

Modes of Operation

Structure types: The *CrystalGrower* visualiser is capable of rendering all structure types input into the *CrystalGrower* simulation package. Structures are first constructed using the data file with the .vis file extension.

Visualisation methods within the visualiser can be separated into three main operating modes (Figure 1) : tiles, net (average spheres) and net (atoms and bonds). Each mode type refers to the type of data read into the program and the shapes displayed on the screen. Each data type has a slightly different set of options for visualisation methods discussed in later sections.

Tiles mode (Figure 1, top) constructs and displays natural tiles at the coordinates listed in the XYZ coordinate file produced by the *CrystalGrower* simulation package. All coordinates in the .vis and .XYZ files are scaled to the *a* unit cell parameter of the structure being studied. Tiles are always centred at the origin of the simulation space before being translated to their final positions contained in the .XYZ file. This method is most frequently applied for framework materials, where any atom type at a tile vertex is interchangeable (i.e. there is no explicit atom type that should exist at this coordinate as with ionic crystals such as NaCl). Natural tiles are displayed as filled polyhedral faces, and are useful for studying crystal surface terminations and terrace heights to be compared to AFM data.

Net mode can be split into two subtypes: average spheres and atoms and bonds; both mode types share similarities but are discussed separately. The average spheres (Figure 1, Bottom, Left) mode was developed first and therefore possesses a limited number of the visualisation methods discussed later. Rather than reading in coordinates for tile vertices and faces, this mode reads in only the central coordinate of a molecule / ion in a unit cell.

Reading the XYZ coordinates file, the visualiser then translates to the listed positions and draws a sphere. The sphere's size is equal for all molecules and its radius is equal to half the distance between the centre of each species (which is then averaged across all molecules / ions). This drawing method is well suited for simple molecular crystals of one species type but is less suited for multicomponent crystals (e.g. MOFs and ionic crystals). This mode is now a legacy mode, and can only be accessed by deselecting "Keep Original Structure" in *ToposPro* when generating a structure file.

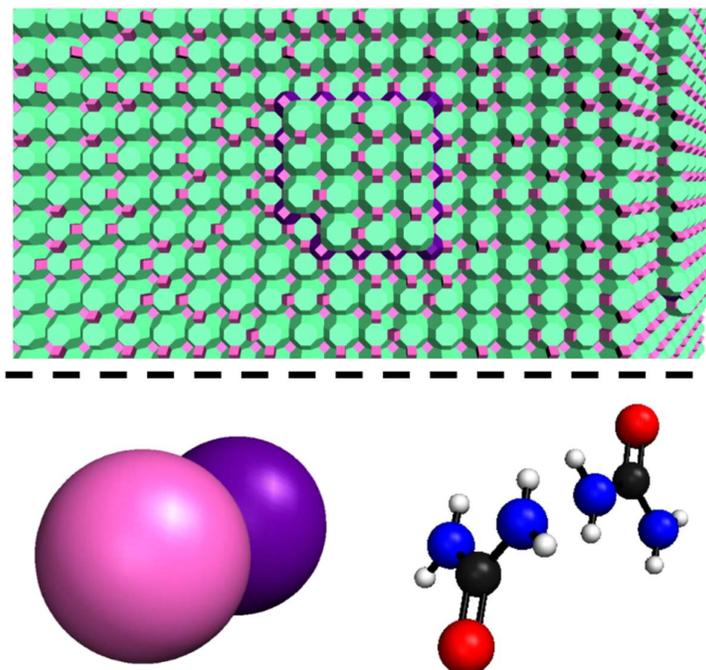


Figure 1 Top: An image captured of an LTA crystal visualised with the visualiser. The operating mode displayed is referred to as “tiles” mode, with natural tiles constructed from polygon faces.
Bottom, Left: Two urea molecules displayed in the molecular (average spheres) operating mode.
Right: The same two urea molecules displayed in the molecular (atoms and bonds) operating mode.

Atoms and bonds mode (Figure 1, Bottom, Right) is a recent large-scale modification to the net mode within the visualiser. This mode reads in additional information for molecular or ionic crystal structures output by *CrystalGrower*, including: atom types, atom positions, bond types and bond positions within molecular or ionic species. Identically to previous modes, upon reading in the XYZ coordinates file from *CrystalGrower*, the visualiser translates to each position then draws the required species as listed. Molecules are built one atom type at a time, then connected by their interactions. Atoms are constructed as spheres with radii defined by a database within the visualiser for each of the current 118 element types (H – Og), with an additional element “X” for growth modifiers (size based on the radius used for Kr). The radius of each subsequent atom type is larger than the previous by a scaling factor of 20% of the radius of the sphere representing hydrogen. Bonds are constructed using a cylinder or multiple offset cylinders, with end caps drawn as flat disks.

The visualiser currently supports five bond types: single, double, triple, dashed and dotted bonds. By default all bonds are set as single when output from *CrystalGrower*, however users

can edit their .vis files to access the additional bond types for improved visualisation (see Output Files section on .vis files for further details). Aligning bonds along the correct axis requires rotational matrix calculations in addition to translational calculations, increasing the complexity of the visualisation process – which requires some additional computation. This mode offers vast improvements over the average spheres visualisation mode and is well suited for drawing more complex multi-component crystals e.g. MOFs and ionic crystals. This mode can still visualise molecules as average spheres and requires additional data to be output from the *CrystalGrower* simulation package including bond and atom data. Due to this, structures simulated prior to the addition of this mode would require repetition specifying the new output format.

Figure 2 illustrates the general procedure each of these modes follow (molecular average spheres mode skips steps two and three in this procedure). Discussed in greater detail the steps in displaying a simulated crystal are as follows:

1. A data file is read into the visualiser, listing the coordinates of species defined relative to the unit cell origin (scaled to the *a*-parameter of the unit cell). The object is then centred at the origin of the unit cell by subtracting the average of the coordinates (i.e. the central coordinate of the molecule or tile) from all coordinates in the object.
2. An object is constructed using:
 - Polygons for natural tiles, constructed face-by-face (using the GL_TRIANGLE, GL_QUAD, GL_POLYGON and GL_TRIANGLE_FAN commands in OpenGL).
 - Spheres, cylinders and disks for net structure atoms and bonds mode (using the gluSphere, gluCylinder, and gluDisk commands in OpenGL).
3. The constructed object is saved as a display list.
4. Coordinate data along with species type are read in from the XYZ data file output by *CrystalGrower*.
5. The visualiser translates to the listed coordinates, then calls the required display list (tiles and molecular atoms and bonds) or an average sized sphere using gluSphere (molecular average spheres).
6. All of the display lists that are the same object type (but repeated in several locations) are now grouped together as a new display list. This can be thought of as a large display list constructed of many smaller display lists. Each object type in the crystal (e.g. different tile / molecule / atom or bond types) will have a large display list.

7. These large lists (of lists) are all called, combining to construct the full crystal structure and displayed on the screen to the user.

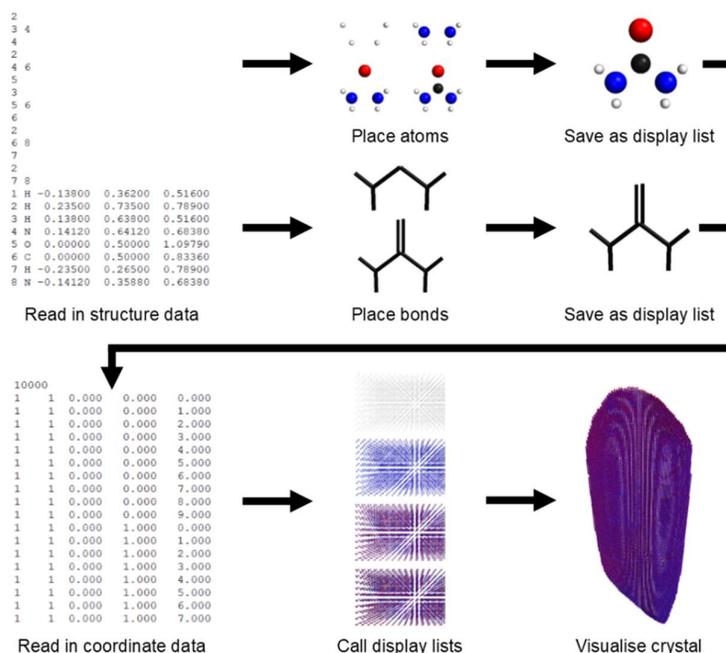


Figure 2: A diagram demonstrating the process for visualising a structure using the molecular (atoms and bonds) operating mode. The coordinates and types for the atoms within a urea molecule are read in, along with bond types between pairs of atoms. This is used to construct display lists for each atom and bond type, which are then saved and called at the locations defined in the XYZ coordinates file. Combining these lists together will result in the full simulated crystal being displayed for study.

All options for loading structures and coordinates are found under the “File” drop-down menu on the visualiser toolbar. The visualiser will automatically detect the type of structure which is being loaded and will use the correct objects to assemble the structure. Clicking the “Load data file” option will open a file explorer dialog box filtering files by the “.vis” file extension allowing the user to locate their data file and load it into the program. Users can then open the “File” drop-down menu again and select “Load coordinates”. Clicking this option will also open a file explorer dialog box, but will instead filter files by the “.XYZ” file extension. All file explorer filtering modes can be disabled by the user if their structure or coordinate files do not possess the “.vis” or “.XYZ” file extension. These can be disabled by clicking the drop-down menu in the file explorer window and selecting the option “All Files (*)”.