

Manipulation of Structures

Structure manipulation: Users can interact with the displayed crystal via the mouse or through a number of hotkeys. The crystal can be rotated, translated, recoloured and in some cases resized to display in the manner required by the user.

Once a structure is constructed and visualised, the user has several options for manipulating the simulated crystal. The user can rotate a crystal in real-time in 3D (provided the simulation is of a reasonable data size), orienting the crystal any required direction (Figure 4, Left). Additionally, the user can translate the crystal along either the X, Y or Z directions to place the crystal in a position they desire and zoom in / out to study features of interest (Figure 4, Right).

By default, the mouse is set in rotation mode, meaning the user can simply click the **left mouse button** and move the mouse to rotate the crystal about either the X or Y axis, or click the **right mouse button** to rotate the crystal about the Z axis. Additionally, the user can use a set of keyboard commands (**UP , DOWN, LEFT, RIGHT, + or – while holding SHIFT**) to rotate by 5 degree increments about the X, Y or Z axis. By holding **SHIFT, CTRL or both of these keys simultaneously**, the user can control the size of the rotational increments. Keyboard commands exist for translational operations (**W, A, S, D, Z and X** – for the X, Y and Z directions, respectively), including the ability to change the translational increments by holding **SHIFT, CTRL or both of these keys**. A full summary of key bindings can be found at the end of this manual section.

In addition to the default mouse mode (rotation), the user can change the mouse mode to translation or scale mode. By selecting translation mode, holding the left mouse button and

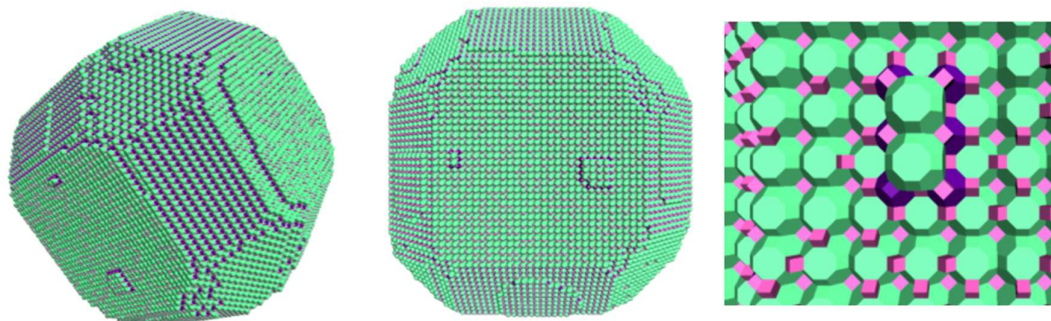


Figure 4, Centre: An LTA crystal located at the default viewing position, along the z axis at an automatically calculated distance. **Left and Right:** The same LTA crystal rotated in 3D space, and translated along the X, Y and Z axes.

moving the mouse will translate the crystal along the X or Y directions. Scale mode will instead translate the crystal in the Z direction while the left mouse button is held, allowing the user to zoom in or out using only the mouse. Mouse mode options are located in the “Mouse Mode” drop-down menu on the visualiser toolbar. An additional rotation option which uses a quaternion instead of Euler angles is available if users select “View > Enable Quaternion Rotation”

The user also can set the boundaries of the screen buffers, deciding how far backwards and forwards the buffer zone extends. This effectively decides the distance an object can extend in the Z direction before being cut off, either towards the screen (the near buffer) or extending away from the screen (the far buffer). These buffers are controlled independently giving the user more options for displaying their simulation results (Figure 5). The far buffer can be moved closer or further away from the screen with **CTRL + SHIFT + J** and **CTRL + SHIFT + K** respectively, whereas the near buffer can be moved closer or further away from the screen by pressing **CTRL + SHIFT + N** and **CTRL + SHIFT + M** respectively. Many of these options were inspired by the controls available within VMD (Visual Molecular Dynamics).⁶

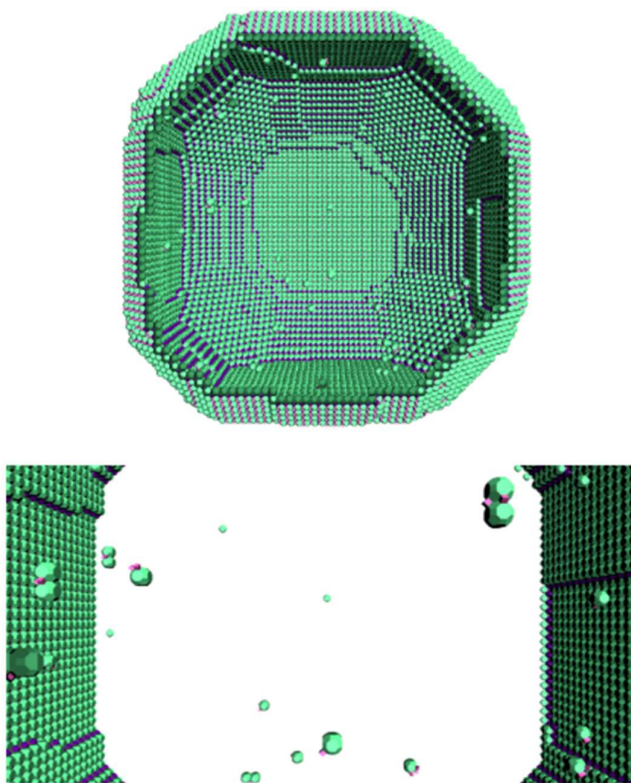


Figure 5, Top: An LTA crystal with the near screen buffer moved to cut off a portion of the crystal nearest the screen. **Bottom:** The same LTA crystal, zoomed in through the front face of the crystal, with the far screen buffer moved to cut off a portion of the crystal far away from the screen.