

Simulation States and Reset Commands

Saving states and resetting: Custom visualiser states allows users to save their work on recolouring and manipulating the displayed crystal. These states can be loaded later when revisiting the structure, or be used as good starting points for movies. Reset commands are available to quickly restore the display to its default state.

Due to the effort required to orient a simulated crystal in desired positions for image recording, a feature was added to save custom simulation states. This feature grants the user the ability to save all details from a state (or scene) for a single simulation and load it at will. Details recorded include: rotation angles in degrees (for X Y and Z), translation values (also for X, Y and Z), colouring mode selection, custom colours and custom sphere scaling values. Users are able to record any number of states for any given simulation; however, states recorded for one simulation can only be used with simulations of the same structure type i.e. if the data (.vis) files are identical for a both simulations. Structures are considered as identical if they have the same structure file generated from ToposPro and have been run in the same simulation mode. For example, a “growth modifier” simulation would have a slightly different .vis file to a “normal” simulation even with the same ToposPro structure file, as the former accounts for the additional modifier species in the system.

Options for saving and loading custom states are found under the “File” drop-down menu on the visualiser toolbar. State files are saved with the “.stat” file extension to reduce clutter when searching for states to load, and are filtered by this file type when selecting “Load State”. As with other file explorer menus, this filter can be removed by clicking the drop-down box listing

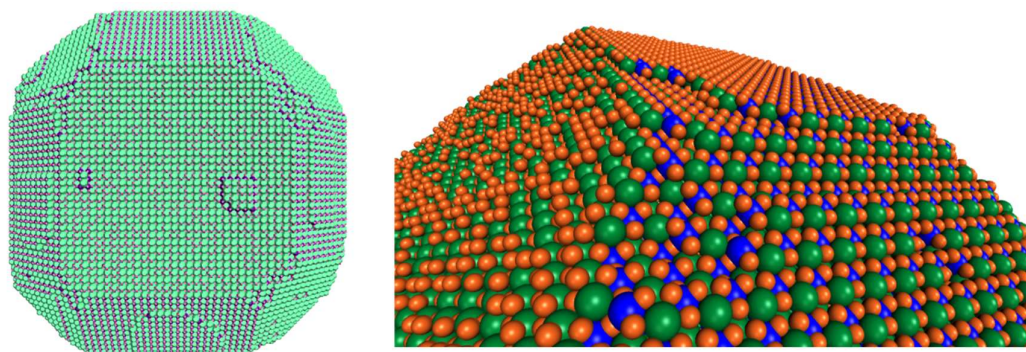


Figure 12, Left: An LTA crystal rendered in the visualiser with all settings set to system defaults.

Right: The same LTA simulation with custom colours, sphere scaling, viewing settings all saved as a custom state that can be loaded at will.

“.stat” and selecting “All Files (*)”. This tool is useful for all types of simulations, as users can find areas of interest on their simulated crystals, save them for later and revisit them at will. An example of a saved state is shown in Figure 12.

Reset commands have also been added to the visualiser toolbar under the heading “Reset”. The user can reset all translation values to zero by selecting “Reset > Reset View > Reset Translation” or all rotation values to zero by selecting “Reset > Reset View > Reset Rotation”. Options also exist to reset all sphere and bond scaling to their default values “Reset Sphere + Bond Scaling” and to reset depth buffers to their starting positions “Reset Depth Buffers” without changing any other parameters. Users can decide to reset all simulation parameters to their starting values with “Reset All Parameters”.

Finally, users can use the keyboard shortcut CTRL + SHIFT + R to reset the simulation view (rotation and translation) to their starting values. This differs to the “Reset Translation” and “Reset Rotation” commands as the parameters are not reset to zero but to the values calculated upon loading the simulation.