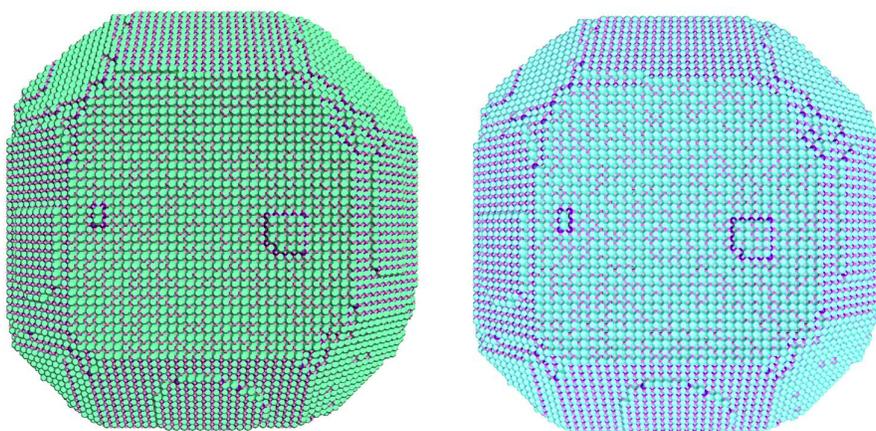


## Lighting

**Lighting controls:** Two lighting schemes are available in the visualiser which can be controlled by the user. Lights can be turned on or off within their schemes.

Lighting is crucial for improving the look of visualisation programs. Usually divided into the categories of diffuse, specular and ambient, the balance between these types of lighting affect the colours displayed on the screen and give an element of depth to a 2D projection. Diffuse and specular lighting both correspond to light that comes from a directional source, whereas ambient light has no directional source and instead illuminates equally in all directions. Specular and diffuse light differ in their reflective properties; specular light will reflect primarily in one direction, while diffuse light will reflect equally in all directions.

Within the visualiser, species colours are generally defined by the diffuse light they reflect, with the colour reflected being the colour that appears on the screen. Specular light is used to give the white “shine” effect seen on objects when rotated towards a light source e.g. the shine from a snooker ball. Ambient light is used sparingly within the program, as raising it too high will give everything a washed-out look. Lights in OpenGL can be treated as points with X, Y and Z coordinates, or treated as directional sources where the light position is defined simply as a vector (effectively placing the light source at a distance of infinity).



**Figure 11:** An LTA crystal displayed in the visualiser with differing lighting schemes. **Left:** The “standard” lighting scheme, generally giving the best results. This scheme was primarily inspired by VMD’s lighting settings. **Right:** The more blue-toned “3dt” scheme inspired by the 3dt program settings. Each scheme has four and three toggleable lights, respectively, along with an additional weak light coming from behind the crystal, to eliminate shadows caused by incorrect normal direction calculations.

Two separate lighting schemes exist within the visualiser. The first scheme was inspired by the lighting settings in VMD, which uses 4 directional light sources that are all coloured white. The second scheme was inspired by the settings found in 3dt, which instead uses three directional sources with one light causing the structure to exhibit a blue glow. All lights in the same scheme can be switched on or off independently, however lights from both schemes cannot be mixed. This is due to OpenGL possessing a limited number of lights that can be assigned.

In addition to the four or three light sources, both schemes possess an additional “lighting correction” which is a weak light source shining from behind the crystal. This correction is used to light some tile surfaces with negative curvature that are frequently entirely in shade, which can give the visualised structure undesired strips of shadow running the entire length of the crystal. All lighting options are controlled through the “Lighting” drop-down menu on the visualiser toolbar. Options for each lighting schemes are separated into further drop-down menus under the options “Standard” and “3dt”. A comparison of the available lighting schemes is shown in Figure 11.