

List of Menu Options

This section will present a comprehensive guide of all menu options and their functions within the current version (v1.69) of the visualiser (options that open drop-down menus are shown in italics, while indents show if an option is part of a drop-down menu):

<u>Menu Option</u>	<u>Description</u>
File	
Open Data File	Opens a file explorer window to locate data files (.vis) for objects to construct crystals.
Load Coordinates	Opens a file explorer window to locate coordinate (.XYZ) files for all structure types.
Save Image	Opens a file explorer window to capture the current screen within the visualiser and save it as an image file (.bmp).
Save All Frames	Opens a file explorer window to define a location and filename to save an image of each frame from the current multi-frame simulation.
<i>Process a Directory</i>	Drop-down menu for processing entire folders of XYZ files.
Single Image	Opens a file explorer window to select a folder / directory to process. Selecting a coordinate (.XYZ) file will instruct the visualiser to cycle through all coordinates files within the same folder and enact the "Save all Frames" option. A data file must be loaded prior to running this option. All XYZ files in the folder must have the same .vis file.

Cycle Species Types	<p>Opens a file explorer window to select a folder / directory to process. Selecting a coordinate (.XYZ) file will instruct the visualiser to cycle through all coordinate files within the same folder, open the simulation and cycle through all species types one by one. A single image is saved for each selected species type keeping the viewing distance and angles consistent for the entire directory. A data file must be loaded prior to running this option.</p>
<i>Process + Rotate Movie</i>	<p>Drop-down menu for processing entire folders of XYZ files and produce short movies rotating about a single axis.</p>
About X	<p>Opens a file explorer window to select a folder / directory to process. Selecting a coordinate (.XYZ) file will instruct the visualiser to cycle through all coordinate files within the same folder and save 8 images of the crystal rotating around the X axis. The final frame of multi-frame simulations will be used for the rotation. A data file must be loaded prior to running this option. Axes are defined relative to the current viewing angle of the crystal via Euler angles.</p>
About Y	<p>Same as previous option but rotation about the Y axis.</p>

About Z	Same as previous option but rotation about the Y axis.
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Load State	Opens a file explorer window to open a state (.stat) file. The parameters recorded in this file will be read into the visualiser and the simulation scene will be set to match these values. A data file and coordinates file must be loaded prior to loading a state file. Simulations of the same structure types (i.e. simulations with the same .vis files can share .stat files).
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Save Colour File	Opens a file explorer window to save a colour (.col) file. This will save all custom colours currently selected in the visualiser in RGBA format.
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Save Current State	Opens a file explorer window to save a stat (.stat) file. All values required to recreate the current visualiser scene will be written to this file to be loaded when required.
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Exit	Quits the visualiser after user confirmation (Yes/No).
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Drawing

<i>Tile Crystals</i>	Drop-down menu for drawing options related to crystals constructed from natural tiles.
Points	Toggle to display structure as points (On/Off).
Layers Tiles	Display natural tiles and colour using layer colouring. (Default drawing mode for tile crystals with layer information).
Type Tiles	Display natural tiles and colour using tile type colouring. (Default drawing mode for tile crystals without layers information).
Block Colour Tiles	Display natural tiles and colour all types with a single block colour.
Layers Spheres	Display spheres and colour using layer colouring. Sphere size can be determined by tile size (default) or use the average sphere radius.
Type Spheres	Display spheres and colour using tile type colouring. Sphere size can be determined by tile size (default) or use the average sphere radius.
Block Colour Spheres	Display spheres and colour all types with a single block colour.
Avg. Sphere Size On/Off	Toggle between displaying spheres with radii controlled by tile size or a single average radius across all tiles.

<i>Net Crystals</i>	Drop-down menu for drawing options related to crystals partitioned as simplified nets.
Points	Toggle to display structure as points (On/Off).
Layers Molecules	Display molecules as atoms and bonds and colour using layer colouring.
Atom Type Molecules	Display atoms and bonds and colour using atom type colouring.
Block Colour Molecules	Display molecules as atoms and bonds and colour all atom types with a single block colour.
Layers Spheres	Display molecules as average sized spheres and colour using layer colouring. (Default drawing mode for net structures with layers information).
Type Spheres	Display spheres and colour using molecule type colouring. Spheres are all an average radius calculated by measuring the distance between species and filling the space. (Default drawing mode for net structures with no layers information).
Block Colour Spheres	Display molecules as spheres and colour all types with a single block colour.
Show Bonds	Checkbox to enable or disable bonds (note, this is a global option and will control all bonds separately to their status).

Show Atoms	Checkbox to enable or disable atom display (note, this is a global option and will control all atoms separately to their status).
Avg. Sphere Size On/Off	Toggle between displaying spheres with radii controlled by species size or a single average radius across all tiles. (Currently has no effect on net crystals)
Change Sphere Size	Checkbox to show that resizing spheres is selected – CTRL and + / CTRL and - will enlarge / reduce spheres.
Change Sphere Resolution	Checkbox to show that resolution scaling is selected – CTRL and + / CTRL and - will increase / reduce sphere resolution.

Colouring

Custom Colours	Toggles between custom colours or default colours. Custom colours are retained until changes are made or the visualiser is closed, allowing users to switch back and forth between custom and default colours.
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Change All Colours (Load File)	Opens a file explorer window to load a custom colours (.col) file. The currently displayed colours will switch to the RGBA values listed in the colour file.
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Change Single Colour	Opens a colour picker window allowing the user to select a single custom colour. The colour selected in this window will change the colour of the currently selected species (i.e. tile, sphere, atom or bond).
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<i>Background Colour</i>	Drop-down menu for altering the background colour.
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Black	Changes the background colour to black.
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White	Changes the background colour to white.
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Red	Changes the background colour to red.
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Green	Changes the background colour to green.
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Blue	Changes the background colour to blue.
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Custom	Opens a colour picker window allowing the user to select a custom colour for the background.
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Mouse Mode

Rotate Mode

Switches the mouse behaviour to control rotation. Left clicking and moving the mouse controls rotation about the X and Y directions, whereas right clicking and moving the mouse controls rotation about the Z direction only.

Scale Mode

Switches the mouse behaviour to control scaling. Left clicking and moving the mouse controls the zoom level (i.e. translation in the z direction).

Translate Mode

Switches the mouse behaviour to control translation. Left clicking and moving the mouse controls translation in the X and Y directions.

Render Movies

<i>Rotate Clockwise</i>	Drop-down menu to create simple clockwise rotation movies. Axes are currently fixed to the orthogonal simulation axes.
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Around X	Create a movie of clockwise rotation about the X axis. An image is taken every ten degrees, resulting in a movie of 37 frames.
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Around Y	Same as previous option but rotation about the Y axis.
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Around Z	Same as previous option but rotation about the Z axis.
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Around XY	Same as previous option but rotation about the XY axis.
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Around XZ	Same as previous option but rotation about the XZ axis.
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Around YZ	Same as previous option but rotation about the YZ axis.
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Around XYZ	Same as previous option but rotation about the XYZ axis.
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<i>Rotate Anticlockwise</i>	Drop-down menu to create simple anticlockwise rotation movies. Axes are currently fixed to the orthogonal simulation axes.
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Around X	Create a movie of anticlockwise rotation about the X axis. An image is taken every ten degrees, resulting in a movie of 37 frames.
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Around Y	Same as previous option but rotation about the Y axis.
Around Z	Same as previous option but rotation about the Z axis.
Around XY	Same as previous option but rotation about the XY axis.
Around XZ	Same as previous option but rotation about the XZ axis.
Around YZ	Same as previous option but rotation about the YZ axis.
Around XYZ	Same as previous option but rotation about the XYZ axis.
<i>Flight Path</i>	Drop-down menu for creating movies between viewpoints (i.e. a flight path from one viewpoint to another).
<i>Rotation, Translation</i>	Drop-down menu for creating flight path movies where the first half of the movie is solely a rotational transition, whereas the second half is solely a translational transition.
20 Frames	Create a movie of 20 frames. 10 frames of rotation followed by 10 frames of translation. 20 images will be saved at a location defined by the user through a file explorer window. "Flight_Path" will be appended to all filenames. A starting and ending viewpoint must be selected before selecting this option.

40 Frames	Same as previous option, but 40 frames. 20 frames of rotation followed by 20 frames of translation.
60 Frames	Same as previous option, but 60 frames. 30 frames of rotation followed by 30 frames of translation.
80 Frames	Same as previous option, but 80 frames. 40 frames of rotation followed by 40 frames of translation.
100 Frames	Same as previous option, but 100 frames. 50 frames of rotation followed by 50 frames of translation.
120 Frames	Same as previous option, but 120 frames. 60 frames of rotation followed by 60 frames of translation.
<i>Translation, Rotation</i>	Drop-down menu for creating flight path movies where the first half of the movie is solely a translational transition, whereas the second half is solely a rotational transition.
20 Frames	Create a movie of 20 frames. 10 frames of translation followed by 10 frames of rotation. 20 images will be saved at a location defined by the user through a file explorer window. "Flight_Path" will be appended to all filenames. A starting and ending viewpoint must be selected before selecting this option.
40 Frames	Same as previous option, but 40 frames. 20 frames of translation followed by 20 frames of rotation.

60 Frames	Same as previous option, but 60 frames. 30 frames of translation followed by 30 frames of rotation.
80 Frames	Same as previous option, but 80 frames. 40 frames of translation followed by 40 frames of rotation.
100 Frames	Same as previous option, but 100 frames. 50 frames of translation followed by 50 frames of rotation.
120 Frames	Same as previous option, but 120 frames. 60 frames of translation followed by 60 frames of rotation.
<i>Translation + Rotation</i>	Drop-down menu for creating flight path movies where the translational and rotational transitions occur at the same time. (Preferred method).
10 Frames	Create a movie of 10 frames. 10 images will be saved at a location defined by the user through a file explorer window. "Flight_Path" will be appended to all filenames. A starting and ending viewpoint must be selected before selecting this option.
20 Frames	Same as previous option, but 20 frames.
30 Frames	Same as previous option, but 30 frames.
40 Frames	Same as previous option, but 40 frames.
50 Frames	Same as previous option, but 50 frames.
60 Frames	Same as previous option, but 60 frames.

Take Most Direct Path

Checkbox to enable direct path calculation.
The visualiser will take the most direct path between points (e.g. if the rotation angle in one direction is greater than 180 degrees, it will instead rotate in the opposite direction).

Lighting

<i>Standard</i>	Drop-down menu for controlling light status with lighting setting inspired by VMD.
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Light 0	Toggle light 0 on or off.
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Light 1	Toggle light 1 on or off.
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Light 2	Toggle light 2 on or off.
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Light 3	Toggle light 3 on or off.
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Light Correction	Toggle lighting corrections. Surfaces occasionally have their lighting inverted when calculating the curvature of a surface. This setting will toggle a weak light behind the crystal to remove patches of darkness when viewing crystals. Generally improves tiles visualisation, not usually required for spheres.
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<i>3dt</i>	Drop-down menu for controlling light status with lighting setting inspired by 3dt.
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Light 0	Toggle light 0 on or off.
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Light 1	Toggle light 1 on or off.
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Light 2	Toggle light 2 on or off.
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Light Correction	Toggle lighting corrections.
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View

Set Starting Viewpoint	Saves current camera position and rotation as the starting viewpoint for flight path movies.
Set Ending Viewpoint	Saves current camera position and rotation as the ending viewpoint for flight path movies.
Display Axes xyz	Display orthogonal axes in the bottom-left corner of the visualiser window. X – red, Y – green and Z – blue.
Display Axes abc	Display crystallographic axes in the bottom-left corner of the visualiser window. Axes are defined by the non-primitive unit cell of the crystal structure loaded in the .vis file a – red, b – green and c – blue.
Scale Axes to Unit Cell	Scale size of axes relative to unit cell parameters. All are defined relative to a.
Display Overlay	Toggle text overlay on / off.
Change Overlay Colour	Open a colour wheel to change the colour of overlay text.
Display Full Overlay	Display additional overlay information.
Add Overlay Background	Add a white rectangle as background for the overlay text.
Enable Quaternion Rotation	Switch calculation method for the rotational matrices. Uses a quaternion instead of Euler angles.

Reset

<i>Reset View</i>	Drop-down menu for reset options.
Reset Rotation	Resets all rotation values to 0.
Reset Translation	Resets all translation values to 0
Reset Sphere + Bond Scaling	Resets all sphere and bond scaling to default (scaling factor of 1.0).
Reset Depth Buffers	Reset depth buffers back to their default positions.
Reset All Parameters	Resets all parameters to their default values when opening the simulation for the first time.

Help

Controls	A list of hotkeys for user reference.
Manual	A link to the <i>CrystalGrower</i> website page containing this manual section and links to YouTube videos.
About	Information on authors and visualiser version.
Cite CrystalGrower	A link to the <i>CrystalGrower</i> website homepage. Links to papers and downloads for reference managers are available.
