL key.
   The cursor will show a **+** symbol indicating that the selected item(s) will be copied.
5. Release the *left mouse button*.
6. If you are copying multiple items, on the dialog checking if you want to copy them, click *Yes*.

Sorting the documents in a project

You can use the Project Explorer to sort documents and folders in your project.

> **Tip:** Folders are always displayed before documents, irrespective of any sorting applied.

When you move project documents and folders using the Project Explorer, the corresponding items on the hard disk are also moved.

To sort documents and folders

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

Or:

- Click the *Sort* arrow  on the Project Explorer toolbar and choose the type of sorting to apply, options are:
  - Date Created
  - Name

  The type of sorting currently applied is indicated by the dropdown list tick mark.

> **Tip:** Click the *Sort* button a second time to switch to the other sorting type.

Renaming documents and folders

You can use the Project Explorer to rename project documents and folders. When a project document or folder is renamed, the corresponding item is renamed on the hard disk.

To rename a project document or folder

1. Right-click on the document or folder you want to rename in the Project Explorer.
2. Select *Rename* from the shortcut menu.
3. Enter a new name for the document or folder and press ENTER, or press ESC to cancel editing.

or

1. Select the document or folder you want to rename in the Project Explorer.
2. Click the document or folder name to begin editing.
3. Enter a new name for the document or folder.

or

1. Select the document or folder you want to rename in the Project Explorer.
2. Press F2 to begin editing.
3. Enter a new name for the document or folder.

Deleting documents and folders

You can use the Project Explorer to remove documents and folders from a project. When a project document or folder is deleted, it is either sent to the Recycle Bin or removed from the hard disk.

If the document you are trying to delete is currently displayed in a viewer, the viewer will be closed.

To send documents or folders to the Recycle Bin

1. Select the documents or folders you want to delete in the Project Explorer.
2. Press the DELETE key.

or

1. Right-click on the document or folder you want to delete in the Project Explorer.
2. Select *Delete* from the shortcut menu.

or

1. Select the documents or folders you want to delete in the Project Explorer.
2. Click the *Delete* button  on the Project Explorer toolbar.

> **Tip:** To delete documents without sending them to the Recycle Bin, hold down the SHIFT key while pressing the DELETE key, right-clicking in the Project Explorer, or clicking the toolbar button.

Exporting documents

You can export Materials Studio documents in a wide range of formats using the *Export...* command on the File menu.

To export a structure

1. Make sure that the document containing the structure you want to export is the active document.
2. Select *File | Export...* from the menu bar to open the Export dialog.
3. Select the type of file to generate from the *Save as type* dropdown list.
4. If you select one of the following structure formats, click the *Options...* button to select format-specific options:
   - Cerius2 Structure Files (*.msi)
   - InsightII Molecule Files (*.car; *.cor)
   - Materials Studio 3D Mesoscale Files (*.msd)
5. Navigate to the location where you want to save the exported file and specify the *File name*.
6. Click the *Save* button.

To export an image

1. Make sure that the document containing the structure you want to export is the active document.
2. Select *File | Export...* from the menu bar to open the Export dialog.
3. Select Structure Bitmap (*.bmp) from the *Save as type* dropdown list.
4. Click the *Options...* button to open the Bitmap Export Options dialog.
5. Specify the size of the image to generate and click the *OK* button.
6. Navigate to the location where you want to save the exported file and specify the *File name*.
7. Click the *Save* button.

To export a movie

1. Make sure that the document containing the structure you want to export is the active document.
2. Select *File | Export...* from the menu bar to open the Export dialog.
3. Select Movie Clip (*.avi) from the *Save as type* dropdown list.
4. Click the *Options...* button to open the AVI Export Options dialog.
5. Specify the frames to use, the speed, the size of the frame, and the quality.
6. Click the *OK* button.
7. Navigate to the location where you want to save the exported file and specify the *File name*.
8. Click the *Save* button.

To export to an earlier Materials Studio version

1. Make sure that the document containing the structure you want to export is the active document.
2. Select *File | Export...* from the menu bar to open the Export dialog.
3. Select one of the following from the *Save as type* dropdown list, depending on the document being exported:
   - Materials Studio 3D Atomistic Files (*.xsd)
   - Materials Studio 3D Atomistic Trajectory Files (*.xtd)
   - Materials Studio 3D Atomistic Collection Files (*.xod)
   - Materials Studio Study Table Files (*.std)
4. Click the *Options...* button to open the XSD/XTD/XOD Export Options or STD Export Options dialog.
5. Specify the Materials Studio version format in which to save the file, options are:
   - 8.0
   - 7.0
   - 6.1
   - 6.0
   - 5.5
   - 5.0
6. Navigate to the location where you want to save the exported file and specify the *File name*.
7. Click the *Save* button.

Tip: If the document you are exporting contains objects that were not supported in the *Export version* selected, the generated file will not contain those objects and a warning will be displayed.

Opening a folder in Windows Explorer

You can use the Project Explorer to open Windows Explorer for the folder containing any item.

To open a folder in Windows Explorer

1. Right-click on the file or folder you wish to view in the Project Explorer.
2. Select *Open Containing Folder* from the shortcut menu.

A Windows Explorer is opened for the folder which contains the currently select file or folder.

Note: A Windows Explorer cannot be opened for the project root.

Project Explorer toolbar

The *Project Explorer* toolbar allows you to manage your Materials Studio projects.

Project Explorer toolbar

It contains the following command buttons:

 **Open:** Opens the selected document(s) in the appropriate Materials Studio viewer(s).

 **Delete:** Deletes the selected document(s) and folder(s) from the project and from the disk.

 **New Folder:** Creates a new folder with the default name `New Folder` in the selected folder. Enter a new name for the folder and press ENTER, or press ESC to cancel editing.

 **Refresh:** Refreshes the content of the Project Explorer.

 **Sort:** Sorts the contents of the Project Explorer. Click the dropdown arrow to choose the sort criteria, options are:

- Date Created
- Name

> **Tip:** Folders are always displayed before documents, irrespective of any sorting applied.

 **Help:** Displays help information about the Project Explorer.

Project Explorer shortcut menu

The *Project Explorer* shortcut menu is displayed when you right-click on an item in the Project Explorer. Depending on the context, it contains some of the following commands:

New: Displays a submenu of commands for creating new items.

> **Note:** The *New* command is only available when right-clicking on the project root or a folder in the Project Explorer.

The *New* submenu commands are:

-  **Folder:** Creates a new folder in the current location.
-  **3D Atomistic Document:** Creates an empty 3D Atomistic document in the current folder. The new document is displayed in the 3D Viewer.
-  **3D Mesoscale Document:** Creates an empty 3D Mesoscale document in the current folder. The new document is displayed in the 3D Viewer.
-  **Text Document:** Creates an empty text document in the current folder. The new document is displayed in the Text Viewer.
-  **HTML Document:** Creates an empty HTML document in the current folder. The new document is displayed in the Text Viewer.
-  **Grid Document:** Creates an empty grid document in the current folder. The new document is displayed in the Grid Viewer.
-  **Study Table Document:** Creates an empty study table document in the current folder. The new document is displayed in the Study Table Viewer.
-  **3D Atomistic Collection Document:** Creates an empty 3D Atomistic Collection document in the current folder. The new document is displayed in the 3D Viewer.
-  **Perl Script Document:** Creates a script document containing a standard MaterialsScript header in the current folder. The new document is displayed in the Script Viewer.
-  **Forcefield Document:** Creates a forcefield document containing a *Dummy forcefield type* in the current folder. The new document is displayed in the Forcefield Viewer.

 **Import...:** Displays the Import Document dialog. Browse to the document you want to import, then click the *Import* button. The document is imported into the current folder.

> **Note:** The *Import* command is only available when right-clicking on a folder in the Project Explorer.

 **Open:** Opens the selected document(s) in the appropriate viewer(s). If a document is already open but hidden behind other windows, it will be brought to the front.

Insert Into: Imports the selected document into the currently active document. The contents of the selected document are inserted into the active document without replacing the current contents.

> **Note:** The *Insert Into* command is only available for certain specific combinations of source and target document types.

Open Containing Folder: Opens the folder containing the selected document in Windows Explorer.

 **Delete:** Removes the selected document(s) and/or folder(s) from the project. When a project document or folder is deleted from the project, it is also removed from the hard disk.

Rename: Enables you to rename the selected project document or folder.

Note: The *Rename* command is only available when a single item is selected in the Project Explorer.

 **Copy:** Copies the currently selected document or folder to the clipboard.

 **Paste:** Pastes the contents of the clipboard to the current location in the project.

 **Refresh:** Refreshes the content of the Project Explorer.

 **Properties:** Displays a standard Windows Properties dialog box for the selected document or folder.

Documents which contain saved module settings have additional menu items for tools that can be used to view the stored module settings. Selecting one of these opens the corresponding tool and displays the module settings stored in the document.

Working with project settings

Some tools in the Materials Visualizer and all Materials Studio modules have default settings for certain parameters. These settings are created when you change the parameters in question from their default values and then save the project. The Settings Organizer dialog allows you to create a template project containing your preferred settings for new projects and also to share your tool and module settings between different projects.

About the template project

The template project governs the initial state of all the configurable parameters for the Materials Visualizer tools and Materials Studio modules in new projects. For example, if you wanted to change the default charge equilibration method from QEq to Gasteiger in all new projects that you create in future, you would make the appropriate change on the Charges dialog, then export the *Charges* settings from the current project into the template project using the Settings Organizer dialog. Thereafter, whenever you created a new project, the Charges dialog would always be set to use Gasteiger charge equilibration you specified rather than the default of QEq value set by Accelrys.

By default, an empty template project (`Normal.stp`) is created within your Windows user profile, for example, `C:\Documents and Settings\[user name]\Application Data\Accelrys\Materials Studio\[version]\Templates\Normal.stp`.

Using settings from external projects

There can be times when a group of related settings that you have are suitable to a certain type of work and you may wish to re-use them in another project. The Settings Organizer dialog allows you to import some or all of the settings from one or more external project into your current project, thus saving you the time and effort of continually reconfiguring your settings whenever you want to perform certain types of calculation.

Setting project defaults

Materials Studio allows you to alter the default settings of many parameters for some Materials Visualizer tools and all the Materials Studio modules by creating a template project that governs the initial state of all these configurable parameters in new projects. This means that you only need to set all your preferences once for your template project. Thereafter, whenever you create a new project, your preferred settings will automatically be imported and applied, overwriting the default values set by Accelrys. You can also transfer settings between projects, including the template project, allowing you rapidly to configure your projects.

To set up a template project

1. Open the project containing the settings that you wish to transfer to the template project.
2. Open the template project using the *Saved settings in external project* entry box. The template project (`Normal.stp`) is automatically created in the location defined on the Locations tab of the Options dialog. If you have previously customized any settings in the template project, they will be shown in the *Saved settings in external project* tree view. If you are altering the template project for the first time, this field will be blank.
3. Select the settings that you wish to transfer from the *All settings in current project* tree view and click the *Save >>* button. Any existing settings defined for the template project will be overwritten by the transferred settings.

   Tip: The *All settings in current project* and *Saved settings in external project* fields support multiple selection. Select multiple items by holding down the CTRL key and clicking on them individually or by holding down SHIFT and selecting the first and last items in a range. Alternatively, click and drag to the right of the tree view items to describe a rectangular selection region or click on a parent item to select all its children.

4. Repeat steps 1-3 to export further settings to the template project from other projects. If you make any errors, you can return settings in the template project to their Accelrys default values by selecting the appropriate settings in the *Saved settings in external project* tree view and clicking the *Delete* button.

Tip: It is also possible to manually configure parameter settings in the template project by opening it in the normal way, displaying the dialog containing the parameters you wish to set, and then closing the dialog. Your preferences will be saved in the template project and will be applied to any new projects you create subsequently.

To exchange settings with an external project

1. Open a project that you wish to transfer settings into or out from.
2. Select an external project that you wish to transfer settings into and out of from the *Saved settings in external project* dropdown list. Alternatively, click the ... button to display the Choose Project dialog and browse to an external project, then click the *Open* button.
3. If you wish to export settings from the current project to the external project, select the settings that you wish to transfer from the *All settings in current project* tree view and click the *Save >>* button. Any existing settings defined for the external project will be overwritten by the transferred settings.

   Tip: The *All settings in current project* and *Saved settings in external project* fields support multiple selection. Select multiple items by holding down the CTRL key and clicking on them individually or by holding down SHIFT and selecting the first and last items in a range. Alternatively, click and drag to the right of the tree view items to describe a rectangular selection region or click on a parent item to select all its children.

4. If you want to import settings from the external project into the current project, select the settings that you wish to transfer from the *Saved settings in external project* tree view and click the *<< Load* button. Any existing settings defined for the current project will be overwritten by the transferred settings.
5. If you wish to return settings in the external project to their Accelrys default values, select the appropriate settings in the *Saved settings in external project* tree view and click the *Delete* button.

   Note: Unlike the *<< Load* and *Reset* buttons, the action of the *Delete* button cannot be undone; however, the deleted files can be restored from the Windows Recycle Bin if necessary. The action of the *Save >>* button cannot be undone.

6. If you want to return any settings in the current project to the default values set by Accelrys, select the appropriate settings in the *All settings in current project* tree view and click the *Reset* button.

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.

All settings in current project: Displays all the settings that are present in the current project. The settings are organized into two folders: the *Modules* folder contains module settings and the *Visualizer* folder contains settings for Materials Visualizer tools. The exact contents of the folders are dependent on the modules and tools that are available in your installation. Double-clicking in this window will transfer settings in exactly the same way as clicking the *Save >>* button.

Saved settings in external project: Select an external project from which to import customized settings from the dropdown list. The dropdown list shows the template project, if you have created one, and the 10 most recently accessed projects. Alternatively, enter the path to a project file (`.stp`) directly into the field or click the ... button to display the Choose Project dialog and browse to an external project. Double-clicking in this window will transfer settings in exactly the same way as clicking the *<< Load* button.

Tip: The *All settings in current project* and *Saved settings in external project* fields support multiple selection. Select multiple items by holding down the CTRL key and clicking on them individually or by holding down SHIFT and selecting the first and last items in a range. Alternatively, click and drag to the right of the tree view items to describe a rectangular selection region or click on a parent item to select all its children.

Save >>: Copies the selected settings in the current project into the specified external or template project, overwriting any existing settings.

<< Load: Copies the selected settings in the specified external into the current project, overwriting any existing settings.

Reset: Returns the selected settings in the current project to the default values set by Accelrys. Projects may also be reset by pressing the DELETE key while in the *All Settings in Current Project* view.

Delete: Removes the selected settings from the specified external project, restoring the settings to the default values set by Accelrys. Pressing the DELETE key while in the *Saved settings in external project* has the same action.

Note: The *Save >>*, *<< Load*, and *Delete* buttons are enabled only if an external project is displayed in the *Saved settings in external project* field.
Unlike the *<< Load* and *Reset* buttons, the action of the *Delete* button cannot be undone; however, the deleted files can be restored from the Windows Recycle Bin if necessary. The action of the *Save >>* button cannot be undone.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Tools	Settings Organizer*

Common Visualizer operations

The Materials Visualizer provides the core modeling and visualization capabilities for Materials Studio. It allows you to visualize 3D models with a variety of display styles, labels, and measurement tools.

Viewing documents

Data are presented in Materials Studio through several types of document views. The following viewers are available:

- 3D Viewer
- Chart Viewer
- Grid Viewer
- Script Viewer
- Study Table Viewer
- Text Viewer

Selecting objects

Most operations in Materials Studio act upon whichever objects are selected in the active document.

When a document is made active, its contents are implicitly selected, and operations act upon all of the objects in the document. To refine the selection, groups of objects or individual objects can be selected before running an operation.

Selection simply allows you to mark objects to be worked on at a particular moment in time. If you don't want to lose information about selection of objects in a 3D Atomistic document, you can save them as a set. A set stores data about which objects are selected and allows you to recreate the same selection in the future.

Selected objects are indicated graphically in the user interface for as long as they are in a selected state. For example, selected objects in a 3D Atomistic document are colored yellow.

Editing documents

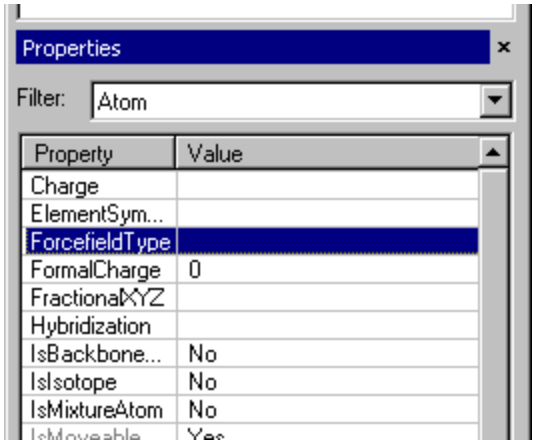
The *Edit* menu contains a variety of commands that you can use to edit documents. The commands that are available vary depending on whether the active document is 3D, Text, Grid, or Chart.

> **Note:** The *Edit* menu is context-sensitive: the choice of commands displayed depends on the document type that is currently active.

Available commands include Undo and Redo, *Cut*, *Copy*, *Paste* and *Delete*, as well as *Select all*.

Viewing and editing properties

You can use the Properties Explorer to view or edit the properties of selected items in an active document window, including 3D, Chart, Grid, and Text documents. You can work with all the objects in the document window (with no individual objects selected), or one or more selected objects. Since there are a large number of properties for most types of object, the Properties Explorer defaults to show the more interesting properties. Properties that cannot be edited are disabled.



Properties Explorer

To edit object properties

1. Choose *View | Explorers | Properties Explorer* to open the Properties Explorer. *Filter* lists the types of object that are in the selection.
2. Select an object type to see properties only for objects of that type. A property will only have a displayed value if all objects have the same value for that property. Choose All to show properties for all the selected objects; if you selected more than one type of object, the list contains only those properties that are common to all the objects in the selection.
3. Double-click on a property to display an editing dialog. The dialog that appears depends on the property type.

Tip: To show all the properties for the selected objects, select All from the *Filter* list.

Saving and document operations

The *File* menu contains a variety of commands that you can use to create, import, open, and save documents and projects.

To create a new document

1. To create a new document, select *File | New...* from the main menu.

   A window will appear containing a list of the types of document that you can create, such as *3D Atomistic*, *Text*, and *HTML*.
2. Select one of the document types by clicking on its icon, and then click the *OK* button.

   A new view window will open within Materials Studio, containing a view of the new document. An entry for the new document will also appear in the Project Explorer.
3. You can use the Project Explorer to give the document a new name. You can also create a new document by using the toolbar or shortcut menu in the Project Explorer.

To open an existing project document

1. If the document you want to open is visible within the Project Explorer then simply double-click on its entry. The document will open in a new viewer window. If the document is already open, but perhaps hidden behind other windows, it will pop to the front.
2. If you can't see the document you want to open in the Project Explorer, then select *File | Import...* from the main menu. A file browser dialog will appear and enable you to locate the document you want to open.
3. Browse to the project folder, locate the document, select it by clicking on it, and then click the *Import* button. The document will open in a new viewer window. If the document is already open, but perhaps hidden behind other windows, it will pop to the front.

To open multiple project documents

1. Select the documents you want to open using the Project Explorer.
2. Right-click on one of the selected documents and click *Open*.

To save a document

You should periodically save changes that you have made to the documents with which you are working. The *File* menu contains several commands that you can use to save changes to documents.

Save: Saves changes that have been made to the active document.

Save As: Saves the active document with a new name, for which you will be prompted. The document can be saved only within the project folder and in the Materials Studio file format for this document type.

Export: Exports the active document to a location outside of the project using any of the export file formats supported by Materials Studio.

When you close a document that has unsaved changes, you will be asked by Materials Studio whether you want to save those changes. You will also be prompted if you close Materials Studio or open a different project when you have documents with unsaved changes open.

Printing

Materials Studio can generate print output from any of its viewers. The printed page is a copy of what is seen on the screen. The resolution of printed output is determined by the view type, *Printer Setup* settings, and the printer settings.

Print resolution

The resolution of the printed image of a 3D structure can be adjusted using the *Low*, *Medium*, and *High* Quality buttons in the *File | Printer Setup | Properties | Advanced* option. A low quality printout uses one-fourth the resolution of the printer, medium quality uses one-half, and high quality uses the full resolution of the printer.

Sending output to the printer

1. To print the contents of the current view, choose *File | Print* from the menu bar.
2. In the standard Print dialog box, choose the printer in the *Printer Name* field. If necessary, click the *Properties* button to change the settings for the current printer.

Note: Graphics are produced as bitmaps, even if generated for PostScript output.

Note: High quality printing may require several minutes.

Sharing Materials Studio data

Materials Studio data can be shared with many other desktop applications either by copying and pasting to and from the clipboard or by importing and exporting documents as files. The following topics contain details about sharing data with various applications.

Sharing with Microsoft Office products

Clipboard sharing

To copy 3D structures

It is simple to use the clipboard to transfer an image of a 3D structure from Materials Studio into Microsoft Office products such as MS Word, MS Excel, and MS Powerpoint.

1. Once you have the structure at a size and aspect ratio that suits you, choose *Edit* | *Copy* from the main menu.
2. Then, in the Office product, choose *Edit* | *Paste* to insert the bitmap.

To copy charts and grids

Both images and data may be copied to the clipboard from Materials Studio Chart and Grid Viewers, and pasted into MS Office products.

In this case, since text and multiple graphics formats are copied to the clipboard, choose *Edit* | *Paste Special* from the Office product's menu bar to specify the format that you wish to paste.

File sharing

Certain files are suitable for data interchange between Materials Studio and Microsoft Office products.

Materials Studio Document Type	Format	Import/Export	MS Office Product
3D Model	Bitmap (`.bmp`)	Export only	MS Word, MS Excel, MS Powerpoint
Chart	Bitmap (`.bmp`), Windows Enhanced Metafile (`.emf`)	Export only	MS Word, MS Excel, MS Powerpoint
	Comma delimited (`.csv`)	Export only	MS Excel
Table	Comma delimited (`.csv`)	Import and Export	MS Excel
Text	ASCII text (`.txt`)	Import and Export	MS Word, MS Excel
HTML	HTML (`.html`, `.htm`)	Import and Export	MS Word, MS Excel, MS Powerpoint

Sharing with Accelrys programs

Clipboard sharing

It is possible to use the clipboard to transfer a 3D structure from Materials Studio to Discovery Studio and vice versa.

1. Choose *Edit* | *Copy* from the menu bar or press CTRL + C in the application containing the structure you wish to transfer.
2. In application you wish to transfer the structure to, select *Edit* | *Paste* from menu bar or press CTRL + V to insert the structure.

To copy part of the structure, select the portion you want to copy before performing the copy/paste steps described above.

File sharing

The table below provides guidance on the file formats that are suitable for data interchange between Materials Studio and other Accelrys software.

Document type	File format	Materials Studio	Discovery Studio	Cerius^2	Insight II	Pipeline Pilot
3D structure	.msi	Import/Export	Import	Import/Export	N/A	Import/Export
	.car/.mdf	Import/Export	Import	Import/Export	Import/Export	Import/Export
	.mol2	Import/Export	Import/Export	N/A	N/A	Import/Export
	.xtl	Import	N/A	Import/Export	Import/Export	N/A
	.mol	Import/Export	Import/Export	Import/Export	Import/Export	Import/Export
	.pdb	Import/Export	Import/Export	Import/Export	Import/Export	Import/Export
	.cif	Import/Export	Import	Import	N/A	Import/Export
	.xyz	Import	Import/Export	N/A	N/A	N/A
	.xsd	Import/Export	N/A	N/A	N/A	Import/Export
3D trajectory	.trj/ `.msi`	Import	N/A	Import/Export	N/A	Import/Export
	.his/ `.car`	Import/Export	N/A	Import/Export	Import/Export	Import/Export
	.xtd	Import/Export	N/A	N/A	N/A	Import/Export
Chart	.tbl (tabular)	Import	N/A	Import	Import/Export	N/A
Study Table	.std	Import/Export	N/A	N/A	N/A	Import/Export

Pipeline Pilot

Pipeline Pilot is a powerful tool capable of manipulating and analyzing large quantities of scientific data. Structures exported by Materials Studio can be used as input for various Pipeline Pilot collections in the following formats:

- ACX
- CAR
- CIF
- MDL
- MOL
- MOL2
- MSI
- PDB
- RES
- SD
- SDF
- XSD
- XTD

For more information on Pipeline Pilot and the Materials Studio Collection please contact BIOVIA Support.

Discovery Studio

Nonperiodic 3D structure data may be shared between Materials Studio and Discovery Studio using `.mol`, `.mol2`, `.sd` or `.pdb` files. Periodic 3D structure data may be transferred from Materials Studio to Discovery Studio using `.msi`, `.car`, `.mdf`, `.pdb` or `.cif` files.

Multiframe documents, such as trajectories, and documents containing periodic structures can be exchanged using the `.mol2` format. Standard Materials Studio trajectories (`.xtd` file format) can be exported directly as `.mol2` multi-structure files.

The table below provides guidance on the file formats that are suitable for data interchange between Materials Studio and Discovery Studio.

From	To	File formats to use
Discovery Studio	Materials Studio	`.mol`, `.mol2`, `.sd`, `.pdb`, `.xyz`
Materials Studio	Discovery Studio	`.msi`, `.car`, `.mol`, `.mol2`, `.sd`, `.cif`, `.pdb`

PDB Import Options dialog

Materials Studio can import files in the PDB format. Select *File | Import...* from the main menu.

By default, a crystal is not generated when a PDB file is imported. This is because of the typically large size of PDB entries, which would lead to very long import times. To specify that a crystal should be built on import, select Protein Data Bank Files (*.pdb, *.ent) from the file types dropdown list for the *File name* and click the *Options...* button to open the PDB Import Options dialog.

Load all frames: Specifies that all frames of the PDB document will be imported into a single XSD document.

Note: A PDB file can contain multiple MODEL records with various structures. By default, only first of those records is imported and displayed. If the *Load all frames* box is checked, all records will be imported.

Automatically build crystal: Specifies that a crystal should automatically be generated on import.

Note: In the case of PDB files containing data where the structure was determined by a technique other than crystallography, the CRYST1 record contains a = b = c = 1.0, alpha = beta = gamma = 90 degrees, space group = P 1, and Z = 1. In these cases, a crystal will not be built, regardless of whether the *Automatically build crystal* box is checked.

Lattice orientation: The PDB file format specification assumes that the crystal cell is oriented with A along the X axis of the Cartesian system, and with B in the XY plane, unless otherwise specified. However, some applications write the file assuming a different orientation. As the atom coordinates are given within the Cartesian framework, this is highly significant. The *Lattice orientation* control allows the specification of a different orientation option for the import.

Tip: If A along X, B in XY plane is not appropriate for the file you are importing, then the next most likely lattice orientation is C along Z, B in YZ plane.

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

Cancel: Closes the dialog without updating any settings.

Help: Displays the Help topic in a browser.

Note: The chosen import options specific to each file type are retained and applied every time the Import Document dialog is used.

Access methods

Menu	*File* | *Import*, choose Protein Data Bank Files (*.pdb, *.ent) from the file types dropdown list for *File name* and then click *Options...*

Cerius^2

3D structure data can be most easily transferred between Cerius^2 and Materials Studio using the `.msi` format, although `.car`/`.mdf`, `.mol`, `.pdb`, `.cif` and `.xtl` can also be used. For more information about the types of 3D structure data that can be shared, see the detailed entries on `.msi`, `.car`/`.mdf`, `.mol`, `.pdb`, `.cif`, `.xtl` files.

Currently Chart and Grid data cannot be shared between Cerius^2 and Materials Studio.

When reading files generated under Windows into programs running on UNIX, it is advisable to perform a file conversion to remove extraneous characters. When going in the opposite direction, that is, reading UNIX-generated files into Materials Studio, no conversion is required.

Insight II

3D structure data can be most easily transferred between Insight II and Materials Studio using the `.car`/`.mdf` format, although the `.mol`, `.pdb` and `.xtl` formats can also be used. For more information about the types of 3D structure data that can be shared, see the detailed entries on the `.car`, `.mol`, `.pdb` and `.xtl` file formats.

Chart and Grid data can be transferred from Insight II to Materials Studio using the `.tbl` format.

When reading files generated under Windows into programs running on UNIX, it is advisable to perform a file conversion to remove extraneous characters. When reading UNIX-generated files into Materials Studio, no conversion is required.

Sharing with other scientific programs

Clipboard sharing

It is possible to use the clipboard to copy a 3D structure from Materials Studio and paste it into ISIS/Draw as a 2D structure and vice versa.

To copy a structure to or from Materials Studio

1. Choose *Edit* | *Copy* from the menu bar or press CTRL + C in the application containing the structure you wish to transfer.
2. In application you wish to transfer the structure to, select *Edit* | *Paste* from menu bar or press CTRL + V to insert the structure.

To copy part of the structure, select the portion you want to copy before performing the copy/paste steps described above.

File sharing

Data may be shared between Materials Studio and other scientific programs via several file formats supported by Materials Studio. Notably, .cif files can be used to exchange data with the Cambridge Structural Database (http://www.ccdc.cam.ac.uk) and .mol files can be used to exchange data with other programs (http://accelrys.com/products/informatics/cheminformatics/ctfile-formats/no-fee.php).

ISIS/Sketch files (.skc) can be imported into Materials Studio as 3D Atomistic documents (.xsd).

Grid documents can be exchanged between Materials Studio and many other applications in comma-separated format (.csv).

Simple text files (.txt) can be exchanged with word processors such as Notepad.

HTML files (.htm) can be exchanged with web browsers.

Finally, bitmap files (.bmp) can be exported by Materials Studio and read by programs that can process images, for example, Microsoft Photo Editor.

Sharing files between Windows and UNIX

ASCII files (such as the `.msi` and `.car` files) can be viewed using ordinary word processors, such as Notepad on Windows or vi on UNIX. However, there is an important difference between files generated in these two environments: ASCII files generated under the Windows operating system have an extra carriage return (<CR>) at the end of each line, and this can confuse programs on UNIX systems. The converse is not a problem: ASCII files generated under UNIX can be read by Materials Studio without difficulty.

These extra <CR>s may be removed in several ways.

On most Altix systems the command:

```
to_unix input_file output_file
```

will convert the Windows file *input_file* to the UNIX file *output_file*.

On most Linux systems the command:

```
dos2unix input_file
```

will convert the windows file *input_file* to UNIX format.

Alternatively, you can accomplish the same thing using the vi editor. The line edit command:

```
1,$s/^M//
```

will remove all the (<CR>)s.

Note: *^M* signifies CTRL + M and may be entered by typing CTRL + V followed by CTRL + M.

On most Linux systems the line edit command:

```
set ff=unix
```

followed by a file write will convert the file to UNIX format.

Selecting objects and groups of objects

Many operations in Materials Studio operate upon those objects that are selected in the active document.

Note: By convention, when no objects are selected, this is equivalent to all objects being selected. For example, to apply a particular display style to all atoms in a 3D Atomistic document, first ensure that nothing is selected, then apply the atom display style.

Objects in a document are usually selected by using the mouse within a view of that document and these techniques apply to all object types. There are more sophisticated tools provided for selecting atoms, bonds, distances, angles, and torsions in 3D Atomistic documents because of their importance in materials modeling.

Selections may be added to existing selections or entirely replace existing selections.

Note: Once objects in a 3D Atomistic document are selected, the current selection may be stored as a set. Once a set is stored in a 3D Atomistic document, it may be retrieved and its contents selected again at any time.

To deselect all objects in a document

To clear all selections in a document, just click in empty space within a document view or press CTRL + D.

Selecting and deselecting individual objects

Many kinds of objects in Materials Studio documents can be selected, for example, the atoms in a 3D Atomistic document or the markers in a chart document. The usual way to achieve this is simply to place the mouse cursor over the object in the viewer and click with the left mouse button. In some instances, this default selection mechanism is overridden in order to perform a context-specific task (for example, when sketching atoms or adding chart markers). In these cases, it may be necessary to use a selection rectangle or selection lasso in order to select objects, or to use one of the SHIFT or CTRL keys to modulate the left mouse button click, as detailed in the tasks below.

Selected objects in the 3D Viewer are displayed in yellow. In other views, where a white background is the norm, the default system highlight color is used.

Selecting an object, replacing any current selection settings

Click on the object with the left mouse button. Any other selected objects are deselected and the object becomes selected.

Selecting an object, without changing any other selection settings

Click on the object with the left mouse button while holding down the SHIFT key. The object becomes selected, in addition to any objects already selected.

Toggling object selection, without changing any other selection settings

Click on the object with the left mouse button while holding down the CTRL key. The object toggles its selection state (if selected it becomes deselected, and vice versa). All other selected objects remain selected.

Selecting and deselecting groups of objects

As an alternative to picking on an individual object to select it, one or more objects may be selected graphically by describing a region of the view with the mouse. All objects in this region are considered

"picked".

There are two methods of region picking: rectangle and lasso. Lasso picking only applies to objects in 3D views.

Rectangle pick (left mouse button). The starting point of the mouse forms one vertex of a rectangle and the current location of the mouse is the opposite vertex. Use this technique to describe a strictly rectangular region. In the task descriptions below, use the E key to effect a rectangle pick.

> **Note:** The rectangle pick selection mode is the default cursor mode. In other cursor modes the rectangle pick can be used by holding down the E key with the left mouse button.

Lasso pick (left mouse button + Q key). The solid border of the region follows the movement of the mouse and a dashed line connects the location of the cursor with the origin of the selection. Use this technique to describe an arbitrarily-shaped region. In the task descriptions below, use the Q key to effect a lasso pick.

> **Note:** Selected objects in the 3D Viewer are displayed in yellow. In other views, where a white background is the norm, the default system highlight color is used.

Selecting multiple objects, replacing any current selection settings

Describe a region by dragging the mouse with the left mouse button down, or with the left mouse button and the Q key. Release the mouse button to complete the operation. Any other selected objects are deselected and the objects in the described region become selected.

Selecting multiple objects, without changing any other selection settings

Describe a region by dragging the mouse with the left mouse button down, or with the left mouse button and the Q key and the SHIFT key. Release the mouse button to complete the operation. The objects in the described region become selected, in addition to any objects already selected.

Toggling the selection of multiple objects, without changing any other selection settings

Describe a region by dragging the mouse with the left mouse button down, or with the left mouse button and the Q + CTRL keys. Release the mouse button to complete the operation. The objects in the described region toggle their selection state (selected objects become deselected, and vice versa). All other selected objects remain selected.

Selecting similar objects

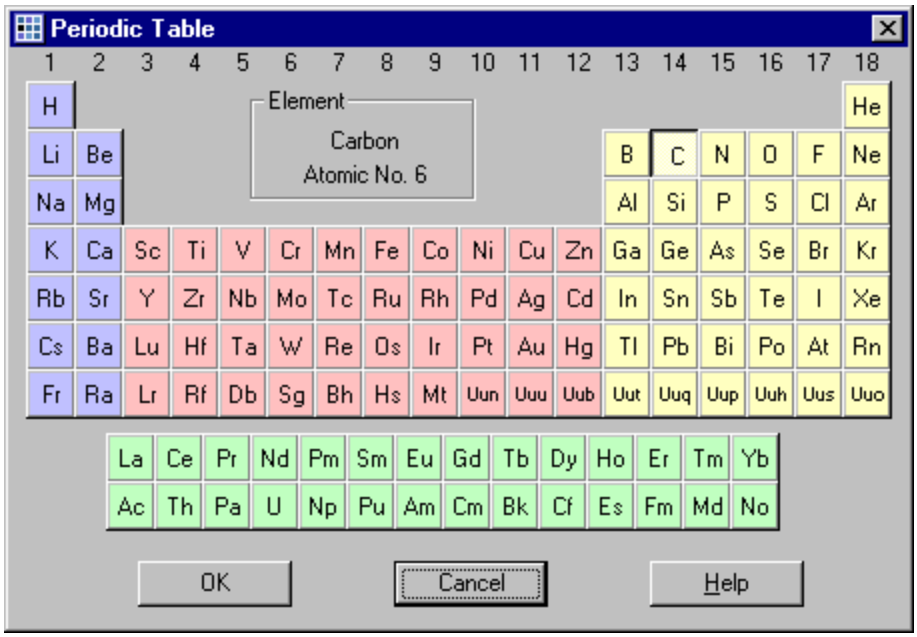
Often, it is convenient to select all objects of a certain type, such as all the hydrogens or all the bonds in a structure.

To select all objects of a certain type

Press and hold the ALT key and double-click on an object. Every object of that type will be selected.

Selecting elements

Materials Studio maintains a list containing common elements and those you have used recently. If an element you require is not in the list, you can add to it in several dialogs and also from the *Document* toolbar. The change you make to this list is applied system wide.



To select an element

1. Choose *Modify | Element Properties* from the menu bar.
2. Type a periodic symbol or atomic number in the *Element* list or click the ... button next to the list and choose an element from the *Periodic Table* dialog.
3. In the dialog, click a *Periodic Symbol* button in the table. The element name and atomic number is displayed.
4. Click *OK* to add the element to the list.

Tip: You can also view the periodic table by choosing *Modify | Modify Element | Periodic Table...*.

Selecting fragments

It is often convenient to select all atoms and bonds connected together in a wholly bonded fragment so that they can be manipulated. If these atoms and bonds are contained in a molecule in a 3D Model document, then this can be achieved by double-clicking (see Selecting by hierarchy). However, this is sometimes not the case, for instance, if the 3D Model document has been imported from a file format that does not store molecules (for example .msi files).

To select a connected fragment of atoms and bonds

1. Select one or more atoms and bonds in the fragment.
2. Right-click in the 3D Viewer window and choose *Select Fragment* from the shortcut menu.

Selecting symmetry images

It is sometimes useful to be able to select all objects in a symmetry system that are related by symmetry. For example, you may wish to color all the facets of a given form in a Morphology crystal habit representation. However, it is not necessarily obvious which facets in a crystal habit belong to the same form. Similarly, selecting related atoms in a crystal manually using the mouse could be difficult. The *Select Symmetry Images* command provides a convenient way to select all the objects that are related by symmetry to the current selection.

To select an object and its symmetry images

1. Select one or more objects which are subject to symmetry.
2. Right-click in the 3D Viewer window and choose *Select Symmetry Images* from the context menu.

Selecting fields, surfaces, segregates, slices, and mesoscale molecules

Depending on the display style chosen, volumetric objects such as fields, isosurfaces, slices, and mesoscale molecules do not always have a representation in the 3D Viewer from which you can pick and select them easily. So, a special control, the Volumetric Selection dialog, provides a convenient tree view of all volumetric objects defined in the current 3D model document.

Selecting volumetric objects

Either, if the objects that you wish to select are visible, select them as described in Selecting objects and groups of objects.

Or, if the objects are invisible or difficult to pick, then:

1. Display the Volume Visualization toolbar by selecting *View | Toolbars | Volume Visualization* from the menu bar.
2. Choose the *Volumetric Selection* tool  on the *Volume Visualization* toolbar to open the Volumetric Selection dialog.

   Note: This button and the associated dialog are enabled only if the current document contains one or more fields.

   The top level of the tree hierarchy shows the fields present in the current 3D model document. Each field can have one or more isosurfaces or slices associated with it, which are displayed by expanding the corresponding node.
3. Select volumetric objects in the tree view by clicking on the  *Field*,  *Atom Volumes Field*,  *Isosurface*,  *Slice*,  *Segregate*,  *Segregator*, or  *Mesoscale Molecules* icons.
4. Perform multiple selections using the SHIFT or CTRL keys.

Renaming volumetric objects

Either:

1. Select a field, isosurface, slice, or set of mesoscale molecules as described above.
2. In the Properties Explorer, change the *Name* property.

Or:

1. Display the Volume Visualization toolbar by selecting *View | Toolbars | Volume Visualization* from the menu bar.
2. Choose the *Volumetric Selection* tool  on the *Volume Visualization* toolbar to open the Volumetric Selection dialog.

   Note: This button and the associated dialog are enabled only if the current document contains one or more fields.
3. If necessary, expand the field nodes to display the slices and isosurfaces associated with that field.
4. Select the field, isosurface, slice, or set of mesoscale molecules in the Volumetric Selection dialog. Click on its name and enter a new name.

Controlling the visibility of volumetric objects

The standard method of controlling visibility of objects in Materials Studio is via the Properties Explorer (see Structure visibility). Since volumetric objects frequently obscure each other, an easier method of controlling visibility for these objects is provided by the Volumetric Selection and Display Style dialogs.

Either:

1. Select one or more volumetric objects and bring up the appropriate tab on the Display Style dialog.
2. Check or uncheck the *Visible* checkbox.

Or:

1. Open the Volumetric Selection dialog as described above.
2. If necessary, expand the field nodes to see slices and isosurfaces associated with each field.
3. Check or uncheck the checkboxes next to the *Field*, *Isosurface*, *Slice*, *Segregate*, *Segregator*, or *Mesoscale Molecules* icons to make the corresponding objects visible or invisible.

Deleting volumetric objects

Either:

1. Select a field, isosurface, slice, or set of mesoscale molecules as described above.
2. In the 3D Viewer, press the DELETE key.

Or:

1. Open the Volumetric Selection dialog as described above.
2. If necessary, expand the field nodes in the tree view to display the slices and isosurfaces associated with each field.
3. Select the volumetric objects to be deleted.
4. Press the DELETE key.

Selecting according to properties

As an alternative to the direct approach of selecting objects using the keyboard and mouse, some objects can be selected based on the value of one or more of their properties. Currently, selection by property is supported only for atoms.

To select all silicon atoms in a large structure using just the mouse would be tedious; instead you can specify the atom property (element) and value (Si) and the Materials Visualizer can select all the Si atoms.

Selecting atoms by property value

1. Ensure that the structure that you wish to work with is in the currently active view.
2. Choose *Edit | Atom Selection* from the menu bar to open the Atom Selection dialog.
3. Choose the property that you wish to use for selection from the *Property* list.
4. Set the selection condition, if it can be set for this property.
5. Fill out any required value parameters for this condition. This might be a limit, a range, or a value.
6. Set the *Selection Mode*, depending on whether you want to:
   - Cancel any existing selection settings and create a new atom selection from atoms in the 3D structure that meet the selection criteria.
   - Create a new atom selection, but only include atoms that meet the selection criteria *and* are currently selected.
   - Add to the atom selection atoms in the 3D structure that meet the selection criteria, but also retain the existing atom selection.
7. Click the *Select* button to apply the selection to the currently active 3D structure.

Selecting by hierarchy

Materials Studio employs a hierarchical description of the data within documents, especially 3D Atomistic documents. For example, atoms and bonds are usually contained within molecules and polymer repeat units are contained within polymer chains. This simplifies the display and manipulation of data within the document. It can often be convenient to select the parent object containing a given object so that they can be manipulated. This can be achieved in two ways:

- Double-click on an object that has already been selected to select its parent and all other objects sharing that same parent.
- Select one or more objects and then right-click within the 3D Viewer window to display the shortcut menu. In the middle of this menu is the command *Select <Type>* [*Name*], where *<Type>* is the category that the common parent of all the currently selected objects belongs to and [*Name*] is the name of this particular common parent. Choosing this command selects the parent object and all other objects sharing this parent.

Tip: You can remove the Molecule or Polymer hierarchy levels from the current selection by right-clicking within the 3D Viewer window and choosing *Remove Molecule Hierarchy* or *Remove Polymer Hierarchy*, as appropriate, from the shortcut menu. This option is only available when such a hierarchy exists in the currently active 3D structure document.

Removing the hierarchy

It may occasionally be useful to remove the formal hierarchy from a 3D Atomistic document. For example, you may wish to redefine the existing hierarchy for a Morphology calculation. The *Remove Molecule Hierarchy* and *Remove Polymer Hierarchy* commands allow you to remove the hierarchy from the current selection.

To remove the Molecule or Polymer hierarchy

1. Select one or more molecular fragments.
2. Right-click within the 3D Viewer window and choose *Remove Molecule Hierarchy* or *Remove Polymer Hierarchy*, as appropriate, from the shortcut menu.

Finding patterns

The following examples illustrate several common uses of the Find Patterns tool.

To find bonded C-H pairs in butane

1. Open a new 3D Atomistic document and either sketch a carbon atom bonded to a hydrogen atom or copy and paste a C-H fragment from an existing document. Save the document as CHPair.xsd.
2. Import the file Examples\Documents\3D Model\butane.msi and save the project.
3. Select *Edit | Find Patterns* from the menu bar to display the Find Patterns dialog. Select CHPair.xsd as the *Pattern document* and choose Element Type as the *Match property*.
4. Ensure that butane.xsd is the active document and click the *Find* button.

A message will appear in the status bar reporting that 10 distinct matches have been found. These are indicated by wireframes around the atoms in question. Materials Studio will create 10 objects, each of which contains a carbon-hydrogen pair.

By editing the element types in the pattern document, different pairs of atoms can be screened. The pairs can be entered into a new set using the Define New Set dialog. This is especially useful for providing input into analytical applications.

A similar procedure can be used to find bond lengths, except that instead of identifying the pairs of atoms involved, the result of the *Find* operation is to create distance measurements.

To find C-H bond distances in butane

1. Open a new 3D Atomistic document and either sketch a carbon atom bonded to a hydrogen atom or copy and paste a C-H fragment from an existing document.
2. Create a distance measurement on the C-H bond and select this measurement object. Save the document as CHPair.xsd.
3. Import the file Examples\Documents\3D Model\butane.msi and save the project.
4. Select *Edit | Find Patterns* from the menu bar to display the Find Patterns dialog. Select CHPair.xsd as the *Pattern document* and choose Element Type as the *Match property*.
5. Ensure that butane.xsd is the active document and click the *Find* button.

Again, a message will appear in the status bar reporting that 10 matches have been found. However, instead of identifying the atoms which match the pattern, distance measurements will be created on the butane molecule for each different C-H bond.

This technique can also be used to find bond angles, torsion angles, centroids, and best fit lines and planes in a molecule. Simply ensure that the relevant measurement is created and selected in the pattern document prior to performing the *Find* operation.

To create a set of solute atoms

1. Import the file Examples\Documents\3D Model\polyoxyethylene_cinnamide.xsd, containing polymer and solute molecules.
2. Select and copy one of the cinnamide solute molecules.
3. Create a new 3D Atomistic document and paste the cinnamide molecule. Rename the document to cinnamide.xsd
4. Undo the selection in both documents.
5. Select *Edit | Find Patterns* from the menu bar to display the Find Patterns dialog.
6. Select cinnamide.xsd as the *Pattern document* and choose Element Type as the *Match property*.
7. Ensure that polyoxyethylene_cinnamide.xsd the active document and click the *Find* button.
8. On completion, right-click in polyoxyethylene_cinnamide.xsd and choose Select Substructure Items from the shortcut menu.
9. Click the *New Sets...* button on the Find Patterns dialog to open the Define New Set dialog.
10. For Name enter Cinnamide and click the *OK* button.

Atom Selection dialog

When a 3D document is active you can display the Atom Selection dialog from the *Edit* menu. This dialog allows you to select atoms in the structure based upon the properties of those atoms. The dialog controls are described below.

Select by Property: Determines the property to be used as the basis of the selection. The frame below this dropdown list contains a set of controls appropriate for the specification of the value or values to be used in the selection process. The following table lists the possible settings of the *Property* dropdown list and details the frame contents for each property.

Property	Action	Frame contents
Element	Select atoms based on their element type.	Single element selected: ■ The selection criterion dropdown list is set to either Is or Is Not. A single element symbol in the *element* text box determines the element type for atom selection. Note that an atomic number may be entered instead of an element symbol. The … button displays a periodic table from which an element may be chosen. The periodic table is kept synchronized with the element that appears in the *element* text box. Multiple elements selected: ■ The selection criterion dropdown list is set to either Is One Of or Is Not One Of. One or more element symbols in the *element* text box, delimited by commas, determine the set of elements to be used for atom selection. Note that atomic numbers may be entered instead of or in addition to element symbols. The … button displays a periodic table from which the elements may be chosen (use the CTRL key to make multiple element selections in the periodic table panel). The periodic table is kept synchronized with the elements that appear in the *element* text box.
Name	Select atoms based on their assigned name.	The search string entered in the text box after *matches* determines which atoms are selected. The text may be a precise atom name to search for, or else a name that includes wild-card characters to make the search more flexible. A ***** character represents any number of matching characters of any value. A **?** character represents a single character of any value. As an example, "C*" will match with any atom name that starts with a "C". And "C?" will match with any two-character atom name that begins with a "C". **Note:** If the target string actually contains one of the following special characters, you should precede it with a backslash (****) to ensure that it is not confused with the matching syntax. **?*+\.^[]$&()**

Property	Action	Frame contents
Charge	Select atoms based on their charge value.	The *selection criterion* dropdown list specifies the test to be made in determining whether an atom's charge value dictates that the atom be selected or not. Comparison case: ■ The comparison is one of Equal To, Greater Than, Less Than, Greater Than Or Equal To, Less Than Or Equal To, Inclusive Range, or Exclusive Range. A simple test is made against the number in the *charge value* text box. Range case: ■ An atom is selected if its charge value falls between two limits. An Inclusive Range test includes values at the limits. An Exclusive Range test does not include values at the limits. The value limits to be used are specified in the *lower charge value* and *upper charge value* text boxes.
Connected	Select atoms connected to those that are currently selected.	There are no further criteria to specify.
Bond Count	Select atoms based upon the number of atoms that are attached to it.	The *selection criterion* dropdown list specifies the selection test to be made using an atom's attached atom total. Comparison case: ■ The comparison is one of Equal To, Greater Than, Less Than, Greater Than Or Equal To, Less Than Or Equal To, Inclusive Range, or Exclusive Range. A simple test is made against the number in the *bond order value* text box. Range case: ■ An atom is selected if the number of attached atoms falls between two limits. An Inclusive Range test includes values at the limits. An Exclusive Range test does not include values at the limits. The range limits to be used are specified in the *lower bond count value* and *upper bond count value* text boxes.
Attached Bond Type	Select atoms based upon the bond type of its attached bonds.	The *attached bond type* dropdown list is set to one of a predefined list of bond order values: Single, Double, Partial Double, Triple. The *selection criterion* dropdown list specifies whether the atoms to be selected should have bonds of the chosen bond order type or not have any bonds of that type.

Property	Action	Frame contents
Forcefield Type	Select atoms based on their assigned forcefield type.	The search string entered in the *forcefield name* text box determines which atoms are selected. The text may be a precise forcefield name to search for, or else a name that includes wild-card characters to make the search more flexible. A ***** character represents any number of matching characters of any value. A **?** character represents a single character of any value. As an example, "H*" will match with any atom name that starts with an "H". And "H?" will match with any two-character atom name that begins with a "H". **Note:** If the target string actually contains one of the following special characters, you should precede it with a backslash (\) to ensure that it is not confused with the matching syntax. **?*+\.^[]$&()**
Hybridization	Select atoms based on their hybridization value.	The *hybridization value* dropdown list is set to one of a predefined list of hybridization values: Linear, Trigonal, Tetrahedral, SquarePlanar, TrigonalBipyramid, SquarePyramid, Octahedral, No hybridization. The *selection criterion* dropdown list specifies whether the atoms to be selected should be of the chosen hybridization type or not of that type.
Is Backbone Atom	Select atoms based on whether they are polymer backbone atoms or not.	The two possible values to act as the selection criterion for this property are True and False. The *selection criterion* dropdown list specifies whether the atoms to be selected should be those marked as backbone atoms or those not marked as backbone atoms.
Radial Distance	Select atoms based on their 3D distance from a point in space or from currently selected atoms.	The *distance* textbox value is the distance in Å to be used as the limit for radial distance determinations. The *selection criterion* dropdown list specifies whether all atoms that lie within this distance or outside of it are selected. If the Selected atoms radio button is set, then an atom lies within the radial distance if its 3D distance from the closest of the selected atoms is within the specified value. If the Location radio button is set, then an atom lies within the radial distance if its 3D distance from the *location coordinates* is within the specified value.

Property	Action	Frame contents
X Coordinate	Select atoms based on the value of their X coordinate.	The *selection criterion* dropdown list specifies the selection test to be made using an atom's axis coordinate. Comparison case: ■ The comparison is one of Equal To, Greater Than, Less Than, Greater Than Or Equal To, Less Than Or Equal To, Inclusive Range, or Exclusive Range. A simple test is made against the number in the *coordinate value* text box. Range case: ■ An atom is selected if its coordinate axis value falls between two limits. An Inclusive Range test includes values at the limits. An Exclusive Range test does not include values at the limits. The range limits to be used are specified in the *lower coordinate value* and *upper coordinate value* text boxes.
Y Coordinate	Select atoms based on the value of their Y coordinate.	
Z Coordinate	Select atoms based on the value of their Z coordinate.	
Relative X	Select atoms based on their position relative to the currently selected atoms, along the X axis.	A range is specified for the distance from selected atoms along the axis, in terms of the upper and lower bounds for the search. The *selection criterion* dropdown list specifies whether all atoms within this range or outside of it should be selected.
Relative Y	Select atoms based on their position relative to the currently selected atoms, along the Y axis.	
Relative Z	Select atoms based on their position relative to the currently selected atoms, along the Z axis.	
Contains Core Hole	Select atoms based on whether their electronic configuration contains a core hole.	There are no further criteria to specify.

Selection mode: These three radio buttons offer flexibility in defining which population of atoms are analyzed as potential candidates for selection, and how the new selection interacts with atoms already selected.

- Create a new selection from all visible atoms - In this mode, any selected atoms are deselected, and all of the visible atoms in the 3D structure are taken as candidate atoms for the new selection.

  Note: The current selection is lost even if no new atoms are selected.

- Select from the existing selection - In this mode, only atoms that are already selected are taken as candidates for selection. Effectively, this causes deselection of atoms that do not meet the selection criteria.

  Tip: This mode allows you to "and" two selections together. For example to select all Si atoms with a charge greater than 0.0, first select all Si atoms in a model, then switch the selection mode to Select from the existing selection, and run the charge selection operation.

- Add to the existing selection - In this mode, the current selection is untouched, and all of the atoms in the 3D structure are taken as candidate atoms for the new selection.

  Tip: This mode allows you to "or" two selections together. For example to select all atoms whose names begin with S or Fe, first select all atoms in a model whose name matches "S*", then switch the selection mode to Add to the existing selection, and run the name selection operation again using "Fe*".

Select All: Selects all atoms in the active model.

Deselect All: Deselects all objects in the active model.

Select: Selects atoms in the active model according to the specified property and values.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Edit	Atom Selection*

Edit Sets dialog

The Edits Sets dialog allows you to create, display, and modify sets in the active 3D Atomistic document. You can display the Edit Sets dialog using the *Edit Sets* command on the Edit menu when a 3D Atomistic document is active.

Note: The Edit Sets dialog is only available when a 3D Atomistic document is active.

A set is a list of objects in a particular 3D Atomistic document. Each set in a document should be given a unique name so that it may be readily identified for future retrieval. You can select atoms or other objects in the 3D Atomistic document using one of the available selection techniques and then create a set that contains all the selected objects. At a later date, you can recreate the selection from the contents of the named set, instead of having to recreate the selection from scratch.

Note: Objects may be included in more than one set.

Note: Any objects deleted from a document are automatically removed from any set that includes them.

The Edit Sets dialog contains a list of all the sets defined in the current 3D Atomistic document. Select sets from this list and use the buttons on the right to perform the following operations:

New...: Provides access to the Define New Set dialog, which allows you to create and name a new set made up of the currently selected objects in the active 3D Atomistic document.

Set names must be unique within a particular 3D Atomistic document. Duplicate names will be rejected.

> **Note:** The *New...* button is enabled only when one or more objects are selected in the active 3D Atomistic document.

Delete: Deletes the selected set or sets, but not the objects contained in them.

> **Note:** The *Delete* button is enabled only when one or more sets are selected on the Edit Sets dialog.

Select: Selects the objects in the selected set or sets in the active 3D Atomistic document.

> **Note:** The *Select* button is enabled only when one or more sets are selected on the Edit Sets dialog.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Edit	Edit Sets*

Define New Set dialog

The Define New Set dialog allows you to create and name a set containing the selected objects in the active 3D Atomistic document. If the set is to be made up entirely of particles, then you can make it visible in the 3D Viewer.

Name: Specify the name for the new set.

> **Note:** Set names must be unique in a particular 3D Atomistic document. Duplicate names will be rejected.

Show set: When checked, indicates that the set will be made visible when it is created. Default = checked.

> **Note:** Only sets consisting entirely of atoms can be made visible.

OK: Creates a new set with the specified name and closes the dialog.

Cancel: Closes the dialog without creating a set.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Edit	Edit Sets	New...*

Find Patterns dialog

The Find Patterns dialog allows you to search a specified structure or trajectory document for a structural motif defined in another structure document. You can display the Find Patterns dialog using the *Find Patterns* command on the Edit menu when a 3D Atomistic (`.xsd`) or 3D Atomistic Trajectory document (`.xtd`) is the active document.

Note: The Find Patterns dialog is only available when a 3D Atomistic or 3D Atomistic Trajectory document is active. The process of finding patterns will only be carried out if this document contains atoms or beads.

Some step-by-step examples of how to use the Find Patterns functionality are provided in the Finding patterns topic.

Pattern document: Select the structure document to be used as pattern document from the dropdown list. Only documents that are currently open are listed.

The pattern document contains the motif or pattern you wish to search for in the target document. The pattern document must meet a number of criteria:

- It must be a 3D Atomistic document
- It must contain at least one atom or bead
- It must contain a single fragment
- It must be nonperiodic

The pattern document may contain geometry measurement objects, such as distance, angle, torsion measurements, centroids, best fit planes, and lines. By selecting such a measurement object prior to executing the *Find* operation, equivalent measurement objects for each match will be created in the target document. The new objects will be selected in the target document on completion. If atoms are selected in the pattern document, substructure objects comprising only those atoms will be created in the target document, for each match, and selected on completion. If nothing is selected in the pattern document, then substructure objects comprising all equivalent atoms or beads will be created. Substructure objects are visualized by green cages around the comprising atoms or beads when unselected.

Note: If a selection is made in the pattern document it may only contain atoms *or* beads *or* a single measurement object. Selections containing both atoms and measurements, or more than one measurement, are not allowed. The Property Explorer can be used to list the types of objects in the current selection.

Pattern documents can be generated using the sketching tools in the Materials Visualizer or by copying molecules or molecular fragments from another document.

The target document is the currently active structure or trajectory document that will be searched for the motif contained in the pattern document. The search domain is the whole of its structure or, if a selection is made, only those atoms or beads in the selection. Selections of objects other than atoms or beads will cause the *Find* operation to fail. Both periodic and nonperiodic target documents can be searched. If the pattern document contains beads then the target document must also contain beads.

Match property: Select the atom or bead property that will provide the basis of a match from the dropdown list. Available options are:

- ElementType (default for pattern documents containing atoms)
- ForcefieldType
- Name
- None
- BeadTypeName (default for pattern documents containing beads)

When None is selected, Materials Studio looks for topologically identical arrangements of atoms.

The ElementType option is only applicable to patterns of atoms and the BeadTypeName option is only available if the pattern document contains beads.

Find: Initiates the pattern matching operation.

A *Find* operation will create new objects in the target document, which will be selected on completion. For each match of the pattern found an object is created. The type of object created depends on the type of object selected in the pattern document. If, for instance, an angle measurement was selected in the pattern document, then, for each match found between the pattern and the target, an equivalent angle measurement will be created in the target document. Likewise, if a centroid was selected in the pattern document, a new centroid for each match is created in the target document. In case atoms were selected in the pattern document, then a substructure object comprising those atoms will be created in the target document. If nothing is selected in the pattern document, then a substructure object comprising all atoms or beads will be created in the target document. Substructure objects are visualized by green cages around the comprising atoms or beads when unselected.

Find | Copy Script: Converts the current settings to a script and copies the script to the clipboard. Refer to the Generating scripts topic for more information on using sections of scripts generated from a dialog.

New Sets...: Provides access to the Define New Set dialog, which allows you to create a set from the current selection. The purpose of this button is to facilitate creation of sets containing the results of the pattern-matching operation.

> **Note:** To create a set of the matched atoms or beads comprised by the substructures, rather than a set of substructure objects, you must first change the selection. With the substructures selected, right-click in the target document and choose Select Substructure Items from the shortcut menu. With the new selection, when defining a new set, it will contain the matched atoms or beads.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Edit	Find Patterns*

Viewing and displaying 3D structures

Every document opened by Materials Studio creates a View based on its file type. 3D structures are presented to the user in a 3D Viewer.

In a 3D Viewer, you can:

- Change the display attributes of various types of objects
- Rotate, translate, and zoom your view of the structure
- Change the structure's position and orientation
- Define a center of rotation
- Animate a structure
- Label objects
- Change the color of the document background or objects in the document
- Control lighting, depth cueing, and graphical quality
- View and customize the display of fields and other volumetric data

Basic tasks and methods

The Materials Visualizer's 3D Viewer displays 3D model documents within a 2D Materials Studio window. The mapping from the 3D document coordinate space to the 2D screen coordinate space is controlled by the 3D Viewer "view transform". Modifying the view transform lets you rotate, translate, and zoom your view of the structure. Note that this does not change the coordinates of objects within the 3D model document. If you want to do this, see Measuring and changing geometry and Changing position and orientation. Materials Studio allows the 3D Viewer to be in one of several modes in which mouse actions control various aspects of the view. Buttons on the 3D Viewer toolbar allow you to switch among modes.

Mode	Effect
Translation	Translates the structure to another screen location
Rotation	Rotates view around the screen X and Y axes
Zoom	Changes the magnification of the view

Translating the 3D View

3D Viewer translation mode is activated by clicking the *Translation* button  on the 3D Viewer toolbar.

In translation mode, you can translate the view of the current 3D structure by dragging the mouse while clicking the left mouse button.

Structures can also be translated when other 3D Viewer modes are active using the following mouse and key combinations:

To	Press
Pan view	Middle mouse drag
Pan view	Mouse wheel drag

To	Press
Pan view	ALT + Right mouse drag
Pan view left	ALT + LEFT arrow
Pan view right	ALT + RIGHT arrow
Pan view up	ALT + UP arrow
Pan view down	ALT + DOWN arrow

Note: The arrow key translation rate can be set using the Movement dialog.

Rotating the 3D View

3D Viewer rotation mode is activated by clicking the *Rotation* button  on the 3D Viewer toolbar.

In rotation mode, you can rotate the current 3D structure by dragging the mouse while clicking the left mouse button.

Structures can also be rotated when other 3D Viewer modes are active using the following mouse and key combinations:

To	Press
Trackball rotation	Right mouse drag
Rotate about X	X + Right mouse drag
Rotate about Y	Y + Right mouse drag
Rotate about Z	Z + Right mouse drag
Rotate view about X 45° clockwise	Up arrow
Rotate view about X 45° counterclockwise	Down arrow
Rotate view about Y 45° clockwise	Left arrow
Rotate view about Y 45° counterclockwise	Right arrow

Note: The arrow key rotation angle can be set using the Movement dialog.

Changing the 3D View magnification

3D Viewer zoom mode is activated by clicking the *Zoom* button on the 3D Viewer toolbar: 

In zoom mode you can magnify the view of the current 3D structure using left-mouse click + drag.

Structures can be zoomed when other 3D Viewer modes are active using the following mouse and key combinations:

- Mouse wheel spin
- Left mouse click + Right mouse click + drag
- Left mouse click + R key + drag
- Plus key (+) on numeric keypad (Zoom in)
- Minus key (-) on numeric keypad (Zoom out)

Monitoring the scale

You can monitor the scale of the current view using the Scale Ruler.

1. Right-click in the 3D Viewer and select *Display Options* from the shortcut menu.
2. Select the *Legends* tab of the Display Options dialog.
3. Check the *Show scale bar* checkbox.

Setting position and orientation

The 3D Viewer toolbar contains a number of buttons for defining the position and orientation of the view:

3D Viewer toolbar

To	Click
Return the view to the original orientation	*Reset View* button
Center the view on the entire structure	*Recenter* button
Center the view on the selected items	*Recenter* button
Orient the view such that a near-planar fragment is presented parallel to the plane of the screen	Select *View Onto* from the dropdown list associated with the *Recenter* button
Orient the view such that a near-planar fragment is presented horizontally	Select *View Across* from the dropdown list associated with the *Recenter* button
Orient the view along the major axis of near-linear fragment	Select *View Across* from the dropdown list associated with the *Recenter* button
Orient the view across the major axis of a near-linear fragment	Select *View Onto* from the dropdown list associated with the *Recenter* button
Orient the view along the length of a selected bond	Select *View Across* from the dropdown list associated with the *Recenter* button
Orient the view across the length of a selected bond	Select *View Onto* from the dropdown list associated with the *Recenter* button
Fit a structure to the current view	*Fit to View* button

Note: The orientation of the fragment generated by *View Onto* and *View Across* is dependent on the initial orientation of the fragment (the smallest, acute, angle is used to orientate the fragment, and this angle will depend on the initial configuration).

Defining a center of rotation

Use the *Recenter* button  on the 3D Viewer toolbar to define the center of rotation.

To	Use
Center on selected items	Select the items and click the *Recenter* button
Center on the entire structure	Select all (or none) and click the *Recenter* button

Animating structures

Using the animation controls, you can play back a series of frames from a calculation, for instance, from a molecular dynamics run.

You can read a trajectory (a series of frames meant to be animated) from a `.trj`, `.his`, or `.arc` file. The Common file formats topic contains more information about these files.

- To read a `.trj`, you must also have the corresponding `.xtd` file.
- To read a `.his`, you must also have the corresponding `.car` file.

Whenever the active document has frame information, the Animation toolbar is enabled. If the *Animation* toolbar is not visible, you can display it using the *Toolbar* command on the View menu.

When you play an animation, information about the frame that is currently displayed appears in the status bar at the bottom of the Materials Studio window. By default, animations play starting at frame 1 and proceeding to the last frame, but you can control the direction, speed, and starting point using the animation controls accessible from the *Animation* toolbar.

Animations may be exported in Microsoft's Movie Clip (AVI) format.

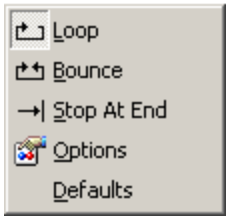
Animation controls

The animation controls allow you to animate 3D Atomistic and Mesoscale Trajectory files containing multiple geometries or orientations of a structure. Typical examples include the series of configurations output from a Forcite molecular dynamics run or the series of snapshots of a mesoscale system produced by a MesoDyn simulation.

Animation toolbar

The Animation toolbar allows you to control the animation of 3D Atomistic and Mesoscale Trajectory files in the 3D Viewer. It also provides access to the Animation Mode dropdown list, which allows you to control how the current animation is played and to set various animation options and defaults.

Animation Mode dropdown list



Animation Mode dropdown list

Loop: Replays the animation continuously, beginning at either the first or the final frame.

Bounce: Replays the animation continuously by reversing direction upon reaching the first and final frames.

Stop At End: Plays the animation once, stopping at either the first or the final frame.

Options: Displays the Animation Options dialog, which provides further options for controlling the animation of the current trajectory.

Defaults: Displays the Animation Defaults dialog, which allows you to specify the settings that will be used when new animations are created.

Making movies

Materials Studio can export trajectory files as Microsoft Movie Clip (`.avi`) files. Movies are made by stepping through the frames of a trajectory frame sequence. The 3D Viewer records bitmaps of each displayed frame and then assembles them into an AVI stream.

To export a trajectory

1. Choose *File | Export...* from the menu bar to display the Export dialog.
2. Navigate to the location that you wish to save the file to and then specify a name for the movie in the *File name* field.
3. Select Movie Clip (*.avi) from the *Save as type* dropdown list.
4. If you wish to specify particular frames for inclusion/exclusion, to adjust the playback speed, or to alter the movie quality settings, click the *Options...* button to display the Export AVI dialog and make the appropriate changes.
5. Click the *Export* button on the Export dialog.

Animation Options dialog

The Animation Options dialog provides you with further options for controlling the animation of the current trajectory and also allows you to select the frames that are displayed.

Current frame: Specify a frame number and press the TAB key to manually move to a particular frame in the trajectory or use the spin controls to display the next or the previous frame in the sequence.

Start frame: Specify the starting position in the frame sequence for the animation. This will be the first frame that is seen when the trajectory is played in a forward direction.

End frame: Specify the end position in the frame sequence for the animation. This will be the last frame that is seen when the trajectory is played in a forward direction.

Step size: Specify the number of frames in each step of the animation sequence. Setting this parameter to a value greater than one means that some frames will be skipped and not displayed during playback.

Playback speed: Specify the playback speed for the animation using the slider control. This parameter controls the delay before the next frame in the sequence is displayed.

Playback style: Select the style of playback for the animation from the dropdown list. Available options are:

- Loop - replays the animation continuously, beginning at either the first or the final frame
- Bounce - replays the animation continuously by reversing direction upon reaching the first and final frames
- Stop At End - plays the animation once, stopping at either the first or the final frame

Recalculate atom visibility every frame: When checked, indicates that the visibility of atoms in a periodic structure will be redetermined after every frame on the basis of the coordinates of the atoms.

Note: The *Recalculate atom visibility every frame* option is enabled only if the current document contains a periodic structure.

Help: Displays the Help topic in a browser.

Access methods

Toolbar	 / *Options*

Animation Defaults dialog

The Animation Defaults dialog allows you to specify the default settings that will be used when new animations are created. These default settings are a subset of the options available on the Animation Options dialog.

Note: The settings specified on the Animation Defaults dialog are not applied to new trajectory documents created by Forcite Dynamics calculations.

Playback speed: Specify the playback speed for the animation using the slider control. This parameter controls the delay before the next frame in the sequence is displayed.

Playback style: Select the style of playback for the animation from the dropdown list. Available options are:

- Loop - replays the animation continuously, beginning at either the first or the final frame
- Bounce - replays the animation continuously by reversing direction upon reaching the first and final frames
- Stop At End - plays the animation once, stopping at either the first or the final frame

Recalculate atom visibility every frame: When checked, indicates that the visibility of atoms in a periodic structure will be redetermined after every frame on the basis of the coordinates of the atoms. This option has no effect on nonperiodic structures.

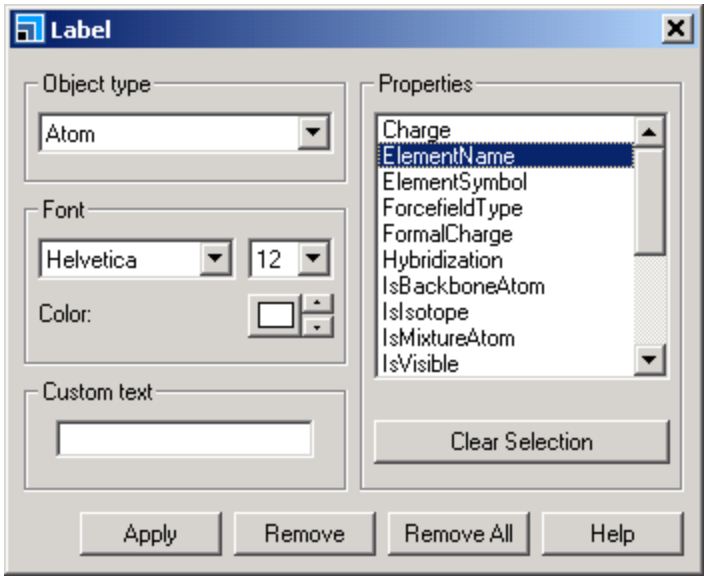
Help: Displays the Help topic in a browser.

Access methods

Toolbar	 / *Defaults*

Labeling structures

Labeling structures is performed using the Label dialog.



Label dialog

Labels are text strings showing either structure element properties or custom text strings entered by the user. Labels depicting properties are dynamic, such that they always reflect the current value of the 3D document. Multiple labels may be displayed simultaneously, drawn as a column of text strings within the 3D View.

Label dialog

The *Label* dialog allows creation of property labels and custom text labels.

Object type: Lists the types of objects in the current structure. The list of *Properties* is updated depending on the object type selected.

Font: Controls in this area specify the typeface, type size and color of the label text.

Available typefaces are Helvetica, Times, and Courier.

Available type sizes (in points) are 8, 12, 16, and 24.

The *Color* control accesses the Microsoft Common Color Control for color selection. Spinners control the brightness.

Custom text: Allows you to enter a character string to be displayed as the label.

Properties: Lists properties that can be used as the basis for labels. Use the SHIFT or CTRL key with the mouse to select multiple properties. Hold down CTRL and click the mouse to toggle a selection. *Clear Selection* clears all the selections.

Clear Selection: Deselects any highlighted properties in the list.

Remove All: Removes all labels.

Remove: Removes all labels belonging to selected objects of type *Object Type*.

Apply: Creates labels on selected objects of type *Object Type*.

Help: Displays the Help topic in a browser.

Access methods

Menu	*View	Label*
Shortcut menu	*Label*

Structure display colors

You can control the color of structures in a 3D model document. Periodic table elements are each assigned default colors and the default document background is black. These assignments can be modified and you can also color other objects. Using the selection features of Materials Studio, you can select and then color objects:

- individually
- by a property that you may select
- by grouping objects into sets

Many of the View and Sketcher dialogs in the 3D Viewer offer the ability to color objects.

Default element colors

The default element colors can be edited using the Element Properties dialog.

Atoms in all structures will be displayed with the appropriate element color unless an atom has been explicitly set to another color, for example, by using the atom coloring functionality on the Atom tab of the Display Style dialog.

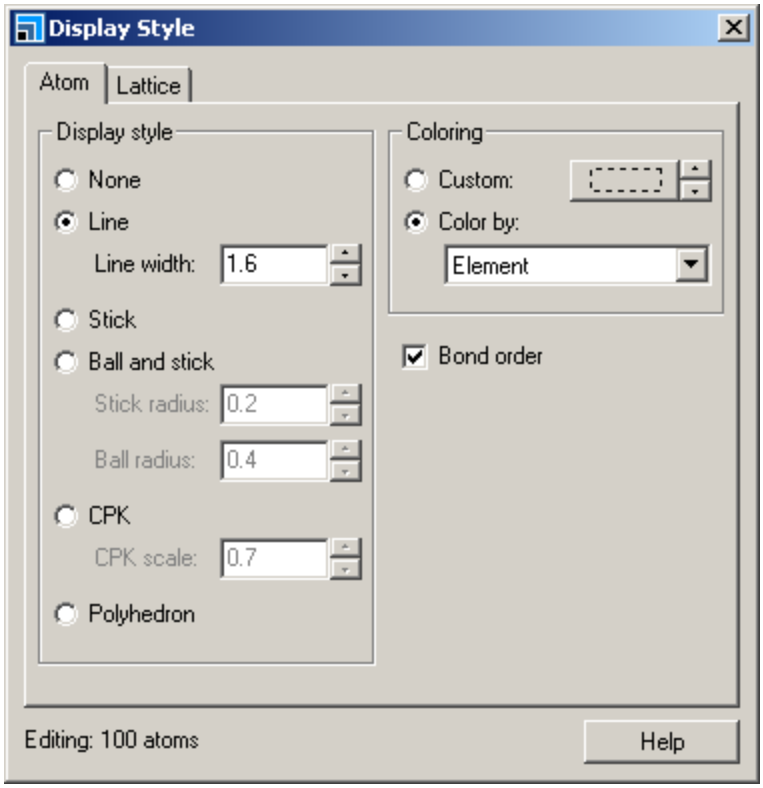
To set an atom's color back to its element default value, use the *Color By* option on the Atom tab on the Display Style dialog.

Coloring selected objects

The ability to color objects is available within Materials Studio. All structure elements are given a default color, usually defined by the type of atomic element. Many structure elements can be given a custom color or colored by a specific property.

All objects have the property *Color*, which is shown in the Properties Explorer. Double-clicking on the *Color* property in the Properties Explorer displays the Microsoft Common Color Control, which allows you to select a display color.

The Display Style dialog makes use of a color control  . Clicking this displays the Microsoft Common Color Control so you can select a color. The spin controls allow you to directly modify the brightness of the selected color.



Display Style dialog, Atom tab

The following operations can be performed using the controls on the Display Style dialog:

To	Click
Select a color	Color chooser
Brighten the color	Up spin control
Darken the color	Down spin control

Note: For certain volumetric objects (fields, isosurfaces, and slices), more sophisticated color maps can be defined. See Viewing volumetric objects for details.

Background color

The background color in 3D Viewer documents is controlled from the *Backgrounds* tab of the Display Options dialog.

The Display Options dialog makes use of a color control so you can select a background color.

Color control

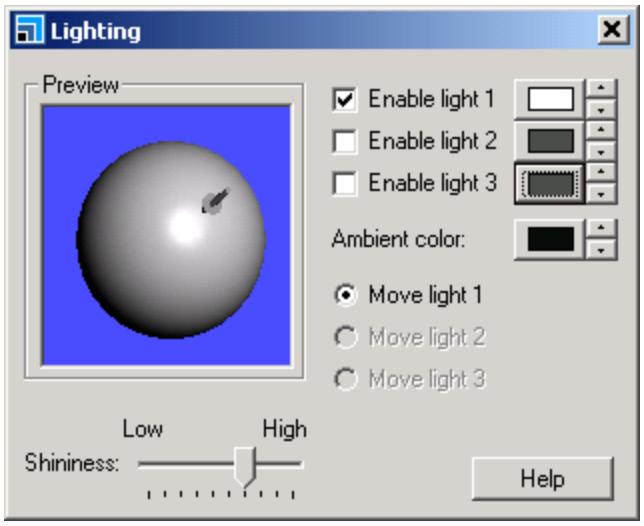
The background may also be filled with a color spectrum or user-supplied image. Refer to the Display Options dialog for more information on texturing the 3D Viewer background.

Access methods

Menu	*View	Display Options*
Shortcut menu	*Display Options*

Lighting control

Lighting structures within 3D views is performed by the Lighting dialog. The Lighting dialog allows you to control the position, color, and shininess of as many as three light sources.



Lighting dialog

The dialog allows control of the following light environment properties:

- Number of light sources (up to 3)
- Light Position
- Diffuse Color
- Ambient intensity
- Shininess

From the Lighting dialog, the following operations can be performed:

To	Press
Enable a light	Check an *Enable light* checkbox
Select which light to position	Select a *Move light* radio button
Set the light direction	Click and drag left mouse in *Preview* window
Select a light color	Click a color select button
Set the shininess	Drag the *Shininess* slider

Access methods

Menu	*View	Lighting*
Shortcut menu	*Lighting*

Lighting dialog

The Lighting dialog controls the lighting environment of solid structures within a 3D Viewer document. The lighting affects the rendering of spheres, cylinders, ellipsoids, and surfaces. The lighting control will have no effect on a structure with *Display Style* set to Line.

Preview: Controls the direction of light sources. The preview sphere is a control that allows interactive positioning of light directions. Click and drag with the left mouse button to modify the direction of the current light. You can control selection of the current light using *Move light*.

Move light: Specifies the current light. Only one light can be current at a given time. The current light is positioned using the *Preview*.

Enable light: Enables the light. The color of the light is controlled using the color buttons to the right of the Enable option.

Ambient color: Controls the color (intensity) of the ambient light.

Shininess: Controls the shininess of the structures within the 3D Viewer. Setting this control to High produces intense specular highlights.

> **Tip:** Graphic display related problems can sometimes be remedied by disabling the hardware accelerated video driver. Check the *Disable hardware acceleration* checkbox on the *Tools | Options | Graphics* tab. Changing this setting will not effect the use of graphics by other software installed on your machine.

Help: Displays the Help topic in a browser.

Access methods

Main menu	*View	Lighting*
Shortcut menu	*Lighting*

Overlaying structures

Materials Studio allows you to view structures or defined groups of atoms in the same 3D Cartesian space, but keep them separate in other respects (for example, physical interaction). This allows you to, for example, view structures in close proximity or overlay them on one another, making small differences in geometry easier to identify. A separate document type, the 3D Atomistic Collection document (.xod) is defined to accommodate this activity.

Each structure or group of atoms in a collection document is known as a physical system. Physical systems are defined when the atoms or structures they contain are initially brought into the collection document. The introduction of the physical system into the data hierarchy within 3D Atomistic Collection documents means that you can, for example, color atoms according to the physical system to which they belong, allowing you to differentiate a series of similar structures so that trends are easier to identify. System properties (such as the number of atoms, chemical formula and dipole moment) are also defined on the physical system.

Physical systems do not interact; this allows atoms in different physical systems to be in close proximity without affecting each other. As a result, you can, for example, calculate hydrogen bonds for a structure within a particular physical system without atoms and molecules in other physical systems influencing the calculation.

Creating collections

Collections can be created by inserting structures from a study table containing structure cells or by simply opening an empty 3D Atomistic Collection document and adding physical systems, as detailed in the Basic operations with collections topic.

To create a collection

Either extract structures from a study table:

1. Select cells containing structures in a study table and right-click.
2. Choose *Extract To Collection* from the shortcut menu.

Or create an empty collection document:

1. Select *File | New...* from the menu bar or click the *New* button  on the toolbar and select *3D Atomistic Collection Document* from the New Document window.
2. Alternatively, click on the options arrow associated with the *New* button  and select *3D Atomistic Collection Document* from the dropdown list or right-click on the project in the Project Explorer and select *New | 3D Atomistic Collection Document* from the shortcut menu.

Basic operations with collections

Physical systems can be added to collection documents by inserting files containing 3D structures (`.xsd`, `.msi`, `.car`/`.cor`, `.acx`, `.res`/`.ins`, `.mol`/`.mdl`, `.pdb`/`.ent`, `.skc`). Structures can also be copied from individual frames of 3D Atomistic Trajectory documents (`.xtd`). Files in the `.sd` and `.his` formats must be brought into Materials Studio in the form of study tables before any structures they contain can be extracted into a collection.

Fragments or partial structures can be inserted from a 3D atom-based document by copying and pasting.

To add physical systems to a collection

Either insert the contents of an entire structure file:

1. Select *Edit | Insert From...* from the menu bar or click the *Insert From File* button  on the toolbar.
2. In the Insert into Active Document dialog, navigate to the appropriate file and click the *Insert* button.

Alternatively,

1. Select the documents to insert in the Project Explorer.
2. Right-click on one of the selected documents.
3. Select *Insert Into* from the shortcut menu.

Or copy and paste a structure or fragment from a 3D atom-based document:

1. Open the appropriate 3D atom-based document (`.xsd`, `.xtd`, or `.xod`) and select the atoms you wish to insert into the collection.
2. Select *Edit | Copy* from the menu bar, click the *Copy* button  on the toolbar, or press CTRL + C.
3. Make a pre-existing `.xod` file the active document and select *Edit | Paste* from the menu bar, click the *Paste* button  on the toolbar, or press CTRL + V.

If there are many physical systems in a 3D Atomistic Collection document, it can be difficult to visually separate objects in individual systems so that they can be manipulated. The easiest way to select a physical system is to use the Physical Systems dialog, which provides a convenient view of all physical systems defined in the currently active 3D Atomistic Collection document.

To select physical systems

1. Ensure that a 3D Atomistic Collection document containing one or more physical systems is the active document.
2. Choose *View | Physical Systems* from the menu bar to display the Physical Systems dialog.

   Note: The Physical Systems dialog is enabled only if the current document is a 3D Atomistic Collection document containing at least one physical system.

3. Select the physical systems in the list on the Physical Systems dialog by clicking on the *Physical System* icons. Multiple selections can be made using the SHIFT or CTRL keys.

Alternatively, physical systems can be selected using selection by hierarchy or, if the physical system to be selected is not in close proximity to any others, region selection can be used.

Physical systems are most easily removed from a 3D Atomistic Collection document using the Physical Systems dialog, although the standard methods for deleting objects from 3D model documents can also be applied.

To remove physical systems from a collection

1. Ensure that a 3D Atomistic Collection document containing one or more physical systems is the active document.
2. Choose *View | Physical Systems* from the menu bar to display the Physical Systems dialog.

   Note: The Physical Systems dialog is enabled only if the current document is a 3D Atomistic Collection document containing at least one physical system.

3. Select the physical systems that you wish to delete in the list on the Physical Systems dialog by clicking on the *Physical System* icons. Multiple selections can be made using the SHIFT or CTRL keys.
4. Press the DELETE key.

Alternatively,

1. Manually select the physical systems you wish to remove from the collection.
2. Press the DELETE key, select *Edit | Delete* or *Edit | Cut* from the menu bar, right-click and select *Delete* from the shortcut menu, or click the *Cut* button  on the toolbar.

To rename physical systems

1. Ensure that a 3D Atomistic Collection document containing one or more physical systems is the active document.
2. Choose *View | Physical Systems* from the menu bar to display the Physical Systems dialog.

   Note: The Physical Systems dialog is enabled only if the current document is a 3D Atomistic Collection document containing at least one physical system.

3. Click on the name of the physical system that you wish to rename in the list on the Physical Systems dialog and enter the new name.

Alternatively,

1. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
2. Make the 3D Atomistic Collection document containing the physical system to be modified the active document and manually select the physical system you wish to rename.
3. Set the *Filter* on the Properties Explorer to Physical System using the dropdown list.
4. Double-click on *Name* in the Properties Explorer to display the Edit Name dialog.
5. Enter the new name and click the *OK* button.

Generally, the visibility of objects in Materials Studio is controlled by altering the value of the *IsVisible* property using the Properties Explorer. Since physical systems frequently obscure one another, it is often more convenient to use the Physical Systems dialog to control the visibility of physical systems.

To adjust the visibility of physical systems

1. Ensure that a 3D Atomistic Collection document containing one or more physical systems is the active document.
2. Choose *View | Physical Systems* from the menu bar to display the Physical Systems dialog.

   Note: The Physical Systems dialog is enabled only if the current document is a 3D Atomistic Collection document containing at least one physical system.

3. Check or uncheck the checkboxes next to the *Physical System* icons  to make the corresponding physical systems visible or invisible.

Note: When a physical system is made invisible, all the objects that comprise the system also become invisible. However, the visibility property of the component objects is not changed, so that when you make the physical system visible again, only the objects that were visible before become visible again. This also means that certain dialogs, such as the Display Style dialog, may indicate that an object is visible when it cannot actually be seen in the 3D Viewer because it is part of a physical system that is invisible.

You can extract physical systems from a 3D Atomistic Collection document to separate `.xsd` files.

To extract physical systems to separate files

1. Manually select the physical systems that you wish to extract from the collection.
2. Right-click in the 3D Atomistic Collection document and select *Extract to Atomistic Documents* from the context menu.

Note: The extracted `.xsd` files will be placed into the active folder within the current project.

Working with collections

Many of the operations that can be performed on structures in 3D Atomistic documents act in exactly the same way when applied to structures in 3D Atomistic Collection documents. For example:

- View transformation - You can translate, rotate, and zoom in on structures in collection documents. This enables you to overlay a sequence of structures (for example, from a molecular dynamics simulation) one upon another, making small changes in geometry throughout the series easy to identify.
- Setting display styles - You can alter the way structures are rendered in collection documents. This enables you to display structures in different colors so that they are easier to distinguish when they are overlaid on one another.
- Labeling - You can label structures in collection documents. This enables you to highlight areas of interest in particular structures.
- Adding measurements - You can measure distances and angles in structures in collection documents. This enables you numerically to display changes in geometry in a sequence of structures (for example, from a molecular dynamics simulation).

Tip: In order for them to operate correctly, certain functions within Materials Visualizer need to be performed one-by-one on individual physical systems within a 3D Atomistic Collection document rather than on the entire contents of the collection document at the same time, these include: Sketching and editing structures, Manipulating Atoms and Bonds (Add Atoms, Calculate Bonds, Calculate Close Contacts, Calculate Hydrogen Bonds), Clean, Symmetry (Show Symmetry, Lattice Parameters, Find Symmetry, Make P1, Unbuild Crystal, Nonperiodic Superstructure, Supercell, Redefine Lattice, Primitive Cell, Conventional Cell), Build/Rebuild Crystal, Build Vacuum Slab, Build/Rebuild Surface, Constraints, Charges (Atomic Charge Assignment, Charge Group Definition/Calculation/Removal), Volumes and Surfaces, and Find Patterns.

Note: None of the module applications act on collection documents. In addition, the following Materials Visualizer functions have not yet been enabled for collection documents: Find Equivalent Atoms, Reaction Preview, Vibrational Analysis, Polymer Builder, Build Layer, Cleave Surface.

Physical Systems dialog

The Physical Systems dialog lists all the physical systems present in the currently active 3D Atomistic document. A 3D Atomistic Collection document may contain multiple physical systems. Other 3D Atomistic documents can contain only one physical system.

The Physical Systems dialog allows you to select, rename, and control the visibility of physical systems, even if they are currently invisible, obscured, or otherwise difficult to select in the 3D Viewer.

Click on an entry in the Physical Systems dialog to select the corresponding physical system.

Check or uncheck the checkboxes to control the visibility of the physical systems. When a checkbox is checked, objects in the physical system that are defined as visible will be shown in the 3D Viewer. When a checkbox is unchecked, all objects in the physical system will be hidden in the 3D Viewer, whether or not the objects are themselves defined as visible.

The name of each physical system is displayed next to the visibility control checkbox. If no name has been assigned to the physical system, the default name <Physical System> may be displayed. To rename a physical system, click on the existing or default name, then enter the new name.

You can delete physical systems from the currently active 3D Atomistic Collection Document by selecting the relevant physical system in the Physical Systems dialog and pressing the DELETE key.

Help: Displays the Help topic in a browser.

Access methods

Menu	*View	Physical Systems*
Shortcut menu	*Physical Systems*

Visualizing volumes

Materials Visualizer provides a range of powerful tools for viewing and analyzing volumetric data, such as fields, isosurfaces, slices, and mesoscale molecules. Many Materials Studio applications generate fields (particle densities, potentials, etc.) 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 generated can be imported via the `.msi` and `.grd` file formats.

In Materials Studio, you can:

- View periodic and nonperiodic fields and surfaces.
- Create and customize isosurfaces for arbitrary fields, individually controlling their display style, color, and transparency.
- Create 2D projections of a field onto slices of arbitrary position and orientation.
- Create high quality color maps and contour maps of field values on isosurfaces and slices using a variety of color schemes.
- Use the Properties Explorer to view and modify the properties of fields, isosurfaces, slices, and mesoscale molecules.
- Use standard Materials Studio operations to move, copy, paste, or otherwise manipulate fields, isosurfaces, slices, and mesoscale molecules.
- Control apparent depth effects, lighting, resolution, graphical quality, and visibility for volumetric objects in the same manner as for atoms and molecules.

Periodic and nonperiodic fields

Materials Studio allows you to visualize both periodic and nonperiodic fields. For periodic fields, the field value is invariant under periodic translations. The field volume in this case is identical to the periodicity volume.

Changing the field display range

1. Display the Volume Visualization toolbar using the *View | Toolbars* menu.
2. Click the *Volumetric selection* button  on the *Volume Visualization* toolbar to display the Volumetric Selection dialog.
3. Select one or more fields using the Volumetric Selection dialog.
4. Select the Field tab on the Display Style dialog.
5. Modify the display range using the *Min* and *Max* entry fields for the *1st*, *2nd*, and *3rd* axis spanning the field volume. For periodic fields, the display range is arbitrary - for nonperiodic fields, the display range must be within 0.00 and 1.00.

Note: The field display range also affects the display of isosurfaces and slices associated with the currently selected field.

Note: The periodicity of the field is independent of the periodicity of the lattice. Hence, changing the lattice display range on the Lattice tab of the Display Style dialog has no effect on the field display range, and vice versa.

Changing the field display style

1. Select one or more fields and choose the *Field* tab on the Display Style dialog.
2. Choose either the Empty, Dots, or Volume display style.
3. Use the *Quality*, *Dot size*, and *Transparency* controls to customize the chosen display.
4. Check the *Show box* checkbox if you wish a box to be drawn around the field volume.

Changing the field display color

1. Select one or more fields and choose the *Field* tab on the Display Style dialog as above.
2. Choose either Custom coloring or Color by field values.
3. If you chose *Custom* coloring, click the color button to display the Microsoft Common Color Control. Use the spinners to adjust the brightness.
4. If you chose to *Color by field value*, use the Color Maps dialog to specify how to map field values onto colors.
5. To modify lighting conditions, use the Lighting dialog.
6. To modify resolution, depth cue, and background, use the Display Options dialog.

Note: You can also modify field properties by selecting the field and then using the Properties Explorer. See Field, surface, slice and mesoscale molecule properties for details.

Creating and using field probes

Field probes allow you to view and edit the values of a field and to see the gradient of the field at a specific point.

A field probe is represented by a selectable probe object that indicates the point on the field where the measurement is being taken. The position of the probe is given by the *ProbePosition* property in the Properties Explorer. A sphere indicates the actual position of the probe and the arrow connected to the sphere shows the magnitude and direction of the field gradient. The field probe object takes its color from the point on the field that it is measuring. If there are no field data at the selected position or if the specified display range is such that the value in question is not mapped, the field probe will not be displayed.

Field probes can be moved by selecting them and:

- Dragging the mouse while holding SHIFT, ALT, and the right mouse button.
- Using the tools on the 3D Movement toolbar and the Movement dialog.
- Editing the *ProbePosition* property in the Properties Explorer.

There are two modes of operation for field probes in Materials Studio, the properties of which are summarized in the table below. The field probe mode can be set by editing the *ProbeMode* property in the Properties Explorer.

Mode	Position measured	*FieldValue* property
NearestGridPoint	At field grid point closest to selected position	Editable

Mode	Position measured	*FieldValue* property
LinearInterpolate	At selected position	Read-only (value interpolated from surrounding grid points)

Creating field probes

1. Open a 3D structure document containing field data. If the document contains more than one field, you may wish to select the field to be measured using the Volumetric Selection dialog.
2. Click the *Create Probe* button  on the Volume Visualization toolbar. If the currently active 3D structure document contains more than one field and you did not select a field in step 1, the Choose Field On Which to Create Probe dialog will be displayed. If this is the case, select the field to be measured from the list on the dialog and click the *OK* button.

Editing field values using a probe

1. Select a field probe in the currently active 3D structure document.
2. If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.
3. Set the *Filter* on the Properties Explorer to Field Probe using the dropdown list.
4. Double-click on *ProbeMode* in the Properties Explorer to display the Edit ProbeMode dialog.
5. Select NearestGridPoint from the dropdown list and click the *OK* button.
6. Move the probe to the desired position using one of the methods listed above.
7. Double-click on *FieldValue* in the Properties Explorer to display the Edit FieldValue dialog.
8. Enter the new value and click the *OK* button.

Creating and customizing isosurfaces

Materials Studio enables you to create isosurfaces for arbitrary periodic and nonperiodic fields. You can create isosurfaces for several fields at once, and you have a wide range of control over the display style and color used to draw the isosurface.

Creating isosurfaces

1. Display the Volume Visualization toolbar by selected *View | Toolbars* from the menu bar.
2. Click the *Create Isosurface* button  on the Volume Visualization toolbar.
3. If no field is selected and the currently active 3D Model document contains more than one field, you are asked to select the fields to isosurface on the Choose Fields to Isosurface dialog. Alternatively, you could have selected the fields to be isosurfaced on the Volumetric Selection dialog prior to creating the isosurface.
4. An isosurface appears in the 3D Viewer - the default isovalue used is the mean value of the field.
5. In the Properties Explorer, modify the *IsoValue* to shift the surface to higher or lower field values.
6. Customize the isosurface as described below.

Note: When creating isosurfaces on segregates the surface isovalue is obtained from the segregator, rather than using the segregate field mean.

Changing the isosurface display range

1. Click the *Volumetric Selection* button  on the *Volume Visualization* toolbar to display the Volumetric Selection dialog.
2. Select one or more fields using the Volumetric Selection dialog.
3. Open the Display Style dialog and select the Field tab.
4. Modify the display range using the *Min* and *Max* entry fields for the *A*, *B*, and *C* axis spanning the field volume. For periodic fields/isosurfaces, the display range is arbitrary. For nonperiodic fields/isosurfaces, the display range must be between 0.00 and 1.00.

Note: The periodicity of the field/isosurface is independent of the periodicity of the lattice. So changing the lattice display range on the Lattice tab of the Display Style dialog has no effect on the isosurface display range, and vice versa.

Changing the isosurface display style

1. Select one or more isosurfaces and choose the Isosurface tab on the Display Style dialog.
2. Choose either the Dots or Solid display style.
3. Use the *Dot size* and *Transparency* controls to customize the chosen display.
4. Set the display style to *Solid* and map a field in the *Mapped field* dropdown list.
5. Check the Banded checkbox to give the isosurface a banded appearance. See the glossary for details.
6. Select +/- from the *Type* dropdown list to display the reverse side isosurface in a different color.

Changing the color of the isosurface

1. Select one or more isosurfaces and choose the *Isosurface* tab on the Display Style dialog.
2. If you wish to color the isosurface according to the mapped field, choose the field to use for the color map from the *Mapped field* dropdown list.
3. Choose either *Custom* coloring or *Color by mapped field*. See Color and contour mapping for details on coloring and contouring the isosurface according to the values of the mapped field on the surface. If you are viewing a legacy surface imported from a different modeling application, choose *Original colors*.
4. If you chose *Custom* coloring, click the color button to display the Microsoft Common Color Control. Use the spinners to adjust the brightness.
5. If you chose to *Color by mapped field*, use the Color Maps dialog to specify how to map field values onto colors.
6. To swap the inside and outside of the isosurface, uncheck the *High values inside* checkbox.
7. To modify lighting conditions, use the Lighting dialog.
8. To modify resolution, depth cue, and background, use the Display Options dialog.

Note: You can also modify isosurface properties by selecting the isosurface and then using the Properties Explorer. See Field, surface, slice and mesoscale molecule properties for details.

Creating and customizing segregates

Materials Studio enables you to divide periodic and nonperiodic fields into regions or segregates. The boundary between these regions is a surface of constant value. You can create segregates for several fields at once, and you have a wide range of control over the criteria used to select segregates, their display style, and colors.

Creating segregates

1. Display the Volume Visualization toolbar using the *View* | *Toolbars* menu.
2. Click the *Create Segregates* button  on the Volume Visualization toolbar.
3. If no field is selected and the currently active 3D Model document contains more than one field, you are asked to select the fields to segregate on the Choose Fields to Segregate dialog. Alternatively, you could have selected the fields to be segregated on the Volumetric Selection dialog prior to creating the segregator.
4. Segregates appear in the 3D Viewer - the default isovalue used is the mean value of the field.

Changing constraints

1. Right-click anywhere in the active document and select *Display Style* to open the Display Style dialog, then select the Segregate tab.
2. In the *Constraints* section modify the *Isovalue* to shift the dividing value up and down.
3. Use the *Values* dropdown list to only generate segregates with values above or below the isovalue.
4. Use the *Connectivities* dropdown list to display only isolated or accessible regions.

Changing the segregate display style

1. Select one or more segregates and choose the Segregate tab on the Display Style dialog.
2. Choose either the Dots or Volume display style.
3. Use the *Dot size* and *Quality* controls to customize the display of dots, or the *Quality* and *Transparency* to control the volume display.

Changing the segregate coloration

1. Select one or more segregates and choose the Segregate tab on the Display Style dialog.
2. Choose *Custom* coloring to give all these segregates a single color of your choice, *Color by field values* to map the values to a range of colors or *Color by segregate* to give each segregate a different single color.
3. When *Custom* coloring is used, clicking on the color button displays the Microsoft Common Color Control. Use the spinners to adjust the brightness. See Color and contour mapping for further details.
4. For the *Color by field values* selection, the Color Maps dialog can be used to specify how to map field values onto colors.

Note: You can also modify segregate properties by selecting the segregate and then using the Properties Explorer. See Field, surface, slice, segregate, and mesomolecule properties for details.

Creating and customizing slices

Materials Studio enables you to create color maps of field values on 2D slices for arbitrary periodic and nonperiodic fields. You can create such slices for several fields at once, you can move and rotate the slices using standard Materials Studio mouse and keyboard actions, and you have a wide range of control over the display style and coloration used to draw the slice.

Creating slices

1. Display the Volume Visualization toolbar using the *View | Toolbars* menu.
2. To create a slice *through a set of objects* (for example atoms, bonds), select those objects in the 3D view, then click the *Create Slices* button  on the Volume Visualization toolbar. If the selected objects do not all lie in a plane, the slice is created as a best fit to the selected objects. If no objects are selected, this is equivalent to all objects in the model being selected.

   OR, to create a slice *aligned with one of the planes* delimiting the field volume, choose one of the *Parallel to* items from the dropdown list to the right of the *Create Slices* button  .
3. If nothing is selected and the currently active 3D model document contains more than one field, you are asked to select the fields to slice on the Choose Fields to Slice dialog. Alternatively, you could have selected the fields to be sliced on the Volumetric Selection dialog prior to creating the slice.
4. A slice appears in the 3D view. The area is chosen so that all points within the visible field volume intersecting with the slice plane form part of the slice.
5. Check the *Frame* checkbox to draw a frame around the slice edges.
6. Position and realign the slice as described below.

Positioning and realigning slices

To realign slices using the *Fit Slices* tool

1. Display the *Volume Visualization* toolbar using the *View | Toolbars* menu.
2. To align a slice *through a set of objects* (for example atoms, bonds), select the objects in the 3D view, then click the *Fit Slices* button  on the Volume Visualization toolbar. If the selected objects do not all lie in a plane, the slice is realigned as a best fit to the selected objects. If no objects are selected, this is equivalent to all objects in the model being selected.

   OR to reposition a slice *so that it is aligned with one of the planes* delimiting the field volume, choose one of the *Parallel to* items from the dropdown list to the right of the *Create Slices* button  .
3. If nothing is selected and the currently active 3D model document contains more than one slice, you are asked to select the slices to align on the Choose Slices to Align dialog. Alternatively, you could have selected the slices to be aligned prior to clicking the *Fit slices* button.

To realign slices using the mouse

1. Select the slice.
2. Translate and rotate the slice as described in Changing positions, using standard Materials Studio mouse and keyboard actions. The slice position and center of rotation are indicated by a cross-hair symbol in the 3D view when the slice is selected.

Note: If you wish to align the slice along a precisely known crystallographic direction, you can also use the Properties Explorer to specify slice position and slice normal. See Field, surface, slice and mesoscale molecule properties for details.

Changing the slice display style

1. Select one or more slices and choose the Slice tab on the Display Style dialog.
2. Choose either the Empty, Dots, or Solid display style.
3. Use the *Dot size*, *Quality*, and *Transparency* controls to customize the chosen display.
4. If you chose the *Solid* display style, you can achieve a banded appearance of the colors on the slice by checking the Banded checkbox.

Changing the slice coloration

1. Select one or more slices and choose the *Slice* tab on the Display Style dialog as above.
2. Choose either Custom coloring, or Color by field values.
3. If you chose *Custom* coloring, click the color button to display the Microsoft Common Color Control. Use the spinners to adjust the brightness.
4. If you chose to *Color by field value*, use the Color Maps dialog to specify how to map field values onto colors.
5. To modify lighting conditions, use the Lighting dialog.
6. To modify resolution, depth cue, and background, use the Display Options dialog.

Color and contour mapping

Color and contour maps provide an intuitive and visually attractive way of displaying variations of field values across a surface or slice. Materials Studio allows you to combine the use of colors and contours in the display of all volumetric objects (fields, isosurfaces, and slices).

Defining the color map

1. Select the volumetric object (field, slice, isosurface) which you want to define a color map for, and ensure that it is visible.
2. For color mapping isosurfaces, ensure that a *Mapped field* has been defined on the Isosurface tab of the Display Style dialog.
3. Ensure that *Color by mapped field* or *Color by field values* is selected on the appropriate tab of the Display Style dialog.
4. Display the Volume Visualization toolbar using the *View | Toolbars* menu.
5. To display the Color Maps dialog, click the *Color Maps* button  on the *Volume Visualization* toolbar. Alternatively, right-click and choose *Color Maps* from the shortcut menu.
6. On the Color Mapping tab of the Color Maps dialog, choose a color spectrum from the options in the *Spectrum* dropdown list.
7. Using the *From (To)* entry fields, specify the field values to map onto the colors on the left and right of the color range chooser. Min, max, and mean field values for the field being mapped are accessible via the arrows to the right of these entry fields.
8. Any change to the coloring options on the Color Maps dialog immediately results in a change to the 3D view.
9. Values outside the *From (To)* range are either drawn in the same color as the leftmost (rightmost) color shown on the color range chooser or they are not drawn at all. To toggle between these two alternatives, click on the arrow (double bar) to the left (right) of the color range chooser.
10. If you have chosen *Solid* display style for a slice or isosurface, using the *Banded* display option often results in a smoother appearance of the color map.
11. You can now add contours as described below.

Note: By default, the color map ranges specified by the *From (To)* entry fields are derived from the mapped field, as described in the Color map defaults table below.

Excluding colors - contour maps

You can create contours on your isosurface or slice by excluding field value ranges from the color map.

1. Follow steps 1 - 6 above.
2. With the mouse, hover over the Color range chooser, and from the tooltip shown identify the color band (field range) that you wish to be excluded from the color map.
3. Click on the color band - a vertical dashed line will appear on top of it in the color range chooser, and an appropriate contour may show up on the isosurface or slice.
4. Reactivate an excluded band by clicking on it again.
5. Drag the mouse across several color bands to exclude/reactivate larger ranges.

Note: You can define contours not only if you have opted to *Color by mapped field* or *Color by field values* on the appropriate tab of the Display Style dialog, but also if you have chosen a *Custom* color. In this case, the color range chooser displays the single custom color selected and contours can be defined as above.

Displaying color map legends

For any volumetric object (field, isosurface, or slice) for which you have defined a color map, you can also specify that this color map (i.e., the association between field values and colors) is displayed alongside the 3D view in the 3D viewer.

1. Follow the steps above to generate a color or contour map
2. On the Legend tab of the *Color Maps* dialog, check the *Show legend* checkbox.
3. Control the *Size*, *Font*, *Tick count*, and *Text color*.
4. If you do not wish a caption with the name of the mapped field to be shown above the color map legend, uncheck the *Show caption* box.
5. If you do not wish excluded color bands to be shown on the color map legend, uncheck the *Show exclusions* box.

If the color at the top or bottom of the color map legend is *arrow shaped*, that last color also applied to any field values outside the maximum or minimum. If the top or bottom of the color map is *a straight line*, any field values outside the range are not colored. This behavior is controlled by the Color range chooser on the Color Mapping tab.

Color map defaults

The table below illustrates the default color maps (ranges, exclusions, etc.) chosen for fields mapped onto slices and surfaces. To assist workflow, color maps for fields mapped onto slices (surfaces) are inherited from any previous slices (surfaces) for which a color map for the same field has already been defined. This ensures that, for example, several slices through the same field will by default use the same color-value mapping, so the colors/contours on different slices are comparable.

The example assumes two fields A and B:

Volumetric object	Mapped field	Color map default
Slice A1	A	Field A Minimum (Maximum)
Slice A2	A	copied from Slice A1

Volumetric object	Mapped field	Color map default
Slice A3	A	copied from Slice A2
Slice B1	B	Field B Minimum (Maximum)
Surface A1	A	Field A Mapped Minimum (Maximum)
Surface A2	A	copied from Surface A1
Surface A3	A	copied from Surface A2
Surface B1	B	Field B Mapped Minimum (Maximum)

Selecting fields, surfaces, segregates, slices, and mesoscale molecules

Depending on the display style chosen, volumetric objects such as fields, isosurfaces, slices, and mesoscale molecules do not always have a representation in the 3D Viewer from which you can pick and select them easily. So, a special control, the Volumetric Selection dialog, provides a convenient tree view of all volumetric objects defined in the current 3D model document.

Selecting volumetric objects

Either, if the objects that you wish to select are visible, select them as described in Selecting objects and groups of objects.

Or, if the objects are invisible or difficult to pick, then:

1. Display the Volume Visualization toolbar by selecting *View | Toolbars | Volume Visualization* from the menu bar.
2. Choose the *Volumetric Selection* tool  on the *Volume Visualization* toolbar to open the Volumetric Selection dialog.

   Note: This button and the associated dialog are enabled only if the current document contains one or more fields.

   The top level of the tree hierarchy shows the fields present in the current 3D model document. Each field can have one or more isosurfaces or slices associated with it, which are displayed by expanding the corresponding node.
3. Select volumetric objects in the tree view by clicking on the  *Field*,  *Atom Volumes Field*,  *Isosurface*,  *Slice*,  *Segregate*,  *Segregator*, or  *Mesoscale Molecules* icons.
4. Perform multiple selections using the SHIFT or CTRL keys.

Renaming volumetric objects

Either:

1. Select a field, isosurface, slice, or set of mesoscale molecules as described above.
2. In the Properties Explorer, change the *Name* property.

Or:

1. Display the Volume Visualization toolbar by selecting *View | Toolbars | Volume Visualization* from the menu bar.
2. Choose the *Volumetric Selection* tool  on the *Volume Visualization* toolbar to open the Volumetric Selection dialog.

   Note: This button and the associated dialog are enabled only if the current document contains one or more fields.
3. If necessary, expand the field nodes to display the slices and isosurfaces associated with that field.
4. Select the field, isosurface, slice, or set of mesoscale molecules in the Volumetric Selection dialog. Click on its name and enter a new name.

Controlling the visibility of volumetric objects

The standard method of controlling visibility of objects in Materials Studio is via the Properties Explorer (see Structure visibility). Since volumetric objects frequently obscure each other, an easier method of controlling visibility for these objects is provided by the Volumetric Selection and Display Style dialogs.

Either:

1. Select one or more volumetric objects and bring up the appropriate tab on the Display Style dialog.
2. Check or uncheck the *Visible* checkbox.

Or:

1. Open the Volumetric Selection dialog as described above.
2. If necessary, expand the field nodes to see slices and isosurfaces associated with each field.
3. Check or uncheck the checkboxes next to the  *Field*,  *Isosurface*,  *Slice*, *Segregate*,  *Segregator*, or  *Mesoscale Molecules* icons to make the corresponding objects visible or invisible.

Deleting volumetric objects

Either:

1. Select a field, isosurface, slice, or set of mesoscale molecules as described above.
2. In the 3D Viewer, press the DELETE key.

Or:

1. Open the Volumetric Selection dialog as described above.
2. If necessary, expand the field nodes in the tree view to display the slices and isosurfaces associated with each field.
3. Select the volumetric objects to be deleted.
4. Press the DELETE key.

Field, surface, slice, segregate, and mesomolecule properties

Most manipulations of fields, isosurfaces, and slices can be performed using the Display Style dialog or the Volume Visualization toolbar. As with other Materials Studio objects, it is also possible to view and manipulate properties of volumetric objects using the Properties Explorer.

Common properties

IsVisible: Turn the visibility of the selected object on or off.

Name: Change the name of the selected object.

Style: Shows the display style of the selected object. This is a non-editable field.

Field properties

FieldMax, FieldMean, FieldMin: Show the maximum, mean, and minimum value of the field within the field volume.

FieldPeriodicity: Shows the number of dimensions in which the field is periodic (0 for a nonperiodic field).

FieldStandardDeviation: Shows the standard deviation of the field from its mean value.

GridSize: Shows the size of the grid used to store the grid values in the three dimensions used to store the grid.

Isosurface properties

EnclosedVolume: Shows the volume enclosed by the isosurface, within a single repeat unit. The volume is calculated by counting the number of grid points whose value is above (or below) the isovalue. The setting *High values inside* on the Isosurface tab of the Display Style dialog determines whether grid points above or below the isovalue are counted. Visually, the volume is that which is on the gray side of the isosurface. In a 3D atom-based document, the volume is in units of $Å^3$.

SurfaceArea: Shows the area of the isosurface, within a single repeat unit. In a 3D atom-based document, the area is in units of $Å^2$.

HasMappingField: Indicates whether or not a mapped field has been specified for this isosurface.

IsInsideVisible: If *No*, indicates that the inside of the isosurface should not be rendered at all, i.e., it will appear completely transparent. For open surfaces, this usually results in an incorrect visual appearance. For closed surfaces, you can use this property to remove a spurious bright "halo" which appears at the edge of the isosurface under some lighting conditions. See also Tips and Tricks.

IsIsoValueInRange: If No, indicates that the specified isovalue lies outside the range of values of the field. Hence, no isosurface is visible.

IsIsoValueMirrored: If Yes, displays a mirrored isosurface for the negative isovalue. Corresponds to the +/- selection from the *Type* dropdown list on the Isosurface tab on the Display Style dialog.

IsoValue: Displays the isovalue for the isosurface. The isovalue can be edited via the *Isovalue* entry field on the Isosurface tab on the Display Style dialog.

SurfaceMappedMax, SurfaceMappedMean, SurfaceMappedMin: Show the maximum, mean, and minimum values of the mapped field on the surface.

Slice properties

SliceCrystalDirection: For periodic fields only, the "Miller indices" of the slice, i.e., the projection of the slice normal onto the reciprocal lattice vectors. The resulting indices are arbitrarily normalized to one. Use this property to create a slice plane that lies within a particular Miller plane.

SliceCrystalPosition: The slice position expressed in fractional coordinates.

SliceMappedMax, SliceMappedMean, SliceMappedMin: Show the maximum, mean, and minimum values of the field on the slice plane.

Segregate properties

FieldMax, FieldMean, FieldMin: Show the maximum, mean, and minimum value of the field in the field volume.

FieldStandardDeviation: Shows the standard deviation of the field from its mean value.

FieldVolume: The volume of this segregate.

FieldVolumeFractional: The fraction of the total volume of the field occupied by this segregate.

SegregateConnectivity: Whether this segregate is accessible or isolated.

Segregator properties

IsoValue: Displays the isovalue dividing segregates. The isovalue can be edited using the *Isovalue* entry field on the Segregate tab of the Display Style dialog.

SegregateConnectivities: The connectivity filter for segregates. This filter can be edited using the *Connectivities* entry field on the Segregate tab of the Display Style dialog.

SegregateValues: The value filter for segregates, controlling whether only segregates with values higher or lower than the isovalue should be available. This filter can be edited using the *Values* entry field on the Segregate tab of the Display Style dialog.

SegregateVolumeMin: The minimum volume of the segregates generated, in $Å^3$. This filter can be edited using the *Minimum size* entry field on the Segregate tab of the Display Style dialog.

Mesomolecule properties

BeadFormulaPerMesoMolecule: Shows the numbers of each bead type present in a single mesoscale molecules object.

NumBeadsPerMesoMolecule: Shows the total number of beads present in a single mesoscale molecules object. Typical values are of the order of 10.

NumMesoMolecules: Shows the number of mesoscale molecules within a single mesoscale molecules object. Typical values are of the order of 100-1000.

Volume visualization dialogs

Volume visualization tasks in Materials Studio can be performed using dialogs which can be accessed from the Volume Visualization toolbar.

Volumetric Selection dialog

The Volumetric Selection dialog allows you to select, rename, and control the visibility of fields, isosurfaces, slices, and mesomolecules, even if they are currently invisible, obscured, or otherwise difficult to select in the 3D Viewer.

The Volumetric Selection dialog shows a tree view of all the volumetric objects (fields, isosurfaces, slices, and mesoscale molecules) in the current 3D structure document. To see the slices and isosurfaces defined for a field, expand the corresponding field node by clicking on the + symbol.

You can delete volumetric objects displayed in the tree view using the DELETE key.

The view can be resized by dragging the edges of the dialog.

Each entry shows:

Visibility control: When checked, makes the corresponding object visible in the 3D Viewer.

Icon: Selects the corresponding object (one of *Field*, *Atom Volumes Field*, *Field Probe*, *Isosurface*, *Slice*, *Segregate*, *Segregator*, or *Mesoscale Molecules*) in the 3D Viewer. Hover the mouse cursor over the icon to see a tool tip.

Name: The name of the volumetric object. To rename, click on the name, then type in the new name.

> **Note:** Many objects in 3D structure documents have automatic names. To revert to an automatic name, just remove the custom name.

Help: Displays the Help topic in a browser.

Access methods

Toolbar	

Segregate Analysis dialog

The *Segregate Analysis dialog* analyses the distribution of properties in the selected segregates, or all segregates in the document if there is no selection. As each segregate contributes one point to the distribution, the analysis is most useful when applied to a large number of segregates.

Current options for all documents containing segregated fields are:

- Segregate size - plots probability against the segregate volume.
- Segregate major axis - plots probability against the major axis length of a fitted ellipsoid.
- Segregate radius (best-fit sphere) - plots probability against the sphere radius.
- Segregate separation - plots probability against the distance between segregates.

For atomistic documents Å are the unit of length. For mesoscale documents this varies.

> **Note:** The fitted ellipsoid is determined from unweighted moment analysis of the segregate shape. The segregate sphere radius is defined to be the geometric mean of the radii of these ellipsoids.

Number of bins: Defines the number of bins to use for analysis values.

Analyze: This button is only active if a segregated field is available in the active document.

Help: Displays the Help topic in a browser.

Access methods

Toolbar		*Analyze Segregated Field*

Color Maps dialog

The Color Maps dialog contains the following tabs:

- Color Mapping: Allows you to specify how field values will be mapped onto colors for volumetric objects, to define a different color map for each volumetric object, and to create contour maps.
- Legend: Allows you to control the display of color map legends in the 3D Viewer.

Access methods

Toolbar	
Shortcut menu	*Color Maps*

Color Mapping tab

The *Color Mapping* tab on the Color Maps dialog allows you to specify how you wish to map field values onto colors for volumetric objects (i.e., fields, isosurfaces, and slices). You can define a different color map for each volumetric object, and you can also create contour maps by specifying field value ranges excluded from the color map.

Note: The settings on this tab reflect common settings for all currently selected *and visible* volumetric objects, or, if nothing is selected, all visible volumetric objects in the currently active 3D model document. A setting will only have a displayed value if it is the same for all selected (and visible) volumetric objects, or, if nothing is selected, if it is the same for all visible volumetric objects in the model. If the current selection does not include a visible volumetric object or if no visible volumetric objects are present in the model, all controls on this tab are disabled. See Selecting fields, surfaces, slices and mesoscale molecules for details on how to select volumetric objects and how to control their visibility.

From (To): Use these entry fields to specify the field values which map onto the left-most (right-most) color of the color range chooser. Use the spinners to increment the field values. The right arrow to the right of the entry fields opens a menu showing a variety of special field values:

- Field Maximum (Mean, Minimum): The global maximum (mean, minimum) value of the mapped field.
- Mapped Field Maximum (Mean, Minimum): The maximum (mean, minimum) value of the mapped field on the selected isosurface or slice.

Color range chooser: This control shows color bands and how they map onto field values. Click anywhere on the color range to exclude individual value ranges (color bands) from the color map - such exclusions will not be drawn and are shown as vertical dashed lines in the color range chooser. Exclusions can be used to generate contour maps.

To reactivate an excluded range, simply click on it again. Drag the mouse across several color bands to exclude/reactivate larger ranges. To identify the value range which a particular color band corresponds to, use the mouse to hover over the color band. A small tooltip window will be displayed showing the range.

Color range chooser

 **Continue/exclude below:** Click on the left arrow to crop, or exclude, field values below the minimum specified, or click on the left double bar to re-enable the left-most color for all such field values.

 **Continue/exclude above:** Click on the right arrow to crop, or exclude, field values above the maximum specified, or click on the right double bar to re-enable the right-most color for all such field values.

Spectrum: Allows you to choose between different color schemes.

Bands: For each color scheme, you can specify the number of color bands you wish to generate. Each color band corresponds to a range of field values. The maximum number of color bands allowed is 128.
Help: Displays the Help topic for the current tab.

Access methods

Toolbar		*Color Mapping*
Shortcut menu	*Color Maps*	*Color Mapping*

Legend tab

The *Legend* tab on the Color Maps dialog allows you to control the display of color map legends in the 3D Viewer. A separate legend can be displayed for each volumetric object (field, isosurface, or slice) with

an associated color map.

Note: The settings on this tab reflect common settings for all currently selected *and visible* volumetric objects, or, if nothing is selected, all visible volumetric objects in the currently active 3D model document. A setting will only have a displayed value if it is the same for all selected (and visible) volumetric objects, or, if nothing is selected, if it is the same for all visible volumetric objects in the model. If the current selection does not include a visible volumetric object or if no visible volumetric objects are present in the model, all controls on this tab are disabled. See Selecting fields, surfaces, slices and mesoscale molecules for details on how to select volumetric objects and how to control their visibility.

Show legend: If checked, color map legends are shown alongside the structural model in the 3D view.

Size: The size of the color map legend.

Font: The font used for labeling the color map legend.

Tick count: The number of tick marks with field values shown alongside the color map legend.

Text color: The color of the text used to annotate the color map legend in the 3D view.

Show caption: If checked, the name of the volumetric object that corresponds to a color map legend is displayed above the map.

Show exclusions: If checked, exclusions (contours) defined on the color range chooser of the Color Mapping tab are shown on the color map legend.

Access methods

Toolbar	 | *Legend*
Shortcut menu	*Color Maps* | *Legend*

Choose Slices To Align dialog

The Choose Slices To Align dialog is displayed when there is more than one slice present in the currently active 3D structure document and none of these was selected when you clicked the *Fit Slices* button  on the Volume Visualization toolbar. You are presented with a list of slices that can be aligned. Select a one or more slices, then click the *OK* button.

Tip: You can avoid displaying this dialog by explicitly selecting one or more slices using the Volumetric Selection dialog before clicking the *Fit Slices* button.

OK: Aligns the selected slices and closes the dialog.

Cancel: Closes the dialog without aligning the slices.

Help: Displays the Help topic in a browser.

Access methods

Toolbar	

Choose Fields To Isosurface dialog

The Choose Fields To Isosurface dialog is displayed when there is more than one field present in the currently active 3D structure document and none of these was selected when you clicked the *Create*

Isosurfaces button  on the Volume Visualization toolbar. You are presented with a list of fields for which an isosurface can be created. Select one or more fields, then click the *OK* button.

> **Tip:** You can avoid displaying this dialog by explicitly selecting one or more fields using the Volumetric Selection dialog before clicking the *Create Isosurfaces* button.

OK: Creates an isosurface for the selected field(s) and closes the dialog.

Cancel: Closes the dialog without generating any isosurfaces.

Help: Displays the Help topic in a browser.

Access methods

Toolbar	

Choose Fields To Segregate dialog

The Choose Fields To Segregate dialog is displayed when there is more than one field present in the currently active 3D structure document and none of these was selected when you clicked the *Create Segregates* button  on the Volume Visualization toolbar. You are presented with a list of fields for which a segregate can be created. Select one or more fields, then click the *OK* button.

> **Tip:** You can avoid displaying this dialog by explicitly selecting one or more fields using the Volumetric Selection dialog before clicking the *Create Segregates* button.

OK: Segregates the selected field(s) and closes the dialog.

Cancel: Closes the dialog without segregating fields.

Help: Displays the Help topic in a browser.

Access methods

Toolbar	 / *Create Segregates*

Choose Fields To Slice dialog

The Choose Fields To Slice dialog is displayed when there is more than one field present in the currently active 3D structure document and none of these was selected when you clicked the *Create Slices* button  on the Volume Visualization toolbar. You are presented with a list of fields for which a slice can be created. Select one or more fields, then click the *OK* button.

> **Tip:** You can avoid displaying this dialog by explicitly selecting one or more fields using the Volumetric Selection dialog before clicking the *Create Slices* button.

OK: Slices the selected field(s) and closes the dialog.

Cancel: Closes the dialog without creating any slices.

Help: Displays the Help topic in a browser.

Access methods

Toolbar	

Choose Fields On Which To Create Probe dialog

The Choose Fields On Which To Create Probe dialog is displayed when there is more than one field present in the currently active 3D structure document and none of these was selected when you clicked the *Create Probe* button  on the Volume Visualization toolbar. You are presented with a list of fields for which a probe can be created. Select one or more fields, then click the *OK* button.

> **Tip:** You can avoid displaying this dialog by explicitly selecting one or more fields using the Volumetric Selection dialog before clicking the *Create Probe* button.

OK: Creates a probe on the selected field(s) and closes the dialog.

Cancel: Closes the dialog without creating any probes.

Help: Displays the Help topic in a browser.

Access methods

Toolbar	

Choose Fields for Distribution Creation dialog

The Choose Fields for Distribution Creation dialog is displayed when there is more than one field present in the currently active 3D structure document and none of these was selected when you clicked the *Field Distribution* button  on the Volume Visualization toolbar. You are presented with a list of fields for which a field distribution can be created. Select one or more fields, then click the *OK* button.

> **Tip:** You can avoid displaying this dialog by explicitly selecting one or more slices using the Volumetric Selection dialog before clicking the *Field Distribution* button.

OK: Creates a field distribution chart for the selected field(s) and closes the dialog.

Cancel: Closes the dialog without creating a chart.

Help: Displays the Help topic in a browser.

Access methods

Toolbar	

Tips and tricks for volume visualization

These suggestions are provided to allow you to take actions to optimize your interactive experience when analyzing large datasets. The general theme is to reduce the graphics workload until the desired view orientation is achieved. Printing and exporting to bitmaps should always be performed at high quality settings, so it may be necessary to reset several of these options prior to (and after) printing or bitmap export.

Interactivity

Enable fast-render-on-move and make use of Dots display style whenever possible.

Large field datasets produce high resolution isosurfaces. Interactivity during the viewing of high resolution graphical objects requires hardware accelerated graphics capabilities.

To optimize response by the graphics processor, ensure the fast-render-on-move option is enabled. This allows the drawing of lower resolution objects (or dots) during operations where the user is rotating or zooming a structure in the 3D View.

Selecting the Dots display style for large objects can greatly improve the response of the graphics processor. Drawing partially transparent large surfaces in the Solid display style is extremely graphics-intensive. Keeping the transparency value at zero (fully opaque) until the desired view orientation is achieved provides a much faster refresh rate.

Enable banding if you have hardware accelerated texture mapping.

The Banded display style allows Materials Studio to make use of texture mapping capabilities. If your system has hardware accelerated texture mapping, enabling the Banded option will provide better visual quality and faster interactive rendering speed.

If your system does not have hardware accelerated texture mapping, disable banding until the desired view orientation is achieved.

Printing and export of bitmaps of large surfaces in the Banded style will be very slow.

Use volume display style of large fields only when extreme visual quality is required.

The rendering of large fields in the volume display style requires significant graphics resources. Very high-end graphics hardware is required for smooth interactive rendering of large fields in the volume display style. Setting the quality level to Low or Lowest may allow interactive frame rates.

In order to better see the field with the quality set to low values, you may need to increase the opacity by sliding the transparency to the left.

Printing and export of bitmaps of fields in the volume display style will be very slow.

Transparency

Use light background colors.

Use a light colored background color or texture bitmap for optimum viewing of translucent objects such as isosurfaces or fields displayed using the volume style, using the Display Options dialog.

Object visibility

Tidying up the view - hide rather than delete.

When you are working with several objects, say slices or isosurfaces, but using only one or two at the moment, turn off the visibility of the others rather than closing them. See Volumetric Selection dialog.

Removal of spurious "halo" around isosurfaces

Use IsInsideVisible property to remove spurious halo around the edge of an isosurface

Under some lighting conditions, you may observe a spurious bright halo appearing where the isosurface and background meet. This is an artifact arising from the rendering of the inside of an isosurface. If your isosurface is completely closed, you may be able to remove this artifact by selecting the isosurface and changing the *IsInsideVisible* property to No. See also Field, surface, slice and mesoscale molecule properties.

Glossary for volume visualization

Color Map: A map relating field value ranges and colors. In a color map, the full range of field values is subdivided into a range of so-called bands. Each band is then assigned a unique color.

Contour: A line on top of a surface (such as a slice or isosurface) characterized by a constant value of the field being mapped onto that surface.

Field: A set of numeric values defined at each point in the field volume. Internally, Materials Studio stores fields as a set of values defined at each point of a regularly spaced grid filling the field volume. If required, field values at arbitrary points are obtained through interpolation.

Field axes: The three axes spanning the field volume.

Field volume: The 3D volume where a field is defined. Materials Studio requires the field volume to be a parallelepiped defined by three field axes.

Isosurface: A surface formed by points whose field values are identical. Isosurfaces can be closed or open, finite or infinite, connected or disconnected, depending on the field and on the isovalue.

Isovalue: The value of a field characterizing the points of an isosurface.

Mesoscale molecule set: A grouping of mesoscale molecules which share identical topology. The molecules or beads that make up those molecules cannot be selected individually.

Miller indices: The projections of the slice normal onto the reciprocal lattice vectors $\mathbf{a}^* = (\mathbf{b} \times \mathbf{c})/V$, $\mathbf{b}^* = (\mathbf{c} \times \mathbf{a})/V$, and $\mathbf{c}^* = (\mathbf{a} \times \mathbf{b})/V$, where V is the volume spanned by the lattice vectors **a**, **b**, and **c**. By construction, the Miller plane <100> thus corresponds to a plane parallel to the plane spanned by the **b** and **c** lattice vectors, and similarly for <010> and<001>.

Periodic field: A field whose value is invariant under a periodic translation. Materials Studio supports 2D and 3D periodicity, see periodic fields for details.

Segregate: A subregion of a field. Segregates are created and managed by a segregator.

Segregator: Divides a field into a number of subregions or segregates whose boundaries are defined by an isovalue. Filtering may be applied so only regions which are accessible or isolated, or have values higher or lower than the isosurface are created.

Slice: A plane used to generate a 2D cut through a 3D field. A slice is characterized by the slice position and the slice normal. Materials Studio chooses the visible size of the slice such that all points lying both within the visible field volume and on the slice plane are visible.

Slice crystal direction: The Miller indices of a slice, arbitrarily normalized to 1.

Slice normal: A normalized vector describing the direction perpendicular to the slice plane.

Slice position: The position of a point on the slice plane. Only the position along the slice normal affects the positioning of the slice in the 3D view.

Volume display style: A descriptive name for a field display style where the field is visualized as a semi-transparent "fog", colored according to field values. In the graphics community, this technique is also called "Direct", "Ray-casting", or "Volume Rendering".

Display Style dialog

The Display Style dialog allows you to control the way in which structures displayed in the 3D Viewer are rendered. You can also interact with the 3D Viewer to improve display and interpretation of the data in the current 3D model document.

The Display Style dialog can contain some or all of the following tabs:

- Atom: Allows you to control the rendering style and color of atomistic structures.
- Bead: Allows you to control the rendering style and color of structures composed of beads.
- Lattice: Allows you to control the rendering style, range, and color of crystal lattices.
- Reciprocal: Allows you to control the rendering style and color of reciprocal lattices.
- Molecule: Allows you to control the rendering style, color, and transparency of molecules.
- Molecule Interaction: Allows you to control the rendering style and color of interactions between molecules.
- Habit: Allows you to control the rendering style, color, and transparency of crystal habit data.
- Measurement: Allows you to control the rendering style, color, and transparency of measurements.
- Temperature Factor: Allows you to control the scaling, color, and transparency of thermal ellipsoids.
- Miller Plane: Allows you to control the rendering style, color, and transparency of Miller planes and their periodic and symmetry images.
- Field: Allows you to control the rendering style, range, and color of fields.
- Segregate: Allows you to control the rendering style, range, and color of segregates.
- Isosurface: Allows you to control the characteristics of isosurfaces derived from a field.
- Slice: Allows you to control the characteristics of slices derived from a field.
- Mesoscale Molecules: Allows you to control the rendering style, range, and color of mesoscale molecules.
- Vector: Allows you to control the rendering style, size, and color of vectors.
- Electrode: Allows you to control the rendering style, size, and color of electrodes.

Note: Only tabs that are relevant to the objects in the currently active document will be displayed in the Display Style dialog.

Help: Displays the Help topic for the current tab.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style*
Toolbar	
Shortcut menu	*Display Style*

Atom tab

The *Atom* tab allows you to control the rendering style and color of atomistic structures.

Display style

None: When selected, indicates that atoms and bonds will not be displayed.

Line: When selected, indicates that atoms and bonds will be rendered as lines. Non-bonded atoms will be displayed as jacks.

Line width: Specify the width, in pixels, of the lines used to represent atoms and bonds when employing the *Line* display style.

Stick: When selected, indicates that atoms and bonds will be rendered as solid cylinders, or sticks. Non-bonded atoms will be displayed as spheres.

Ball and stick: When selected, indicates that atoms will be rendered as solid spheres, or balls, and bonds will be rendered as solid cylinders.

Stick radius: Specify the radius of the cylinders used to represent atoms and/or bonds when employing the *Stick* or *Ball and stick* display styles. The *Stick radius* must always be less than or equal to the *Ball radius*.

Ball radius: Specify the radius of the spheres used to represent atoms when employing the *Ball and stick* display style.

CPK: When selected, indicates that atoms will be rendered as spheres with radii that are related to the van der Waals (vdW) radii of the atoms.

CPK scale: Specify the scale factor to be applied to the atomic radii when employing the *CPK* display style.

Polyhedron: When selected, indicates that solid coordination polyhedra are drawn around cations, with the number of corners corresponding to the coordination number, as defined by the bonding connectivity.

Coloring

Custom: When selected, indicates that custom coloring will be used for atoms and bonds. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Color by: When selected, indicates that atoms and bonds will be colored according to the property selected from the dropdown list. Available options are:

- Element
- Forcefield Type
- Charge
- Charge Group
- Backbone
- Repeat Unit
- Linear Chain
- Motion Group
- Constraint
- Molecule
- Physical System

Note: When coloring atoms by their constraints, unconstrained atoms are shown in gray, whereas fixed atoms are shown in red.

Tip: Except for coloring by element type, the atom coloring will not be updated dynamically if the atom properties are modified. In order for the atom coloring to reflect current property values correctly, it is recommended that you recolor the atoms whenever any changes to their properties are made.

Bond order: When checked, indicates that bonds will be displayed in a way that reflects their bond order or type. This control is disabled when the display style is set to *None*, *CPK* or *Polyhedron*.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Note: Default settings for the rendering style of atoms and bonds in 3D structure documents can be specified using the Default Atom Style dialog. However, the default coloring scheme for atoms cannot be altered.

Access methods

Menu	*View	Display Style	Atom*
Toolbar		*Atom*
Shortcut menu	*Display Style	Atom*

Bead tab

The *Bead* tab allows you to control the rendering style and color of structures composed of beads.

Display style

None: When selected, indicates that beads and bead connectors will not be displayed.

Line: When selected, indicates that beads and bead connectors will be rendered as lines. Beads without linkages will be displayed as jacks.

Dot and line: When selected, indicates that beads will be rendered as dots and bead connectors will be rendered as lines.

Line width: Specify the width, in pixels, of the lines used to represent beads and bead connectors when employing the *Line* or *Dot and line* display styles.

Stick: When selected, indicates that beads and links between beads will be rendered as solid cylinders, or sticks. Unlinked beads will be displayed as spheres.

Ball and stick: When selected, indicates that beads will be rendered as solid spheres, or balls, and bead connectors will be rendered as solid cylinders.

Stick radius: Specify the radius of the cylinders used to represent beads and/or connectors when employing the *Stick* or *Ball and stick* display styles. The *Stick radius* must always be less than or equal to the *Ball radius*.

Ball radius: Specify the radius of the spheres used to represent beads when employing the *Ball and stick* display style.

CPK: When selected, indicates that beads will be rendered as spheres with radii that are related to the radii of the beads.

CPK scale: Specify the scale factor to be applied to the beads radii when employing the *CPK* display style.

Coloring

Custom: When selected, indicates that custom coloring will be used for beads and bead connectors. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Color by: When selected, indicates that beads and bead connectors will be colored according to the property selected from the dropdown list. Available options are:

- Bead Type
- Forcefield Type
- Charge
- Constraint
- Molecule
- Physical System

Note: When coloring beads by their constraints, unconstrained beads are shown in gray, whereas fixed beads are shown in red.

Tip: Except for coloring by bead type, the bead coloring will not be updated dynamically if the bead properties are modified. In order for the bead coloring to reflect current property values correctly, it is recommended that you recolor the beads whenever any changes to their properties are made.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Bead*
Toolbar	 *| Bead*
Shortcut menu	*Display Style	Bead*

Lattice tab

The *Lattice* tab allows you to control the rendering style, range, and color of crystal lattices.

Display style

The controls in this section allow you to adjust the range of atoms and other objects that are displayed in periodic systems. Periodic systems are considered to be infinite in extent. These controls govern the finite portion of the structure that is to be displayed.

Style: Select the rule by which atoms are to be made visible. Available options are:

- Default - Atoms will be made visible according to the center of geometry of connected sets of atoms, so that only complete molecules are shown. If the structure forms an infinite network, this rule is modified so that visibility in the direction of the network is simply controlled by the atom coordinates. This gives a display representation that should be suitable for most types of structure.
- In-Cell - Atoms in the structure will be made visible purely according to their coordinates. A small tolerance is used when calculating the set to be displayed, hence, in the display of a single cell, it is possible to have an atom displayed together with a translational copy of itself.
- Original - Each atom will be displayed in its original location, together with copies formed by applying each of the operators of the symmetry group. Translational copies of these are added according to the integer values of the *Range* parameters.
- None - Display of atoms in the structure and the lattice will be turned off.

Range: Specify the range of space in which atoms are to be made visible by entering *Min* and *Max* values for each of the three crystallographic directions, *A*, *B*, and *C*. Fractional values can be entered, allowing

display of just a portion of a cell. Negative values are also permitted. The spin controls increase or decrease the relevant value by 1.00, regardless of whether it is an integer or not.

Lattice

The controls in this section allow you to adjust the way in which a periodic lattice is represented.

None: When selected, indicates that the lattice will not be displayed.

Dashed line: When selected, indicates that the lattice will be rendered using dashed lines.

Line: When selected, indicates that the lattice will be rendered using solid lines.

Line width: Specify the width, in pixels, of the lines used to represent the lattice when employing the *Dashed* or *Solid* display styles.

Stick: When selected, indicates that the lattice will be rendered using solid cylinders, or sticks.

Stick radius: Specify the radius of the cylinders used to represent the lattice when employing the *Stick* display style.

Color: Select a color to be used for the lattice. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Label axes: When checked, indicates that axes will be labeled, if displayed.

> **Tip:** The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View* | *Display Style* | *Lattice*
Toolbar	 | *Lattice*
Shortcut menu	*Display Style* | *Lattice*

Reciprocal tab

The *Reciprocal* tab allows you to control the rendering style and color of reciprocal lattice elements.

Display style

The controls in this section allow you to select whether to display elements of the reciprocal space and how to map it onto the displayed coordinate system.

Display reciprocal lattice: When selected the reciprocal lattice will be displayed.

Scale: Specify the relative scaling of the reciprocal lattice with respect to the atomistic data for documents where both are displayed together. Reciprocal lattices are frequently displayed along with the atomistic structural data from which they were derived. These two sets of data are defined in different coordinate systems.

Paths

The controls in this section allow you to adjust the way in which a high-symmetry path in the Brillouin zone is represented.

Line type: Select the style of line to display, options are:

- None - the path will not be visible
- Solid - the path will be rendered using solid lines
- Dashed - the path will be rendered using dashed lines

Line width: Specify the width, in pixels, of the lines used to represent the path. This is not available if the *Line type* control of the Paths is set to None.

Color: Select a color to be used for the path. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted. This is not available if the *Line type* control of the Paths is set to None.

Brillouin zone

Display style: Select the style of line to display, options are:

- None - the Brillouin zone will not be visible
- Solid - the Brillouin zone will be rendered using solid lines
- Dashed - the Brillouin zone will be rendered using dashed lines

Line width: Specify the width, in pixels, of the lines used to represent the Brillouin zone when employing the *Dashed* or *Solid* display styles. This is not available if the *Display style* of the Brillouin zone is set to None.

Color: Select a color to be used for the Brillouin zone. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted. This is not available if the *Display style* of the Brillouin zone is set to None.

Transparency: Specify the degree of transparency of the Brillouin zone display using the slider control. Moving the slider to the right increases the transparency of the Brillouin zone, while moving it to the left increases its opacity. This is not available if the *Display style* of the Brillouin zone is set to None.

Display axes: When selected the axes of reciprocal lattice will be displayed.

> **Tip:** The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View | Display Style | Reciprocal*
Toolbar	 *| Reciprocal*
Shortcut menu	*Display Style | Reciprocal*

Molecule tab

The *Molecule* tab allows you to control the rendering style, color, and transparency of molecules.

For some structures, explicit Molecule objects may have been defined to group atoms into chemical molecular units. By default, these units are not displayed in the 3D view and only their atoms may be seen.

Display style

None: When selected, indicates that molecules will not be displayed.

Polyhedron: When selected, indicates that molecules will be rendered as polyhedra. The vertices of the polyhedra are defined by the locations of the atoms contained within each molecule.

Ellipsoid: When selected, indicates that molecules will be rendered as ellipsoids covering the approximate extent of the atoms contained in each molecule.

Coloring

> **Note:** Symmetry is not respected when coloring molecules, making it possible to color different symmetry images independently.

Color: Select a color to be used for molecules. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Transparency: Specify the degree of transparency of molecules using the slider control. Moving the slider to the right increases the transparency of the molecules, while moving it to the left increases their opacity.

> **Tip:** The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Molecule*
Toolbar	 *| Molecule*
Shortcut menu	*Display Style	Molecule*

Molecule Interaction tab

The *Molecule Interaction* tab allows you to control the rendering style and color of interactions between molecules.

Molecule interactions are pairings of formal Molecule objects. They are used by the Morphology module to define crystal graphs.

Display style

None: When selected, indicates that molecule interactions will not be displayed.

Dashed line: When selected, indicates that molecule interactions will be rendered as dashed lines.

Line: When selected, indicates that molecule interactions will be rendered as solid lines.

Line width: Specify the width, in pixels, of the lines used to represent molecule interactions when employing the *Dashed line* or *Line* display styles.

Stick: When selected, indicates that molecule interactions will be rendered as solid cylinders, or sticks.

Stick radius: Specify the radius of the cylinders used to represent molecule interactions when employing the *Stick* display style.

Coloring

> **Note:** Symmetry is not respected when coloring interactions, making it possible to color different symmetry images independently.

Custom: When selected, indicates that custom coloring will be used for molecule interactions. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Color by energy: When selected, indicates that molecule interactions will be colored according to their bond energy. Within the current selection, the strongest will be colored blue and the weakest colored red. The colors will be smoothly graduated between these two extremes for interactions with intermediate bond energies.

Note: The interaction coloring will not be updated dynamically if the energies are re-evaluated. In order for the interaction coloring to reflect current property values correctly, it is recommended that you recolor the molecule interactions whenever any changes to their bond energies have been made.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Molecule Interaction*
Toolbar	 *| Molecule Interaction*
Shortcut menu	*Display Style	Molecule Interaction*

Habit tab

The *Habit* tab allows you to control the rendering style, color, and transparency of crystal habit data.

Display style

Habit data consist of facets and growth faces. Facets are created from the intersections of the growth faces nearest the growth center. Consequently, each facet has an associated growth face, however, the reverse is not necessarily true. Facets are displayed as a solid plane. The edges between facets are shown as lines. Growth faces are indicated by an arrow normal to the plane, with its base on the plane.

Show facets: When checked, indicates that habit facets will be made visible.

Show edges: When checked, indicates that habit edges will be made visible.

Show growth faces: When checked, indicates that growth faces will be made visible.

Arrow size: Specify the relative size of the arrows used to represent growth faces. Default = 0.10.

Note: The *Show facets*, *Show edges*, *Show growth faces*, and *Size* controls all respect the symmetry of the system. Thus, if one facet, edge, or growth face has its visibility altered by these controls, all the symmetrically equivalent facets, edges, or growth faces will be affected in the same way.

Habit size: Specify the relative scaling of the habit data with respect to the atomistic data for documents where both are displayed together. Habit data are frequently displayed along with the atomistic structural data from which they were derived. These two sets of data are defined in different coordinate systems.

Coloring

Habit facets share their coloring attributes (color and transparency) with the associated growth faces. Thus, these options affect both types of object (depending on their visibility).

Note: Symmetry is not respected when coloring growth faces and edges, making it possible to color different faces or edges independently.

Facet color: Select a color to be used for growth faces and facets. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Transparency: Specify the degree of transparency of growth faces or facets using the slider control. Moving the slider to the right increases the transparency of the growth faces or facets, while moving it to the left increases their opacity.

Edge color: Select a color to be used for edges. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Habit*
Toolbar	 *| Habit*
Shortcut menu	*Display Style	Habit*

Measurement tab

The *Measurement* tab allows you to control the rendering style, color, and transparency of measurements. Measurements include distance, angle, and torsion monitors.

Display style

None: When selected, indicates that measurements will not be displayed.

Line: When selected, indicates that measurements will be rendered in the default manner, using lines and arcs.

Label measurement: When checked, indicates that measurements will be annotated with their current values.

Coloring

Custom: When selected, indicates that custom coloring will be used for measurements. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Color by: When selected, indicates that measurements will be colored according to the property selected from the dropdown list. Available options are:

- Type
- Constraint

Note: When coloring measurements by their constraints, unconstrained measurements are shown in gray, whereas fixed measurements are shown in red.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Measurement*
Toolbar	 *| Measurement*
Shortcut menu	*Display Style	Measurement*

Temperature Factor tab

The *Temperature Factor* tab allows you to control the scaling, color, and transparency of thermal ellipsoids.

Add: Adds thermal ellipsoids to any of the selected atoms that have non-zero temperature factors. If no atoms are selected in the currently active document, thermal ellipsoids are added to all atoms with non-zero temperature factors.

Remove: Removes the selected thermal ellipsoids. If no selection is made, all of the thermal ellipsoids in the currently active document are removed.

Scale factor: Specify the scale factor that determines the rendering size of thermal ellipsoids on screen. Thermal ellipsoids are drawn at a size corresponding to a certain probability, which the scale factor can be used to vary. See the Thermal ellipsoid scaling topic for more details.

Transparency: Specify the degree of transparency of thermal ellipsoids using the slider control. Moving the slider to the right increases the transparency of the ellipsoids, while moving it to the left increases their opacity.

Show hatched octant: When checked, indicates that thermal ellipsoids will be displayed with the forward-facing octant cut away.

Coloring

Custom: When selected, indicates that custom coloring will be used for thermal ellipsoids. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Color by atom: When selected, indicates that thermal ellipsoids will be colored according to the color of the atom to which they are attached.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Temperature Factor*
Toolbar	 *| Temperature Factor*
Shortcut menu	*Display Style	Temperature Factor*

Miller Plane tab

The *Miller Plane* tab allows you to control the rendering style, color, and transparency of Miller planes and their periodic and symmetry images.

Display style

None: When selected, indicates that Miller planes will not be displayed.

Outline: When selected, indicates that Miller planes will be rendered by showing only the outline of the visible portion of the plane.

Filled: When selected, indicates that Miller planes will be rendered by showing a solid plane.

Show periodic images: When checked, indicates that the set of periodic images of the selected Miller plane will be shown.

Show symmetry images: When checked, indicates that the set of symmetry images of the selected Miller planes will be shown.

Note: The set of planes that is shown at any time is the set of all possible planes that intersect the current lattice display range, subject to the settings of the *Show periodic images* and *Show symmetry images* options for the specific structure.

It is possible, especially if both the *Show periodic images* and *Show symmetry images* checkboxes are unchecked, that none of the Miller planes that should be visible will intersect with the lattice display range. If this is the case, it is recommended that you check the *Show periodic images* checkbox.

Halo size: Specify the extent, in Å, by which the selected Miller plane should extend beyond the lattice display range.

Coloring

Color: Select a color to be used for Miller planes. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Transparency: Specify the degree of transparency of Miller planes using the slider control. Moving the slider to the right increases the transparency of the planes, while moving it to the left increases their opacity.

Note: If you set the *Display style*, *Color*, or *Transparency* when a set of parallel planes or a family of symmetry-related planes is in scope, the new settings will be applied to all planes in the set or family, regardless of whether they are currently visible or not. Hence, if the lattice display range is increased or the planes are moved, the new planes that come into view will be rendered using these new settings.

However, if you alter the *Display style*, *Color*, or *Transparency* settings after individually selecting one or more Miller planes, the new settings will be applied only to the planes that are in scope. This means that if the lattice display range is increased or the planes are moved, the new planes that come into view will be rendered using the previous settings and not the new ones.

Tip: The *Editing* field at the bottom of the dialog shows the number of Miller planes, sets of parallel planes, and families of symmetry-related planes that are in scope in the currently active document. When nothing is selected, all the families and the planes in the current display range in the document are deemed to be in scope.

Access methods

Menu	*View	Display Style	Miller Plane*
Toolbar	 *| Miller Plane*
Shortcut menu	*Display Style	Miller Plane*

Field tab

The *Field* tab allows you to control the rendering style, range, and color of fields.

See Selecting fields, surfaces, slices, and mesoscale molecules for details on how to select fields.

Display style

Visible: When checked, indicates that fields (including any surrounding boxes) will be made visible, regardless of any other settings on the *Field* tab.

Show box: When checked, indicates that a box will be drawn around the visible field volume. The visible field volume can be modified using the Display range controls.

Empty: When selected, indicates that fields will not be displayed. Any surrounding boxes will continue to remain visible.

Dots: When selected, indicates that fields will be rendered as randomly spaced dots. By default, dots are shown wherever the field is defined, but you can restrict the display to regions of space with field values that fall within a specified range using the Color Maps dialog.

Quality: Set the quality of the field rendering when employing the *Dots* display style. This setting determines the density (number) of dots shown - the higher the field quality, the greater the number of dots. Available options are:

- Lowest
- Low
- Medium
- High
- Highest

Dot size: Specify the size of the dots used to render the field when employing the *Dots* display style. Allowed values are integers ranging from 1 to 9.

Volume: When selected, indicates that fields will be rendered as a semi-transparent fog. This is also known as direct visualization of the field and is particularly useful when coloring the field *By field values*. Hardware limitations may adversely affect interactive performance while in this mode. Use the Color Maps dialog to restrict the display to regions of space with field values within a specific range.

Quality: Set the quality of the field rendering when employing the *Volume* display style. In general, a higher quality results in the field having a smoother appearance, at the expense of slower performance. Available options are:

- Lowest
- Low
- Medium
- High
- Highest

Transparency: Specify the degree of transparency of fields when employing the *Volume* display style using the slider control. Moving the slider to the right increases the transparency of the fields, while moving it to the left increases their opacity.

Coloring

Custom: When selected, indicates that custom coloring will be used for fields. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Color by field values: When selected, indicates that field values will be mapped to colors according to the settings specified on the Color Maps dialog, which also controls whether or not a color map legend is displayed alongside the field.

Display range

Specify the proportions of fields, isosurfaces, and slices that are displayed along the directions defining the field volume by entering *Min* and *Max* values for each of the three directions. Fractional values can be entered, allowing display of just a portion of the field volume. Negative values are also permitted. For nonperiodic fields, both the *Min* and *Max* values must lie between 0.00 and 1.00. The spin controls increase or decrease the relevant value to the next half-integer (i.e., 0.50, 1.00, 1.50, etc.). The actual value shown may deviate slightly from a half-integer, since the field volume is discretized into a finite number of points (voxels) and the display range is rounded to match the nearest voxel.

Note: For periodic systems, the field display range is independent of the display range specified on the Lattice tab. As a result, the visible part of the field can be set independently of the visible part of the 3D structure.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Field*
Toolbar	 *| Field*
Shortcut menu	*Display Style	Field*

Segregate tab

The *Segregate* tab allows you to control the rendering style, range, and color of segregates.

See Selecting fields, surfaces, segregates, slices, and mesoscale molecules for details on how to select segregates.

Display style

Visible: When checked, indicates that segregates (including any surrounding boxes) will be made visible, regardless of any other settings on the *Segregate* tab.

Show box: When checked, indicates that a box will be drawn around the visible segregate volume. The visible segregate volume can be modified using the Display range controls.

Empty: When selected, indicates that segregates will not be displayed. Any surrounding boxes will remain visible.

Dots: When selected, indicates that segregates will be rendered as randomly spaced dots. By default, dots are shown wherever the segregate is defined, but you can restrict the display to regions of space with segregate values that fall within a specified range using the Color Maps dialog.

Quality: Set the quality of the segregate rendering when employing the *Dots* display style. This setting determines the density (number) of dots shown - the higher the segregate quality, the greater the number of dots. Available options are:

- Lowest
- Low
- Medium
- High
- Highest

Dot size: Specify the size of the dots used to render the segregate when employing the *Dots* display style. Allowed values are integers ranging from 1 to 9.

Volume: When selected, indicates that segregates will be rendered as a semi-transparent fog. This is also known as direct visualization of the segregate and is particularly useful when coloring the segregate *By field values*. Hardware limitations may adversely affect interactive performance while in this mode. Use the Color Maps dialog to restrict the display to regions of space with segregate values within a specific range.

Quality: Set the quality of the segregate rendering when employing the *Volume* display style. In general, a higher quality results in the segregate having a smoother appearance, at the expense of slower performance. Available options are:

- Lowest
- Low
- Medium
- High
- Highest

Transparency: Specify the degree of transparency of segregates when employing the *Volume* display style using the slider control. Moving the slider to the right increases the transparency of the segregate, while moving it to the left increases their opacity.

Coloring

Custom: When selected, indicates that custom coloring will be used for segregates. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Color by field values: When selected, indicates that field values will be mapped to colors according to the settings specified on the Color Maps dialog, which also controls whether or not a color map legend is displayed alongside the segregate.

Color by segregate: When selected, indicates that each segregate will be colored with a different solid color.

Constraints

Isovalue: Defines the limits of the segregates displayed, the *FieldMean* isovalue is used by default.

Values: Choose whether the segregates generated should contain field values that are Low or High relative to the Isovalue. All values can also be used. Changing the limit will return the display styles to their defaults as new segregate objects are created.

Connectivities: Choose whether to display segregates that are Accessible or Isolated or to display All segregates. Changing the connectivities will return the display styles to their defaults as new segregate objects are created.

Minimum size: Defines the minimum volume of the segregates generated.

> **Tip:** The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Segregate*
Toolbar		*Segregate*
Shortcut menu	*Display Style	Segregate*

Isosurface tab

The *Isosurface* tab allows you to control the characteristics of isosurfaces derived from a field.

See Selecting fields, surfaces, slices, and mesoscale molecules for details on how to select isosurfaces.

Display style

Visible: When checked, indicates that isosurfaces (including any surrounding frame) will be made visible, regardless of any other settings on the *Isosurface* tab.

Dots: When selected, indicates that isosurfaces will be rendered as randomly spaced dots. By default, dots are shown wherever the field is defined, but you can restrict the display to regions of the isosurface with field values that fall within a specified range using the Color Maps dialog.

Dot size: Specify the size of the dots used to render the isosurface when employing the *Dots* display style. Allowed values are integers ranging from 1 to 9.

Solid: When selected, indicates that isosurfaces will be rendered as filled triangles. Hardware limitations may adversely affect interactive performance while in this mode.

Banded: When checked, indicates that isosurfaces will be subdivided into uniformly colored regions, each of which will correspond to a range of values in the mapped field. This results in 'bands' of uniform color across the surface. The number of different colors is determined by the *Bands* setting on the Color Maps dialog. This checkbox is enabled only if a mapped field has been chosen for each of the currently selected isosurfaces. See the glossary for more details.

Transparency: Specify the degree of transparency of isosurfaces when employing the *Solid* display style using the slider control. Moving the slider to the right increases the transparency of the isosurfaces, while moving it to the left increases their opacity.

Note: If the *Solid* display style is chosen, the inside of the isosurface is usually rendered in gray. However, choosing the *Banded* rendering mode means that the inside of the isosurface will appear in the same color as the outside. This is an artifact of OpenGL.

High values inside: When checked, indicates that the specified rendering settings will be applied to the outside of the isosurface. If unchecked, reverses the rendering styles of the inside and outside of the isosurface. By default, it is assumed that decreasing field values indicate the outside of the isosurface. The inside is uniformly colored gray, unless the Banded display style is selected.

Coloring

Custom: When selected, indicates that custom coloring will be used for fields. Clicking on the color controls provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted. If *+/-* is selected from the Isovalue dropdown list, the second color control becomes active and enables you to individually control the color of the positive and negative isosurfaces.

Original colors: When selected, indicates that isosurfaces will be rendered in the original colors that they were generated with. This option is enabled only for legacy surfaces, i.e., surfaces generated in a different modeling environment and subsequently imported into Materials Studio. At present, only surfaces imported into Materials Studio in the `.msi` file format can be displayed.

Color by mapped field: When selected, indicates that each point on the isosurface will be colored according to the value of the mapped field at this point. Field values of the mapped field are mapped to colors according to the settings specified on the Color Maps dialog, which also controls whether or not a color map legend is displayed alongside the 3D view. This option is enabled only if a mapped field has been chosen for each of the currently selected isosurfaces.

Mapped field: Select a field to use for the color map when employing the *Color by mapped field* coloring mode from the dropdown list. Selecting a mapped field while in another coloring mode automatically resets the coloring mode to *Color by mapped field*.

Generation

Isovalue: Specify the field value at which the isosurface is drawn and select the way in which it is generated from the dropdown list.

Type: Specify the type of isosurface to display. Available options are:

- normal - A single surface is generated at the specified *Isovalue*.
- accessible - A surface is generated that encloses those regions which are externally accessible. External accessibility is determined by a flooding algorithm that fills from the external faces of the field.

  If the *High values inside* checkbox is checked, flooding is allowed to pass through regions below the *Isovalue*. Conversely, if the *High values inside* checkbox is unchecked, flooding is blocked from passing through regions below the *Isovalue*.
- +/- - Two surfaces are generated, one at the specified *Isovalue* and one at the corresponding negative value.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Isosurface*
Toolbar	 *| Isosurface*
Shortcut menu	*Display Style	Isosurface*

Slice tab

The *Slice* tab allows you to control the characteristics of slices derived from a field.

See Selecting fields, surfaces, slices, and mesoscale molecules for details on how to select slices.

Display style

Visible: When checked, indicates that slices (including any surrounding frame) will be made visible, regardless of any other settings on the *Slice* tab.

Show frame: When checked, indicates that a frame will be drawn around the visible slice area. The visible field volume can be modified using the Display range controls on the *Field* tab.

Empty: When selected, indicates that slices will not be displayed. Any surrounding frames will continue to remain visible.

Dots: When selected, indicates that slices will be rendered as randomly spaced dots. By default, dots are shown wherever the field is defined, but you can restrict the display to regions of the slice with field values that fall within a specified range using the Color Maps dialog.

Quality: Set the quality of the slice rendering when employing the *Dots* display style. This setting determines the density (number) of dots shown - the higher the slice quality, the greater the number of dots. Available options are:

- Lowest
- Low
- Medium
- High
- Highest

Dot size: Specify the size of the dots used to render the slice when employing the *Dots* display style. Allowed values are integers ranging from 1 to 9.

Solid: When selected, indicates that slices will be rendered according to the currently specified coloring mode.

Banded: When checked, indicates that slices will be subdivided into uniformly colored regions, each of which will correspond to a range of values in the mapped field. This results in 'bands' of uniform color across the surface. The number of different colors is determined by the *Bands* setting on the Color Maps dialog. See the glossary for more details.

Transparency: Specify the degree of transparency of slices when employing the *Solid* display style using the slider control. Moving the slider to the right increases the transparency of the slices, while moving it to the left increases their opacity.

Coloring

Custom: When selected, indicates that custom coloring will be used for slices. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Color by field values: When selected, indicates that field values will be mapped to colors according to the settings specified on the Color Maps dialog, which also controls whether or not a color map legend is displayed alongside the slice.

> **Tip:** The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Slice*
Toolbar	 *| Slice*
Shortcut menu	*Display Style	Slice*

Mesoscale Molecules tab

The *Mesoscale Molecules* tab allows you to control the rendering style, range, and color of mesoscale molecules.

See Selecting fields, surfaces, slices, and mesoscale molecules for details on how to select mesoscale molecules.

Display style

Visible: When checked, indicates that mesoscale molecules will be made visible, regardless of any other settings on the *Mesoscale Molecules* tab.

Show beads: When checked, indicates that bead positions in mesoscale molecules will be made visible.

Show bonds: When checked, indicates that bead-bead bonds in mesoscale molecules will be made visible.

Dot and line: When selected, indicates that beads in mesoscale molecules will be rendered as dots and bead-bead bonds will be rendered as lines.

Dot size: Specify the size of the dots used to represent beads when employing the *Dot and line* display style. Allowed values are integers ranging from 1 to 9.

Line width: Specify the width of the lines used to represent bead-bead bonds when employing the *Dot and line* display style. Allowed values are integers ranging from 1 to 9. The *Line width* must always be less than or equal to the *Dot size*.

Ball and stick: When selected, indicates that beads in mesoscale molecules will be rendered as solid spheres, or balls, and bead-bead bonds will be rendered as solid cylinders, or sticks.

Stick radius: Specify the radius of the cylinders used to represent bead-bead bonds in mesoscale molecules when employing the *Ball and stick* display style. Allowed values are numbers greater than 0.05. The *Stick radius* must always be less than or equal to the *Ball radius*.

Ball radius: Specify the radius of the spheres used to represent beads in mesoscale molecules when employing the *Ball and stick* display style. Allowed values are numbers greater than 0.05. Values larger than 1.0 are permitted, but produce unphysical images.

Coloring

Custom: When selected, indicates that custom coloring will be used for mesoscale molecules. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Bead: When selected, allows you to individually specify the color and visibility of each bead type present in the mesoscale molecules. Clicking on the controls in the *Color* column provides access to the Microsoft Common Color Control for color selection.

Note: In cases where the same bead type appears in more than one type of mesoscale molecule in the system, it is possible for it to be represented by more than one color or to be visible in some molecules and invisible in others. In these circumstances, the *Color* setting and the *Visible* checkbox for that bead will become indeterminate.

Display range

Specify the proportion of a simulation cell that is displayed by entering *Min* and *Max* values for each of the three directions that define the simulation cell volume. Fractional values can be entered, allowing display of just a portion of the cell. Negative values are also permitted. The spin controls increase or decrease the relevant value to the next half-integer (i.e., 0.50, 1.00, 1.50, etc.).

Note: The mesoscale molecules display range is independent of the display range specified on the Field tab. As a result, the visible part of the mesoscale simulation cell can be set independently of the visible parts of the associated density fields.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Mesoscale Molecules*
Toolbar	 *| Mesoscale Molecules*
Shortcut menu	*Display Style	Mesoscale Molecules*

Vector tab

The *Vector* tab allows you to control the visual characteristics of vectors.

Display style

- None - When selected, indicates that vectors will not be displayed.
- Line - When selected, indicates that vectors will be displayed as lines.
- Arrow - When selected, indicates that vectors will be displayed as 3D arrows.

Coloring

Color: Select a color to be used for the selected vectors. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Scaling

When using scaling, the size of the displayed vector is related to the magnitude of the vector property. Without scaling, all vectors will appear the same size, indicating the direction but not the size of the vector. Options are:

- No scaling - The length of the line is fixed and will not vary with the magnitude of the vector. Applies to *Line* style only
- Scale length - The length of the symbol increases with the magnitude of the vector, but its width is constant. Applies to both *Line* and *Arrow* styles
- Scale size - Both length and width of the arrow head and shaft increase with the magnitude of the vector. Applies to *Arrow* style only
- Scale head - The size of the arrow head increases with the magnitude of the vector, but the shaft remains short. Applies to *Arrow* style only

Fixed length: Specifies the length of the symbol when not using scaling, in Å.

Scale factor: Controls the size of the symbol when using scaling. Increase the scale factor to increase symbol size. The displayed length of the vector is the product of the vector size and the scale factor, in Å.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Vector*
Toolbar		*Vector*
Shortcut menu	*Display Style	Vector*

Electrode tab

The *Electrode* tab allows you to control the rendering style and color of electrodes.

Display style

Show wire: When checked, indicates that electrode wires will be made visible.

Show repeat arrow: When checked, indicates that an arrow will be shown on visible electrode wires. The arrow indicates the periodic repeat direction of the wire.

Arrow scale: Specify the relative size of the arrows used to represent the periodic repeat direction of the wire. At a scale of 1.0, the arrows show the actual repeat distance of the wire. Default = 1.0.

Show tip: When checked, indicates that electrode tips will be made visible.

Coloring

Wire color: Select a color to be used for electrode wires. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted. This also controls the color of the repeat arrow.

Transparency: Specify the degree of transparency of electrode wires using the slider control. Moving the slider to the right increases the transparency of the wires, while moving it to the left increases their opacity.

Tip color: Select a color to be used for electrode tips. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

Transparency: Specify the degree of transparency of electrode tips using the slider control. Moving the slider to the right increases the transparency of the tips, while moving it to the left increases their opacity.

Note: Not all electrodes have tips. The tip controls are disabled if a tip is not present.

Note: For periodic systems, the display range of the electrode part is dependent upon the display range specified on the Lattice tab.

Tip: The *Editing* field at the bottom of the dialog shows the number of items that are in scope in the currently active document. When nothing is selected, all the contents of the document which are in the current display range are deemed to be in scope.

Access methods

Menu	*View	Display Style	Electrode*
Toolbar	 *| Electrode*
Shortcut menu	*Display Style	Electrode*

Display Options dialog

The Display Options dialog allows you to control the way in which 3D structures are rendered in the 3D Viewer and how they are printed or exported as bitmapped output.

The Display Options dialog contains the following tabs:

- Graphics: Allows you to control the viewing transform, rendering quality and depth cueing in 3D model documents.
- Legends: Allows you to control legends in 3D model documents.
- Backgrounds: Allows you to control the background color or background images in 3D model documents.

Help: Displays the Help topic for the current tab.

Access methods

Menu	*View	Display Options*
Shortcut menu	*Display Options*

Graphics tab

The *Graphics* tab of the Display Options dialog controls viewing transform, rendering quality, and depth cueing in 3D Viewer documents.

Projection

Orthographic: Specifies an orthographic viewing transform. An orthographic projection maps objects directly onto the screen without affecting their relative size. This projection is used when the image needs to reflect the measurements of objects.

Perspective: Specifies a perspective viewing transform. You can control the field of view angle using *Angle*. The perspective projection matches how you see things in daily life. Perspective makes objects that are further away appear smaller.

Angle: Controls the view angle used in the *Perspective* projection. Range = 5 to 120°.

Quality

Allows control over the rendering quality of the 3D View. This slider control trades visual quality against interactive performance.

> **Tip:** The quality setting is used for both on-screen and printed output, which should be similar in appearance. The influence of the quality setting depends on the available graphics support on the machine. The Resolution and graphical quality topic provides more information about the quality setting.

Depth cue: Enables depth cueing. You can control depth cue intensity using *Depth cue intensity*.

Fast render on move: Enables dynamic level-of-detail switching while the 3D Viewer is performing a move operation. This is a performance optimization for improving interactive usability of Materials Studio.

Optimized lights: Enables optimization of lighting calculations. This control may cause rendering artifacts on some graphics hardware, therefore its default value is unselected.

Depth cue intensity: Controls the rate at which the background color fades. A high value appears as a strong fade and so emphasizes viewer depth. The Depth Cue color is always the same as the background color, which is set from the *Background* tab on the *Display Options* dialog.

Access methods

Menu	*View	Display Options	Graphics*
Shortcut menu	*Display Options	Graphics*

Legends tab

The *Legends* tab of the Display Options dialog provides control of legends in 3D Viewer documents.

Show axis indicator: Enables the display of the axis indicator in the lower right-hand corner of the 3D Viewer.

Show scale bar: Enables the display of the scale ruler at the bottom of the 3D Viewer. The scale ruler will not be shown if a *Perspective* projection is used.

Units: Select the units to be used for the scale bar legend. Available options are:

- Angstrom
- nanometer

> **Note:** The units selected here affect only the legend for the scale bar. They do not affect any other coordinate or distance information.

Color: Select a color to be used for the scale bar. Clicking on the color control provides access to the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted.

> **Note:** The color map legends for volumetric visualization are controlled by the Color Maps dialog.

Access methods

Menu	*View	Display Options	Legends*
Shortcut menu	*Display Options	Legends*

Backgrounds tab

The *Backgrounds* tab of the Display Options dialog provides control of background color or images in 3D Viewer documents.

Solid color: Allows you to select the background color using the Microsoft Common Color Control. Spinners control the brightness. This color is also used as the Depth Cue color.

Image texture: Allows you to select a background image. Images may be added to the list by using the *Browse...* button. This version of Materials Studio allows only 24-bit uncompressed BMP format images as background textures.

Browse...: Provides access to the Open Background Image dialog allowing you to select any 24-bit uncompressed bitmap (`.bmp`) image file to use as a background for the 3D Viewer.

Note: Enabling background images may severely affect interactive performance on some machines. It is recommended that this feature be used only during bitmap export, AVI export and printing if the graphics system does not support texture mapping hardware acceleration.

Users can create their own background using a paint program such as Microsoft Paint. Ensure the *Save as type* is set to 24-bit Bitmap.

Access methods

Menu	*View	Display Options	Backgrounds*
Shortcut menu	*Display Options	Backgrounds*

Motion modes

You can turn on and off moving displays of 3D models using the Rock & Roll toolbar. Clicking one of the command buttons on the toolbar turns on the associated motion mode. Clicking the button again turns it off. There are three different motion modes available:

 **Spin:** Spins the current 3D model continuously around the virtual Y axis.

 **Rock:** Spins the current 3D model part of a revolution around the virtual Y axis, first in one direction and then in the other.

 **Roll:** Spins the current 3D model continuously around the virtual X axis.

Note: The *Spin*, *Rock*, and *Roll* motions of the 3D model are relative to the virtual axes and not the axes of the 3D model (as represented by the axis legend). The virtual axes represent the axes of the screen. For example, the Y axis runs vertically, parallel to the face of the screen. Since the virtual axes also run through the center of the 3D Viewer document, spinning, rocking, or rolling an off-center model gives the visual impression that it is "orbiting" the virtual axis.

While the 3D View is rocking, rolling, or spinning, you can also use other tools, commands, or mouse actions to make selections, change the display, sketch, etc. However, the selection lasso, selection rectangle, and zoom rectangle operations are disabled while the 3D View is in motion.

Apparent depth effects

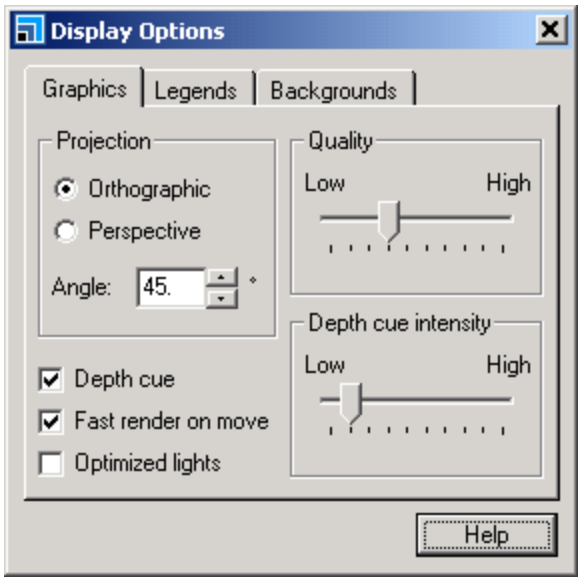
Depth effects in the 3D Viewer are controlled from the Display Options dialog.

The Display Options dialog provides a *Depth Cue* checkbox and a *Depth Cue Intensity* slider. Enable depth cueing by clicking on the checkbox then drag the slider to control the intensity of the depth cue.

The Depth Cue color is set by the *Solid Color* button on the Backgrounds tab of the *Display Options* dialog.

Resolution and graphical quality

The graphical quality of the 3D View is controlled from the Display Options dialog. Visual quality is dependent on the precision of the 3D representation. A structure drawn with high resolution cylinders will appear smooth with more accurate lighting as compared with a structure drawn with a low resolution. Quality settings are used for on-screen, printed, and bitmapped image output, which should be similar in appearance.



Display Options dialog

The *Quality* slider defines the tessellation complexity of some graphics features in the 3D View. The majority of graphics cards support Open GL shaders, which are used by default. Using shaders, both the quality and speed of graphics in Materials Studio are now higher and largely independent of the *Quality* setting. In the absence of shaders, the *Quality* setting adjusts the tessellation complexity of spheres and cylinders. The *Quality* setting has no effect on lines, fields, surfaces, or slices. The *Quality* setting always has an effect on ellipsoids, transparent spheres, and cylinders.

Note: On some systems, increasing the quality may greatly affect interactive performance, as it increases the work placed on the graphics subsystem. It is recommended that the highest values of the quality range be limited to times when the user is creating bitmapped output or printing.

Tip: Graphic display related problems can sometimes be remedied by disabling the hardware accelerated video driver. Check the *Disable hardware acceleration* checkbox on the *Tools | Options | Graphics* tab. Changing this setting will not affect the use of graphics by other software installed on your machine. Also consider checking for available updates of the graphics driver from your graphics card vendor.

Structure visibility

You can control the visibility of structures in a 3D document. All of the objects have a property "IsVisible" which can be inspected in the Properties Explorer. For all objects currently visible in the 3D Viewer, IsVisible has a Yes value. All other objects have a value of No. Most types of object are visible by default. To hide any objects in the scene, select them and then modify the IsVisible property to the value No. In many cases you can similarly modify the IsVisible property to the value Yes to show previously hidden objects.

For systems subject to symmetry, Materials Studio makes automatic choices for the visibility of individual objects from time to time. The user has control over the choice of visibility scheme within the Lattice tab of the Display Style dialog. In addition, the user can make temporary alterations to the choice of visible objects by editing their IsVisible property, as described above.

Note that the visibility reverts to the automatic scheme at the following times:

- when changes are made on the Lattice tab of the Display Style dialog
- during a crystal build, rebuild or unbuild
- following a Find Symmetry operation
- when changing between primitive and conventional lattice choices
- when retrieving server results within some Materials Studio applications

Producing grayscale images

These guidelines give advice on how to produce publication quality grayscale images using Materials Studio.

Tip: If you plan to modify the image with a paint program after exporting it from Materials Studio, uncheck the *Show axis indicator* checkbox on the Legends tab of the Display Options dialog. Post-processing will likely degrade the appearance of the axis indicator - you can easily add an axis indicator using the paint program.

Optimizing the display of the image

Your choice of background and color and your presentation of the image will affect the quality of the final grayscale output. Use the Display Style, Display Options, and Lighting dialogs to set the following parameters. These dialogs are accessible via the *View* menu and from the shortcut menu that appears when you right-click in a 3D structure document.

Choosing colors

For the best results, set the background to a light color and maximize the quality settings.

To set the stage for a molecule

1. Choose *View | Display Options* from the menu bar to display the Display Options dialog.
2. Select the Backgrounds tab and set the background to a *Solid color*, such as white or light gray, using the color chooser.
3. Select the Graphics tab. Set the *Quality* to *High* using the slider control and uncheck the *Depth cue* checkbox.

Representing atoms, bonds, and lattices

Use different atom sizes and contrasting shades of gray so that the structure is readily apparent in the absence of color.

To exchange colors for shades of gray in a molecule

1. Choose *View | Display Style* from the menu bar to display the Display Style dialog.
2. Select the Atom tab and change element colors to distinct shades of gray using the *Coloring* controls.
3. Vary the size of each element and bond type to provide a visual distinction between them using the *Ball radius* and *Stick radius* slider controls.
4. Select the Lattice tab (if available) and set the lattice color to one that is visible against the chosen background using the color chooser. For the best results, set the lattice *Line width* to 1 pixel.

Note: Only tabs that are relevant to the objects in the currently active document will be displayed in the Display Style dialog. Hence, if your document does not contain a periodic structure, the *Lattice* tab will not be available.

Adjusting the lighting

Lighting controls are located on the Lighting dialog. Your choice of lighting parameters, such as light source positioning and color and ambient light color, can greatly enhance your final image.

To optimize lighting conditions

1. Choose *View | Lighting* from the menu bar to display the Lighting dialog.
2. It is advisable to use only one light source, so ensure that the *Enable light 2* and *Enable light 3* checkboxes are unchecked.
3. Click and drag on the *Preview* sphere to place the light source where it best highlights your structure's areas of interest. Set the color of the light source using the color chooser next to the *Enable light 1*. White or light gray will provide the best results.
4. Choose an ambient color that provides a moderate contrast with the color of the light source. The *Ambient color* control specifies the color of shadowed areas.

Tip: Setting the *Shininess* to a high value using the slider control will enhance the appearance of your image.

Managing image dimensions

When you are ready to export the image, estimate the desired size of the final image and calculate the image dimensions in pixels.

To produce the image in the desired dimensions

1. Decide what size, in inches, you want the final image to be.
2. Determine the resolution of the printed image in dpi (dots per inch).
3. Calculate the dimensions of the final image, in pixels, by multiplying the vertical image size (inches) by the vertical resolution (dpi), and the horizontal image size (inches) by the horizontal resolution (dpi). For example, if you want your finished image to be 3 × 4 inches and your printer's resolution is 600 dpi, the final image will be 1800 × 2400 pixels.

   Tip: If you plan to use a paint program to further manipulate the image, export the image from Materials Studio as a `.bmp` file at *twice* the desired final image size. In the paint program, resize the image by 50% using a smoothing filter.
4. Choose *File | Export...* from the menu bar to display the Export dialog.
5. Select Structure Bitmap (*.bmp) from the *Save as type* dropdown list, then click the *Options...* button to display the Bitmap Export Options dialog.
6. Uncheck the *Use current window size* checkbox and specify the final image dimensions, in pixels, in the appropriate fields.

Modifying the image with a paint program

Use a paint program if you want to resize and annotate images created in Materials Studio and to convert the `.bmp` files Materials Studio generates into other graphical image formats. These functions are more versatile in paint programs than they are in Materials Studio.

You can move straight to printing if your image does not require resizing, annotation, or conversion.

To resize and annotate the image

1. Open the `.bmp` file in the paint program and resize the image as required, using a smoothing filter.
2. Annotate the image if desired, adding in lattice axis labels, for example.

To convert to another image format

Save the image in a lossless image format such as `.tif`.

Printing the image

If you have used a paint program to modify the image, print the image directly from the paint program.

If you are printing directly from Materials Studio, use the highest available print quality setting.

To set the print quality in Materials Studio

1. Choose *File | Page Setup...* from the menu bar to display the Page Setup dialog.
2. Select the Page Layout tab and click the *Advanced Options...* button to display the Advanced Printer Options dialog.
3. Set the *Print quality* to *High*.

Default Atom Style dialog

The Default Atom Style dialog allows you to specify default settings for the rendering style of atoms and bonds in 3D structure documents. Default atom display settings are applied by many tools including when:

- Sketching in a new 3D Atomistic document or adding to an existing 3D structure document a new fragment that is not connected to any of the existing fragments
- Importing structure files in formats other than the standard Materials Studio formats (for example, `.msi` files)
- Adding atoms to a crystal or surface
- Creating new structures using the polymer and nanostructure builders.

> **Note:** Since sketching using invisible atoms would clearly be impractical, the *None* option in the *Display style* section of the dialog is permanently disabled.

Line: When selected, indicates that atoms and bonds will be rendered as lines. Non-bonded atoms will be displayed as jacks.

Line width: Specify the width, in pixels, of the lines used to represent atoms and bonds when employing the *Line* display style.

Stick: When selected, indicates that atoms and bonds will be rendered as solid cylinders, or sticks. Non-bonded atoms will be displayed as jacks.

Ball and stick: When selected, indicates that atoms will be rendered as solid spheres, or balls, and bonds will be rendered as solid cylinders.

Stick radius: Specify the radius of the cylinders used to represent atoms and/or bonds when employing the *Stick* or *Ball and stick* display styles. The *Stick radius* must always be less than the *Ball radius*.

Ball radius: Specify the radius of the spheres used to represent atoms when employing the *Ball and stick* display style.

CPK: When selected, indicates that atoms will be rendered as spheres with radii that are related to the van der Waals (vdW) radii of the atoms.

CPK scale: Specify the scale factor to be applied to the atomic radii when employing the *CPK* display style.

Polyhedron: When selected, indicates that solid coordination polyhedra are drawn around cations, with the number of corners corresponding to the coordination number, as defined by the bonding connectivity.

> **Note:** These settings are honored to different degrees by the various tools which create atoms within Materials Studio.

> **Note:** Since the default coloring scheme for atoms cannot be altered, the controls in the *Coloring* section of the dialog are permanently disabled.

Bond order: When checked, indicates that bonds will be displayed in a way that reflects their bond order or type. This control is disabled when the display style is set to *CPK* or *Polyhedron*.

Access methods

Menu	*Modify | Default Atom Style*

Working with charts

Materials Studio allows you to display 2D charts in the Chart Viewer. Each chart may contain one or more sets of data created by Materials Studio or loaded from one of several different file types. Four chart types are supported: scatter, line, bar, and dendrogram. Scatter and line charts can also show *chart markers* which note points of significance in the chart.

You can also transfer the content of the chart view between different Windows applications. You can save data from a chart document in the internal data format, or in other standard formats. In addition, the chart image can be saved or copied in several graphical formats.

While it is possible to copy information freely from the Chart Viewer, this version of Materials Studio supports only limited functionality for pasting chart markers into a chart document. On scatter or line charts, you can delete unwanted graphs and chart markers from a document using the Chart Viewer's shortcut menu.

With the Chart Viewer, you can focus on regions of specific interest by using the zoom and pan operations.

Managing chart documents

Chart documents can be generated by reading data directly from an existing XCD, TBL, or ASC file using the Import dialog, or by creating them manually within a Materials Studio module.

You can save underlying chart data in internal XCD or comma-separated value (CSV) format, or save the chart image in bitmap (BMP) or enhanced metafile (EMF) format.

Loading and saving chart documents

To open an existing chart document that is not already part of the current project

- Choose *File | Import...* and select an XCD, TBL, or ASC file.

To save chart data to your project

- Choose *File | Save As...* to save the data in internal XCD format.

To save chart data outside of the project

1. Choose *File | Export...*.
2. To save the chart *data* select either the internal XCD or comma-separated value (CSV) format.
3. To save the chart *image* select either bitmap (BMP) or enhanced metafile (EMF) format.

Editing the chart document

To select data, either:

- Double-click on a point in the series you want to select.
- Click and drag a box around the data to select.
- Right-click and choose *Select All* from the shortcut menu.

The selected data in the chart is highlighted in red.

To remove selection:

- Click outside the selection in the Chart Viewer.
- Right-click and choose *Deselect All* from the shortcut menu.

To hide scatter or line graphs

- Uncheck the checkbox in the legend for the data set that you want to hide.

To delete scatter or line graphs

1. Uncheck the checkboxes in the legend for the data sets that you want to delete. Check the checkboxes for the data sets you want to keep.
2. Right-click and select *Delete Hidden Graphs* from the shortcut menu.
3. In the dialog that appears click *Yes* to confirm deletion.

Copying and pasting

To copy chart data

1. Choose *Edit | Copy*. Provided that no chart markers are selected, *Copy* copies the (x,y) chart data.
2. In another application choose *Edit | Paste* or *Paste Special*.

This operation allows you to copy the chart data into a spreadsheet application or into a Materials Studio grid document.

To copy the chart image

1. Choose *Edit | Copy*.
2. In another application either open the saved file or choose *Edit | Paste Special* and select a graphics format.

To paste marker data into scatter or line charts

- Right-click in the chart window and choose *Paste Markers*.

Note: The *Paste Markers* menu item is disabled if the clipboard does not hold suitable text.

Materials Studio interprets data as "markers" only if the data exist in the form of one or two columns of numeric data. When the data consist of a single column of numbers, Materials Studio interprets it as the x value of the marker and assigns a default y value based on the data in the chart. When the data is in the form of two columns of numbers, the values in the leftmost column are assumed to represent the x-value and those in the right the corresponding y-values.

The format of the data is checked for errors only when the operation is attempted.

To copy marker data from scatter or line charts

1. Select the markers whose details you wish to copy (see Chart mouse and keyboard actions for details on how to select markers).
2. Right-click and choose *Copy Markers* from the shortcut menu. This copies the (x,y) data of the selected markers. This operation is useful in order to insert marker data into spreadsheet applications or into a Materials Studio grid document.

Printing

To print the chart image

- Choose *File | Print...*.

Basic tasks and methods for the Chart Viewer

The Chart Viewer allows you to customize your view of chart data. You can modify the chart view using both translation and zoom operations. These operations are applied only to the view of the data and do not affect the underlying chart document.

In addition to customizing the chart view, you can enter *marker mode* and add chart markers to scatter and line graphs, marking features of interest. Chart markers can be used to flag features of the plot that you would like to be visible in other views.

In selection mode, you can select data points in a scatter or line graph. For a graph related to a trajectory, picking an individual point will cause the corresponding trajectory frame to be displayed. For a scatter graph derived from a study table, selecting one or more points will cause the corresponding rows of the study table to be selected.

You can enter *cluster cursor mode* in a dendrogram plot to add a cluster cursor to the dendrogram. You can then position the cluster cursor to see the effect of different clustering parameters.

The Chart Viewer can be in one of several modes in which mouse actions control various aspects of the view. Buttons on the Chart Viewer toolbar allow you to switch between the different modes.

Chart Viewer toolbar

Mode	Effect
Selection	Allows for point and marker selection
Translation	Translates the chart, adjusting the axes as necessary.
Zoom	Zooms chart by expanding and contracting the x- and/or y-axis scale.
Marker	Allows addition of new chart markers.
Cluster cursor	Allows for positioning a cluster cursor

Selection in the chart view

Data points and chart markers can be selected either by simple mouse actions when in selection mode or by one of a number of default operations common to all modes.

Selection mode

Enter selection mode by clicking the *Selection Mode* button on the Chart Viewer toolbar.

Selection Mode button

When in selection mode, you can select an individual point or marker by left-mouse-clicking on it (this will clear the previous selection). Selection of multiple data points or markers can be performed using a left-mouse-button drag in the chart window.

Holding down the SHIFT key while performing a selection causes the selected items to be added to the previous selection. Holding down the CTRL key toggles the selection state of the chosen items.

Translating the chart view

Your view of the chart data can be translated either by a simple left-mouse-button drag performed when in Translation mode or by one of a number of default operations common to all modes. The effect of a translation can be thought of as moving a frame of a fixed size over the data.

Translation mode

Enter translation mode by clicking the *Translation* button on the Chart Viewer toolbar.

Translation button

When in translation mode, the view of the chart can be moved by performing a left-mouse-button drag in the chart window.

Other modes

In fact, charts can be translated while in any mode by using the following mouse operations:

- Middle mouse button click + drag
- Mouse wheel click + drag

In addition to these dragging operations, users can use the arrow keys or the Chart Viewer's scrollbars to translate the view.

Zooming the chart view

The user's view onto the chart data can be zoomed either by a simple left-mouse-button drag performed when in zoom mode or by one of a number of default operations common to all modes.

Zoom mode

Enter zoom mode by clicking the *Zoom* button on the Chart Viewer toolbar.

Zoom button

When in zoom mode, the view of the chart can be zoomed by performing a left-mouse-button drag in the chart window. This will scale both the x- and the y-axes of the chart according to the magnitude and direction of the mouse cursor movement.

Furthermore, the zoom can be constrained either to the x- or the y- axis in one of two ways. First, by holding down the X or the Y key while left dragging, the zoom is applied to the corresponding axis. Secondly, by holding down the CTRL key, the zoom is applied only to the axis parallel to the *initial* direction of movement of the mouse cursor.

Other modes

In fact, chart views can be zoomed while in other modes by using the following mouse and keyboard operations:

- Using the *+* and - keys on the numeric keypad
- Mouse wheel rotation
- Left-and-right mouse-button drag

These zooms can again be constrained by using the X and Y keys, as described above.

In addition, by holding down the R key and performing a left-mouse-button drag in the Chart Viewer, you can define a rectangular area to zoom to.

Using markers in the chart view

Points of special significance in a chart can be indicated by *chart markers*. Such points may be used, for example, to denote the peaks in a powder pattern to be used as a basis for further calculations. In the current release of Materials Studio, chart markers appear in the chart as blue lines perpendicular to the x-axis. Chart markers can be applied to the chart manually, programmatically, or by copy-and-paste from an appropriate source.

Marker mode

Enter marker mode by clicking the *Marker* button on the *Chart Viewer* toolbar.

Marker button

When in marker mode, a new marker can be added to the chart by clicking the left mouse button in the chart view. However, if you click the left mouse button when the mouse cursor is over an existing marker - a fact reflected by the "highlighting" of the marker - instead of adding a new marker you can now drag that marker to a new position. By holding down the CTRL key at the same time as you drag the chart marker, the marker's position will automatically snap to any data point within a few pixels of the mouse cursor.

Other modes

When in selection mode, individual markers can be selected by left-clicking on them. Several markers may be selected at once by using left-click drag to encompass them. This will also select any other content within the dragged boundary. Either of these methods may be combined with SHIFT to add the markers to the existing selection, or with CTRL to toggle the selection of the markers. Left double-clicking on any marker will select all markers.

Editing charts with the Properties Explorer

Tip: If the Chart document contains more than one chart, each chart's features can be edited separately. The Properties Explorer filter will allow you to select Chart or Chart 2 for example.

Note: If the Properties Explorer is not visible, select *View | Explorers | Properties Explorer* from the menu bar to display it.

To edit any chart features you must make the Chart the active document.

To edit the chart title

1. Set the *Filter* on the Properties Explorer to Chart using the dropdown list.
2. Double-click on *Title* in the Properties Explorer to display the Edit multi-line string property dialog.
3. Enter the new chart title and click the *OK* button.
4. Double-click on *Font* in the Properties Explorer to display the Edit font property dialog.
5. Change the font face and size and click the *OK* button.

To edit an axis label

1. Set the *Filter* on the Properties Explorer to X axis or Y axis using the dropdown list.
2. Double-click on *Title* in the Properties Explorer to display the Edit multi-line string property dialog.
3. Enter the new chart title and click the *OK* button.
4. Double-click on *Font* in the Properties Explorer to display the Edit font property dialog.
5. Change the font face and size and click the *OK* button.

To edit an axis limit

1. Set the *Filter* on the Properties Explorer to X axis or Y axis using the dropdown list.
2. Double-click on *Max* or *Min* in the Properties Explorer to display the Edit floating point property dialog.
3. Enter the new axis limit value and click the *OK* button.

Note: The extents of the chart can only be increased within reasonable limits. The increase in size is generally limited as the difference between the current maximum and minimum of a given axis.

To edit chart markers

1. Select the chart marker(s) that you wish to edit.
2. Set the *Filter* on the Properties Explorer to Chart Markers using the dropdown list.
3. Double-click on *IsUsed* in the Properties Explorer to display the Edit Boolean property dialog.
4. Choose whether to use markers and click the *OK* button.
5. Double-click on *X* or *Y* in the Properties Explorer to display the Edit floating point property dialog.
6. Change the X or Y position of the markers and click the *OK* button.

Note: If you have selected more than one chart marker changing the Y property will make all markers the same height. Changing the X property will place all markers at the same location on the X axis and should usually be avoided.

To show point coordinates

The crosshair displays the x and y coordinates of points that are close to the mouse position.

1. Right-click on the chart to display the context menu.

   The *Show Crosshair* item is checked or unchecked depending on whether the crosshair is currently visible or not.
2. Click the *Show Crosshair* item to toggle the visibility of the crosshair.

Using point selection to view related data

A point in a chart can be selected by clicking on the point while in *Selection mode*. Multiple points can be selected by holding the left mouse button and dragging the mouse cursor to create a bounding box for selection. Point selection is most useful when working with a chart that is associated with a trajectory file, such as those created by DMol^3, or one that has been created from a study table.

When a single data point is selected on a chart associated with a trajectory, the corresponding trajectory frame is displayed.

When data points are selected on a chart associated with a study table, the corresponding rows of the study table become selected.

Using cluster cursor mode to identify clusters

A cluster cursor is drawn as a vertical line over a dendrogram graph while in *chart cluster cursor mode*. Cluster cursor mode is useful for identifying the number of clusters at a given depth of a dendrogram.

To enter cluster cursor mode

1. Click the *Chart Cluster Cursor Mode*  button on the Chart Viewer toolbar to enter cluster cursor mode.
2. Click and drag on the cluster cursor within the chart. As you drag the cursor, labels identifying the clusters are drawn above the dendrogram branches. In addition the number of clusters at the given depth is shown.

Chart mouse and keyboard actions

Default modes and tool modes

Certain mouse and keyboard actions are available regardless of the Chart Viewer's tool mode. These are labeled as **Default** actions in the following table, and can be used in any tool mode. Other mouse and keyboard actions are specific to a particular tool mode, and may behave very differently between modes.

Default modes

The actions described in this section can be performed in any tool mode.

View transform

To	Press
Reset to original view	HOME
Translate View	Middle mouse drag
Translate View	Mouse wheel drag
Translate View	Cursor keys
Translate View	Scroll bars
Translate View	T + Left mouse drag
Page Translate View	CTRL + Cursor keys
Zoom	Left-and-right mouse drag
Zoom In	+ (on keypad)
Zoom Out	- (on keypad)
Zoom In	Mouse wheel up
Zoom Out	Mouse wheel down
Zoom X-scale	X + zoom operation
Zoom Y-scale	Y + zoom operation
Zoom with Zoom Rectangle	R + Left mouse drag

Selection

Note that selection applies to data points and chart markers.

To	Press
Select All	CTRL + A
Clear selection	CTRL + D

Editing

To	Press
Copy selected markers	CTRL + C
Delete selected markers	DELETE
Move marker	Middle mouse drag a selected marker

Tool modes

The actions described in the following tables can be performed only in the specified tool modes, and may behave very differently in other tool modes.

Selection mode

The Selection mode actions described here apply to data points and chart markers.

Selection mode cursor

To	Press
Select object	Left mouse click
Select objects in rectangle	Left mouse click and drag
Select whole series	Double left mouse click

Combine these actions with: CTRL to toggle selection or SHIFT to add to the selection.

Zoom mode

The actions described in this table apply only in Zoom mode.

Zoom mode cursor

To	Press
Zoom	Left mouse drag
Constrained Zoom	CTRL + Left mouse drag
Zoom X-scale	X + Left mouse drag
Zoom Y-scale	Y + Left mouse drag

Translation mode

The actions described in this table apply only in Translation mode.

Translation mode cursor

To	Press
Translate	Left mouse drag

Marker mode

The actions described in this table apply only in Marker mode.

Marker mode cursor

To	Press
Add marker	Left mouse click on background

To	Press
Highlight marker	Hover mouse cursor over existing marker
Move marker	Left mouse drag the highlighted marker
Snap marker to nearest data point	CTRL + Move marker

Cluster cursor mode

The actions described in this table apply only in Cluster cursor mode.

Cluster mode cursor

To	Press
Position the cluster cursor	Left mouse click and drag the cluster cursor

Working with forcefields

A number of Materials Studio modules use classical forcefields, for example Forcite, Polymorph and Blends. A forcefield defines the potential energy surface or energy expression, which governs particle interactions as the sum of analytical terms. The analytical terms that contribute to the forcefield are functions of the coordinates of one or more particle(s). Each expression also has a parametric dependence which is determined by the type of particles involved in an interaction. These parameters are typically stored and read from a forcefield file. Materials Studio allows you to view, add, remove, and edit these parameters (for non-licensed forcefields).

Creating and editing forcefields

Materials Studio has a number of standard forcefields that can be used in a variety of situations. However, it may be the case that a specific set of compounds is not well modeled by one of the standard forcefields and it is desirable to modify an existing forcefield or develop a custom forcefield for this case. Materials Studio allows you to create, view, and edit a forcefield document, against which a simulation job can be run.

To create a new forcefield

The basic steps in creating a new forcefield are as follows:

1. Create a new forcefield document (for example, by selecting *New...* from the *Files* menu).
2. A new Forcefield Viewer will be displayed with four tabs. On the Summary tab, you can add information about the purpose of the forcefield, the origin of the parameters, the compounds it applies to, and so on.
3. Define the forcefield types to be used in interaction sequences on the Types tab.
4. Define the forcefield interactions by first specifying the forcefield type sequence that defines the interaction, then selecting the functional form that is to be used, and finally setting the parameters of the interaction on the Interactions tab.
5. If necessary, define the forcefield type equivalences on the Equivalences tab. Typically, the default equivalences are satisfactory. Only if a complex forcefield, such as pcff or cvff, is being edited do these values require changes.

To run a simulation against a new forcefield

To make a new forcefield available to module jobs, go to the Energy tab of the module Calculation dialog and on the forcefield dialog select the browse option. The Choose Forcefield dialog will be displayed. This allows you to add the new forcefield to the forcefield selection list.

Managing forcefield documents

Forcefield documents contain energy expression parameter tables and related information. The characteristics of a simulation using a given forcefield can be altered or extended by loading the forcefield document and editing its contents.

To open an existing forcefield document that is not already part of a project

1. Choose *File | Import...* and select *Materials Studio Forcefield Files (*.off)* from the list of file types.
2. Browse to the location of the forcefield file you wish to import.
3. Select the file and click the *Import* button, or double-click on the file.

To create a copy of a standard forcefield document

1. Choose *Modules | Forcite | Forcefield Manager*.
2. Select the standard forcefield of interest and click >> to import the forcefield into the project.

Note: The standard forcefields distributed with Materials Studio cannot be edited in place. A copy must first be made by importing the desired forcefield into a project.

To create an empty forcefield document

- Select *File | New...* from the menu bar and select *Forcefield Document*.

To save a forcefield document to your project

- Select *File | Save As...* from the menu bar, enter a file name for the forcefield file and click the *Save* button.

To save a forcefield document outside your project

1. Choose *File | Export...*.
2. Select the *Materials Studio Forcefield Files (*.off)* format, browse to the desired location and click the *Export* button.

Editing a forcefield document

To edit the forcefield description, forcefield types, interactions, and equivalences

1. Select a tab for the appropriate data and edit the data directly.
2. Change the description, types, interactions, or equivalences settings.
3. To save the forcefield data, choose *File | Save* from the menu bar.

Note: To run a simulation with the new forcefield, the simulation model must have the forcefield types of the new forcefield applied. For a new forcefield, there are no forcefield typing rules and forcefield types have to be added manually.

Once the model has been prepared, a simulation can be initiated in the same way as a regular job.

To edit a standard forcefield

Copies of some of the standard forcefields can also be edited. Use the forcefield manager to make a copy of a standard forcefield and then add, delete, or amend the forcefield types and interactions as required. This new version of the standard forcefield must be added to the forcefield selection list on the *Energy* tab of the module's calculation dialog before it can be used.

Note: When a forcefield type is created, an attempt is made to determine the most appropriate element based on the forcefield type name. If this attempt fails, the default element value is assigned, "X". Such a forcefield type will not be listed on the *Preparation Options dialog* for modules because only forcefield types with known chemical element values can be assigned using this dialog. A forcefield type which has an element value of "X" can be made visible on the module's *Preparation Options dialog* by changing it to an appropriate value on the Types tab of the Forcefield Viewer.

To run a simulation against a modified standard forcefield

Running a simulation with a modified forcefield differs from using a new forcefield in that, if no new forcefield types have been defined, automatic typing can be applied using the existing forcefield typing rules. If a mixture of existing and new forcefield types is required then the existing types can be calculated and the new forcefield types must be applied manually.

Printing

It is not possible to print a forcefield document.

Editing the forcefield description

The Summary tab of the Forcefield Viewer allows you to edit the description of the forcefield.

Editing a forcefield's description

1. Open a forcefield in the Forcefield Viewer.
2. On the Summary tab you can edit any of the text presented, or add further information to it. For example, you could detail the history of changes to the file.

Editing forcefield types

The Types tab of the Forcefield Viewer allows you to view, select and edit forcefield types.

Forcefield types specify the local environment of a particle and determine how that particle will contribute to a given interaction it participates in. Many forcefields have a large number of forcefield types, but the system being simulated may only use a much smaller subset of these types.

To display the forcefield types

To assist in editing forcefield types, the Forcefield Viewer allows you to filter the displayed types by name or based on a selected model.

1. Open a forcefield in a Forcefield Viewer.
2. On the Types tab either:
   - Check the *Filter by selection in* checkbox and, from the dropdown list, select the document in the current project which contains the structure whose forcefield types you wish to view or edit.
   - Specify a search template in the *Filter* cell at the top of the types column for the forcefield type you wish to edit. The filter is not case sensitive, but the full name must be entered. The wildcard character * can be used in combination with other characters to extend the search. For example, the template C* will filter for all forcefield types beginning with C.

   These filters may be used in combination, so the template filter can be applied to the results of a selection filter. This is useful if the document contains many different forcefield types.
3. Click the *Properties...* button to open the Forcefield Type Properties dialog. Use the checkboxes on the list to switch on and off the display of the properties of the forcefield types.

To edit a forcefield type

On the Types tab of the Forcefield Viewer you can edit any of the properties displayed except the *Type*.

1. When you have the forcefield types of interest and their properties displayed, click in the cell for a property of a forcefield.
2. *Description*, *ElementSymbol*, and *Charge* are text boxes and you can enter any suitable text.
3. For *Hybridization* select one of the options from the dropdown list.
4. If a property that you want to edit is not displayed, use the Forcefield Type Properties dialog to switch the display on.
5. Some properties, such as the *van der Waals Form*, have additional parameters that you can view or modify. To view these parameters, choose the functional form that you wish to view or edit from the dropdown list in the yellow filter cell. The parameters for the selected functional form are displayed and you can edit their values.

To create a new forcefield type

1. Scroll to the last row of the list of forcefield types and click in the empty *Type* cell, enter the name for your new forcefield type here. When you have entered a new name and moved away from this cell it will no longer be editable.
2. Enter a *Description* and any other properties you wish to define.
3. The new forcefield type will be added to the forcefield document saved in your project.

Note: When a forcefield type is created an attempt is made to determine the most appropriate element based on the forcefield type name. If this attempt fails the default element value, X, is assigned.

To delete a forcefield type

- Select the row for the forcefield type to be deleted and press the DELETE key.

Editing forcefield interactions

The Interactions tab of the Forcefield Viewer allows you to view, select, and edit forcefield interactions.

The energy expression that describes the potential energy surface is constructed by adding together interactions that are defined by a given forcefield. Interactions are defined by their topology and the forcefield type sequence of the particles involved in the interaction. Interactions can be classified into sets, grouped together in terms of the physical origins and geometrical measures used to calculate the potential energy and related quantities. Examples of these sets are Bond Stretch, Torsion, and van der Waals interactions.

To display the forcefield interactions

The forcefield viewer allows you to view interactions by set:

1. Open a forcefield in a Forcefield Viewer.
2. On the Interactions tab, select an interaction set from the *Show interaction* dropdown list.

To filter the interactions displayed

Some forcefields can have a large number of forcefield interactions, but the system being simulated may only use a much smaller subset of these. To assist in editing the interactions the Forcefield Viewer allows you to filter the displayed interactions by forcefield type sequence, by a selected model, by functional form or using a combination of all three.

1. Check the *Filter by selection in* checkbox and, from the dropdown list, select the document in the current project which contains the structure whose forcefield types should be used. Only the interactions with a forcefield type sequence that contains a type assigned to the model will be displayed.
2. Specify a forcefield type sequence template in the row labeled *Filter* and press the ENTER key to apply the filter.
   The forcefield type sequence for an interaction is defined in the columns labeled **F*x***. The wildcard symbol "*" can be used in combination with other characters to define a search template. If interactions have been previously filtered based on a model, the forcefield type sequence template will be applied to the filtered set.
3. Select a *Functional form* from the dropdown list in the first cell of the column. The parameters for the selected functional form will be displayed in new columns showing their current values.

Tip: If *Filter by selection in* is checked and no interactions are visible, check that the atoms in the model used as the filter have forcefield types defined, and that these types correspond to types in the forcefield being edited. You may be able to use a forcefield engine such as Forcite to automatically assign forcefield types to the atoms in a model.

To edit a forcefield interaction

Interactions can be edited to change the functional form and the parameters:

1. Select a *Functional form* from the dropdown list. If you select *All* or *Ignore*, or if there are no forcefield type sequences using the selected functional form, no parameters will be available for editing.
2. To alter a given parameter, select the cell containing the parameter and enter the desired value, press the ENTER key.

Note: The forcefield type sequence cannot be edited for an existing interaction. To alter forcefield types you must create a new interaction with the desired sequence, set the parameters and then delete the existing interaction.

Note: Almost all interaction sets contain the functional form *Ignore*. This functional form allows specific interactions to be excluded from the energy expression. This can be useful in a variety of circumstances, including the development of a new forcefield when all the parameters are not immediately available, or when an existing forcefield does not have all the parameters for a set of compounds and only approximate calculations are required. In these situations ignoring terms will allow the calculation to proceed. If required, a whole set of interactions can be excluded, using the checkboxes on the Forcefield Preferences dialog.

To create a new forcefield interaction

A new forcefield interaction can be created using the first empty row of the forcefield editor:

1. Set the forcefield type sequence by selecting the forcefield types from the *Fx* dropdown list, or type them in directly.
2. Select the *Functional form* from the dropdown list. Columns for the parameters for the selected functional form will displayed with their current values.
3. Change the parameters to the desired values.

Note: An explicit van der Waals interaction between two forcefield types can be defined by selecting van der Waals from the *Show interaction* dropdown list.
However, van der Waals interaction parameters are often generated from particle properties and defined combination rules. The combination rule can be specified on the Forcefield Preferences dialog and the particle properties are accessible on the Types tab. Explicitly defined parameters take precedence over generated parameters when the energy expression is created.

To delete a forcefield interaction

- Select the row that specifies the interaction to be deleted and press the DELETE key.

Tip: For interactions which have multiple groups of parameters for their functional forms you may not wish to delete an entire interaction. In order to remove a group of parameters from an interaction select each of parameters in the group and delete their values, the group will no longer be applied for the interaction.

Editing forcefield equivalences

The Equivalences tab of the Forcefield Viewer allows you to view, select and edit forcefield equivalences.

Forcefield equivalences together with the step down rules provide a formal mechanism of assigning interaction terms defined in the forcefield document to topological terms in the structure to construct the energy expression .

To display the forcefield equivalences

To assist in editing forcefield types, the Forcefield Viewer allows you to filter the displayed types by name or based on a selected model.

1. Open a forcefield in a Forcefield Viewer.
2. On the Equivalences tab either:
   - Check the *Filter by selection in* checkbox and, from the dropdown list, select the document in the current project which contains the structure whose forcefield types you wish to view or edit.
   - Specify a search template in the *Filter* cell at the top of the types column for the forcefield type you wish to edit. The filter is not case sensitive, but the full name must be entered. The wildcard character * can be used in combination with other characters to extend the search. For example, the template C* will filter for all forcefield types beginning with C.

   These filters may be used in combination, so the template filter can be applied to the results of a selection filter. This is useful if the document contains many different forcefield types.

To edit a forcefield equivalence

On the Equivalences tab of the Forcefield Viewer you can edit any *Level* (up to a maximum of 4) of the equivalences.

1. When you have the forcefield type equivalences of interest and their properties displayed, click in the cell for a level of equivalence for the forcefield type.
2. Click in the cell for the appropriate *Level* and select the forcefield type label from the dropdown list. This defines an equivalence between the forcefield type for the row and the type selected for the current level.
3. Click the *More...* button to open the Forcefield Preferences dialog. Interactions (and therefore equivalences) can be added and removed and the advanced properties for the selected interactions can be edited.

Note: When a forcefield type is created it is automatically equivalenced to itself and then to X. This should be adequate for most situations.

To delete a forcefield type equivalence at a specific level

- Click in the cell for the appropriate level and press the DELETE key.

Note: If an equivalence level is deleted and there are further equivalences, these are moved up to fill the gap.

Forcefield dialogs

Certain tasks involving forcefield documents in Materials Studio can be performed using dialogs that can be accessed from the Interactions, Equivalences, and the Types tabs of the Forcefield Viewer.

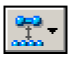
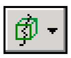
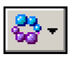
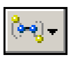
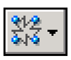
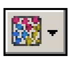
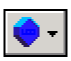
Choose Forcefield dialog

Custom forcefields can be used with a number of applications. The *Choose Forcefield* dialog allows you to control which custom forcefields are displayed as part of the active forcefield list, helping to keep the active forcefield list shorter and easier to navigate.

Select the custom forcefield that you would like to add to the active forcefield list from the document chooser.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Modules | [Module name] | Calculation | Energy | Forcefield | Browse...*
Toolbar	 *| Calculation | Energy | Forcefield | Browse...*  *| Calculation | Energy | Forcefield | Browse...*  *| Calculation | Energy | Forcefield | Browse...*  *| Calculation | Energy | Forcefield | Browse...*  *| Calculation | Energy | Forcefield | Browse...*  *| Calculation | Energy | Forcefield | Browse...*  *| Calculation | Energy | Forcefield | Browse...*  *| Calculation | Energy | Forcefield | Browse...*  *| Calculation | Energy | Forcefield | Browse...*

Forcefield Preferences dialog

The *Forcefield Preferences* dialog is displayed when the *More...* button is clicked on the Interactions or Equivalences tabs of a Forcefield Viewer and allows the selection of advanced properties that are not related to specific forcefield types or terms in the energy expression.

Interactions

Bond stretch: Determines whether bond stretches are used in applying and assigning the forcefield.

Angle bend: Determines whether angle bends are used in applying and assigning the forcefield

Torsion: Determines whether torsions are used in applying and assigning the forcefield.

Inversion: Determines whether inversions are used in applying and assigning the forcefield.

van der Waals: Determines whether van der Waals interactions are used in applying and assigning the forcefield.

Hydrogen Bond: Determines whether hydrogen bonds are accounted for in applying and assigning the forcefield.

Electrostatic: Determines whether electrostatics are used in applying and assigning the forcefield.

Stretch stretch: Determines whether the two bond interactions based on three body topology are used in applying and assigning the forcefield.

Stretch bend stretch: Determines whether the interactions between two bonds and one angle bend based on three body topology are used in applying and assigning the forcefield.

Bend bend: Determines whether the two angle bend interactions based on the four body branched topology are used in applying and assigning the forcefield.

Torsion bend bend: Determines whether the interactions between two angle bends and a torsion based on the four body linear topology are used in applying and assigning the forcefield.

Bend torsion bend: Determines whether the interactions between two angle bends and a torsion based on the four body linear topology are used in applying and assigning the forcefield.

Torsion stretch: Determines whether the central bond stretch interaction and a torsion interaction based on the four body linear topology are used in applying and assigning the forcefield.

Stretch torsion stretch: Determines whether the interactions between the two end bond stretches and a torsion based on the four body linear topology are used in applying and assigning the forcefield.

Separated stretch stretch: Determines whether the two end bond stretch interactions based on the four body linear topology are used in applying and assigning the forcefield.

Bond increments: Determines whether bond increment charges are used in applying and assigning the forcefield.

General

Exocyclic torsion scale: Sets the relative factor by which exocyclic torsions are scaled. Default = 1.

Scale torsions about common bond: Determines whether to scale torsions relative to a shared bond.

Scale by number of defined torsions: Determines whether to scale according to the total number of defined torsions.

Exclude van der Waals 1-2 interactions: Excludes van der Waals interactions between bonded particles. Currently, this must be the same as the equivalent electrostatic exclusion.

Exclude van der Waals 1-3 interactions: Excludes van der Waals interactions between particles separated by two bonds. Currently, this must be the same as the equivalent electrostatic exclusion.

van der Waals combination rule: Allows selection of the van der Waals combination rule, options are Arithmetic, Geometric, and Sixth power.

Exclude electrostatic 1-2 interactions: Excludes electrostatic interactions between bonded particles. Currently, this must be the same as the equivalent van der Waals exclusion.

Exclude electrostatic 1-3 interactions: Excludes electrostatic interactions between particles separated by two bonds. Currently, this must be the same as the equivalent van der Waals exclusion.

Relative dielectric constant: Sets the relative factor for the dielectric constant. Default = 1.

Help: Displays the Help topic in a browser.

Access methods

Menu	*File* | *Import...* and select a forcefield document *Interactions* | *More...*
	File | *Import...* and select a forcefield document *Equivalences* | *More...*
Project Explorer	double-click on a forcefield document | *Interactions* | *More...*
	double-click on a forcefield document | *Equivalences* | *More...*

Forcefield Type Properties dialog

The *Forcefield Type Properties* dialog allows you to switch on and off the display of columns on the Types tab of the Forcefield Viewer.

Properties: lists the properties available in the table in the Forcefield Types tab of the Forcefield Viewer, these can include:

- Description
- Hybridization
- Element Symbol
- Charge
- Hydrogen Bond
- van der Waals

If the checkbox for each property is checked, it will be shown in the Forcefield Types table, if it is unchecked its display is disabled.

Help: Displays the Help topic in a browser.

Access methods

Menu	*File* | *Import...* and select a forcefield document *Types* | *Properties...*
Project Explorer	double-click on a forcefield document *Types* | *Properties...*

Working with tabular data

Tabular data can be displayed in either grid or study table documents. Both document types share some common features. These features are described in this section.

Features specific to grid and study table documents are described in the Working with grids and Working with study tables sections, respectively.

Editing tabular data

You can modify the contents of grid or study table documents. It is possible to edit cell values, insert and delete rows and columns, change the column property heading, and copy a cell value into multiple cells within the same column.

To modify the contents of a cell

1. For numeric or textual data, select the desired cell and type in the value. Use the ENTER and TAB keys to navigate to additional cells for modification.
2. To clear the contents of one or more cells, select the cell or cells that you want to clear and press the DELETE key. Alternatively, you can clear the contents of the selected area by right-clicking in it and selecting *Clear Contents* from the shortcut menu.

To insert rows and columns

1. To insert a new column into the table, right-click on a column heading and select *Insert | Left* or *Insert | Right* from the shortcut menu. A new column is inserted on the appropriate side of the selected column.
2. To insert a new row, right-click on a row heading and select *Insert | Above* or *Insert | Below* from the shortcut menu.
3. To insert multiple rows or columns, use multiple selection to indicate the number and location of rows or columns to be inserted, then proceed as described in steps 1 and 2 above.

To delete rows and columns

1. Select the desired row or column by clicking on its row or column heading.

   Tip: Select multiple consecutive rows or columns by holding down the SHIFT key while clicking on the row or column headings. Select non-consecutive rows or columns by holding down the CTRL key while clicking on the row or column headings.
   To clear a selection, that is, to deselect highlighted cells, press the ESC key.

2. With the desired rows or columns selected, right-click on the row or column heading and choose *Delete* from the shortcut menu or select *Edit | Delete* from the menu bar.

To change the column property description

1. Right-click on the column description cell, i.e., the gray cell below the column heading of the column for which you intend to enter a description. Select *Properties* from the shortcut menu. The Column Properties dialog is displayed.
2. Modify the description as required. Click the *OK* button to confirm the change.

To rename a sheet

1. Right-click on the desired sheet tab and select *Rename Sheet* from the shortcut menu. The Rename Active Sheet dialog is displayed.
2. Modify the sheet name as required and click the *OK* button confirm the change.

To insert a sheet

- Right-click on a sheet tab and select *Insert Sheet | Left* or *Insert Sheet | Right* from the shortcut menu. A sheet is inserted on the appropriate side of the active sheet.

To delete a sheet

- Right-click on the desired sheet tab and select *Delete Sheet* from the shortcut menu.

Note: A grid or study table document must always have at least one sheet.

Copying and pasting tabular data

You can copy and paste the contents of grid or study table documents.

To copy data

1. Make a selection by clicking on individual cells or row or column header(s), or by dragging over a block of contiguous cells. Alternatively, select all the cells by clicking on the top left header cell.
2. Select *Edit | Copy* from the menu bar, click the *Copy* button  on the toolbar, right-click on the selected cells and choose *Copy* from the shortcut menu, or press CTRL + C.

Note: Copying can only be performed for a rectangular selection of cells or a discontinuous selection that could be made rectangular by a suitable reordering of rows and columns.

To paste data

1. Select the cell or cells into which you intend to paste the data.
2. Paste the data into the Materials Studio document (or another application) by selecting *Edit | Paste* from the menu bar, by clicking the *Paste* button  on the toolbar, by right-clicking in the new document and choosing *Paste* from the shortcut menu, or by pressing CTRL + V.

Note: Pasting can only be performed for a rectangular selection of cells or a discontinuous selection that could be made rectangular by a suitable reordering of rows and columns.

Modifying the data view

You can customize and manage the view of the underlying data in grid or study table documents.

To resize rows and columns

1. In the row heading column, drag the horizontal boundary between the desired row and the row above it or below it up or down to resize the row as required.
2. Similarly, resize columns by dragging the boundary between column headings.

Row heights and column widths are individually adjustable. Changes made to row heights and column widths are saved when you save the document.

To size columns to fit

To automatically adjust a column to the minimum width, right-click on the column heading and select *Size to Contents* from the shortcut menu. The column description is not taken into account when performing a size to contents.

Tip: If multiple columns are selected, the columns are all adjusted to their minimum widths. To quickly adjust all columns to their minimum widths, right-click in the top left corner of the grid and select *Size to Contents* from the shortcut menu.

Column width modifications are saved when you save the document.

To hide and show columns

1. Select the columns you intend to hide. Right-click on a selected column heading and choose *Hide* from the shortcut menu.
2. To redisplay hidden columns, select the columns on either side of the hidden columns while holding the SHIFT key and select *Unhide* from the shortcut menu. Alternatively, drag the boundary between the hidden and unhidden columns to redisplay the hidden columns.

Column visibility modifications are saved when you save the document.

To lock and unlock columns

1. Select the rightmost column that you wish to be locked or the leftmost that you want to unlock.
2. Right-click on a selected column heading and choose *Lock* or *Unlock*, as appropriate, from the shortcut menu. Alternatively, click the *Lock Columns*  or *Unlock Columns*  buttons on the Study Table Viewer toolbar.

When a column is locked, it remains in view as you scroll around the grid. You can choose different column locking settings for each sheet in the document. Column locking modifications are saved when you save the document.

Sorting data

You can sort the rows in grids and study tables based on the data values in one or more columns. Sorting can be ascending or descending, and can be made case-sensitive or case-insensitive.

To sort rows

1. Select *Tools | Sort Rows...* from the menu bar to open the Sort Rows dialog.
2. On the Sort Rows dialog, choose the column or columns you want to use as the basis for your sort.
3. Select ascending or descending sorting for each chosen column and check the *Case sensitive* checkbox to enable case-sensitive sorting, if required.
4. Click the *OK* button to sort the data.

In many cases only one column will be required to determine the sort and case sensitivity is not important. In these cases, a sort can be conveniently performed using the *Sort Ascending* or *Sort Descending* buttons on the appropriate toolbar, as described below.

To sort rows based on values in a single column

1. Select the column you intend to use as the basis for the sort by clicking on the column header.
2. Click the *Sort Ascending*  or *Sort Descending*  button on the Study Table Viewer toolbar or the Grid Viewer toolbar, as appropriate.

Plotting data

There are many ways of plotting tabular data from a grid or a study table document:

- 1-D - a plot of data value against row number for one or more columns of data.
- Scatter (2-D) - a scatter plot generated from data values from the dependent column against data values from the independent column for one or more columns of dependent data.
- Histogram - a frequency histogram plot of bin frequencies generated from a single column of data.
- Distribution - a probability density function plot generated from one of more columns of input data, with or without smoothing applied.
- Cumulative distribution - a cumulative distribution function plot generated from one of more columns of input data.

To generate a 1-D plot

Either:

1. Select data from a single column that does not contain array data, either the entire column or just selected cells of interest.
2. Click the *Quick Plot* button  on the toolbar to generate a 1-D plot using the current option values from the Plot Graph dialog.
3. The plot is displayed in a new chart document.

Or:

1. Select the column or columns of data you wish to plot. If you wish, you can select specific rows to restrict the scope of the plot.
2. Click on the options arrow associated with the *Quick Plot* button  and select *Plot Graph* from the dropdown list or choose *Tools | Plot Graph...* from the menu bar to display the Plot Graph dialog.
3. Ensure that the *Graph type* is set to 1-D.
4. Check the *Show lines* checkbox if you wish to show lines between data points on the plot.
5. Check the *Flip plot orientation* checkbox if you wish to plot the row numbers along the Y-axis and the data values along the X-axis.
6. Click the *Plot* button.
7. The plot is displayed in a new chart document.

To generate a scatter (2-D) plot

Either:

1. Select the columns of data you wish to plot. You should select the columns for both axes. You can include more than one column on the Y-axis. If you wish, you can select specific rows to restrict the scope of the plot.
2. Click the *Quick Plot* button  on the toolbar to generate a scatter (2-D) plot using the current option values from the Plot Graph dialog.
3. The plot is displayed in a new chart document.

Or:

1. Select the columns of data you wish to plot. You should select the columns for both axes. You can include more than one column on the Y-axis. If you wish, you can select specific rows to restrict the scope of the plot.
2. Click on the options arrow associated with the *Quick Plot* button  and select *Plot Graph* from the dropdown list or choose *Tools | Plot Graph...* from the menu bar to display the Plot Graph dialog.
3. Ensure that the *Graph type* is set to Scatter (2-D).
4. Specify the column to be used for the X-axis of the plot.
5. Check the *Include X variable* checkbox if you wish to include a plot of the X variable against itself (generating a scatter-plot along the line Y = X).
6. Check the *Show best fit line* checkbox if you wish to draw a line of best fit for each of the independent variables on the plot.
7. Check the *Flip plot orientation* checkbox if you wish to plot the independent data along the Y-axis and the dependent data along the X-axis.
8. Click the *Plot* button.
9. The plot is displayed in a new chart document.

To generate a histogram plot

1. Select the column of data you wish to plot. The histogram plot option is available only if just a single column of data is selected, and is not available for array data. If you wish, you can select specific rows to restrict the scope of the plot.
2. Click on the options arrow associated with the *Quick Plot* button  and select *Plot Graph* from the dropdown list or choose *Tools | Plot Graph...* from the menu bar to display the Plot Graph dialog.
3. Ensure that the *Graph type* is set to Histogram.
4. If the selected column contains numeric data, specify the *number of bins* to use.
5. If the selected column contains non-numeric data, it will be treated as categories, and a separate bin will be generated for each unique category.
6. Check the *Flip plot orientation* checkbox if you wish to plot the data values along the Y-axis and the frequency data along the X-axis.
7. Click the *Plot* button.
8. The plot is displayed in a new chart document.

To generate a distribution plot (probability density function) or a cumulative plot (cumulative distribution function)

Either:

1. Select a single column of array data, typically the result of an atomic properties calculation or a geometry measurement model calculation. If you wish, you can select specific rows to restrict the scope of the plot.
2. Click the *Quick Plot* button  on the toolbar to generate a distribution plot or cumulative distribution plot using the current option values from the Plot Graph dialog.
3. The type of plot will be Distribution or Cumulative distribution, depending on which of these was the more recently used.
4. The plot is displayed in a new chart document.

Or:

1. Select the column or columns of data you wish to plot. One or more of the columns can contain array data. If you wish, you can select specific rows to restrict the scope of the plot.
2. Click on the options arrow associated with the *Quick Plot* button  and select *Plot Graph* from the dropdown list or choose *Tools | Plot Graph...* from the menu bar to display the Plot Graph dialog.
3. Ensure that the *Graph type* is set to Distribution or Cumulative distribution, whichever is required.
4. Choose the *bin size* or *number of bins* appropriately for the data to be plotted.
5. If you wish to have smoothed plots, set a value for *Smoothing width* appropriate to the data and bin parameters. The value for this is a compromise between smoothing out noise and possible loss of genuine features in the data.
6. Choose whether you want to plot just the raw binned data, or just the binned data after smoothing, or both. Set the *Plot(s) to show* value accordingly.
7. If you have multiple columns of data selected, ensure that you have chosen your desired setting for the *Treat multiple columns* parameter.
8. Click the *Plot* button.
9. The plot is displayed in a new chart document.

Coloring data by value

You can color selected cells in a grid or study table document based on their numeric data values. Color can be applied by considering the entire selection, selected columns on an individual basis, or by using a custom data range.

To color data by value

1. Select the cells you wish to color based on their data values.
2. Select *Tools | Color By Value* from the menu bar to display the Color By Value dialog.
3. Choose appropriate options for the value range and color scheme.
4. Click on *Apply* to color the selected cells based on their data value according to the specified settings on the dialog.
5. Click the *Remove* button to reset the color of the selected cells to the default color (white).

Note: If any of the selected cells is of a non-numeric type, for example, containing structure or textual data, they will be omitted from the coloring process. If none of the selected cells contain any suitable data, a warning will be displayed.

Formatting cells

You can change the formatting of numeric data displayed in grid or study table documents.

To set the cell format

1. Select the cells for which you wish to change the display format.
2. Select *View | Format Cells* from the menu bar to open the Format Cells dialog.
3. Choose the format type and the precision (if applicable) you want to use.
4. Click the *Apply* button to apply the new display format to the selected cells.

Table dialogs

Certain tasks involving grid and study table documents in Materials Studio can be performed using dialogs that can be accessed from the Tools menu or the View menu.

Column Properties dialog

The Column Properties dialog displays information about the grid or study table column.

Description: A description of the contents of the column. By default, this is empty. If a study table column represents an output from a model calculation, the description contains information about the model and its output.

Type *(Study Table only)*: The type associated with a column. By default, the column has no type associated with it. If the column represents an output from a model calculation, the type will correspond to the model output type. The type associated with a column is read-only.

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

Cancel: Closes the dialog without updating any settings.

Access methods

Shortcut menu	*Properties*

Sort Rows dialog

The Sort Rows dialog allows you to control the criteria used to order rows during a sort. If a number of rows have the same value in the primary sort column, the values in a second and third column may be used to determine the order.

Sort by column: Specifies the primary column to use in ordering the rows.

Then by column: Specify the second and third columns to use in determining the order of any rows that have the same value in the primary column.

For each column specified, the values can be arranged in *Ascending* or *Descending* order.

Case sensitive: Specifies whether a case sensitive comparison should be used to determine the ordering of rows. This option applies to all of the chosen columns.

Note: In many cases, only one column will be required to determine the sort and case sensitivity is not important. In these cases, a sort can be conveniently performed using the *Sort Ascending*  or *Sort Descending*  buttons on the appropriate toolbar.

OK: Sorts the rows according to the specified columns and orders and closes the dialog.

Cancel: Closes the dialog without sorting rows.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Tools	Sort Rows...*

Plot Graph dialog

The Plot Graph dialog allows you to create plots from data in one or more columns of the selected grid or study table. Four types of plot are available - 1-D, Scatter (2-D), Histogram and Distribution.

Graph type: Select the type of graph to be generated. Available options are:

- 1-D - a plot of data value against row number.
- Scatter (2-D) - a scatter plot generated from independent data from one column and dependent data from another column(s).
- Histogram - a histogram plot of bin frequencies generated from a single column of data.
- Distribution - a probability density function plot generated from one of more columns of input data.
- Cumulative distribution - a cumulative distribution function plot generated from one of more columns of input data.

There are some differences in the types and quantity of data that can be handled by the different options. For example, Distribution plot and Cumulative distribution plot are the only options that can handle array data from study tables without the need to split the arrays, and Histogram plots can only plot a single column of data.

When the dialog is first opened, the *Graph type* will be set to the most appropriate option, as follows:

- If more than one column of data is selected then *Graph type* will be set to Scatter (2-D).
- If a single column of array data is selected then *Graph type* will be set to Distribution or Cumulative distribution, depending on which of these was the more recently used.
- If a single column of non-array data is selected then *Graph type* will be set to 1-D.

Plot: Generates a chart document containing plots according to the specified settings.

Help: Displays the Help topic in a browser.

1-D plot options

This generates a plot of data value against row number for one or more columns of data. If the data in one of the selected columns is not numeric, that column is treated as categorical data.

Show lines: If this is checked, the plot will have lines added between adjacent data points.

Flip plot orientation: By default, plots are generated with the row values along the horizontal X-axis and the data values along the vertical Y-axis. If *Flip plot orientation* is checked, then the row values will be plotted along the vertical Y-axis and the data values along the horizontal X-axis.

Scatter (2-D) plot options

This generates a scatter plot of data values from the dependent column against data values from the independent column for one or more columns of dependent data. If the data in one of the selected columns is not numeric, that column is treated as categorical data.

X-axis: Specify which of the selected columns to use for the independent data.

Include X variable: Normally the column specified for the independent data will not be included in the set of dependent data columns. If *Include X variable* is checked then the independent data column will be included in the set of dependent data columns.

> **Note:** If you choose the *Scatter (2-D)* option when just a single column of data is selected, then that column will be used for both the independent data and the dependent data regardless of the setting of *Include X variable*.

Show best fit line: If this option is chosen a best fit line is calculated and drawn for each of the dependent variables. The equation of the line will be shown in the legend of the plot. This is drawn only if the dependent data and the independent data are both numeric.

Note: If you choose to plot the response variable against the prediction from a regression model (with the response on the *Y-axis* and the prediction on the *X-axis*), the *best fit line* will be the line Y = X. Similarly, if you choose to plot the residual values (*Y-axis*) against the prediction (*X-axis*), the slope of the *best fit line* will be zero. Conversely, if you choose to plot the prediction (*Y-axis*) against the response (*X-axis*), the slope of the *best fit line* will be the r^2 value of the original regression.

Flip plot orientation: By default, plots are generated with the independent data along the horizontal X-axis and the dependent data along the vertical Y-axis. If *Flip plot orientation* is checked, then the independent data will be plotted along the vertical Y-axis and the dependent data along the horizontal X-axis.

Histogram plot options

This allows you to generate a frequency histogram of the data values of a single column of data. This is achieved by splitting the data range into a specified number of equally spaced bins and adding each data point into the appropriate bin. If the data is not numeric then it is considered to be categorical, and each bin corresponds to a separate unique category.

Note: *Histogram* plots can be generated only from a single column of selected data. If more than one column is selected then the *Plot* button will be disabled.

Likewise, if the single selected column contains array data then the *Plot* button will also be disabled.

Number of bins: Specify the number of bins to use for the histogram. If the selected data is not numeric the *Number of bins* control will be disabled and the number of bins used will be equal to the number of distinct categories represented in the data.

Flip plot orientation: By default, plots are generated with the bin values along the horizontal X-axis and the data frequency values along the vertical Y-axis. If *Flip plot orientation* is checked, then the bin values will be plotted along the vertical Y-axis and the data frequency values along the horizontal X-axis.

Distribution plot and Cumulative distribution plot options

The Distribution plot option allows you to generate a probability density function (pdf) plot from numeric data in one or more columns of a study table or grid. Multiple columns can be treated individually or can have their data combined into a single plot. A smoothed plot can be generated which shows the trends in the pdf by smearing out the peaks in an attempt to reduce the noise.

The Cumulative distribution plot option allows you to generate a cumulative distribution function (cdf) plot from numeric data in one or more columns of a study table or grid. Multiple columns can be treated individually or can have their data combined into a single plot. These plots can also be smoothed.

Distribution plots and Cumulative distribution plots can both process array data from study tables without the need to split the arrays.

Distribution plots and Cumulative distribution plots both share the same set of options.

Bin size for: When selected, indicates that the *bin size* control will be used in conjunction with the range of data values to determine the number of bins to use. The list box allows commonly used settings to be obtained:

- A setting of Distances will give a *bin size* of 0.05, and vice versa.
- A setting of Angles will give a *bin size* of 1.0, and vice versa.
- A setting of Custom indicates that the *bin size* has a value other than 0.05 or 1.0.

Number of bins: When selected, indicates that the *Number of bins* control will be used in conjunction with the range of data values to determine the size of bins to use.

Smoothing width: Specify the width of the smoothing function that will be applied to the binned data for the smoothed plot (if requested).

The *Smoothing width* is the width (specified in multiples of the *bin size*) between the inflection points of the normal distribution function that is to be convolved with the binned data. This also equates to twice the variance of that normal distribution function. The total length of the smoothing function will be *2.0 * Smoothing width*, giving a function that extends to twice the variance on either side of zero.

> **Note:** The value of *Smoothing width* should be chosen with care. Too small a value will fail to smooth the noise apparent in the distribution plot caused by finite sample size. Conversely, too large a value will lose real features of the distribution. The smoothing width will be restricted to the number of data bins used for the raw data binning.
>
> The *Smoothing width* value should also be considered in conjunction with the data set size, the bin size, and the possible errors in the original data values. For most circumstances a value close to the default (3.0) should suffice.

Plot(s) to show: Select the types of plot to be generated. Available options are:

- Raw - the raw binned data is plotted
- Smoothed - the binned data is smoothed before plotting
- Raw and smoothed - both raw and smoothed data are plotted in the same chart

Treat multiple columns: Select the graphs to be generated if data from multiple columns are selected. Available options are:

- Individually - a separate graph (or graphs, if Raw and smoothed is chosen for *Plot(s) to show*) is generated for each column of data selected. However the data is treated as a single data set when determining the *bin size* or *number of bins*.
- As one - all the selected data values contribute to a single set of bins. A single graph (or pair of graphs) will be generated.

Access methods

Menu	*Tools	Plot Graph*
Study Table toolbar	 *| Plot Graph*
Grid toolbar	 *| Plot Graph*

Color By Value dialog

The Color By Value dialog allows you to color selected cells in a grid or study table document based on their numeric data values.

Value range

These options allow you to specify the data range over which to apply the color scheme.

Use range of all selected cells: When selected, indicates that the specified color scheme will be applied based on data values from the entire selection.

Use range of selections in each column: When selected, indicates that the specified color scheme will be applied individually to each selected column.

Custom From/To: When selected, indicates that the specified color scheme will be applied based on the specified custom data range.

When the dialog is first displayed, the fields are initially populated with the minimum and maximum values from the selected cells. These values can then be edited to provide a custom range, either by manually entering values or using the spin controls. Alternatively, clicking on  opens a menu that allows the field value to be updated with the minimum/maximum values from the current selection.

Color scheme

These options allow you to specify the color scheme to be used.

Use the color range choosers to specify the start and end colors. Clicking on the color controls  displays the Microsoft Common Color Control for color selection. The spin controls allow the brightness to be adjusted. The color bar provides a visual representation of the color scheme.

Bands: Specify the number of color bands, up to a maximum of 256. Each color band corresponds to a range of data values, calculated based on a linear scaling.

Gradient: Select the type of color gradient for the color scheme. Available options are:

- Two Color
- Three Color

For a two-color gradient, a linear transition from the start color to the end color is used. For a three-color gradient, white is fixed as the middle color and a linear transition from the start color to white, then from white to the end color is used.

Apply: Colors the selected cells according to the specified settings.

Remove: Removes any color from the selected cells, resetting to the default color (white).

Help: Displays the Help topic in a browser.

Access methods

Menu	*Tools	Color By Value*

Format Cells dialog

The Format Cells dialog allows you to change the formatting of numeric data values in a grid or study table document.

Format: Specify the numeric format to be applied to the selected cells. Available options are:

- General - Numeric non-integer values with very small (<1e-3) or very large (≥1e3) magnitudes, excluding the special case of 0.0, are displayed using scientific format. In this case, the number of figures after the decimal point is 6 for double-precision values and 3 for single-precision values. Other values are displayed using decimal format. In this case, the number of figures after the decimal point is 8 for double-precision values and 4 for single-precision values. Integer values are displayed without a decimal point.
- Numeric - Numeric values with very small (<1.e-3) or very large (≥1.e3) magnitudes, excluding the special case of 0, are displayed using scientific format. Other values are displayed using decimal format. In either case, the *Precision* is the number of figures after the most significant figure.
- Decimal - Numeric values are displayed in the form ±xxx.yyyy. The *Precision* is the number of figures after the decimal point.
- Scientific - Numeric values are displayed with a coefficient and an exponent (i.e., ±x.yyyye±zzz). The coefficient value is between 1 and 10 ($1 \le x \le 9$), except for the special case of 0, for which the coefficient is 0. The *Precision* is the number of figures after the decimal point in the coefficient.

Sample: Shows a sample value formatted using the current settings.

Precision: Specify the precision with which numeric values will be displayed.

Apply: Applies the specified format to the selected cells.

Help: Displays the Help topic in a browser.

Access methods

Menu	*View	Format Cells*

Working with study tables

You can calculate, display, and analyze the properties of 3D structures or other tabular and spreadsheet data in study table documents.

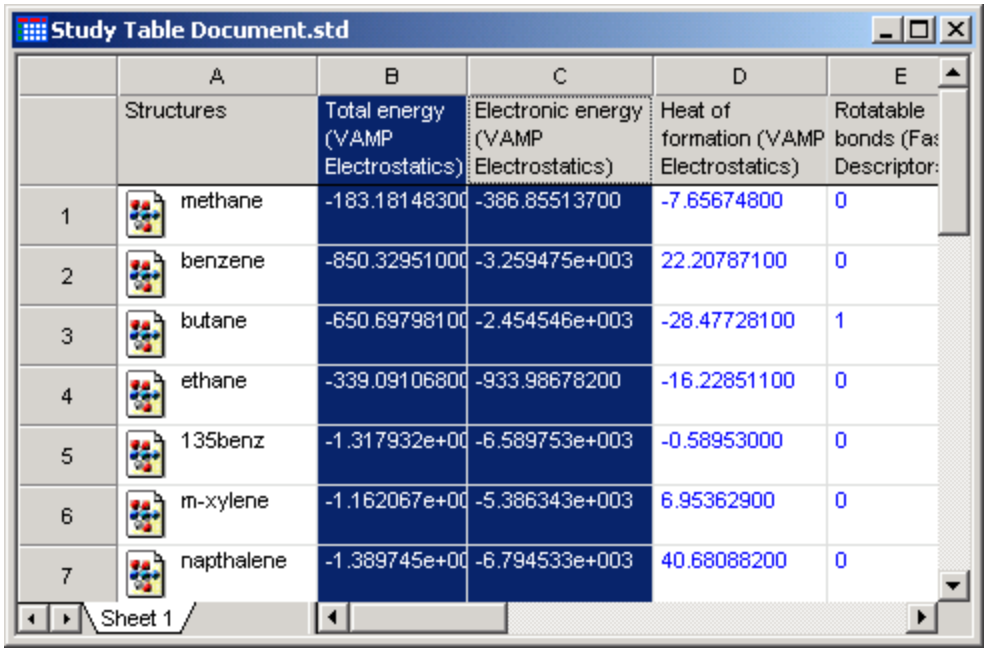
Structural data may be inserted into a study table document and calculations performed to derive properties of those structures. Additional data may be derived by adding functions to the study table or by performing various data analysis operations.

Study tables can also be used to store other document types, such as charts, when output from calculations. In addition, the usual grid editing capabilities for numeric and textual data are supported. Stored document data can be viewed and edited using the detail view.

You can transfer data to and from other Materials Studio documents and different Windows applications, and save the document data in the native study table format.

Managing study table documents

You can populate study table documents by inserting structures or trajectories, or by cutting and pasting data from other Materials Studio documents and other Windows applications. Study table data are saved as `.std` files.



Study Table Viewer showing multiple selection

Loading and saving study table documents

To open a study table document from an existing file

1. Select *File | Import...* from the menu bar, click the *Import* button  on the toolbar, or right-click on the project in the Project Explorer and select *Import...* from the shortcut menu.
2. In the Import Document dialog, navigate to and select an `.std` file.
3. Click the *Import* button.

To create a new study table document

1. Select *File | New...* from the menu bar or click the *New* button  on the toolbar and select *Study Table* from the New Document window.
2. Alternatively, click on the options arrow associated with the *New* button  and select *Study Table Document* from the dropdown list or right-click on the project in the Project Explorer and select *New | Study Table Document* from the shortcut menu.

To save data

- Select *File | Save* from the menu bar or click the *Save* button  on the toolbar to save the underlying data in STD format.

To print the study table

- Select *File | Print...* from the menu bar or click the *Print* button  on the toolbar.

Inserting data into a study table

You can insert data into a study table document using copy and paste. Structures and trajectories may be inserted using the Insert Into Active Document dialog, accessed by clicking the *Insert From File* button  on the *Standard* toolbar or by selecting *Edit | Insert From...* from the menu bar.

Editing study table documents

The Study Table Viewer allows you to easily modify the contents of study table documents. In addition to the tasks described in the Editing tabular data topic, the following tasks are possible for study table documents.

The status of data in a cell is represented by the text color. Calculated data are displayed in **blue**, data that are pending the result of a model calculation are displayed in **red**, and all other data are displayed in **black**.

To modify the contents of a cell

- To edit a document stored in a cell, use the Study Table Detail View.

To split a column of arrays into separate columns

- Right-click on the column description cell and select *Split Arrays* from the shortcut menu. Individual columns for each array element will be inserted into the study table to the right of the original column.

Copying and pasting study table data

To copy data

1. Make a selection by clicking on individual cells or row or column header(s), or by dragging over a block of contiguous cells. Alternatively, select all the cells by clicking on the top left header cell.
2. Select *Edit* | *Copy* from the menu bar, click the *Copy* button  on the toolbar, right-click on the selected cells and choose *Copy* from the shortcut menu, or press CTRL + C.

Note: Copying can only be performed for a rectangular selection of cells or a discontinuous selection that could be made rectangular by a suitable reordering of rows and columns.

To paste data

1. Select the cell or cells into which you intend to paste the data.
2. Paste the data into the Materials Studio document (or another application) by selecting *Edit* | *Paste* from the menu bar, by clicking the *Paste* button  on the toolbar, by right-clicking in the new document and choosing *Paste* from the shortcut menu, or by pressing CTRL + V.

Note: Pasting can only be performed for a rectangular selection of cells or a discontinuous selection that could be made rectangular by a suitable reordering of rows and columns.

Note: When data are transferred from one study table to another, structural and data type information is usually preserved. However, if the copied document is closed before pasting or if the structures are pasted into a column that already has another type, structural information may be lost. In addition, when a calculated column of data is copied and pasted, the information about the model used to perform the calculation is not transferred. This means that, unlike the original data, the data in the pasted column cannot be recalculated.

Note: When data are transferred from a study table to another application or Materials Studio document type, structural and/or data type information may be lost. Structural information may be transferred using the SD file format, if this is supported by the target application, otherwise, only the structure names are transferred.

Study table column type

A column in the study table can be associated with a *Type*. The available types form a hierarchy, all derived from a common base type.

The column type plays several roles:

- When inserting documents to the study table, a column having *structure* type will be used if available in the current selection.
- When adding models to the study table, column types are used to match columns in the study table to model inputs. The Connect Model dialog uses column type to present possible choices for ambiguous model inputs.
- When adding data to a column that already has an associated type, the type is used to attempt a conversion of the added data. If the conversion succeeds, then the converted data values are added to the study table. If the data cannot be converted, the original data values are added to the study table.

To view the type associated with a particular column, right-click on the column description and select *Properties* from the shortcut menu. The Column Properties dialog is displayed, showing the column description and column type.

Study Table Detail View

The Study Table Detail View is used to browse or edit documents in a study table column.

To browse documents

1. Double-click on a document or right-click on a cell in the study table and select *View* from the shortcut menu.
2. Use the *Step Detail View Forwards*  and *Step Detail View Backwards*  buttons on the Study Table Viewer toolbar to browse documents in the study table column. The cell corresponding to the current displayed document is highlighted in the study table.
3. If the current cell contains no document, or an invalid document, the corresponding detail view will be empty.

Note: A number of detail views can be opened on the same study table document or on the same column of a study table document. When the study table is closed, any associated detail views also close.

To edit a document

1. Double-click on a document or right-click on a cell in the study table and select *View* from the shortcut menu.
2. Use the normal functionality available for viewing and editing documents in a 3D Viewer to modify the document as required.
3. Click the *Commit Edit* button  on the *Study Table Viewer* toolbar to commit the edit to the study table.

Note: When you edit a document in a detail view, the study table document is not modified until that edit is committed to the study table. If you perform some action that may result in an edited document being lost, for example, closing the detail view or using *Step Forwards* to move to the next structure, you will be prompted to either commit the edit to the study table document or to discard the edit.

Filtering study table data

Use the *Filter* facility to reduce the volume of data displayed in a study table sheet. This creates a new sheet in the study table that displays only the selected data. You may wish to use this in order to concentrate on only a few important systems from your original set of data or to temporarily remove some unwanted system from the original set of data.

Note: The new filtered sheet is a *view* of the data on the original sheet. Any edits made to data appearing on the new filtered sheet are made to the underlying data and, thus, also appear on the original sheet. Data deleted from the filtered sheet are deleted from the original sheet.

To filter data into another sheet

1. Select the rows, columns, or cells that you wish to be shown in the filtered sheet.
2. Choose *Tools | Filter* from the menu bar or click the *Filter* button  on the Study Table Viewer toolbar.

To filter the inverse of the selected data into another sheet

1. Select the rows or columns that you wish to be omitted from the filtered sheet.

   Note: The *Inverse Filter* functionality is available only when complete rows or columns of data are selected in the study table.

2. Select *Inverse Filter* from the dropdown list associated with the *Filter* button  on the *Study Table Viewer* toolbar.

Tip: In many cases, selection of the important rows may be facilitated by first sorting the rows.

For any filtered sheet, you can display all the data contained in the study table document using the *Show All* command on the dropdown list associated with the *Filter* button  .

Analyzing data in a study table

A number analysis operations, including data reduction, cluster analysis and model building, may be performed on study table data. These operations are accessed from the Statistics menu.

Graphs of study table data may also be produced via the *Quick Plot* button on the Study Table Viewer toolbar.

Inserting documents into a study table

Structures and trajectories can be inserted into a study table from any of the appropriate file formats that are supported in Materials Studio. Chart documents can be inserted into a study table from the XCD native chart document format.

Documents are inserted in a selected column based on the following rules:

- A column will be chosen based on the type of the column being appropriate for the document type, if any exist in the current selection.
- Otherwise, the first column which has not had a type assigned to it, if any exist in the current selection.
- Otherwise, a new column is added to the left of the current selection and the documents are inserted into this new column.

To insert project documents into a study table

1. Ensure that the active document is a study table.
2. In the Project Explorer, select the documents to be inserted.
3. Right-click on one of the documents to be inserted.
4. Select *Insert Into* from the shortcut menu.
5. The documents are inserted into the study table based on the insertion rules listed above.

To insert non-project documents into a study table

1. Ensure that the active document is a study table.
2. Display the Insert Into Active Document dialog by selecting *Edit | Insert From...* from the menu bar or by clicking the *Insert From File* button  on the Standard toolbar.
3. Navigate to the folder containing the document to be inserted into the study table.
4. Supported file formats are displayed in the file type dropdown list for the *File name*. Select the document or documents and click *Insert*.
5. The document or documents are inserted into the study table based on the insertion rules described above.

Note: When inserting 3D structure and chart documents, each cell in the chosen column references a single document. In the case of trajectory documents, however, each cell in the chosen column references a frame of the inserted trajectory document.

Note: Structures and charts in the study table may be browsed and edited using the Study Table Detail View.

Exporting structures from a study table

You can export nonperiodic structures, together with any associated properties, from a study table to an `.sd` file.

When the `.sd` file is written, non-structural data values in named columns are written as named properties attached to the structures with which they share a row. The structures are written to the `.sd` file in row order.

Periodic structures are not supported by the `.sd` format.

In order to transfer a structure from a study table, you can use copy and paste to copy a structure from the study table detail view to a new 3D Atomistic document, which can then be exported in the usual way.

To export structures to an `.sd` file

1. Select the columns containing the structures that you want to export and the columns containing the properties that you want to be associated with these structures in the `.sd` file.
2. Choose *File | Export...* to open the Export dialog.
3. Ensure that Symyx SD Files (*.sd) is selected in the *Save as type* list box before clicking the *Export* button.

Note: If cells are selected in the active sheet, only those structures in the selected cells are exported. If no cells are selected in the active sheet, then all structures in that sheet are exported.

To transfer a structure using copy and paste

1. Select the cell containing the structure you wish to transfer.
2. Right-click on the cell and choose *View* from the shortcut menu to open a study table detail view.
3. While the study table detail view is active, select *Edit | Copy* from the menu bar or click the *Copy* button  on the *Standard* toolbar.
4. Open the New Document dialog by choosing *File | New...* from the menu bar or by clicking the *New* button  on the *Standard* toolbar, and select *3D Atomistic*.
5. With the new 3D Atomistic document as the active document, choose *Edit | Paste* from the menu bar or click the *Paste* button  on the *Standard* toolbar.

Calculating descriptors in a study table

You can calculate descriptors for structures contained in a study table using the *Models dialog*, which is accessible from the *QSAR Models* toolbar.

Calculating descriptors of structural data is a special case of running models.

Defining functions

You can define mathematical expressions and add them to columns of a study table as a function model. This allows expressions of one or more existing columns to be displayed in another column.

The created function model is added to the list of project models. It can then be viewed and applied to any study table document using the Models dialog.

To define a function and add it to the study table

1. Ensure the study table is the active document.
2. Open the Define Function dialog using the *Define Function*  button on the QSAR Models toolbar.
3. Use the Define Function dialog to enter a function expression, and a short name and description if desired.

When you enter an expression to be added to a study table, you should express it in terms of the columns to be used as input to the expression. For example, to evaluate the sum of the data in the columns D and F, enter: D+F.

The supported syntax for functions is described elsewhere.

Supported function expressions

A function expression can consist of variables, operators, functions, and constants.

> **Note:** A variable name cannot contain spaces or underscore characters.

Supported binary operators

- "+" - add
- "-" - subtract
- "*" - multiply, for example 2*a is a valid expression, but 2a is not
- "/" - divide
- "^" - raise to the power
- "&" - string concatenation
- "=" - equal to
- "<" - less than
- ">" - greater than
- "<>" - not equal to
- "<=" - less than or equal to
- ">=" - greater than or equal to

Supported unary operators

- "+" - unary plus
- "-" - unary minus
- "%" - postfix percentage operator

Supported constants

- "pi"

Supported functions of one variable

Trigonometric functions

- "sin"
- "cos"
- "tan"
- "asin" - inverse sine
- "acos" - inverse cosine
- "atan" - inverse tangent

Logarithmic and hyperbolic functions

- "exp" - exponential
- "log" - base 10 logarithm
- "ln" - natural logarithm
- "sinh" - hyperbolic sine
- "cosh" - hyperbolic cosine
- "tanh" - hyperbolic tangent
- "asinh" - inverse hyperbolic sine
- "acosh" - inverse hyperbolic cosine
- "atanh" - inverse hyperbolic tangent

Other simple functions

- "sqrt" - square root
- "abs" - absolute value
- "ramp" - first-order spline function, for example ramp(x) = 0 (x<0), x (x>=0)

Supported functions of more than one variable

The syntax for functions of more than one variable includes a column expansion token, ":". Use of this token interprets the variables as a range for processing. For example, sum(b:e) is equivalent to sum (b,c,d,e). The variables used in such an expansion must correspond to column labels in a study table and the expansion is performed using the column labels convention. Thus, sum(b1:e1) is invalid, whereas sum(y:ac) is valid and expands to sum(y,z,aa,ab,ac).

Note: The separators used in function lists will depend on the configuration of the system locale. In UK/US locales commas are used as separators, for example sum(b,c,d,e) and or(x=y, y<z, w>=1), but these should be translated to semi-colons for European locales: sum(b;c;d;e) and or(x=y; y<z; w>=1) respectively. See also Localization.

Numeric functions

Numeric functions of more than one variable will expand the contents of an array to act on all of the numeric values in the array. Thus, it is possible to specify just a single argument to one of these functions, as long that argument corresponds to an array. Any non-numeric data input to a numeric function will be ignored and will not cause an error.

- "sum" - sum of all numeric values in the specified arguments, for example sum(x,2,3) is equivalent to x+5
- "product" - product of all numeric values in the specified arguments, for example product(3,x,y) is equivalent to 3*x*y
- "min" - lowest of all the numeric values in the specified arguments
- "max" - highest of all the numeric values in the specified arguments
- "mean" - mean of all numeric values in the specified arguments
- "meanpos" - mean of all the positive numeric values in the specified arguments
- "meanneg" - mean of all the negative numeric values in the specified arguments
- "count" - count of all the numeric values in the specified arguments (including the number of numeric array values, if appropriate)
- "countpos" - count of all the positive numeric values in the specified arguments
- "countneg" - count of all the negative numeric values in the specified arguments

Other functions

- "and" - Boolean AND function, for example, and(x=y, y=z)
- "or" - Boolean OR function, for example or(x=y, y<z, w>=1)
- "element" - extracts the nth element from an array, for example element(2,x) gives the second element. Elements may be specified by index or name.

Working with grids

You can display tabular and spreadsheet data in grid documents. These may contain one or more sets of data created by Materials Studio or loaded from one of standard file types supported by the Grid Viewer.

You can transfer the grid data between different Windows applications and save the document data in the grid's native format.

Managing grid documents

You can generate grid documents by reading data directly from an existing `.xgd` or `.csv` file using *File | Import...* on the main menu or create them from scratch within a Materials Studio module. When you save the grid data, the information will always be saved in the Grid Viewer's internal XGD format.

To open a grid document from an existing file

1. Select *File | Import...* from the menu bar, click the *Import* button  on the toolbar, or right-click on the project in the Project Explorer and select *Import...* from the shortcut menu.
2. In the Import Document dialog, navigate to and select an `.xgd` or `.csv` file.
3. Click the *Import* button.

To save data

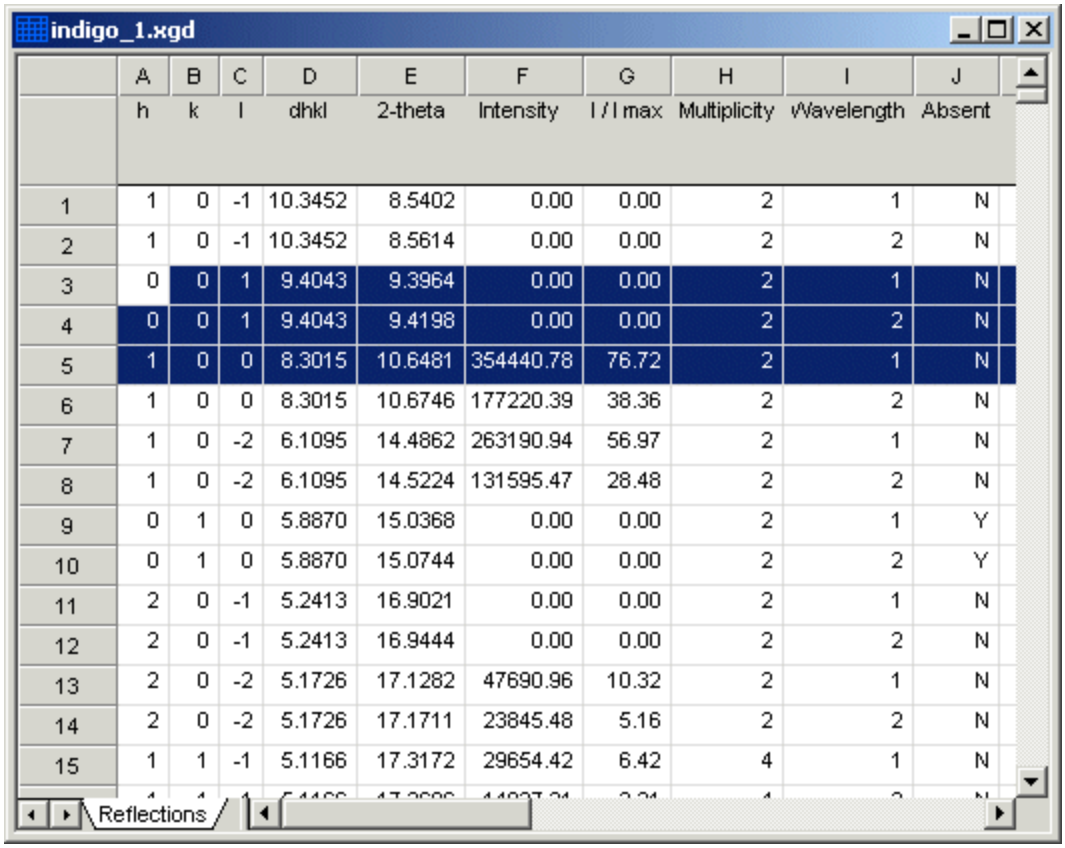
- Select *File | Save* from the menu bar or click the *Save* button  on the toolbar to save the underlying grid data in XGD format.

To create a new grid document

1. Select *File | New...* from the menu bar or click the *New* button  on the toolbar and select *Grid* from the New Document window.
2. Alternatively, click on the options arrow associated with the *New* button  and select *Grid Document* from the dropdown list or right-click on the project in the Project Explorer and select *New | Grid Document* from the shortcut menu.

To copy data

1. Make a selection by clicking on individual cells, row or column header(s), dragging over a block of contiguous cells, or, to select all cells, click the top-left header cell.
2. Select *Edit | Copy* from the menu bar, click the *Copy* button  on the toolbar, right-click on the selected cells and choose *Copy* from the shortcut menu, or press CTRL + C.



	A	B	C	D	E	F	G	H	I	J
	h	k	l	dhkl	2-theta	Intensity	I / I max	Multiplicity	Wavelength	Absent
1	1	0	-1	10.3452	8.5402	0.00	0.00	2	1	N
2	1	0	-1	10.3452	8.5614	0.00	0.00	2	2	N
3	0	0	1	9.4043	9.3964	0.00	0.00	2	1	N
4	0	0	1	9.4043	9.4198	0.00	0.00	2	2	N
5	1	0	0	8.3015	10.6481	354440.78	76.72	2	1	N
6	1	0	0	8.3015	10.6746	177220.39	38.36	2	2	N
7	1	0	-2	6.1095	14.4862	263190.94	56.97	2	1	N
8	1	0	-2	6.1095	14.5224	131595.47	28.48	2	2	N
9	0	1	0	5.8870	15.0368	0.00	0.00	2	1	Y
10	0	1	0	5.8870	15.0744	0.00	0.00	2	2	Y
11	2	0	-1	5.2413	16.9021	0.00	0.00	2	1	N
12	2	0	-1	5.2413	16.9444	0.00	0.00	2	2	N
13	2	0	-2	5.1726	17.1282	47690.96	10.32	2	1	N
14	2	0	-2	5.1726	17.1711	23845.48	5.16	2	2	N
15	1	1	-1	5.1166	17.3172	29654.42	6.42	4	1	N

Grid Viewer showing multiple selection

To paste data

1. Select the cell where you would like the first data item pasted.
2. Paste the data into the Materials Studio document (or another application) by selecting *Edit* | *Paste* from the menu bar, by clicking the *Paste* button on the toolbar, by right-clicking in the new document and choosing *Paste* from the shortcut menu, or by pressing CTRL + V.

To print the grid

- Select *File* | *Print...* from the menu bar or click the *Print* button on the toolbar.

Working with text documents

Materials Studio displays text and HTML documents in the Text Viewer. These documents may be produced directly by Materials Studio (for example, the project log and simulation results), indirectly by Materials Studio (by editing such documents in the Text Viewer) or via external programs. The majority of these documents will have the standard file extensions (`.txt`, `.htm`, `.html`), but other common text-based formats are also recognized (for example, `.out`).

You can transfer text and HTML documents between different Windows applications and save text and HTML documents in their standard formats.

You can edit, cut, copy and paste text into text or HTML documents using the commands available on the Edit menu. You can also insert images into HTML documents.

To display the text viewer

1. Select *File | New...*.
2. Click on *Text* or *HTML* on the *Document* tab.

or

Double-click on an existing text or HTML document in the Project Explorer.

or

Import an existing text or HTML document using *File | Import...*.

Managing text documents

Text and HTML documents can be saved either as part of, or outside of, Materials Studio projects. They are listed in the Project Explorer along with other types of documents such as 3D model, chart, grid and study table documents.

To create a text or HTML document

- Choose *File | New...* from the menu bar, then select *Text* or *HTML* from the *New Document* dialog.

or

- Click the dropdown list next to the *New* button on the Standard toolbar, then click on *Text Document* or *HTML Document*.

To open a text or HTML document that already exists in the current project

- Double-click on the document's icon in the Project Explorer.

To import a text or HTML document to the current project

1. Choose *File | Import...* from the menu bar, or click the *Import* button on the Standard toolbar.
2. Navigate to the file, select it, and click the *Import* button.

To save a text or HTML document to the current project

- Choose *File | Save* from the menu bar, or click the *Save* button on the *Standard* toolbar.

To save a text or HTML document outside the current project

- Choose *File | Export...* from the menu bar.

To copy a text or HTML document

1. Select the text you wish to copy.
2. Choose *Edit | Copy* from the menu bar. Alternatively right-click and choose *Copy* from the shortcut menu.
3. In another application choose *Edit | Paste* or *Paste Special*.

To print a text or HTML document

- Choose *File | Print* from the menu bar.

Editing text documents

You can edit, cut, copy, paste, delete, save, and print text and HTML documents in the Text Viewer.

View modes

Text files opened in the Text Viewer are displayed in Edit Mode. In Edit Mode you can edit, cut, copy, paste, delete, save, and print documents.

HTML Documents are displayed either in Edit Mode or Browse Mode. You can switch between the modes by selecting *Edit Mode* or *Browse Mode* from the Edit menu.

Browse Mode displays documents as they would appear in Internet Explorer, i.e. scripts, links and marquees are live. If you open a URL in the Text Viewer, the document is displayed in View-Only Mode, so the browse and edit modes are not available.

Editing tools

Many of the commands on the File and Edit menus can be used to edit text or HTML documents in the Text Viewer. Editing commands also appear on a shortcut menu when you right-click in the Text Viewer.

You can use tools on the HTML Formatting and HTML Tables toolbars to format HTML documents. Show or hide the toolbars using the *View | Toolbars* dropdown list.

Saving a text or HTML document

To save a text or HTML document to the current project

- Choose *File | Save* or *File | Save As...* from the menu bar.

To save a text or HTML document outside the current project

- Choose *File | Export...* from the menu bar.

Working with Pipeline Pilot Protocols

The Pipeline Pilot Protocols tool allows you to run protocols on a Pipeline Pilot server. You can specify the Pipeline Pilot server and username you want to use to run a protocol, browse available protocols, view protocol and parameter help, and edit protocol parameter values. Materials Studio documents can be used as input for protocol parameters of type URL.

The status of protocol jobs can be monitored and jobs can be stopped and deleted using the Job explorer. On completion, protocol outputs can be downloaded automatically to the Materials Studio project and HTML reports can be displayed in a web browser.

Guidelines for preparing Pipeline Pilot protocols

Although it is possible to run any example protocol using the *Pipeline Pilot Protocols* tool, many of the example protocols provided with Pipeline Pilot are of limited use when run from Materials Studio. Many example protocols do not expose any input parameters at the protocol level and therefore can not be run with different Materials Studio documents as input.

It is, therefore, likely that you will want to add your own protocols. In order to do this, you need access to the Pipeline Pilot Professional Client.

This topic provides guidelines for writing protocols that work well with Materials Studio.

> **Tip:** Only protocols stored on the User tab for the current user or the Protocols/Examples folders in Pipeline Pilot are available in the *Pipeline Pilot Protocols* dialog in Materials Studio.

Transferring documents to the Pipeline Pilot Server

- For a protocol to work with Materials Studio, at least one parameter at the protocol level should be of type "URLType" or "DirectoryType".
  - URLType parameters accept input from a single Materials Studio document
  - DirectoryType parameters accept input from a folder in a Materials Studio project
- Use a *Material Reader* component from the Materials Studio collection to read input from a 3D Atomistic document, 3D Atomistic Trajectory, or 3D Atomistic Collection document in Materials Studio.
- Use a *Study Table Reader* component from the Materials Studio collection to read input from a Study Table document in Materials Studio.
- Use a *Spectrum Reader* component from the Analytical Instrumentation collection to read input from a Chart document in Materials Studio.
- Give input parameters of URLType a name that indicates the type of Materials Studio document that is expected so that users can readily select the correct type of document. For example:
  - Include "Structure", "Molecule", or "Crystal" in the parameter name if a single structure is expected
  - Include "Trajectory" in the parameter name if a trajectory document is expected
  - Include "Chart", "Spectrum" or "Powder Pattern" in the parameter name if a chart document is expected
  - Include "Study Table" in the parameter name if a Study Table document is expected
- Ensure that the protocol functions for a single input file for each URLType parameter. It is not possible to specify more than one input document for an input parameter if it is URLType. If you want a protocol to operate on multiple structures you should use a Study Table document or 3D Atomistic Collection document as input.
- For URLType parameters, if the Pipeline Pilot server is running an older version of Materials Studio than the Materials Visualizer client, then structure, trajectory, collection, and study table documents will be converted to the correct version of Materials Studio supported by the Pipeline Pilot server. If the document contains objects which are not supported by the version of Materials Studio on the Pipeline Pilot server, these will be removed from the documents.
- For DirectoryType parameters, there is no conversion if the Pipeline Pilot server is running a different version to the Materials Visualizer client. This may result in an error in your protocol.

Returning files to your Materials Studio project

- Write output files to the job directory (`$jobdir`). By default, all files in the job directory are returned as results files and will be downloaded to the Materials Studio project when the job finishes.
- Explicitly add output files in subdirectories of the job to the protocol results.
  Refer to the Pipeline Pilot help for the Results tab of the Edit Protocol dialog for more information.
- Avoid writing output files to the user directory. Although, by default, these are returned as results files and downloaded when the job finishes, any dependent files that may be written, for example when writing a trajectory or study table, will not be included.
- Use a *Copy File* component to copy additional output files to the job directory if necessary.
  Many components in the Materials Studio collection save additional output files to an output directory, adding the file path as a property on the data record. This includes temperature charts for molecular dynamics, convergence charts for geometry optimization and density of states, band structure, and optics charts from CASTEP or DMol3. For example, if density of states are requested, the *Energy Calculation (DMol3)* component adds the **MSDMol3_DOSChart** property to the data record, containing the path of the density of states chart file. The simplest way to return such files to Materials Studio is by copying them to the job directory using a Copy File component.
- Use the *Study Table Writer* component to output a large numbers of output structures or structures with additional properties on the data record.
- Use the *Material Writer* component to write each output structure to a different file if only one, or a few, output structures are expected.

Tip: The Pipeline Pilot Connector allows you to connect to servers which may be running previous versions of the Materials Studio Collection. If you run a protocol which uses components from a previous version, objects which are not supported in that previous version will be removed from the copy of the file used for the protocol run.

Note: Submitting jobs on a Pipeline Pilot server with "impersonation" enabled may cause issues with automatic downloading of job results when the protocol is complete.
You are strongly advised to ensure that "impersonation" is disabled on Pipeline Pilot servers where jobs will be submitted from Materials Studio.

Connecting to a server

In order to run a protocol, you need to connect to a Pipeline Pilot Server, specifying a server name, user name and possibly a password.

To connect to a Pipeline Pilot Server

1. Select *Pipeline Pilot Protocols* from the *Tools* menu.
   If you have previously used Materials Studio to connect to a Pipeline Pilot Server, it will attempt to connect with the last used server name and user name. If you are using the Pipeline Pilot Protocols dialog for the first time, or if the last used server is not available, you will be asked to select a Pipeline Pilot Server on the Pipeline Pilot Server Location dialog.
2. Enter the *Server name* and optionally the secure port number separated by a colon, for example `yourppserver:9943`.
   If no port number is specified the default Pipeline Pilot secure port (9943) will be used. Alternatively, select the server from the list of previously used servers.
3. Click the *OK* button.
   If the server is available, Materials Studio will attempt to connect using your Windows user name

and no password. If this succeeds, the Pipeline Pilot Protocols dialog will open, otherwise the Pipeline Pilot Server Authentication dialog will be opened.

4. Enter the appropriate *User name* and *Password*.
5. Click the *OK* button.

To change the current Pipeline Pilot Server

If you have already connected to the server you require you can choose it from the *Server Location* dropdown list on the Pipeline Pilot Protocols dialog. To connect to a new server, follow these instructions.

1. Select *Change Active Server* from the *Tools* menu on the Pipeline Pilot Protocols dialog to open the Pipeline Pilot Server Location dialog.
2. Enter the *Server name* and optionally the secure port number separated by a colon, for example `yourppserver:9943`.
   If no port number is specified the default Pipeline Pilot secure port (9943) will be used. Alternatively, select the server from the list of previously used servers.
3. Click the *OK* button.
   If the server is available, Materials Studio will attempt to connect using your Windows user name and no password. If this succeeds, the Pipeline Pilot Protocols dialog will open, otherwise the Pipeline Pilot Server Authentication dialog will be opened.
4. Enter the appropriate *User name* and *Password*.
5. Click the *OK* button.

To change the current user name

1. Select the *Change User Name* from the *Tools* menu on the Pipeline Pilot Protocols dialog to open the Pipeline Pilot Server Authentication dialog.
2. Specify a *User name* and *Password*.
3. Click the *OK* button.

Note: In order to monitor the status of running protocols or perform other operations on Pipeline Pilot jobs, you need to connect to the Pipeline Pilot Server on which those jobs were run. When you open a project containing existing Pipeline Pilot jobs, you will be asked to specify a password for the each of appropriate servers using the Pipeline Pilot Server Authentication dialog. In this case the *User name* is set to that used when the protocol was run and cannot be changed.

Running a protocol

The Pipeline Pilot Protocols tool allows you to run protocols on a Pipeline Pilot server. Materials Studio documents can be used as input for URL type protocol parameters and protocol outputs can be downloaded automatically to the Materials Studio project.

To run a Pipeline Pilot protocol

1. Open the Pipeline Pilot Protocols dialog and connect to a Pipeline Pilot server if necessary.
2. Select the protocol you wish to run from the list. You can choose from protocols in the Examples folder or the current user's folder on the selected server.
3. More information about the protocol or the protocol parameters is available in the *Details* window.
4. Specify input values in the *Parameters* list.
   Click in a cell to edit its value or to open the appropriate dialog for editing arrays, arrays with legal values, or text parameters.
   For URL type protocol parameters, the input will be taken from a document in the Materials Studio project. The document will be uploaded automatically to the Pipeline Pilot server when the protocol is run.
5. Click the *Run* button to start the protocol.

Note: The *Run* button will be disabled if any enabled parameter has an invalid value. Parameters with invalid values are highlighted in red and disabled parameters are displayed in gray. Hover the mouse over the value to display a tooltip explaining why the value is invalid or disabled.

When a protocol job completes, results files (excluding HTML reports) are downloaded automatically to the results folder in the Materials Studio project if the *Automatically view output* option is checked on the Preferences menu.

In addition, a summary of the job results is written to a text document in the results folder. If the job failed, a file containing the error description is also produced. The location of the results folder for each job is displayed in the job list. Any HTML reports generated are opened in the default web browser.

Note: HTML reports are not downloaded because they often contain content that is only valid on the Pipeline Pilot server. However, the job folder is retained on the Pipeline Pilot server, so the HTML reports can be viewed until the job is explicitly deleted.

Working with jobs

Information about all the Pipeline Pilot protocol jobs that have been run from the current Materials Studio project is displayed, together with Materials Studio Gateway jobs, in the Job explorer. This allows you to monitor the status of running jobs, stop jobs, delete jobs from the Pipeline Pilot server, and view any HTML reports produced by jobs that have been completed.

The jobs list contains the following information:

- *Description* - a text description of the job, including the name of the primary input document (if any) and the name of the protocol
- *Gateway* - the Pipeline Pilot server on which the job was run
- *Status* - the job status
- *Start Time* - the date and time when the job was started
- *Results Folder* - the project path of the folder into which the job results will be downloaded

The job status is continuously monitored and the list is updated automatically while the job is running.

To stop or delete a Pipeline Pilot job follow the instructions given in the Job explorer topic.

Note: After a job has been removed from the Pipeline Pilot server, any HTML reports produced by the job will no longer be available.

Viewing results

When a protocol job completes, results files (excluding HTML reports) are downloaded automatically to the results folder in the Materials Studio project if the *Download results automatically* option on the main Options dialog is selected.

In addition, a summary of the job results is written to a text document in the results folder. If the job failed, a file containing the error description is also produced. The location of the results folder for each job is displayed in the job list on the Job explorer.

Note: HTML reports are not downloaded because they often contain content that is only valid on the Pipeline Pilot server. However, the job folder is retained on the Pipeline Pilot server, so the HTML reports can be viewed until the job is explicitly deleted.

Note: Submitting jobs on a Pipeline Pilot server with "impersonation" enabled may cause issues with automatic downloading of job results when the protocol is complete.
You are strongly advised to ensure that "impersonation" is disabled on Pipeline Pilot servers where jobs will be submitted from Materials Studio.

To view HTML reports produced by a Pipeline Pilot job

1. Select the job you want to view the report for in the Job explorer list.
2. Click the *Remote View* button.

The HTML reports are displayed automatically in the default web browser.

Pipeline Pilot Protocols dialogs

The following topics describe the Pipeline Pilot Protocols dialogs.

Pipeline Pilot Server Location dialog

The Pipeline Pilot Server Location dialog allows you to specify the Pipeline Pilot server to be used for running protocols. This dialog is displayed when you:

- open the *Pipeline Pilot Protocols* dialog for the first time
- select *Change Active Server* from the *Tools* menu on the Pipeline Pilot Protocols dialog

Server location: Specify the server to which Materials Studio should connect. This should be a server name or server name and secure port number separated by a colon, for example `yourppserver:9943`. If no port number is specified the default Pipeline Pilot secure port (9943) will be used. You can enter the name of a new server or choose from a list of previously used servers.

Materials Studio will attempt to connect using the previous user name used for that server, if any, or your Windows user name, and no password. If this fails, the Pipeline Pilot Server Authentication dialog will be opened to allow you to enter a user name and password.

OK: Attempts to connect to the server and closes this dialog.

Cancel: Closes the dialog without changing the server.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Tools | Pipeline Pilot Protocols*
	Tools | Pipeline Pilot Protocols | Tools | Change Active Server

Pipeline Pilot Server Authentication dialog

The Pipeline Pilot Server Authentication dialog allows you to specify the user name and password to be used when connecting to a Pipeline Pilot Server. This dialog is displayed if a password is required to connect to a Pipeline Pilot Server:

- when no server connection is available
- after changing the Pipeline Pilot Server
- when you choose the *Change User Name* option on the *Tools* menu
- when opening an existing Materials Studio project containing previously run Pipeline Pilot jobs

Connection to server: Reports the name and port of the server to which Materials Studio is trying to connect.

If the server is unavailable or authentication fails an error message will be displayed in red below the *Connection to server* report.

User name: Specify the user name for connecting to the Pipeline Pilot Server.

> **Note:** *User name* is disabled if you are reconnecting a previously run job.

Password: Specify the password for connecting to the Pipeline Pilot Server.

OK: Attempts to connect to the server with the specified user name and password and closes the dialog.

Cancel: Closes the dialog without connecting to the server.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Tools	Pipeline Pilot Protocols	Protocols	Tools	Change User Name*

Pipeline Pilot Protocols dialog

The Pipeline Pilot Protocols dialog allows you to setup and run Pipeline Pilot protocols from Materials Studio, you can:

- specify the Pipeline Pilot server on which to run protocols
- select a protocol to be run on the Pipeline Pilot server
- specify protocol parameter values for a calculation

Tools menu

Change Active Server: Provides access to the Pipeline Pilot Server Location dialog for changing or adding the server.

Change User Name: Provides access to the Pipeline Pilot Server Authentication dialog for changing the current users name and password.

Refresh Protocol List: Updates the contents of the protocols available on the current server.

Preferences menu

Automatically View Output: When checked, the output HTML files from the job will be opened automatically in the default browser when the calculation is completed. Default = unchecked.

Notify on Job Completion: When checked, a dialog will be displayed when the job is completed. Default = unchecked.

Protocols explorer

The protocols available on the currently selected server are displayed in a list. The list can be refreshed using the *Tools* menu.

> **Tip:** Click once on a protocol name to view its description in the *Details*. Double-click on a protocol to open it, display its parameters, and make it available to run.

Parameters explorer

The input parameters for the selected protocol are displayed in a list.

- Enabled parameter values can be edited by clicking on them.
- Parameters with invalid values are highlighted in red. Hover the mouse over a value to display a tooltip explaining why the value is invalid.
- Disabled parameters are displayed in gray. Hover the mouse over the value to display a tooltip explaining why the parameter is disabled.
- For URL protocol parameters input will be taken from a document in the Materials Studio project. The document will be automatically uploaded to the Pipeline Pilot server when the protocol is run. When the protocol is selected, the first input parameter of the type URL will be preconfigured to use the active document.
- For Directory protocol parameters input will be taken from a folder in the Materials Studio project. The selected folder and all subfolders will be automatically uploaded to the Pipeline Pilot server when the protocol is run.
- For URL and Directory parameters, click the parameter value to display a dropdown list of all files or folders in the current project which you can select as input for the protocol.
- Array parameters and array parameters with legal values are displayed with a split vertical bar character separating their values.

Click in a cell to edit its value or to open the appropriate dialog for editing arrays, arrays with legal values, or text parameters.

Details

This displays help for the currently selected protocol or parameter. The information displayed is updated when a new protocol is selected. When a parameter is selected information specific to that parameter is displayed.

Server location: Select the Pipeline Pilot server to connect to. To add a new Pipeline Pilot server use the *Change Active Server* function on the *Tools* menu. The Materials Studio collection version on the selected server is reported.

Run: Runs the selected protocol on the Pipeline Pilot server. This button is disabled if no protocol is selected or invalid input values are specified.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Tools	Pipeline Pilot Protocols*

Edit Array Parameter dialog

The Edit Array Parameter dialog allows a new value to be specified for an array parameter. Each array item should be entered on a separate line. The name displayed for the dialog corresponds to the name of the parameter being edited.

Note: Array parameter values are displayed in the parameters list with items separated by a split vertical bar character.

OK: Updates the parameter value and closes the dialog.

Cancel: Closes the dialog without changing the parameter value.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Tools	Pipeline Pilot Protocols* then select a protocol and click the cell containing an array value

Edit Array Parameter With Legal Values dialog

The Edit Array Parameter With Legal Values dialog allows a new value to be specified for an array parameter with legal values. The name displayed for the dialog corresponds to the name of the parameter being edited.

Note: Array parameter values are displayed in the parameters list with items separated by a split vertical bar character.

Select All: Select all allowed items.

Clear All: Clear all items.

OK: Updates the parameter value and closes the dialog.

Cancel: Closes the dialog without changing the parameter value.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Tools	Pipeline Pilot Protocols* then select a protocol and click the cell containing an array value with legal values

Edit Text Parameter dialog

The Edit Text Parameter dialog allows a new value to be specified for a text parameter. The name displayed for the dialog corresponds to the name of the parameter being edited.

OK: Updates the parameter value and closes the dialog.

Cancel: Closes the dialog without changing the parameter value.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Tools	Pipeline Pilot Protocols	Protocol* select a protocol and click a cell containing a text value

Working with client-server systems

When you are working with the Materials Visualizer, some modules run calculations using a separate server program that may even be running on another machine. When a server program is run in this way, it is known as a background *job*. While the job is proceeding, you may continue to work with the Materials Visualizer.

This is all made possible by the client-server architecture of Materials Studio. The client machine is the PC where you are running the Materials Visualizer. The server machine is the one running the calculation (i.e., the server program).

To enable a machine on your network as a server machine, you need to install Materials Studio server components. These include the specific server programs that you need plus a program known as a gateway that runs continuously and provides local management of the server programs and jobs on that machine.

To make a gateway accessible to the client Visualizer, you must register its location with the client PC. Materials Studio includes a server console to provide various gateway management functions of this sort.

Materials Visualizer on the client machine communicates with a server gateway to:

- request information about the installed servers
- launch and/or queue a job
- terminate a job
- check on a job's status

and perform many other operations that allow the client and server to maintain synchronization.

Once a job is launched, you may continue to work with Materials Visualizer on the client machine, and monitor the job running in the background. You can check up on the job progress at any time.

In fact, since the job is running independently of Materials Visualizer, you can even save your project and close down Materials Visualizer, leaving the job running on the server machine. If the server machine is different from the client machine, you may shut down the client PC and start it up again later. When you reload the project, Materials Visualizer automatically reconnects to the job and downloads results if it is completed. Otherwise you may continue to monitor the job progress.

Tips for successful job management

If you are running large jobs or long running jobs or if you encounter communication problems between client and server (for example, as a result of slow connections) there are some settings you can use to improve your experience of running server calculations.

Retain server files

You should always check the *Retain server files* checkbox on the appropriate Job Control Options dialog before a job is started. This is suggested to prevent data loss if you have a slow connection to the remote gateway, a large amount of data will be downloaded, or for long running jobs. This will leave a full copy of the job files on the server machine so that data files may be retrieved at a later time.

If you have used this setting and successfully downloaded your results, you should then remove them from the server.

- In the Job Explorer, right-click and choose *Action* | *Remove* from the shortcut menu.

Download manually

If you have many jobs running or finishing at the same time, it is generally recommended to download them either individually or only a few at a time.

Before running the jobs, choose not to automatically download the results:

- Choose *Tools | Options... | Jobs* from the menu bar, uncheck the *Download results automatically on job completion* checkbox.

Download the results manually as the jobs complete successfully:

- In the Job Explorer, right-click and choose *Action | Download Results* to manually start the download after a job finished.

This is especially useful if you have a slow or non-permanent connection to the gateway as downloads cannot be started at unwanted times.

Request fewer updates less frequently

To reduce the amount of traffic and the communication you can increase the update frequency, reduce the number of updates, or stop them entirely. This can help significantly for slow connections or when many jobs are running in the same project at the same time.

1. Open the *Job Control Options* dialog from the appropriate module's Calculation dialog.
2. Increase the *Update every* setting to wait longer before getting updates to the job files.
3. Uncheck the update checkboxes for:
   - Update structure
   - Update graphs
   - Update textual results

You can stop updates for all running jobs after they have been started:

- In the Job Explorer, right-click and choose *Action | Stop Live updates* from the shortcut menu.

Increase the timeout limit

For slow connections, you can increase the limit after which a given gateway connection is considered to have timed out.

1. Choose *Tools | Server Console* from the menu bar to open the Server Console.
2. Select the relevant gateway, right-click and select *Properties* from the shortcut menu.
3. Choose the *Connection* tab and increase the *Timeout*, 99 seconds should be enough.

   Larger values should be avoided as this may cause a delay in recognizing if the remote gateway has any unforeseen problem.

Working with gateways

A server gateway provides access to the programs installed on a server machine. When you register a gateway from the client PC, all the gateway's server programs are made accessible to the Materials Visualizer installed on that PC.

Server gateways can be managed through a browser or through the Server Console.

The Server Console provides help topics on the options available, including registering and unregistering gateways.

To register a gateway, you need to know the machine name where the gateway is installed and the port number defined for it during installation. On some networks the machine name may not be known to your client PC, and you will have to use the IP address of the machine instead of a network machine

name. An IP address is in the form "nnn.nnn.nnn.nnn", such as "111.222.33.44". By default the port number is 18888, but check with whoever configured the gateway to confirm this information.

Note: Before you reconfigure an existing server to use a different port, delete the old configuration from the server console tree. Then register the new configuration with the new port number. See the Server Console help system for details of these procedures.

Remote gateway browser access

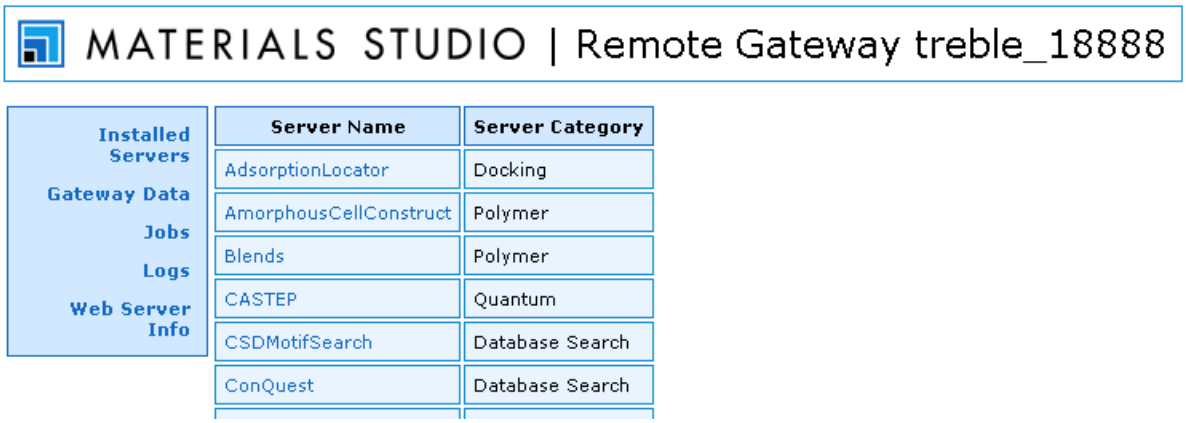
The gateway can be accessed, used to monitor jobs, review any errors, and edit gateway settings through a web browser.

The web browser interface is accessed by entering the URL to the gateway, `http://<gateway>:<port>` (for example, `http://numbercruncher.Accelrys.com:18888`), directly into a web browser or, alternately, by selecting *Remote View* from the *View* menu of the Server Console. From here, clicking on *Gateway Data* in the navigation bar at the side of the view will take you to a page where the relevant configuration data may be viewed and edited. If you are prompted for login details, you should enter the gatekeeper user name and password. If you are not prompted when following the link, you will be required to log in when initiating an edit within the current session. See the Gateway security help topic for more details on administrator security.

To access the gateway using a web browser

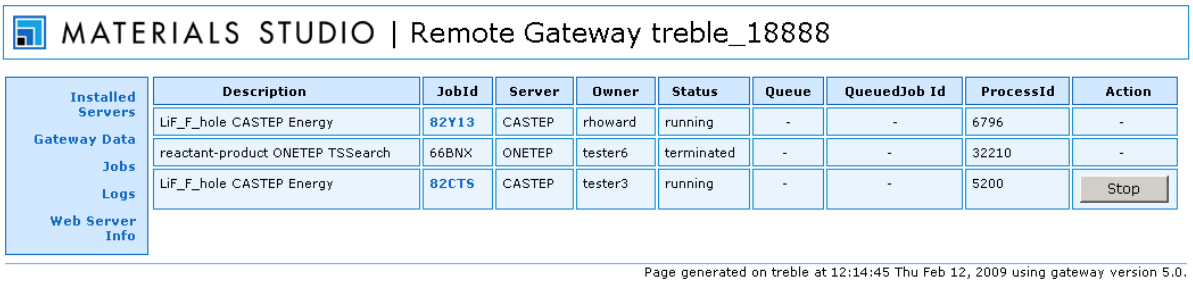
The web pages of the gateway program running on a host machine can be accessed using the *View* modes of the Server Console. However, this information can also be accessed using a standard web browser, such as Microsoft Internet Explorer or Mozilla Firefox. This method enables you to check the status of the gateway and of jobs on the gateway without using the Server Console.

Use a URL of the form `http://<gateway>:<port>`, for example, `http://numbercruncher.Accelrys.com:18888` or `http://localhost:18888`.



To monitor a job

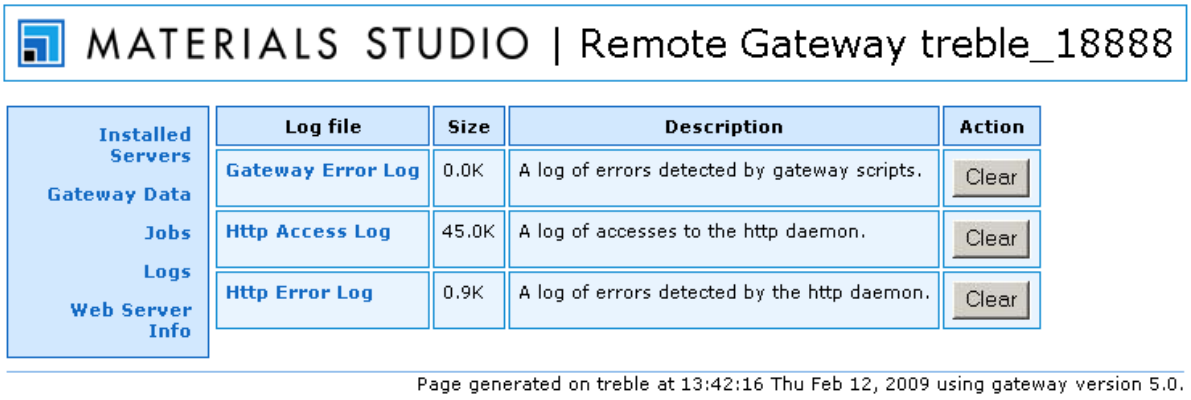
1. In the remote gateway page displayed in a web browser, click the **Jobs** option on the menu. This displays list of all jobs currently running or saved on the server.



   The *Description* of the job, the *Server* on which it is running, its *Owner*, *Status*, *Queue*, and *QueuedJob Id* are reported, along with the *ProcessId*.
2. If the job is running on a remote server, click the **Stop** button to stop the job. The job will be stopped and the files generated will remain on the server.
3. Click on the **JobId** for the job you want to view. A list of all the files generated on the server by the job will be displayed. You can view the contents of the files by clicking on the filenames and save them using the *Save Page As...* option in your browser.
4. Click the **Remove** button to remove files from completed or terminated jobs from the server.

To review logs

1. In the remote gateway page displayed in a web browser, click the **Logs** option on the menu. This displays list of all jobs currently running or saved on the server.



2. Click on the name of the **Log file** to view. This displays a text file in the browser listing all the accesses or errors.
3. To empty a log file, click the **Clear** button.

Working with jobs

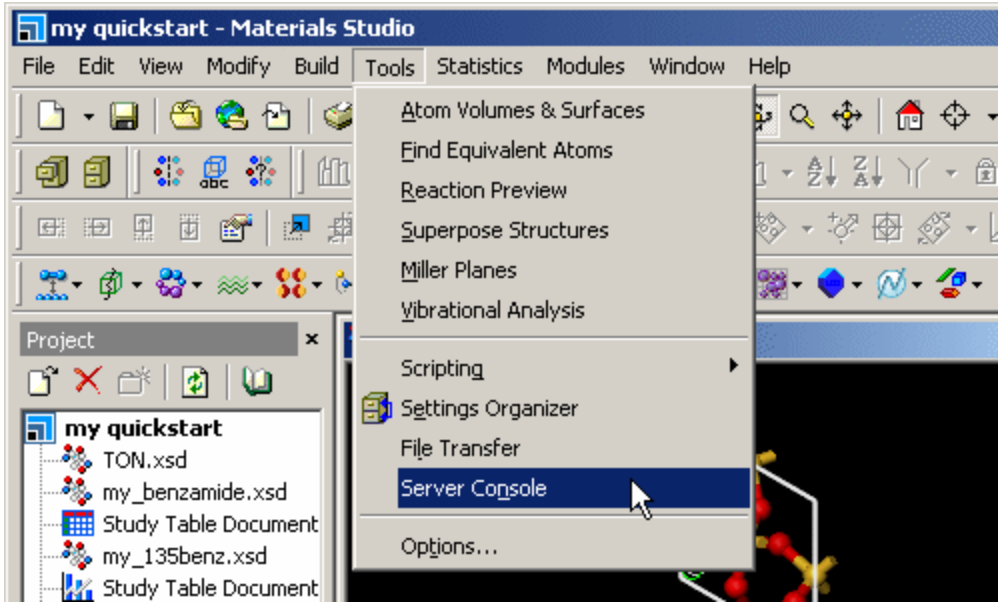
Materials Studio modules use a client-server architecture that allows you to use your PC to control calculations running on a remote computer.

This separation of the client user interface from the server system, where the actual calculation is run, allows you to use a high performance supercomputer to carry out calculations from your Windows desktop PC. It also allows you to make use of spare CPU cycles on other desktop PCs.

Remote jobs are controlled by input files that are generated by Materials Studio when you start a job. The server writes the results of the calculations to various output files, which are downloaded to the appropriate Materials Studio project when the job is completed.

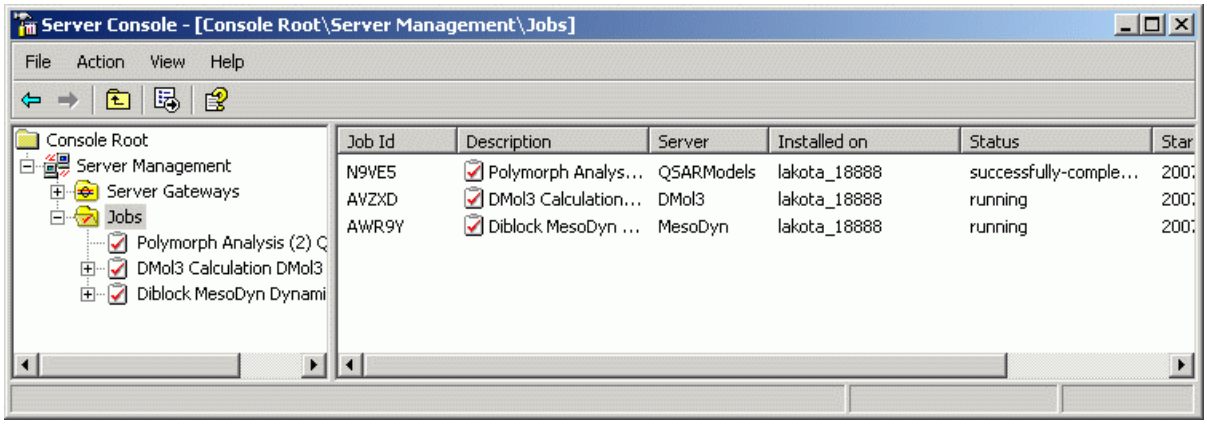
To run a server program, a job is created to represent the running server and its results.

The Materials Studio Server Console provides access to the jobs launched from your client PC. To start the Server Console select *Accelrys | Materials Studio 8.0 Server Console* from the list of programs on the Windows *Start* menu. Alternatively, if you are already running the Materials Visualizer on your PC, choose *Tools | Server Console* from the menu bar.



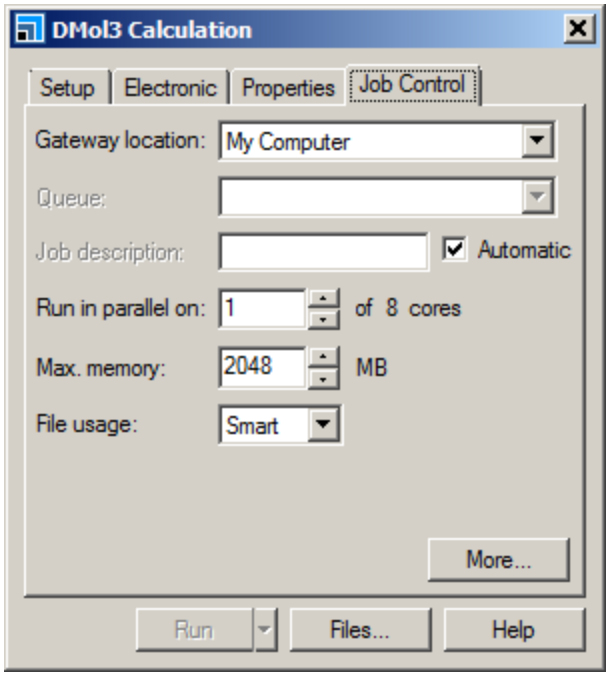
The Server Console provides help topics on the various options available, including the viewing and management of jobs.

Jobs are identified by a *Job ID*, which is reported when a job is launched.



Preparing a job

Before you start a server computation, you have the opportunity to set various job parameters, through the Materials Studio Visualizer. Generally there is a *Job Control* tab with settings related to the job you are about to start. Some of these are specific to the application in question, but some general settings are common to all.



DMol^3 Job Control tab.

1. Choose a **Gateway Location** from the dropdown list, this is the machine on which you want the job to run. All gateways listed support the server program required by this application.

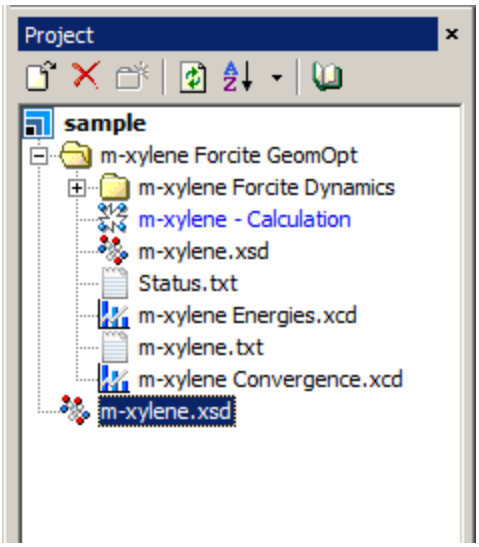
   Tip: If the list is empty or the gateway you require is not present, use the Server Console to check that the gateways are registered correctly. You may need to refresh the gateway information to ensure that the data stored on the client is up to date.

2. Select a **Queue** from the dropdown list of all queues available on the selected gateway.
3. Uncheck the **Automatic** checkbox and enter a **Job description** to use as a part of the overall job description. If not specified, an automatic description is supplied, based on the name of the input data.
4. Click the *More...* button to display the Job Control Options dialog, where you can modify the behavior on job completion. You can choose to retain results files on the server.

   Usually these files are removed when a job completes and the files are transferred to your PC, where they are visible in the Project Explorer. Occasionally it is useful to retain the server files so that they can be used as input to other programs, or to perform diagnostics on a failing job.

Running a job

When you launch a server job, Materials Studio creates a results folder to represent the job data. This may include both input and results, depending on the application. It may also include an application state document to store the settings used for the job. The results folder name is generated using the *Job description* from the module job control settings, or if no description is provided, the name is generated using the name of the document containing the input data.



Materials Studio opens the Job Explorer, which displays basic information about the job. To obtain more detailed information about a server job, double-click on a row in the Job Explorer to open a job log window for the corresponding job.

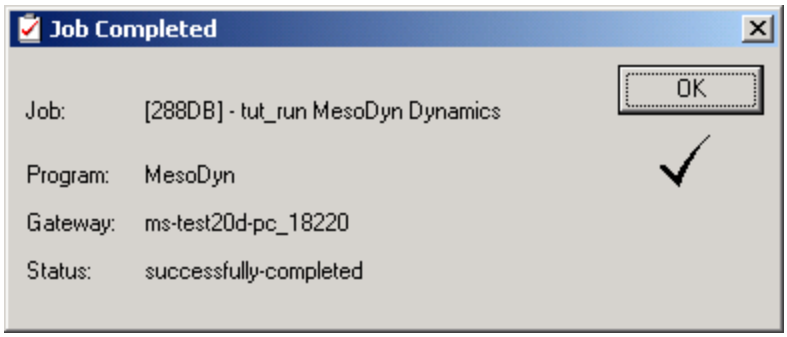
- Initially, the job is in a setup phase, in which job settings are validated and data is transferred to the server environment. The job *Status* displayed is setup.
- When all files have been transferred, the gateway starts the job. The job *Status* displayed is starting.
- If the gateway is running a queuing system the job *Status* displayed is queued.
- When the job has started successfully the job *Status* displayed is running.

Job status is displayed in the Job log window and the Job Explorer.

Note: In addition to queued and running, some queuing systems support additional states, such as suspended, exiting, etc. In the Job log window, these states are all represented by Job Status: running. Log on to the server machine and use queuing system commands to determine the exact state of your job.

For some server codes, such as Amorphous Cell, the status may switch between running and queued several times during job execution. This is expected behavior and occurs because these jobs launch several executables as part of a protocol.

- Intermediate results may be downloaded and Materials Visualizer views updated accordingly, if the application settings are set appropriately.
- If open, the Job log window indicates job completion, displaying Job Status: Completed (OK). If the checkbox marked *Close when Job purged from Gateway, without errors* is checked, the Job log closes at this point, assuming the job was completed successfully. Otherwise, the window will remain open on the screen. Once files have been downloaded, the job is removed, unless you have requested that files be retained on the server once the job is complete.
- If the Job log window is not open when the job finishes, a dialog is displayed indicating the completion status of the job (success or failure). If the original project is not open in Materials Studio at this time, the job results are downloaded the next time you reload the project.



If you shut down your PC before the job completes, you will only be notified of the job completion once you restart Materials Studio. Reload the project from which the job originated to see the final job results.

Network communication problems

When no response is returned by the gateway server, Materials Studio will produce failure messages, such as Server busy, job launch failure or communication failure messages. Materials Studio cannot tell if a gateway server is really down, is busy or if the network communication is very slow. So it will keep trying to connect to the gateway based on the configuration set up when the job was started.

In order to avoid server busy messages when the gateway server is known to be down or failure messages when the job is actually slowly running on the server, the following changes can be made depending on the problem:

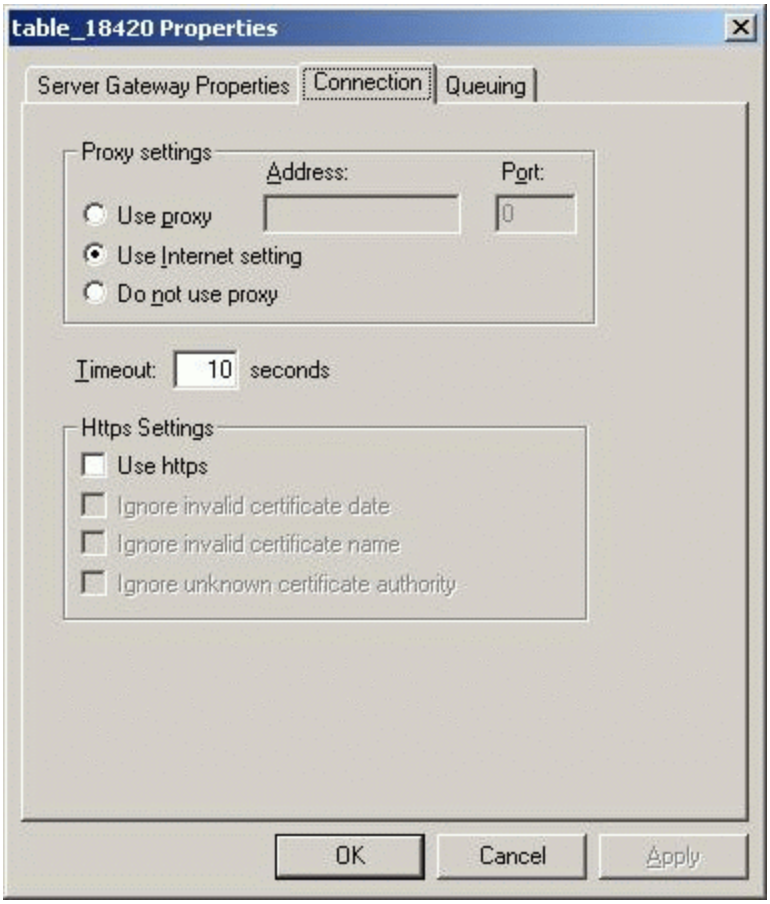
1. **Fast network communication**

   If the network communication is not a problem, the timeout settings can be reduced to achieve quick response, and thus decrease server busy messages.

   - Gateway connection timeout

     This can be reduced so that Materials Studio will wait less time when trying to connect to the gateway server and report promptly. The Gateway connection timeout can be edited through Server Console.

     a. Click on the + icon next to the *Server Management Root* in the console tree, to display the data categories.
     b. Locate the *Server Gateways* item and click on the + icon next to it to expand the tree further.
     c. Select the specific server gateway that you are interested in, and display the shortcut menu for that item.
     d. Click on *Properties* to display the property sheet for that gateway.
     e. Select the *Connection* tab and reduce the *Timeout* in seconds.



2. **Slow network communication**

   Sometimes, the network connection may be very slow when using a remote server, so that Materials Studio may not get a response from the remote gateway server even after time out. You may get server busy, job launch failure or communication failure messages, even though the job may actually be running on the server.

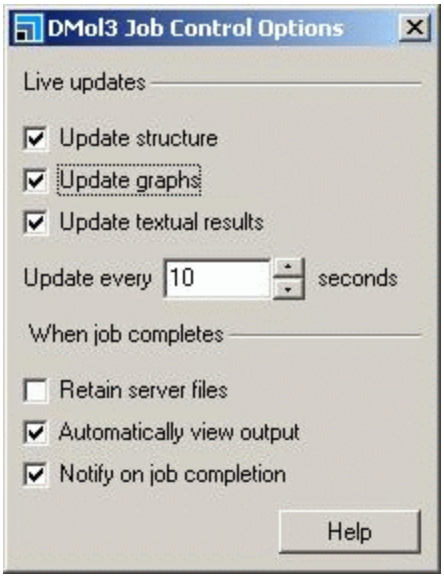
   In the case where a slow response from the server is the problem, some settings can be changed in order to improve the situation.

- Gateway connection timeout

  This timeout can be increased so that Materials Studio waits longer when trying to connect to the gateway server instead of reporting failure immediately. In this case, you may get a Windows system "server busy" message. This will always be displayed until Materials Studio gets a response, or the connection request times out when a failure message will be displayed.

- Live updates

  For all the server modules, Materials Studio has provided a dialog so that the user can configure live updates. This can be accessed by clicking the *More...* button on the *Job Control* tab.

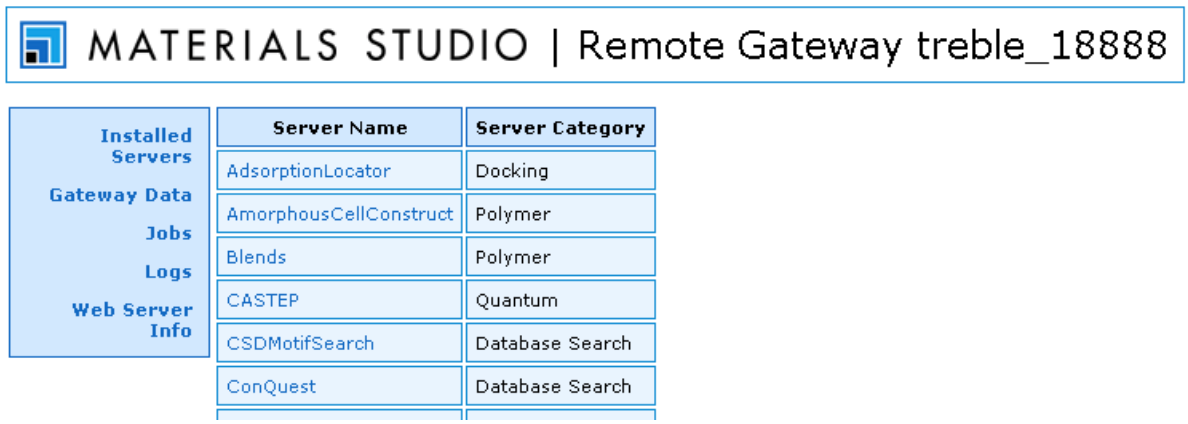


  The default for live updates is to update structure, graphs and textual results every 10 seconds. For some server jobs, the calculation time is long and the data volume is massive. This can cause a bottleneck, leading to a slow network connection to the server machine. In order to avoid this, you should increase the update interval and reduce the number of live update items.

- Minimum Polling Interval

  When a job is submitted to the gateway server, Materials Studio will start a monitoring process. This process queries the gateway server for the job status at a given interval and updates the job status in the job explorer accordingly. For some long calculations, there may be no status changes over short intervals, so this can be increased to reduce network traffic. This is achieved from the gateway server web page, you may need administrative rights:

  a. Go to the gateway interface web page (see the Gateway administration Help topic for more information).
  b. Select *Installed Servers* on the left panel.
  c. Choose a job server from the list displayed.
  d. Click *Edit* on the job server page.
  e. Increase the *MinimumPollingInterval*, this value is in milliseconds.
  f. Save the changes.



Web browser gateway interface

Using job control

Materials Studio runs jobs as background processes on a server. The following tools are provided to set up and control the jobs:

- Use the *Job Control* section on the module dialogs to select the gateway location and job parameters for future jobs.
- Use the Server Console application to add new servers and to monitor multiple jobs.
- Use the Job Explorer to monitor multiple jobs.
- Use the Options dialog to control the automatic downloading of job results.

To set job parameters

1. Set the *Gateway location* and select the *Queue* to which the job will be submitted.
2. By default, the name of the structure is used as the *Job description*. Additional information is appended to this prefix prior to the job being started. However, you may wish to use an alternative description, to distinguish between separate sets of results, for example.
3. If you wish to specify a job name, uncheck the *Automatic* checkbox and enter a new name for the *Job description*.
4. To run the job in parallel, and the module and server provide the opportunity, specify the number of cores to use in the *Run in parallel on* textbox.
5. Click the *More...* button to display the *Job Control Options* dialog.
6. If required, modify the default parameters that control the live updates policy and how completed jobs are reported.

Launching a job

When you start a job, the Job Explorer is displayed automatically. It provides basic information about the job as it progresses. To obtain more detailed information about a server job, double-click on a row in the Job Explorer to open a job log window for the corresponding job.

The job log window contains all of the relevant information about a server job and its current status. It also allows you to stop a job and monitor the transfer of files between the gateway and your PC.

Job completion information

When a job finishes, the results files are transferred from the server to the appropriate results folder in the Project Explorer if the automatic download option was selected on the Options dialog. Materials Studio will report on completion according to the options you have selected. If the automatic download

was turned off, then you can select *Download Results* from the Job Explorer shortcut menu to start downloading the output files.

If the job is small enough that it is completed while the related launch dialog is still open, the completion status will be displayed there, along with any error messages that were generated.

However, if the job is more time consuming, you may wish to exit Materials Studio before the job completes. The next time you start Materials Studio and open the project in which the job was launched, the program will automatically re-establish its connection to the remote job. If the job is still running, live updates will resume. If the job has finished, final results will be downloaded if the automatic download option was selected, as described below.

Jobs for which job completion notification was requested are automatically listed, showing the completion status (success or failure) of each job.

Results files for all completed jobs are transferred from the server and displayed in the Project Explorer. If you checked the *Automatically view output* checkbox on the Job Control Options dialog, the results files are displayed. If an error has occurred, Materials Studio will report this and allow you to examine the project log file.

Tip: When Materials Studio is not running, you can open the Server Console from your desktop to check on job status. Access the Server Console by selecting *Accelrys | Materials Studio 8.0 Server Console* from the list of programs on the Windows *Start* menu.

Monitoring a job

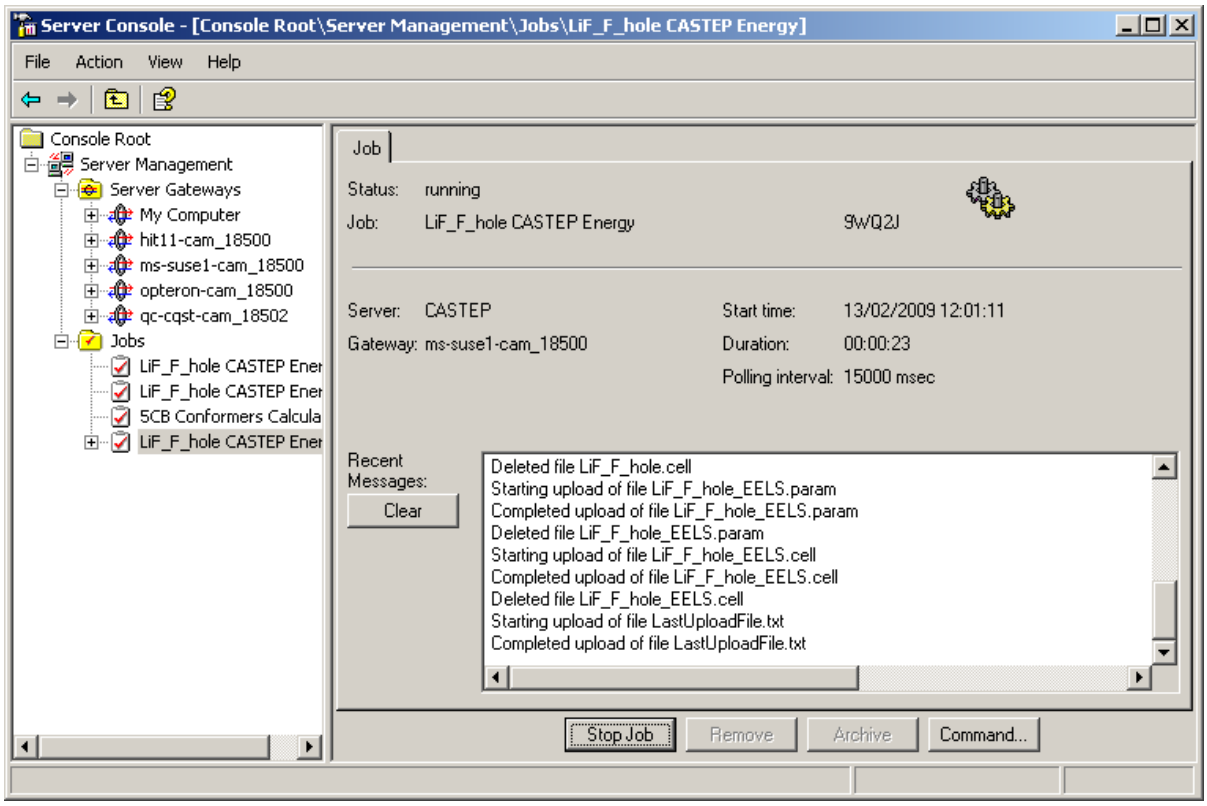
When you launch a server job the Job Explorer is displayed automatically. It provides basic information about each job, as it progresses. To obtain more detailed information about a server job, double-click on a row in the Job Explorer to open a job log window for the corresponding job.

Alternatively, you can also monitor the job at any time using the Server Console.

To open the Server Console

- Choose *Tools | Server Console*.

Tip: When Materials Studio is not running you can open the Server Console from your desktop to check on job status, by selecting *Accelrys | Materials Studio 8.0 Server Console* from the list of programs on the Windows *Start* menu.



Open the *Jobs* node and select the ID of the job to be monitored. The live job information is then displayed in the Server Console results pane.

Job log window

Overview

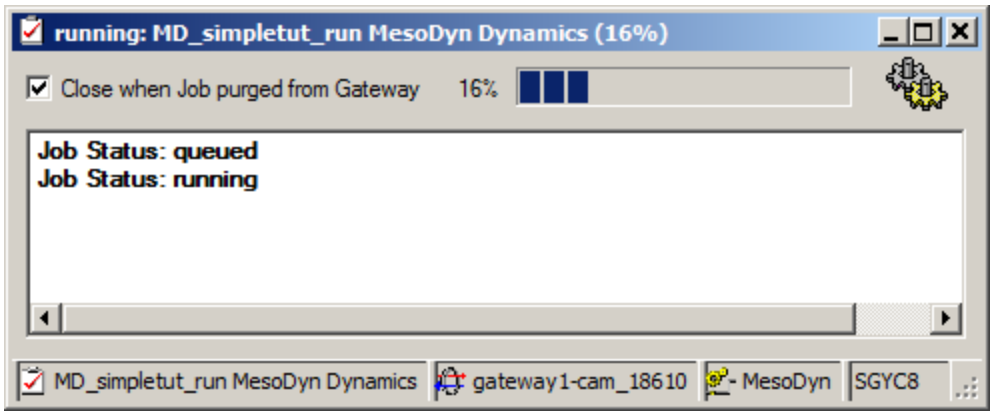
The Job Explorer is displayed automatically when you launch a server job via the gateway. It provides basic information about each job, as it progresses. To obtain more detailed information about a server job, double-click on a row in the Job Explorer to open a job log window for the corresponding job.

The job log window contains all of the relevant information about server job and its current status. Its also allows you to stop a job and monitor the transfer of files between the gateway and your PC.

> **Tip:** Right-click on any *Job Status* message in the job log window to display a shortcut menu. This includes an option to toggle the display of more detailed messages and allows you to copy selected messages to the clipboard, to be pasted into emails or other documents.

Description

The sample below shows the job log window for a MesoDyn dynamics calculation.



The title bar displays the job status and job description.

The status bar at the bottom of the job log window displays the job status and name, the job description, the gateway address and the server program name. It also shows the unique job identifier. This five-character code allows you to locate information about the job using the Server Console in the future.

The *Close when Job purged from Gateway* checkbox allows you to indicate that the job log window should be closed automatically when the job has finished without errors and the files have been removed from the gateway.

The central area of the window shows messages about the job status. These messages are updated automatically as the job progresses.

Additionally, when Powder Solve jobs are running, the central area of the job log window displays:

- the current cycle number
- the lowest R_{wp} found during this cycle so far and the step number it was found

Press CTRL + D or right-click and select *Show message details* from the shortcut menu any job status message to toggle the display of further message details. These message details include information about the transfer of files between your PC and the gateway.

To copy some or all of the displayed messages to the clipboard select them using the mouse (use the SHIFT or CTRL keys for multiple message selection), then press CTRL + C or right-click and select *Copy* from the shortcut menu.

Managing live updates

You can monitor important intermediate results during a remote job.

The Job Control Options dialogs for each module allow you to control the generation of intermediate documents and to set the update frequency. You can view a text document, `Status.txt`, which gives a summary of the calculation as it currently stands. Depending on the job chart documents and 3D Atomistic documents may also be updated during the run.

If live updates have been requested, Materials Studio will transfer the live update documents, containing intermediate results from the server, to the job results directory. Materials Studio attempts to do this at the interval specified in the *Update every* field on the Job Control Options dialog. However, the actual interval between updates is determined by the time it takes to generate new results. The update interval can therefore be significantly longer than the chosen update interval.

Note: All the selected live update documents are transferred to the project folder at the interval specified. For clarity, not all available live update documents are opened automatically. You can select and open any live update documents whose contents you wish to monitor using the Project Explorer.

Note: Intermediate updates can cause problems if the bandwidth of the client-server connection is low, especially when multiple jobs were submitted from the same client. Live updates for a running job can be turned off using the *Stop Live Updates* option on the Job Explorer shortcut menu. Similarly, live updates for a running job can be turned on by selecting *Start Live Updates*.

All live update documents remain in the project folder in the Project Explorer when the job is completed.

If you exit Materials Studio during a run and restart it later, the intermediate update documents will be updated when Materials Studio reconnects to the running job.

To manage live updates

1. Open the Calculation dialog for the module you are using.
2. Select the *Job Control tab*.
3. Click the *More...* button to display the Job Control Options dialog.
4. To receive structure updates, check the *Update structure* checkbox.
5. To receive chart updates, check the *Update graphs* checkbox.
6. To receive textual updates, check the *Update textual results* checkbox.
7. Set the minimum time between live updates by adjusting the value in the *Update every* field.

Viewing job results

If you keep the Materials Visualizer open until the job completes, the results files are moved from the server to the folder created for the job in the Project Explorer. Materials Studio will report on completion according to the parameters you have set.

The Job Explorer will report the completion status of the job. If it is open, the job log window will also report any error messages that are generated by the server program. Otherwise, in most cases, a dialog will appear on the screen to inform you of the fact that the job is now completed.

Job reconnection

If a job runs for a long period of time, you may wish to exit Materials Studio before the job completes. The next time you start Materials Studio, any completed jobs that were initiated in the selected project are automatically reconnected. Any completed jobs are reported by means of a dialog indicating the completion status (success or failure).

If a reconnected job has completed successfully, the files associated with each job are retrieved from the server and displayed in the Project Explorer. Some files may also be displayed in document viewers, depending on the application involved. If an error has occurred, Materials Studio reports the error and allows you to examine the cause of the error in the project log.

If any reconnected jobs are still running, a dialog is displayed from which you can view the Job Explorer to monitor the progress of the running jobs.

Restarting jobs

For some modules, if you click the *Stop Job* button on the job log window and you choose to download the results, you will be able to restart the job from the point at which the calculation was interrupted.

> **Note:** Jobs can only be restarted for these modules: Forcite, Mesocite, Morphology, Polymorph, and Sorption.

To restart a run

1. Open any document in the main results directory for the job you wish to continue.
2. Open the appropriate Calculation dialog. If the calculation was interrupted cleanly and all of the restart files are present, check the *Restart* checkbox.
3. Select a remote gateway and configure other job parameters using the *Job Control* tab.
4. Click the *Run* button to start the job. The restarted job is submitted and executed in exactly the same way as a new run.

A sample remote job run

The sequence of steps that is executed to run a remote job is always the same. When you click the *Run* button the calculation proceeds as follows:

1. Materials Studio communicates with the gateway process to set up a new job.
2. Materials Studio creates the results folder. The results folder name will be generated using the *Job description* specified on the Job Control tab or, if you have left the *Automatic* checkbox checked, the name will be generated using the name of the structure document containing the substrate.
3. Materials Studio opens the Job Explorer. This window contains information about the status of the job and its progress.
4. Materials Studio performs a number of checks on the job settings and input. In addition, all job settings are stored in the results directory.
5. Materials Studio temporarily creates a new project in the job scratch area. This project contains all input files and settings for the remote Materials Studio job. The job project files are transferred to the gateway destination you selected on the *Job Control* tab.
6. When all of the files have been transferred, the gateway starts the job.
7. If you have checked the *Update textual results* checkbox on the Job Control Options dialog, Materials Studio will read intermediate results and update the information on screen and in the relevant file.
8. Alternatively, you may view remote files using the Remote view facility of the Job Explorer. The files are located in the `[seedname]_files/Documents` folder and its subfolders.
9. You can continue to work in Materials Studio, exit the program, or even shut down your PC. It will not affect the calculations you are performing (unless, of course, you are using your PC to run the server application as well as the Materials Studio client).
10. Once the job has finished, Materials Studio will transfer the output files back to your PC, where you can view and edit them, analyze the results, or use them for further calculations.
11. If you have checked the *Retain server files* checkbox on the Job Control Options dialog, Materials Studio will not remove the files from the remote job folder.
12. If you have checked the *Automatically view output* checkbox on the Adsorption Job Control Options dialog, Materials Studio will display the `[seedname].txt` file.
13. If you have checked the *Notify on job completion* checkbox and the job log window is not open, Materials Studio will open a job completion window to notify you of the job status.

14. If you stop an Adsorption Locator job using the *Stop Job* button on the job log window, Materials Studio will offer to download any files produced by the job before it was terminated.

The description given above is somewhat simplified, but provides a reasonable overview of a remote job run.

If a remote job fails

Materials Studio checks most of the data and settings required to perform a remote job prior to launch. If it cannot start the job, error messages are generated detailing the reasons.

However, jobs may sometimes fail for reasons which cannot be checked prior to launch. In such cases, more detailed information about the error may only be available in the `[seedname].txt` report file produced by the job or in the `MatStudioLog.htm` file located in the server-side project directory, `[seedname]_Files`. Other files stored in the directory on the server, for example `MatStudioServer.log`, may also contain further clues. To view the server-side files, you can use the Remote View facility of the Job Explorer.

Below is a list of the most common reasons for jobs to fail. It may help you to identify and fix any problems you have with your remote jobs.

> **Tip:** Select *View* | *Project Log* from the menu bar to see if any error or warning messages have been reported.

Common reasons for a remote job to fail to start

1. Gateway and network communication problems
   - No gateways registered on client.

     The default installation of Materials Studio on a client does not set up the gateway addresses for remote server programs. You can check whether you have gateways registered on your PC using the Server Console. You can also use the Server Console to add gateways.
   - No gateway registered on client that has a suitable server available.

     Jobs require the appropriate module server to be installed. Only server gateways that provide this environment can be selected. You can view the servers available through a particular gateway using the Server Console.
   - Local gateway information out of date.

     The information about which servers are available through a gateway is kept on the gateway itself. When a new gateway is registered on the PC using the Server Console, the list of servers is copied to the client PC. But when a new server is made accessible or removed from a gateway, you will have to refresh the information stored on your PC. You can use the Server Console to refresh the gateway information.
   - Gateway not available.

     If the computer that is running the gateway is switched off or the gateway program is not running, you will not be able to launch jobs on it. Select a different gateway or contact the system administrator of the gateway you want to run the job on. You can test whether a gateway is running using the Server Console.
   - Network failure.

     Materials Studio needs to be able to communicate with a gateway. If this is not possible, it will not be able to launch a job. You can test whether a gateway is running using the Server Console. If you can launch the same job on the same gateway from a different PC, then it may be a problem with your PC. In this case, try rebooting your PC or consult your system administrator.

- Disconnected Server Manager program stopped responding.

  The communication between Materials Studio and the gateways is performed by the Disconnected Server Manager (DSMgr.exe). This program runs in the background and, normally, no output can be observed. However, it may sometimes stop responding, in which case the following symptoms may be observed:

  - No jobs can be started from your PC, but from a different PC the same job can be started on the same gateway.
  - The network connection to the gateway seems OK and you can access the gateway information from an Internet Explorer window with the URL `http://<gateway>:<port>`, for example, `http://numbercruncher.Accelrys.com:18888`.
  - It is not possible to obtain information about any gateway using the Server Console.

  To fix this problem, you will have to exit Materials Studio and end the DSMgr task using the Windows Task Manager. When you restart Materials Studio, the DSMgr will be started automatically.

- User authentication failure for a gateway.

  When a gateway is set at the password level of security, a valid user name and password are required to run a job on such a gateway. If the user name and password supplied cannot be authenticated against the set of users registered for the gateway, the server job will fail to start.

- Job launch failure - network timeout.

  Slow network communications can result in job failure if the gateway timeout setting is not high enough. Try increasing the gateway timeout value if network speed could be causing the job launch failure. Refer to the Server Console help for details on setting the timeout.

2. Client-side problems

- Disk full on client PC.

  Materials Studio creates some files that contain the structure information and job details. If these files cannot be created because the disk is full, the job cannot be started.

  > **Note:** These files are usually created in a temporary file folder, for example, C:\TEMP. You must free up disk space so that these files can be created.

- Job filename too long.

  If a results directory is deeply nested within a number of folders in a project, the default job filename automatically generated by Materials Studio may become longer than the Windows limit of 259 characters. If this happens, you will need to manually assign a shorter filename to the job on the *Job Control* tab before you can run it.

- Unrecognized characters.

  Materials Studio may not recognize some characters that appear in input text boxes. Check these input text boxes, and replace any non-ASCII characters with their closest ASCII equivalents.

3. Server-side problems
   - Disk full on server.

     The module servers need to create files to store the job information and job output data. If these files cannot be created because the disk is full, the job cannot be started. Contact your system administrator to ensure that enough disk space is available on the gateway computer.
   - License failure.

     The use of the server programs is licensed and might only allow a limited number of jobs to be executed concurrently. In this case, you may want to try to run your job on a different gateway or wait until licenses are available again and restart your job.
   - Server process - resources failure.

     If the server has too few resources to execute your job, the job may fail. This can be caused by too many jobs being executed on the server. In this case, you may want to try to run your job on a different gateway or wait until the resources are free again. If the problem occurs frequently, you may want to notify the system administrator of the gateway computer of this problem.

Common reasons for a remote job to fail to finish successfully

1. Server-side problems
   - Out of disk space.

     If the server runs out of disk space while it is running, various errors may occur. You may have to ask the system administrator of the gateway to free up some disk space before trying to run another job.
   - Out of memory.

     If the server machine runs out of virtual memory or swap space when trying to start up a process or while running, various errors may occur. These errors depend on the operating system of the server machine.
   - Communication failure.

     Slow network communications can result in job failure if the gateway timeout setting is not high enough. Try increasing the gateway timeout value if network speed could be causing the job to fail. Refer to the Server Console help for details on setting the timeout.

Common reasons for a remote job to fail to download results

- Process ended without writing the results.

  When the server program encounters problems, it may exit without producing the required output files. You may want to look very carefully at the `[`*`seedname`*`]_Files/Documents/[`*`seedname`*`].txt` file produced by the job for indications of the problem, or, if that file does not exist, at the `[`*`seedname`*`]_Files/MatStudioLog.htm` or `MatStudioServer.log` files, which may contain further clues. To view any remote files, use the Server Console. If neither file exists, you may want to ask the system administrator of the gateway to check whether the disk on the server is full.
- Results folder removed.

  When Materials Studio launches a remote job, it creates a subfolder that will contain the results of the run once the job is finished. This folder must not be renamed, moved, or deleted, since the results cannot then be downloaded. If the files cannot be downloaded, they will not be removed from the server and you can retrieve them individually using the Server Console (or by using the *Save As...* facility of your browser if you are accessing gateway information using the URL).

- Disk full on client PC.

  There needs to be enough free disk space on your PC to store the results files from the remote job. If there is not enough free disk space, the download of the files will fail, although the files will remain stored on the server. After you have freed up some disk space, you can retrieve the files individually using the Server Console.
- Communication failure between client and server during download.

  You can download the output files manually. You need to copy and paste or FTP all the files in the `[seedname]_Files/Documents` folder (located within the server-side job directory) into the client-side job results folder.

Tip: It is important to identify the reason for the failure of a job before taking any action. In most cases, the error message is reported in the report file `[seedname].txt` or in the `MatStudioLog.htm` file located in the server-side project directory `[seedname]_Files`.

Running jobs in standalone mode

The most convenient way of running module calculation is through the Materials Studio interface, which performs all the preparatory tasks required to run remote job. However, in some circumstances, it may be necessary to run a calculation in standalone mode with a set of input files prepared elsewhere, for example for diagnostic purposes or to use a modified input script that expresses a more advanced algorithm.

Note: Not all modules can make use of standalone mode, the exceptions are: Adsorption Locator, Blends, CCDC, Conformers, Morphology, and Sorption.

Each module which makes use of standalone mode requires different input files and produces different results files, you should consult the module help topics for more information on the specific files used by and output by each module.

Overview

There are five distinct steps involved in using Materials Studio to run standalone jobs:

- Generate the input files
- Transfer the input files to the server
- Execute the job
- Download the output files from the server
- Open the output files in Materials Studio

Each step is discussed in more detail below.

Generate the input files

You can create input files using a text editor, such as WordPad on Windows or vi on Linux. However, when the number of input files required is quite large and the information they contain is complex, you should use Materials Studio to generate them for you. You can create the required files using, for example the *Job Files* dialogs.

To create input files using the Job Files dialog

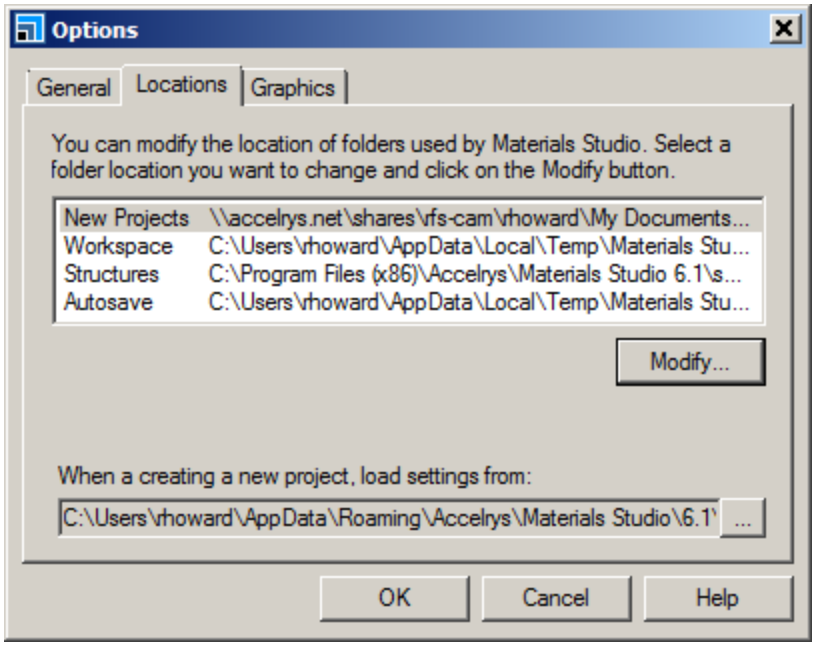
1. Set the appropriate calculation options on the module calculation dialog(s).
2. Click the *Files...* button to open the appropriate Job Files dialog.
3. Click the *Save Files* button. This will save all the files needed to run the job.

Note: You must avoid using special characters (including spaces) in the *seedname* used to identify the job in order to run in standalone mode. Materials Studio automatically substitutes an underscore in place of any special character when transferring files from the client PC to the server using the gateway mechanism, but the files saved on the client PC retain all of the special characters and are therefore unsuitable for use in standalone calculations.

The files created by the Job Files dialog are saved in a new folder in the current project.

To locate the new files

1. Select *Tools* | *Options...* from the menu bar to open the Options dialog.
2. Select the Locations tab.
3. The path displayed under *New Projects* is the top-level project directory. In the example below, this is the `My Documents` directory.



Options dialog

4. In the `New Projects` directory, there are folders for each project. The files which belong to each project are stored in a `Documents` directory in this project folder.
5. The directory structure in each project is shown in the Project Explorer. The hierarchy of folders in the Project Explorer reflects what you will find on the hard drive of your computer.

   Project Explorer example for a Forcite Geometry Optimization job

   In this example, the new input files can be found in the folder `C:\Documents and Settings\<username>\My Documents\Materials Studio Projects\sample Files\Documents\m-xylene Forcite GeomOpt`.

Transfer input files to the server

If you generated the input files manually using a text editor on the server machine, then no file transfer is required. However, if you generated the files on your PC using Materials Studio, you must transfer them to the server before you can start the calculation. If you can access the hard drive of the server machine directly from the client PC, you can use the *Map Network Drive...* option on the Windows

Explorer *Tools* menu to help you transfer the files. This allows you to copy and paste files from one location to another. Alternatively, you can use the hard drive on the server as a location for Materials Studio projects (see above).

If you are unable to access the hard drive on the server, you should use the File Transfer tool to transfer files from the client to the server.

To transfer input files to the server using the File Transfer tool

1. Select the folder containing the input files you wish to transfer using the Project Explorer.
2. Select *Tools | File Transfer* from the menu bar. The File Transfer dialog is displayed.
3. If necessary, supply or update the values for *User name*, *Password*, *Remote host*, *Remote folder*, and *Arguments*.
4. Choose *Upload files to server*.
5. Optionally, check the *Edit script before executing* checkbox. When *Edit script before executing* is enabled, the script generated when you click the *Run* button is opened in a text window immediately after it is created, allowing you to inspect and edit it before it is passed to the FTP client.
6. Optionally, use the *Additional files* option to specify extra files not present in the selected project folder for upload.
7. Click the *Run* button. This generates a script that lists all of the files present in the selected project folder and any additional files specified. The FTP client on the local computer is then launched using the command specified in the *FTP command* text box and the script is executed.
   If you checked the *Edit script before executing* checkbox, a text window containing the script is opened after the script is generated. Make any desired changes, for example remove the names of any files you do not wish to transfer to the remote server, and ensure that you save the updated script. As soon as the text window is closed, the FTP client is launched and the script is executed.

Execute the job

To assist you in running job in standalone mode, a batch/shell file is supplied for each module. It can be found in the directory in which the executables are located, for example `etc/AmorphousCell/bin` in the main Materials Studio directory. These scripts are used to start jobs in standalone mode.

Note that standalone jobs on Linux platforms must be run under the user account which owns the Materials Studio software installation.

> **Note:** For more information on the standalone scripts and the commands they use, consult the help topics for the modules.

Submitting standalone jobs to queues

Standalone jobs can be submitted to queues on Linux servers, provided that the gateway has been properly configured to use a queuing system. See the Installing Materials Studio on a server with a queuing system and Editing gateway data help topics for further information on setting up a gateway with a queuing system.

The shell files for each module, for example at `etc/CASTEP/bin` in the main Materials Studio directory, can be used to run a standalone job through a queuing system. The following syntax should be used:

```
<MS_INSTALL>/etc/<module>/bin/Run<module>.sh  -queue <queuename> <other
parameters>
```

Where `-queue` specifies that the gateway supports a queuing system and the queue to use is defined by the `<queuename>` argument. Additional server parameters such as the number of processors and seednames can also be specified. For example:

```
<MS_INSTALL>/etc/CASTEP/bin/RunCASTEP.sh -queue workq -np 4 Si
```

will submit a CASTEP job to a queue named `workq` to be run on four processor cores using the seedname `Si`.

Refer to the Installing Materials Studio topic for information on the location of the `<MS_INSTALL>` directory.

Download the output files from the server

When the calculation is complete, you must transfer the output files back to your PC for analysis in Materials Studio.

To transfer the output files back to your PC

Transfer the files to the client PC either using copy and paste or the File Transfer tool.

> **Tip:** If you have transferred files into a Materials Studio project folder, but you cannot see them in the Project Explorer, try using the *Refresh* button  to update the Project Explorer.

Open the output files in Materials Studio

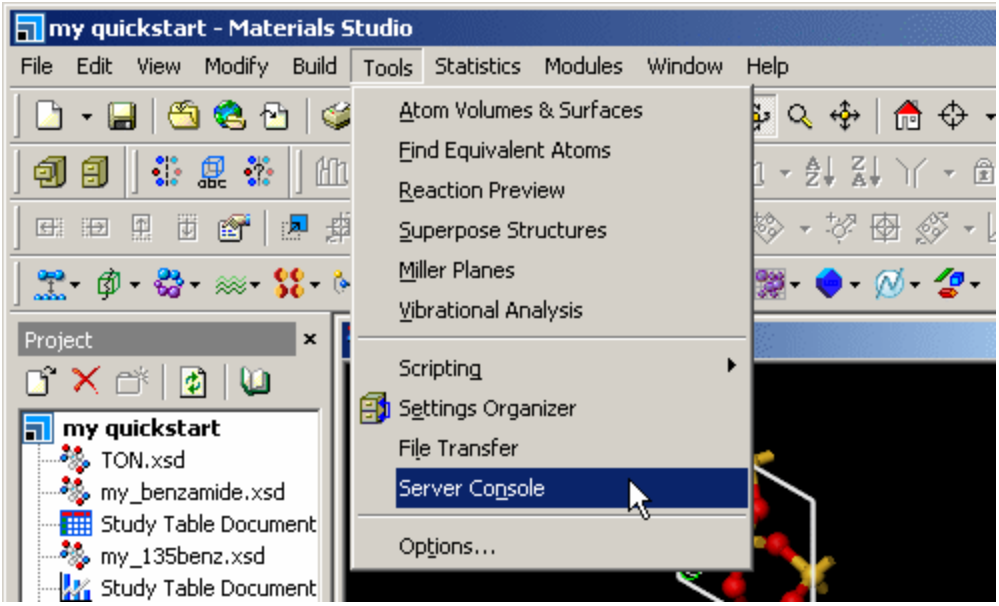
When the output files have been downloaded to your PC, they can be analyzed. Trajectory documents can be animated, text documents can be mined for information, chart documents can be viewed, and structure, study table, or trajectory documents can be examined using the Analysis tools for the module used to run the calculation (Forcite Analysis can be applied to some other module calculation results) or used as input for fresh simulations.

Using the Server Management Console

You can run more than one job at a time on one or more server machines and monitor them using the Server Console. You can use the Server Console to:

- View the currently known servers and active jobs
- View status information on active jobs
- Terminate a job
- Administer the list of server gateways (register, unregister, refresh, etc.)
- Retrieve results files from the server

The Server Console is a separate application that you can open by choosing *Tools | Server Console* from the Materials Studio menu bar. If you use this method, only one Server Console window is displayed.



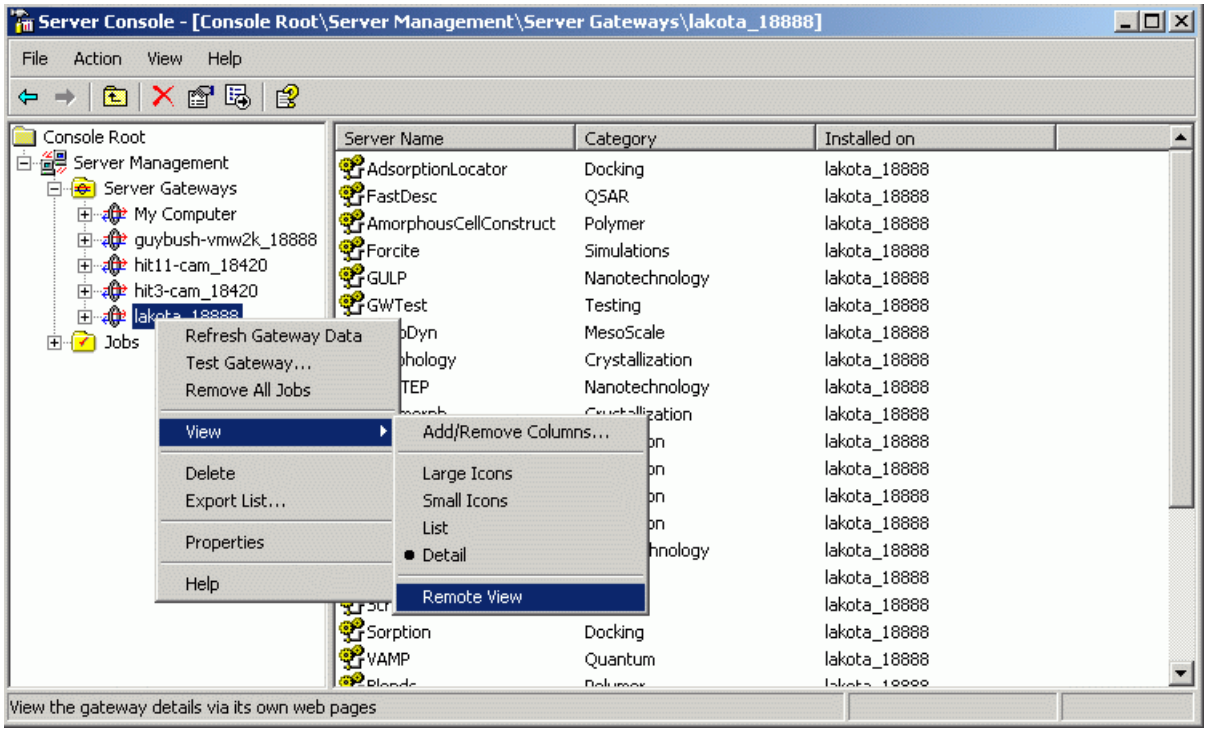
It is also possible to access the Server Console as a separate program, independent of Materials Studio, by selecting *Accelrys | Materials Studio 8.0 Server Console* from the list of programs on the Windows *Start* menu. This method allows you to open multiple Server Console windows.

For further information about using the Server Console, refer to the Help topics accessed from the Server Console *Help* menu. The Server Console Help topics cover all the gateway and job management tasks that you can perform with the console, in addition to more conceptual material on the client-server architecture of Materials Studio.

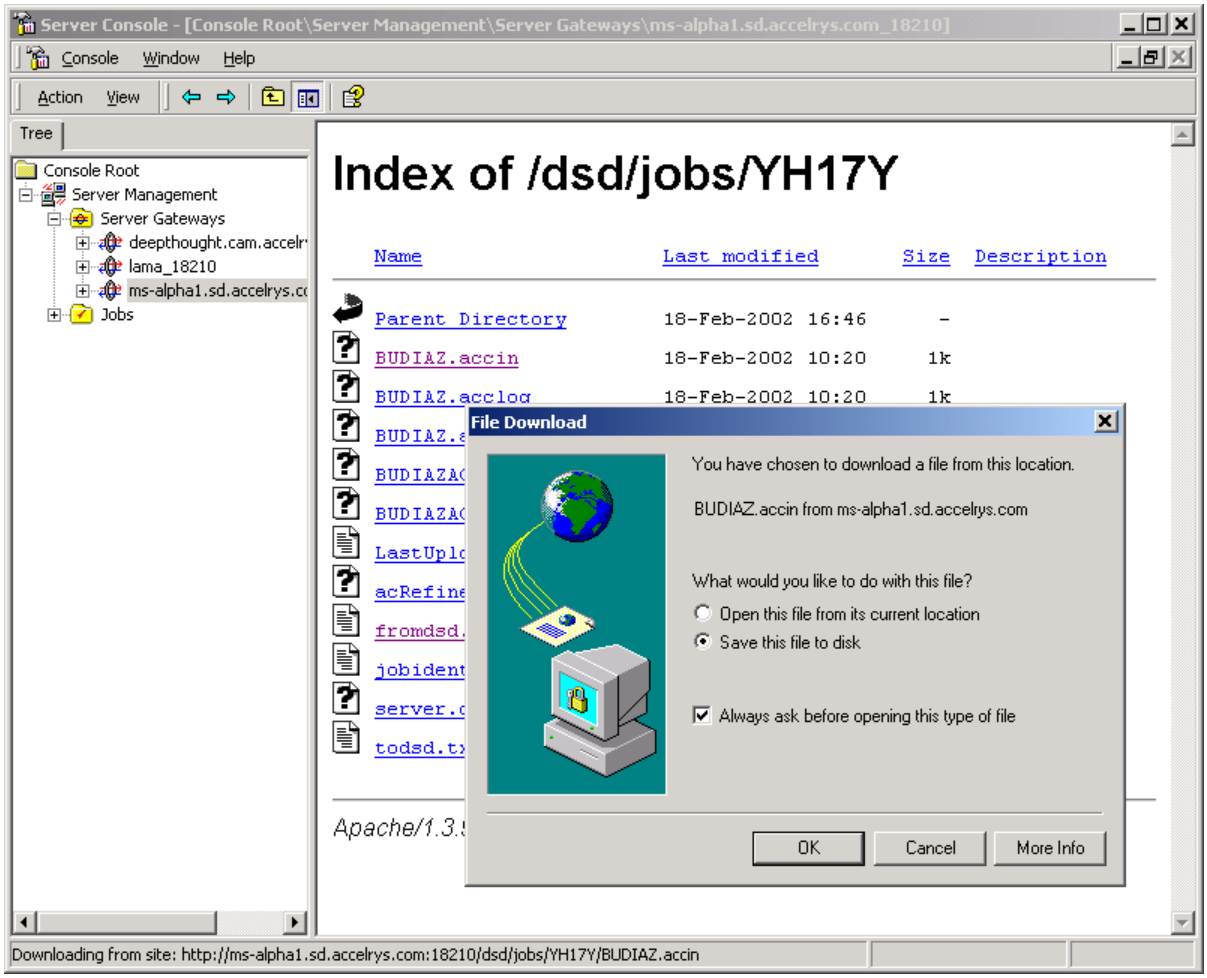
Retrieving results files using the Server Console

Occasionally a job will run to completion successfully but the results files are not downloaded to the client. In such situations the files can be retrieved via the Server Console using the following steps:

1. Open the server gateway folder in the server console explorer and select the gateway from which the files are to be retrieved.
2. Right-click on the gateway and select *View* in the shortcut menu, then *Remote View* on the submenu, as shown below:



3. In the main window the remote view of the server should now be visible. Select the *Jobs* link from the list of links on the right of this window. A list of jobs run on the gateway is displayed. Select the job for which you wish to retrieve files, from this list.
4. A list of the jobs files for that job is displayed in the default web browser. Typically the web browser will display the file contents if you click on a file with the left mouse button and will offer a range of options if you click on a file with the right mouse button. The range of choices should include displaying the file contents and saving the file to your PC. When displaying the file contents, the browser may display the contents in the browser window or open another application on your PC to display the contents. The exact behavior will depend on your browser and the configuration of your PC. When clicking with the right mouse button on a file in Internet Explorer, for example, a dialog will appear which allows you to choose whether to open the file or save it to disk, as illustrated below:



Tip: The job files browser can also be accessed directly through the Job Explorer by right-clicking on the job and selecting *Remote View* from the shortcut menu.

5. Select *Save this file to disk*. A *Save As* dialog is displayed. This allows you to specify the location in which the file will be saved.
6. In general you should download the files into the folder that was created by Materials Studio when the job started. If the *Save As* dialog displays *Text Files* in the *Save as type:* field, you should change this to *All Files* prior to saving the file. This will prevent a `.txt` extension being appended to the file name on download, which would make this file unusable in Materials Studio.

Accessing the Server Management Console

To display the Server Management Console

- Select *Tools | Server Console* from the Materials Studio menu bar.
  Or
- Select *Accelrys | Materials Studio 8.0 Server Console* from the list of programs on the Windows *Start* menu.

Navigating the Server Management Console

To view more or fewer Console Root items

- Click the + icon to expand or the - icon to collapse the console tree.
- Double-click on an item to expand or collapse the tree below it.

To navigate the tree and report views

- Click any item to view its report.
- Use the arrow keys to change to the item before or after the currently selected item.
- Click the  button on the toolbar to go to the parent item.
- Click the  and  buttons on the toolbar to go to the previous or next items.

Exporting information

For any item, except a specific job, the information in the Report View can be exported to a list as a tab or comma-separated text file.

To export a list report

1. Select the item in the console tree whose information you wish to export.
2. Optionally, for a list of jobs, select the rows in the Report View to export.
3. Either:
   - Click the  button.
     Or
   - Right-click and select *Export List...* from the shortcut menu.
     Or
   - Select *Action | Export List...* from the menu bar.
4. On the Export List dialog select the location of the file to create and the *File name*.
5. Choose the *Save as type* from the dropdown list, options are:
   - Text (Tab Delimited) (*.txt) (default)
   - Text (Comma Delimited) (*.csv)
   - Unicode Text (Tab Delimited) (*.txt)
   - Unicode Text (Comma Delimited) (*.csv)
6. For a limited list of jobs, check the *Save Only Selected Rows* checkbox.
7. Click the *Save* button.

Viewing Properties

The properties of each type of item in the console tree can be viewed in the Properties dialog in the Server Management Console.

To view properties

- Click the  button on the toolbar.
- Select *Action | Properties* from the menu bar.
- Right-click in either the console tree or Report View and select *Properties* from the shortcut menu.

To view gateway properties remotely

An Internet browser can be used to view gateway data remotely, or the server console can be used.

1. Select a server gateway in the console tree and either:
   - Select *View* | *Remote View* from the menu bar.
     Or
   - Right-click on the gateway name and select *View* | *Remote View* from the shortcut menu.
     Or
   - Right-click in the Report View and select *View* | *Remote View* from the shortcut menu.

The remote view of the server gateway maintains information about:

- The gateway host machine
- The server programs installed on the host machine
- Any jobs, running, stopped or archived

This information can also be directly exposed through a web page interface accessible using the gateway's http port.

If you know the gateway's host machine name and port number, you can type them into a standard web browser as a URL of the form:

`http://<hostname>:<port>/`

Queuing System Support

Materials Studio allows you to configure a gateway to use a queuing system. This is means that if several jobs are sent to the gateway at the same time, they are not all launched simultaneously. This allows you to optimize the use of the server resources on your network.

For further information on the queuing systems compatible with Materials Studio, their administration, instructions for their configuration, and troubleshooting tips please refer to the "Installing Materials Studio on a server with a queuing system" topic in the Materials Studio online help.

> **Tip:** A queue that allows unrestricted simultaneous jobs can be used to run a high priority job immediately.

To enable/disable the queuing mode of the gateway

You must have Gatekeeper user permissions to carry out this operation.

1. Make sure that a supported queuing system is installed on the server machine and is running.
2. Log in as the Queue Administrator of the system where the gateway is installed. Create and configure the required queues.
3. Add user and group permissions if required. Refer to your queuing system's documentation for details of queue administration tasks.
4. Open a remote view of the gateway and click the *Edit* button.
5. The *Queuing System* dropdown list displays all the queuing systems detected by the gateway. Select [none] if you want to run jobs directly, bypassing the queuing mechanism, or select the required queuing system.
6. Click the *Save* button.
7. Click the queuingsystem link to edit the queuing system configuration file.
8. Click the *Save* button.
9. Close Materials Studio, all Internet browsers, and the Server Console.

Note: When configuring user permissions on password-protected gateways, the username is the name entered when connecting to the gateway. On gateways that are not password-protected, the username is the username of the user currently logged into Windows.

Materials Studio users must refresh gateway data in order to see changes effected by a queue modification. After refreshing, all of a user's available queues will appear on the Queuing tab of the Gateway Properties dialog.

To set the correct number of CPU cores for Linux clusters

You must have Gatekeeper user permissions to carry out this operation.

1. Open a remote view of the gateway and navigate to the Gateway Data page.
2. Click the *Edit* button.
3. In the `cpucorestotal` property, enter the total number of CPU cores available on your cluster.
4. Close Materials Studio, all Internet browsers, and the Server Console.

Using the Report View

The Report View provides detailed information on the child items belonging to the currently selected item in the console tree. The amount of information displayed can be customized, and the display style can be changed.

For jobs the Report View provides interaction with the job while it is running and with the output files when it is complete.

To change the report display style

1. Select any item other than a job in the console tree, then either:
   - Select *View* from the menu bar and choose the display style to use.
     Or
   - Right-click and select *View* from the shortcut menu and choose the display style.

   Available options are:
   - Large Icons
   - Small Icons
   - List
   - Detail
2. When the display style is set to either Large Icons or Small Icons their alignment can be managed. Right-click and choose either *Arrange Icons | Auto Arrange* or *Line up Icons* from the shortcut menu.

To manage a detailed report

When the display style is set to Detail the columns displayed can be managed.

1. Open the Add/Remove Columns dialog, either:
   - Select *View* | *Add/Remove Columns* from the menu bar.
     Or
   - Right-click on the item in the console tree and select *View* | *Add/Remove Columns* from the shortcut menu.
     Or
   - Right-click in the Report View and select *View* | *Add/Remove Columns* from the shortcut menu.
2. Select column names and click the *Add* and *Remove* buttons to change which columns are displayed.
3. Select displayed columns and click the *Move Up* and *Move Down* buttons to change the order of the columns.
4. Click the *Restore Defaults* button to undo all changes and return to the default column display settings.
5. Click the *OK* button to save any changes.

Managing Gateways

Server gateways can be added, removed, edited, updated, and tested through the Server Management Console.

A remote view of each gateway's properties can also be accessed.

To set up a default gateway

A given gateway can be configured so that it is used as the default gateway for a specific server.

1. Open the Server Management Console.
2. Select the *Gateway Server* you wish to configure as a default and expand its list of Server Programs.
3. Right-click on the Server Program which should use this Gateway Server by default and select *Default Server* from the shortcut menu.

Registering a Gateway

The registration of an installed gateway provides access (from this client PC) to all the server programs registered with that gateway. A gateway may be installed on any host machine on the network.

Registering a new gateway

1. Open the Server Management Console.
2. Select the *Server Gateways* item in the console tree.
3. Select *Action | New | Server Gateway* from the menu bar (or right-click and choose *New | Server Gateway* from the shortcut menu).
4. Enter the *URL* and *Port Number* for the new gateway. The default port number is 18888. You should confirm with the gateway administrator; the name and port of the gateway register and whether the gateway has been configured to use the https protocol instead of http.

   Note: The gateway host name can be either the name or the IP address of the machine. Valid port numbers lie between 0 and 65535.

5. Click the *Connection* button to change the default connection properties of the gateway. This expands the dialog to display additional controls. The use of this facility is described below.
6. Before proceeding with the full registration it is recommended that you run a few diagnostic tests to confirm that the information you are providing correctly refers to an installed gateway and that it is up and running. Click the *Run Diagnostics* button to start the tests.
   The tests performed include:
   - Looking up the specified name of the machine to check that it is known on the network
   - Pinging the host machine to check that it is responsive
   - Testing the specified port with some HTTP(S) requests to ensure that the gateway will respond to such requests to create and run jobs

   The dialog is expanded horizontally to display the results of the tests. You can browse these for details of the diagnostics.
7. The overall result (*SUCCESS* or *FAILURE*) is written to the dialog. If the test fails, use the diagnostic information to help you to determine the cause of the problem. A gateway cannot be registered without a valid host name and port. Click the *Cancel* button to close the dialog.
8. If the diagnostics return a *SUCCESS*, click the *OK* button to proceed with the registration process.
9. If this is a password-authenticated gateway and the gateway is configured to be used in conjunction with a queuing system, a dialog may be displayed, asking you to provide your username and password.
10. Once registration is completed, the newly registered gateway and its server programs appear in the console tree.

To configure the connection

1. Choose the type of proxy to use, available options are:
   - Use proxy: Allows you to specify the proxy server and port. Consult with your Network Administrator before using this mode.
   - Use Internet setting: Uses the Internet Explorer default proxy settings.
   - Do not use proxy: Connection to the gateway is established directly, bypassing the proxy server.
2. Specify the *Timeout*, this is the maximum amount of time allowed for one communication request to the gateway to succeed. If the gateway does not respond the request fails. In such cases, Materials Studio attempts several different methods of connecting to the gateway. The timeout limit applies to each attempt. If the machine where the gateway is installed has multiple hostnames, the number of attempts increases. The total timeout is equal to the specified timeout multiplied by the number of attempts. During that time, the user interface may be responding slowly or not responding at all.

   Tip: Use longer timeout values if the gateway is located on a slow network and use shorter values for local gateways.
3. Choose whether to *Use https* protocol (HTTP over SSL) for gateway communication, and if so which certificates to ignore. A self-signed certificate is provided by Accelrys with Materials Studio to get HTTPS gateways working initially. In order to get started all three types of certificate errors should be ignored. With other certificates, different combinations of options may be more suitable. It is recommended that for long-term gateway security the self-signed certificate should be replaced with one obtained from a genuine Certificate Authority.
   - If the *Ignore invalid certificate date* checkbox is checked, errors due to an out-of-date gateway server certificate are ignored. Note that the certificate provided with Materials Studio is only valid for about 1 year from the date of release.
   - If the *Ignore invalid certificate name* checkbox is checked, errors due to a mismatch between the name of the gateway server machine and the name on the certificate will be ignored.
   - If the *Ignore unknown certificate authority* checkbox is checked, errors due to the certificate authority not being known will be ignored.

Unregistering a Gateway

The unregistration of an installed gateway removes access from the client to all the server programs on that gateway.

Unregistering an installed gateway

1. Open the Server Management Console.
2. Select the Server Gateway to unregister.
3. To remove the gateway, either:
   - Select *Action | Delete* from the menu bar.
     Or
   - Right-click the Server Gateway and select *Delete* from the shortcut menu.
     Or
   - Click the  button on the toolbar.
     Or
   - Select the Server Gateways item and delete the gateway from the Report View using one of these methods.
4. The gateway is removed from the set of available gateways, provided that there are no remaining jobs for the gateway. If there are some jobs, you must remove or archive them first.

Testing Gateways

You can run a series of simple tests on a gateway to check that it is accessible to the client machine, and that it can handle http(s) requests.

Testing a server gateway

1. Open the Server Management Console.
2. Select the *Server Gateway* to test.
3. Right-click and choose *Test Gateway...* from the shortcut menu to display the Test Server Gateway dialog.
4. There are two separate tests available. *Test communication* tests that communications are possible to the gateway machine. This test:
   - Looks up the specified name of the machine to check that it is known on the network
   - Pings the host machine to check that it is responsive

   Run job sends an http(s) request to the gateway to run a simple job. If the first test fails, the second is not attempted. You can choose to run one or both of these tests.
5. Click the *Begin Test* button.
6. The progress and results of the test(s) are displayed in the dialog.
7. If you choose to run the simple job test, then you will see the usual job log window displayed while the job is running.

Gateway Test Failure

Gateway test failures can occur for many reasons. The dialog that is displayed when a diagnostic test fails should provide some information to help you understand the nature of the problem.

Typical problems include:

- The gateway is no longer accessible, either because it is not running or the network connection to it is no longer intact.
- The machine where the gateway is running has been reconfigured on the network so that its name or IP address has changed. In this case you will need to register the gateway again with the new information.
- Security failure for a gateway with some level of access control or user security enabled. Either access is not permitted from the client PC or an entered user name could not be authenticated against the set of users registered for the gateway.

Refreshing Gateways

Local information about a server gateway may become out of date in some way, but you can refresh it from the gateway's host machine.

Refreshing a single server gateway's properties

1. Open the Server Management Console.
2. Select the *Server Gateway* to refresh.
3. Right-click and choose *Refresh Gateway* from the shortcut menu to update the local information held for that gateway.
4. If this is a password-authenticated gateway and the gateway is configured to be used in conjunction with a queuing system, a dialog may be displayed, asking you to provide your user name and password.

Refreshing properties of all server gateways

1. Open the Server Management Console.
2. Select the *Server Gateways* item in the console tree.
3. To refresh the information, either:
   - Right-click on the Server Gateways item and choose *Refresh All Gateway Data* from the shortcut menu.
     Or
   - Right-click in the Report View and choose *Refresh All Gateway Data* from the shortcut menu.
     Or
   - Select *Action | Refresh All Gateway Data* from the menu bar.
4. If any of the gateways are password-authenticated and configured to be used in conjunction with a queuing system, a dialog may be displayed, asking you to provide your user name and password.

Failure to Refresh Gateways

A gateway may fail to refresh for a number of reasons:

- The gateway is not running.
- The gateway's host machine is switched off or is off the network.
- The gateway has been reinstalled on a different port. In this case, unregister and reregister the gateway.
- The machine name or IP address has been changed. In this case, unregister and reregister the gateway.
- The gateway has been uninstalled. In this case, unregister (delete) the gateway.

Managing Jobs

The Server Management Console can be used to locate, monitor, communicate with, and stop and remove jobs running on registered gateway servers.

The properties of jobs can also be viewed.

Locating Jobs

To view the progress of a job or to control it in some way, you must first locate the relevant job item in the console tree.

Locating a job by job description

1. Open the Server Management Console.
2. Open the *Jobs* item on the console tree.
3. Check the list of jobs for your job description.

> **Note:** If you do not see your job id, it may have been removed or archived. Additionally, a job only appears in this list if it was created on this PC by the current user.

Locating a job if you do not know the job description

1. Open the Server Management Console.
2. Select the *Server Gateway* in the console tree where the job is running.
3. Choose the Server Program that the job is using, all the jobs that have been created using this server are displayed in the Report View.
4. Use the *Detail* display style to provide more information about each job, which should allow you to locate the job.

Monitoring Jobs

Depending on the server program used, a job may be able to display messages and a percentage completion value that allows you to keep track of how the job is progressing.

Monitoring a job's progress

1. Open the Server Management Console.
2. Locate the job object that you are interested in, as described in Locating jobs.
3. Select the job item that you are interested in, to display the job control panel in the result pane.
4. The job control panel includes a percentage completion bar and a list of messages as they are generated. Note that not all servers provide completion percentages.

Sending a Command to a Job

1. Open the Server Management Console.
2. Locate the job object that you are interested in, as described in Locating a job.
3. In the *Report View* for the job, click the *Command...* button to open the Send Command To Job dialog.
4. Enter the necessary *Command* and any associated *Argument*, then click the *Send* button.

Stopping Jobs

While a job is running, you can request that it be stopped before it has completed.

Stopping a job

1. Open the Server Management Console.
2. Locate and select the *Job* that you are interested in, as described in Locating a job.
3. If the job is running, click the *Stop Job* button to halt the running job. In some cases, partial data may be returned for the computations completed up to that point.

You can request that jobs are automatically removed upon completion. If not, then you will find yourself with a number of completed jobs that you will eventually want to remove or archive, including job configuration information, plus any input or output data files for the job.

To remove a job

1. Open the Server Management Console.
2. Locate and select the *Job* that you are interested in, as described in Locating a job.
3. If the job is in an appropriate phase, click the *Remove* button. Running jobs must be stopped before they can be removed.
4. This operation will attempt to delete all job information on both the client PC and the server gateway. Sometimes you may find that the gateway information for the job cannot be removed. The most likely reasons are:
   - The gateway data has already been removed independently.
   - The job failed during its launch phase, so gateway information for the job was never set up.
   - The gateway is not running currently.
   - You client PC is not connected to the network.

In the first two of these cases, the client-side data is deleted, and a warning is given. In other cases you will be asked whether to proceed with the deletion of just the client-side data. If you do this, you will need to remove the gateway job data independently through the Remote View of the gateway (either through an Internet browser or the Report View).

To remove all jobs

1. Open the Server Management Console.
2. Locate and select the *Gateway Server* that you are interested in.
3. To remove all jobs either:
   - Right-click on the Gateway Server and select *Remove All Jobs* from the shortcut menu.
     Or
   - Right-click in the Report View and select *Remove All Jobs* from the shortcut menu.
     Or
   - Select *Action | Remove All Jobs* from the menu bar.

Archiving a job

Archived data is stored in a job folder named after the job ID, which is placed under a folder named "job-archive". This archived job data can be accessed directly through the file system of the gateway host machine.

1. Open the Server Management Console.
2. Locate and select the *Job* that you are interested in, as described in Locating jobs.
3. If the job is in an appropriate phase, click the *Archive* button to archive the job. Note that running jobs must be stopped before they can be archived.
4. This operation will attempt to delete all job information on the client and move job information on the server gateway. Sometimes you may find that the gateway information for the job cannot be moved. The most likely reasons are:
   - The gateway data has already been removed or archived independently.
   - The job failed during its launch phase, and so gateway information for the job was never set up.
   - The gateway is not running currently.
   - You client PC is not connected to the network.

In the first two of these cases, the client-side data is deleted, and a warning is given. In other cases you will be prompted as to whether to proceed with the deletion of the client-side data. If you do this, you will need to archive the gateway job data independently using direct file system management on the gateway host machine.

Working with queues

This version of Materials Studio allows you to configure a Materials Studio gateway so all jobs submitted to this gateway are fed into a queuing system, instead of being launched instantaneously. This allows you to optimize the use of server resources on your network. Moreover, if you have a Linux cluster, the use of a queuing system is recommended to ensure an even distribution of jobs among the different processors.

Refer to the Installing Materials Studio on a server with a queuing system topic for a full list of supported queuing systems.

Note: Materials Studio supports PBS Pro, OGE, UGE, LSF, and TORQUE on clusters. For parallel execution, CASTEP, DMol^3, Forcite, Mesocite, GULP, MesoDyn, and ONETEP MPI versions are supported for submission on Linux clusters and SMP machines running PBS Pro, OGE, UGE, TORQUE, or LSF. Different versions of these queuing systems may work with Materials Studio, but have not been tested. For the installation and configuration of the queuing system itself, refer to the appropriate documentation.

Once a Materials Studio gateway is configured to work with a queuing system, access and control of jobs submitted to the queuing system are entirely controlled through the Materials Studio interface. The procedures for running and monitoring jobs are the same as those used in the absence of a queuing system. While a job is queued, the *Status* is displayed as queued in the Job Explorer.

Jobs submitted to a gateway that is running a queuing system must be submitted to a queue. Some queuing systems allow the creation of multiple queues with different attributes. You can choose any queue from the list of available queues, using the *Queue* control, which can be accessed from the Job Control tabs of the module calculation dialogs. In DMol^3, for example, select *Modules | DMol3 | Calculation* from the menu bar to display the DMol3 Calculation dialog, then select the *Job Control* tab. Choose a server on which to run the job from the *Gateway location* dropdown list and select the queue to which the job will be submitted from the *Queue* dropdown list.

Note: Third party queuing systems do not check the availability of licenses before attempting to execute jobs from their queue. As a result, if a queue is configured to execute more jobs than there are licenses available, jobs may fail unexpectedly. To prevent this, you should configure your queuing system to execute no more queued jobs than you have licenses. When submitting jobs of different types with different numbers of available licenses, create individual queues for each job type. Alternatively, you can configure your gateway to use the License wait functionality of the license pack - see the Licensing Materials Studio and Gateway administration topics for further details.

Tip: A queue that allows unrestricted simultaneous jobs can be used to run a high priority job immediately.

See Installing Materials Studio on a gateway with a queuing system, Using the Server Console, and the Server Console help system for details of queuing system administration, configuration, installation, and troubleshooting.

Transferring files via FTP

Normally, remote jobs are executed via a Gateway installed on a remote server, as described in the Client-server architecture topic. However, sometimes it is desirable to copy input files to the server and run the remote job manually. You may wish to do this if, for example:

- You prefer to use a secure FTP client to transfer files between computers on your network.
- You wish to access the advanced functionality of certain standalone server codes, for example CASTEP or DMol^3.
- The server you are using is running an operating system which does not support a Gateway.

The File Transfer tool facilitates this operation. It uses an external FTP client to transfer files to and from the remote server.

> **Note:** It may be necessary to configure the File Transfer tool in order for it to work with your local FTP client.

The following describes how to use the File Transfer tool to transfer files to and from the remote server.

To transfer files to the remote server

1. Select the folder containing the input files you wish to transfer using the Project Explorer.
2. Select *Tools | File Transfer* from the menu bar. The File Transfer dialog is displayed.
3. If necessary, supply or update the values for *User name*, *Password*, *Remote host*, *Remote folder*, and *Arguments*.
4. Choose *Upload files to server*.
5. Optionally, check the *Edit script before executing* checkbox. When *Edit script before executing* is enabled, the script generated in the next step is opened in a text window immediately after it is created, allowing you to inspect and edit it before it is passed to the FTP client.
6. Optionally, use the *AdditionalFiles* option to specify extra files not present in the selected project folder for upload.
7. Click the *Run* button. This generates a script that lists all of the files present in the selected project folder and any additional files specified. The FTP client on the local computer is then launched using the command specified in the *FTP command* text box and the script is executed.

   In addition, the following data are written to the project folder when the *Run* button is clicked:

   - User name
   - Host
   - Remote folder

   If you checked the *Edit script before executing* checkbox, a text window containing the script is opened after the script is generated. Make any desired changes, for example, remove the names of any files you do not wish to transfer to the remote server, and ensure that you save the updated script. As soon as the text window is closed, the FTP client is launched and the script is executed.

The files listed in the script are uploaded to the location specified in the *Remote folder* field. Refer to the Remote jobs help for the relevant module to learn how to use the uploaded files to run a standalone job on the server.

To transfer files from the remote server

1. Select the folder containing the files you previously transferred to the remote server using the Project Explorer.
2. Select *Tools | File Transfer* from the menu bar. The File Transfer dialog is displayed.
3. Ensure that the specified *Remote host* and *Remote folder* reflect the location into which you previously uploaded the input files.
4. Choose *Download files from server*.
5. Optionally, check the *Edit script before executing* checkbox. When *Edit script before executing* is enabled, the script generated in the next step is opened in a text window immediately after it is created, allowing you to inspect and edit it before it is passed to the FTP client.
6. To begin the file transfer, click the *Run* button. The FTP client on the local computer is launched using the command specified in the *FTP command* text box.

> **Tip:** By default, the `mget` command is used for downloads. If you do not wish to transfer all of the files present in the remote folder, you should delete the unnecessary files before clicking the *Run* button or edit the download script.

If you checked the *Edit script before executing* checkbox, a text window containing the script is opened after the script is generated. Make any desired changes and ensure that you save the updated script. As soon as the text window is closed, the FTP client is launched and the script is executed.

Configuring file transfer

The File Transfer tool uses the local FTP client installed on your computer. This allows you to adhere to your company security policy and use the FTP client of your choice.

Since different FTP clients are invoked differently, the File Transfer tool may need to be configured in order for it to work with your local FTP client.

The following aliases can be used for the fields in the File Transfer dialog:

Dialog field	Variable name	Description
User name	`$user`	The name to login to the file server.
Password	`$password`	The password for the username if required.
Remote server	`$host`	The location of the FTP server.
Remote folder	`$folder`	The remote folder into or from which to transfer the files.
Arguments	`$arguments`	Any additional arguments
	`$dir`	The current directory.
	`$additionalfiles`	A list of files for the *Additional files* pane in quotation marks, separated by spaces.

These values can be supplied on the command line or they can be included in a script template, thus adjusting the behavior of the File Transfer tool to suit your needs.

Modify the *FTP command* field as required to launch your local FTP client. Use the aliases above, as necessary. For example, if your FTP client accepts the password as an argument, the FTP command may look like this:

```
ftp -p $password
```

The File Transfer tool generates a script file which can be passed to the FTP client using the command line or via a pipe. Refer to your operating system documentation for a more detailed description of pipes and input redirection.

A template used for creating the script header is located in `\share\Resources\FTP\FTP.template`.

You can modify this template to include additional FTP commands. Use the aliases above, as necessary; `open $host`, for example.

Note: The standard Windows FTP client does not accept a password on the command line. Additionally, scripts passed using the `-s:` argument block the FTP client during execution, so you are never prompted for the password. To overcome this problem, the script can be passed to the FTP client via a pipe using the following command:

```
cmd /c type $script | ftp -i
```

The appropriate script header template when using this command is:

```
open $host
$user
```

Alternatively, a more reliable and flexible, but less secure, way is to specify the command line as:

```
cmd /c ftp -i -s:$script
```

The script header template in this case should list a password if one is required by the remote FTP server:

```
open $host
$user
$password
```

To select a file directly from a file explorer, set the command to:

```
explorer $dir
```

File Transfer dialog

Normally, remote jobs are executed via a Gateway installed on a remote server, as described in the Client-server architecture topic. However, sometimes it is desirable to copy input files to the server and run the remote job manually. You may wish to do this if, for example:

- You prefer to use a secure FTP client to transfer files between computers on your network.
- You wish to access the advanced functionality of certain standalone server codes, for example CASTEP or DMol^3.
- The server you are using is running an operating system which does not support a Gateway.

The File Transfer dialog allows you to transfer files to and from a remote server manually using an external FTP client.

Note: It may be necessary to configure the File Transfer tool in order for it to work with your local FTP client.

User name: Specify the name of the FTP user. Typically, an account with this name must exist on the remote server.

Password: Provide the password for the FTP user specified above.

Note: This option is enabled only if the `$password` variable is present in the FTP script header template. See the Configuring file transfer topic for further details.

When this option is disabled, you will be prompted for your FTP password after you click the *Run* button.

Remote server: Specify the name of the remote server to which you wish to transfer files. An FTP server must be running on this computer.

Remote folder: Specify the folder on the remote server into which you wish to place the files you transfer. This folder must already exist.

Arguments: Specify any additional arguments that may be required by your FTP client.

FTP command: Specify the command used to invoke the FTP client on your local machine. The default options are:

- *cmd /c type $script | ftp -i* - This command passes the FTP script to the FTP client via a pipe. It does not require the FTP password to be present in the script.
- *cmd /c ftp -i -s:$script* - This command passes the FTP script to the FTP client via the `-s` argument. In order to use this command, the `$password` variable must be present in the script header template and a password must be entered in the *Password* field on the File Transfer dialog.

Alternatively, you can type any other suitable FTP command into the text box, for example:

- `$dir` is the current directory
- `$additionalfiles` can be used to list files to add to the *Additional files* pane

Upload files to server: Choose this option to upload the specified files to the remote location.

Download files from server: Choose this option to download all of the files present in the remote location.

Edit script before executing: When checked, indicates that the script created when you click *Run* will be opened in a text window before it is executed. This enables you to inspect or modify the script before running it.

Additional files: This option allows you to specify other files not present in the selected project folder that are required as input for your calculation, for example, pseudopotential files for CASTEP jobs.

Add...: Provides access to the Select File(s) To Add dialog, which allows you to select additional files for upload. To add files to the list, navigate to the appropriate folder, select the desired file or files and click the *Add* button. To remove files, select them in the list and press the DELETE key.

Note: This option is enabled only if the *Upload files to server* option is selected.

Run: Creates the specified FTP script, then launches the local FTP client and executes the script.

Cancel: Closes the dialog.

Help: Displays the Help topic in a browser.

Access methods

Menu	*Tools	File Transfer*

Visualizer References

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