

Object Selection and Status

Selecting objects: The visualiser contains functions where species types can be selected and their display can be modified by recolouring, resizing or hiding the species type completely.

By using the SPACE key, the user can cycle between selecting objects displayed on the screen. Repeated presses of the SPACE key will switch between objects by their type, i.e. the first press would select all objects with an assigned type of 1, then type 2 and so on. Selected spheres and tiles are displayed in grey / black on the screen (Figure 9, Top), distinguishing them from other species. Cycling selections with the SPACE key can be used with type, layers and atom and bonds drawing / colouring schemes. Once an object is selected the user can perform several actions, including use of the previously discussed colour picker tool to change a single species' colour. When visualising a structure in molecular (atoms and bonds) mode, the user can also cycle through each bond type that appears by holding SHIFT and pressing SPACE. Selected bonds are highlighted in pale grey to distinguish them from the usual black bonds.

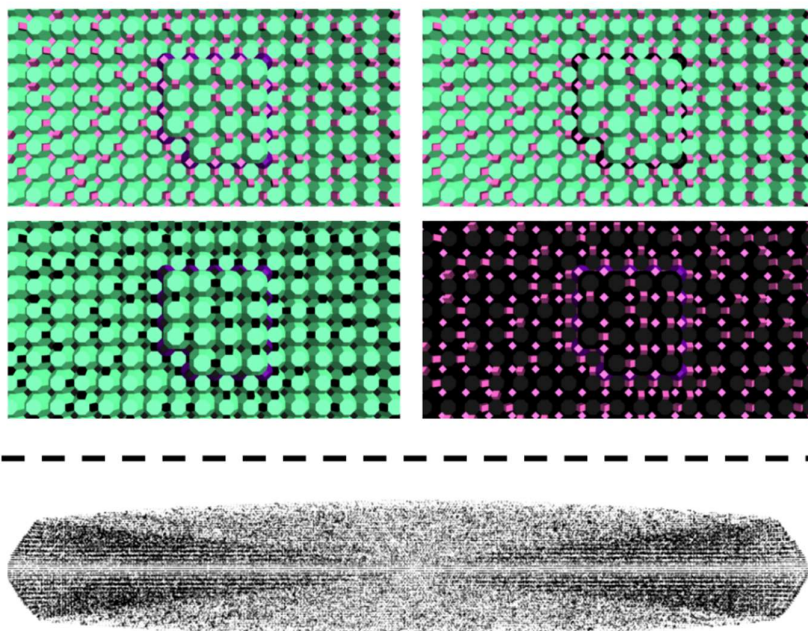


Figure 9, Top, Clockwise from Top Left: An image of an LTA crystal with no species selected, with all t-toc selected, with all t-grc tiles selected, and with all t-cub tiles selected. **Bottom:** An MFI crystal where only one tile type is selected and displayed. Only incomplete tiles will appear in the visualiser, as bulk (fully condensed) tiles are omitted. An hourglass-shaped zoning of defects can be observed.

Selected objects can be toggled on or off by pressing the E key. It will however appear to stay toggled on and displayed in grey / black until the object is deselected or another object is selected. All objects can immediately be toggled off with CTRL + SHIFT + G and toggled on with CTRL + SHIFT + F. Pressing CTRL + SHIFT + SPACE will immediately deselect all objects on the screen, returning the user to the beginning of the selection cycle on both bonds and other objects. Toggling off all objects then cycling through the selection of single species is a useful tool for locating incomplete species within crystals, e.g. hourglass shaped zoning of defects was discovered in the MFI framework in this manner (Figure 9, Bottom). Additionally, this method can be used to locate species that terminate terraces on the crystal surface.

The text overlay will display information about which species are currently selected in the centre of the screen. This label will change dependent on the type of species loaded, along with the total number of species in the system. For atoms and bonds, the element type that is currently selected will be displayed.