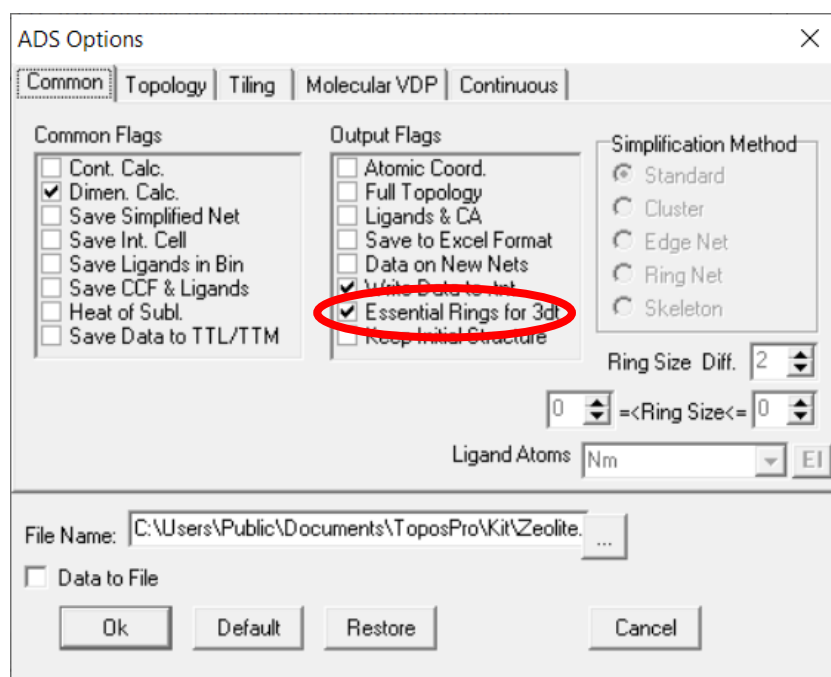


Visualising Tiles with *3dt*

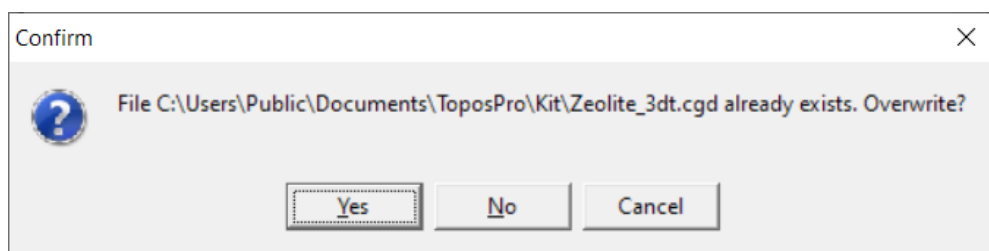
This step-by-step guide will demonstrate how to visualise tile based structures using *3dt*. This can only be used for frameworks where a tiling is calculated i.e. “tile” structures but not “net” structures.

3dt is a visualisation package hosted at <http://www.gavrog.org/>, developed by Olaf Delgado-Friedrichs which visualises tiles and produces very high quality raytraced images for presentations and reports. Enabling certain options in *ToposPro* will output data in the correct format for *3dt*.

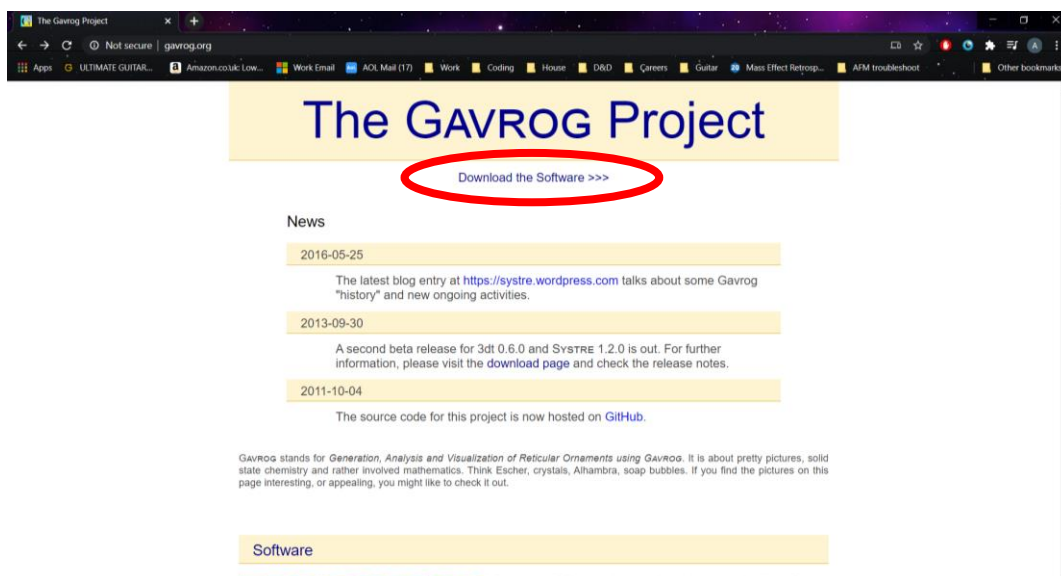
- 1.) Ensure that “Essential Rings for *3dt*” is selected in the ADS options before calculating the tiling.



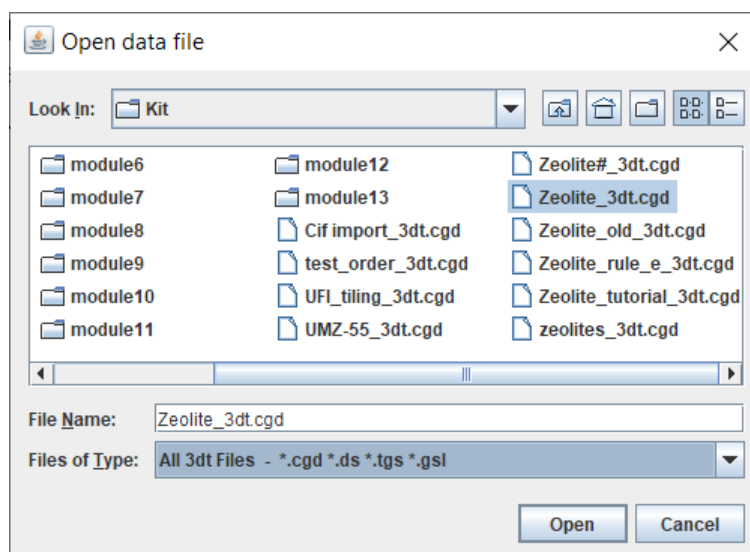
- 2.) After pressing OK and Run to calculate the tiling, a prompt will appear to overwrite the *3dt* file (DatabaseName_3dt.cgd):



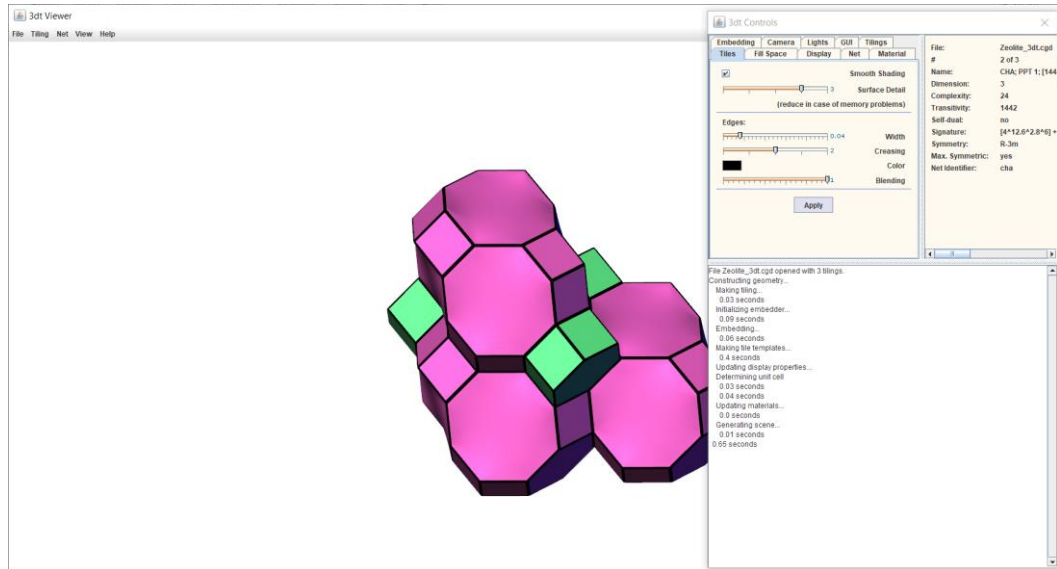
- 3.) Choose “Yes” to completely overwrite the file, or “No” to append the structure to the end of the file. Selecting “Yes” will result in a *3dt* file with only one framework, whereas selecting “No” will result in a *3dt* file containing multiple frameworks which can be switched between.
- 4.) Install *3dt* if it is not installed yet at <http://www.gavrog.org/>. A Java installation is required to run this software.



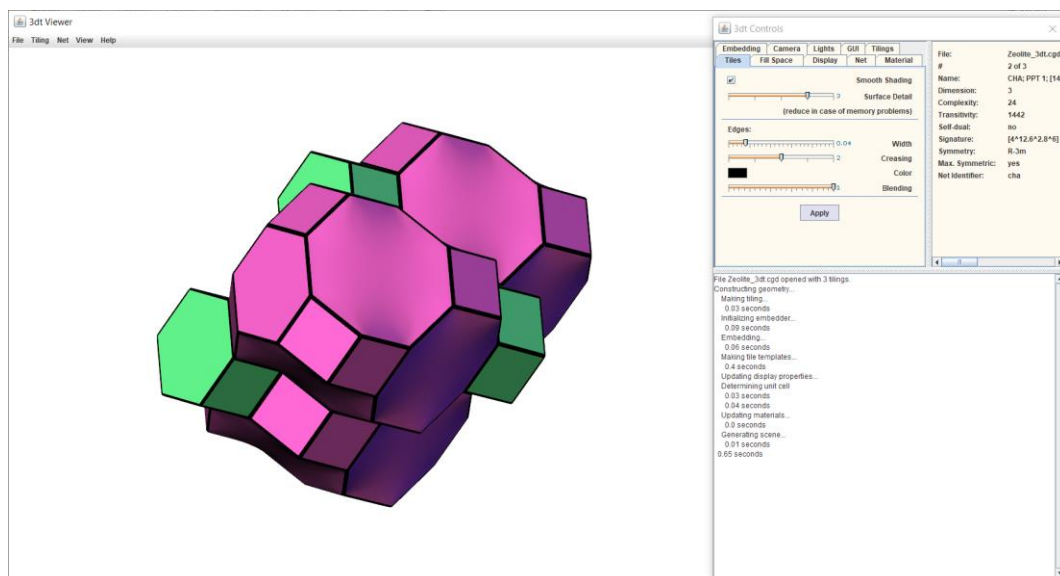
- 5.) Open *3dt*, and use File > Open to find the *.cgd* file generated by *ToposPro*. It will be located in the same folder as the database the tiling calculation was performed in. Filter by “All 3dt Files” to make it easier to locate the file.



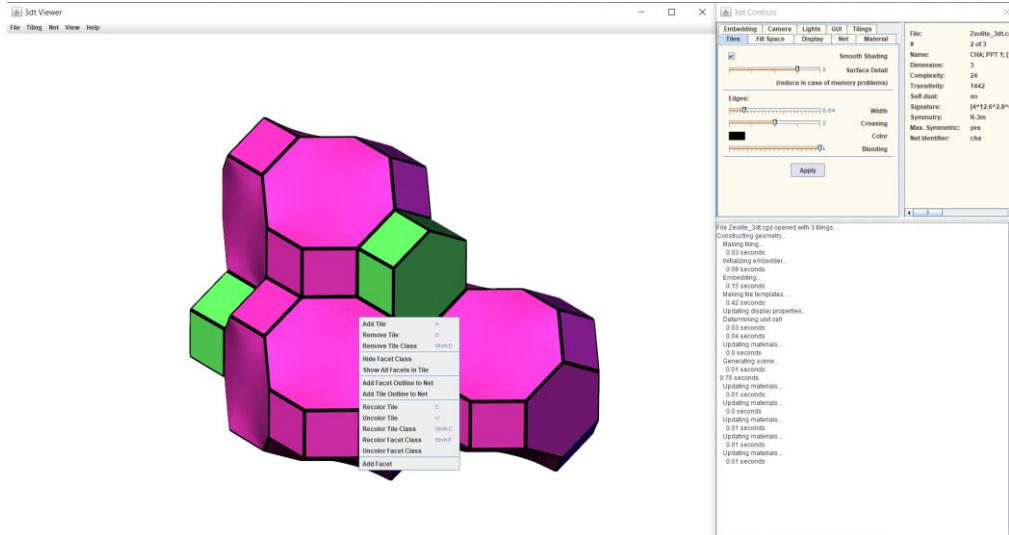
- 6.) Press Open. If the file contains more than one structure or tiling a menu will appear asking which tiling to open first. A valid response is either the tiling number or structure name: e.g. 1 to open the first tiling in the file, or CHA to search for the CHA framework tiling. The tiling will then be displayed:



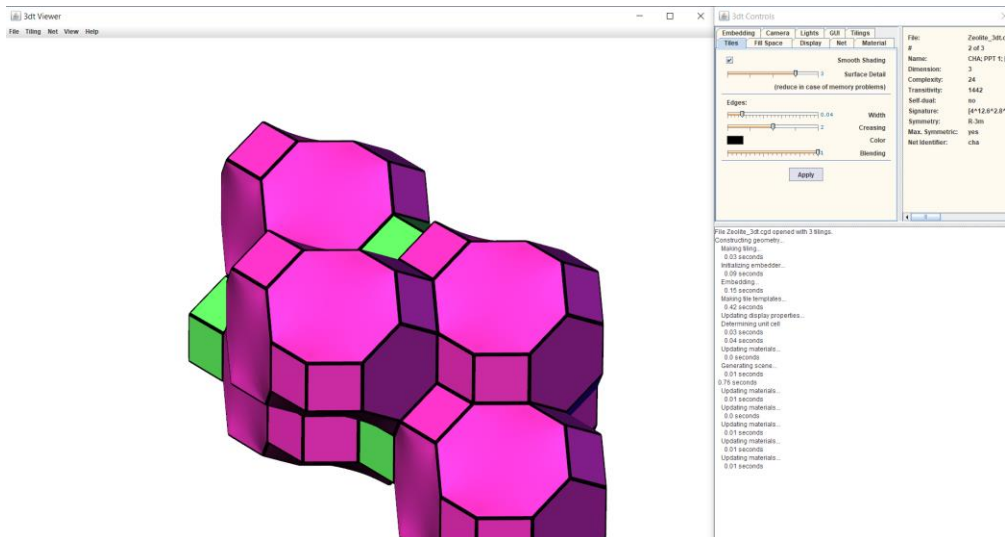
- 7.) Once displayed, the framework can be rotated by left clicking and moving the mouse. Zoom in and out by scrolling the mouse wheel or stretching with two fingers on a trackpad. The framework can also be translated around the screen by holding ALT and left clicking, or by holding the middle mouse button and moving the mouse.



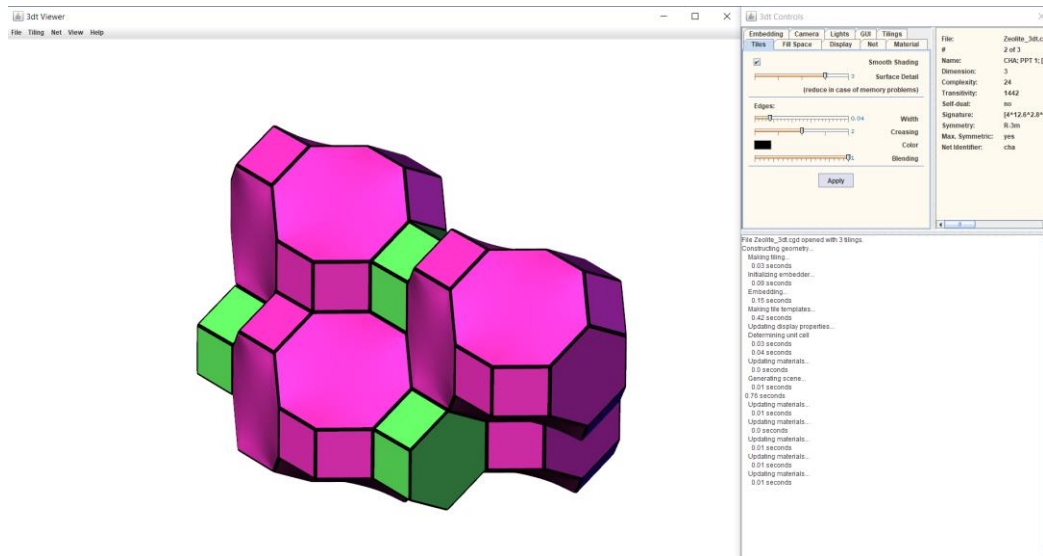
- 8.) Right-clicking a tile results in a pop-up menu appearing, displaying a number of commands that can be used. These include adding and removing tiles, recolouring tiles, removing facets etc.



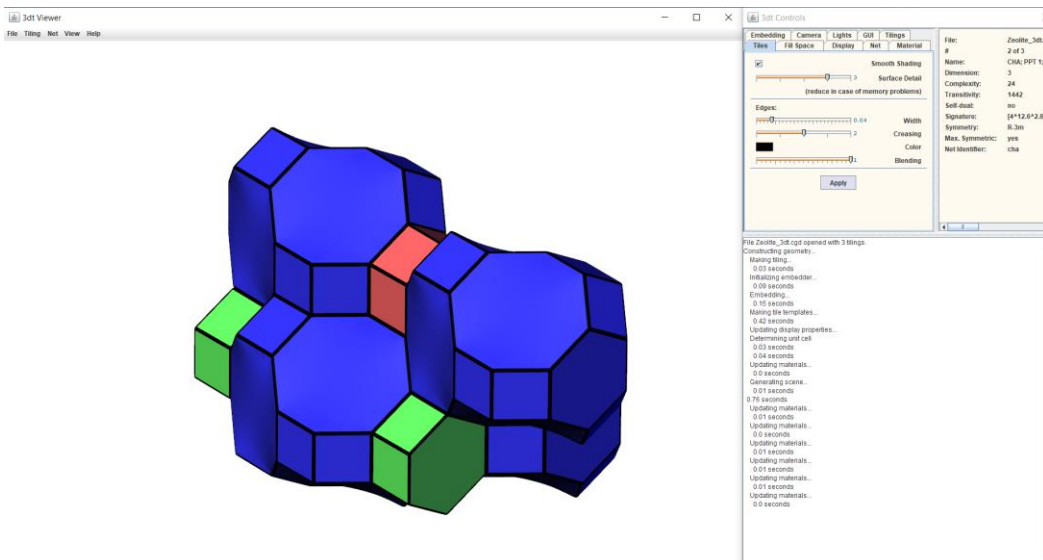
- 9.) Right-clicking and selecting “Add Tile” or pressing A on the keyboard will result in the tile that is connected through the selected face appearing. This process can be repeated to add more and more tiles to the display:



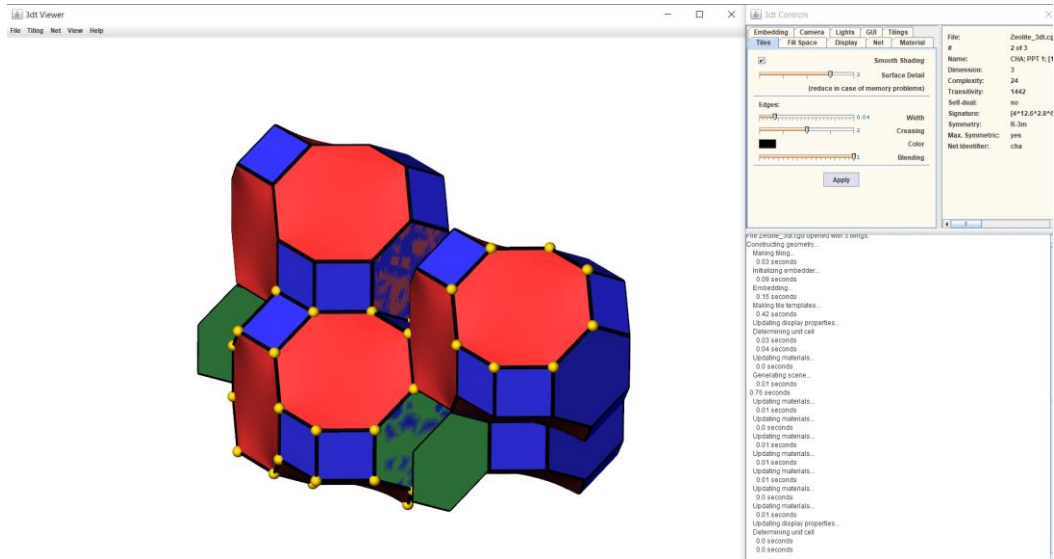
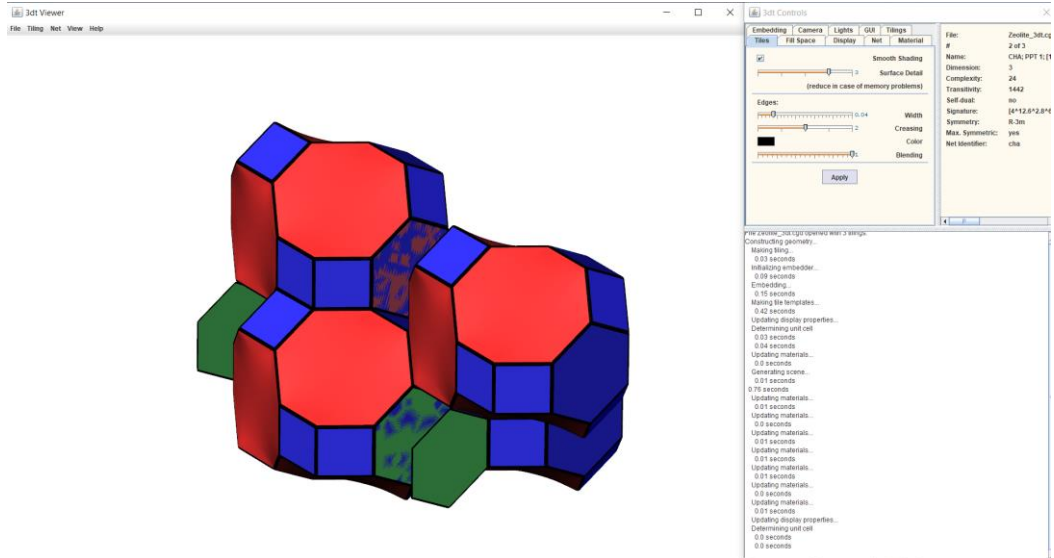
- 10.) Right-clicking and selecting “Remove Tile” or pressing D on the keyboard will delete the selected tile from the display.



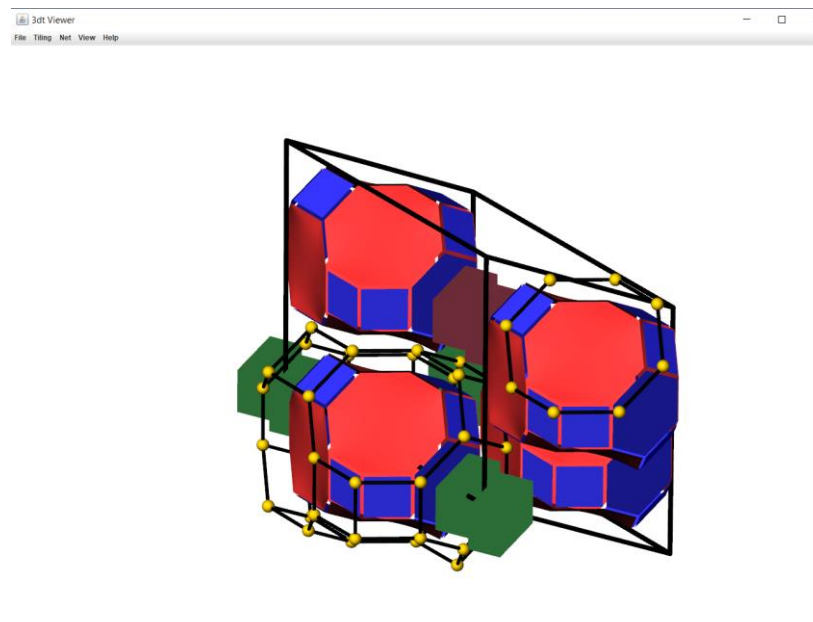
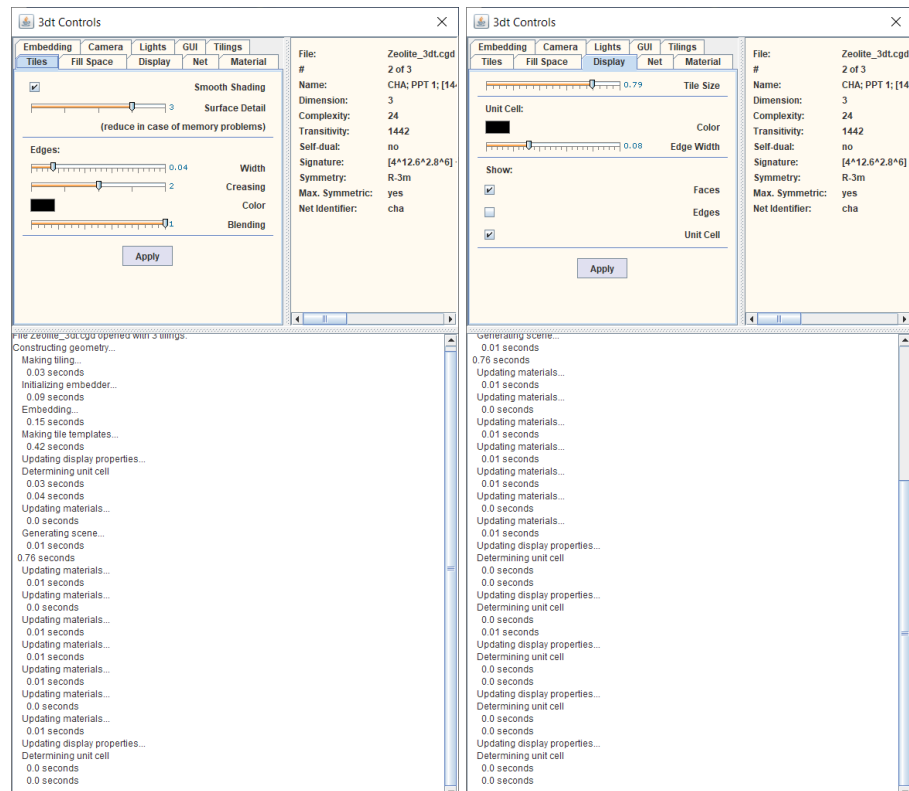
- 11.) Right-clicking and selecting “Recolor Tile” or pressing C on the keyboard will open a colour menu to recolour the selected tile. “Recolor Tile Class” or SHIFT+C on the other hand, will recolour all tiles of the same type simultaneously. Tiles can also be “Uncolored” where they are set to a white / grey colour.



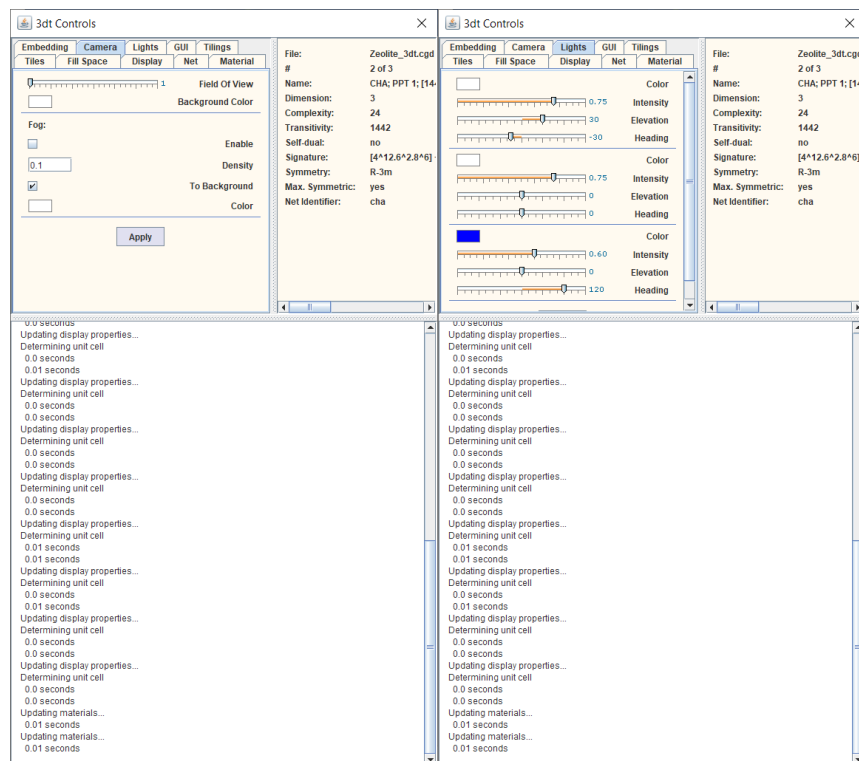
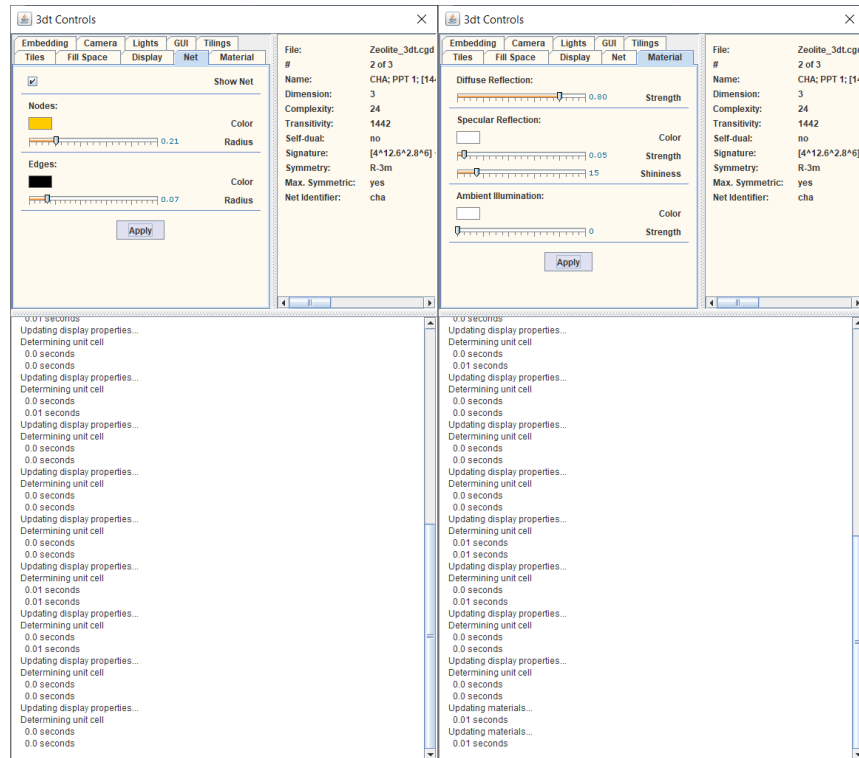
- 12.) Users can also hide, show or recolour certain classes of tile facets / faces. A facet class is a group of facets that are related by symmetry. There are also options to add a crystal net around facets or the tile as a whole. Facet classes can also be “Uncolored” where they are set to a white / grey colour.



- 13.) Moving to the *3dt* controls screen, there are a number of pages for altering how a material is displayed. The “Tiles” window allows users to change the face detailing of tiles along with how tile edges are shown. The “Display” window also has some useful options such as “Tile Size” where users can shrink tiles so they don’t totally fill the space in the structure, along with adding in the unit cell shape. Any changes made in the controls window require pressing the “Apply” button before they are displayed.

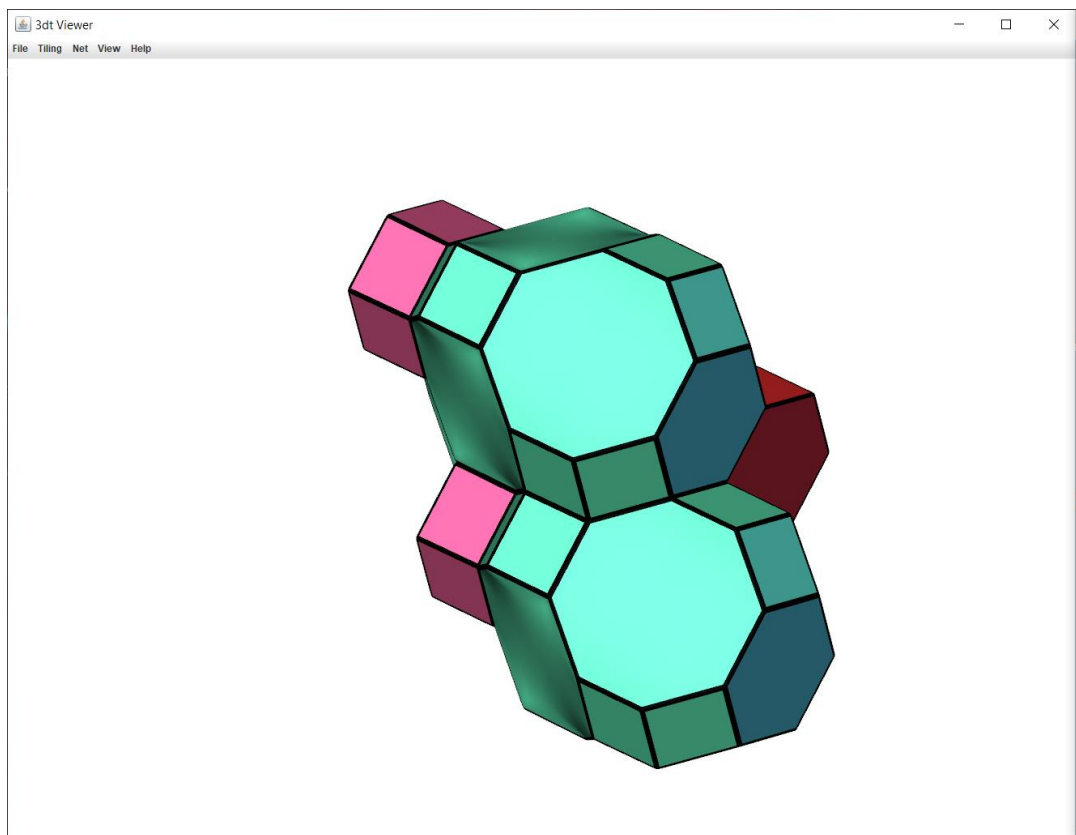


- 14.) Net, Material, Camera and Lights are also useful tabs of the controls window. “Net” allows users to control the display of the nodes and edges of the crystal net, “Material” allows users to alter the reflective behaviour of the tile surfaces and “Camera” gives control over the field of view and background colour, along with adding fog to give an illusion of depth. “Lights” gives control over the multiple lights that give *3dt* its distinct display, light position and colour can be altered.

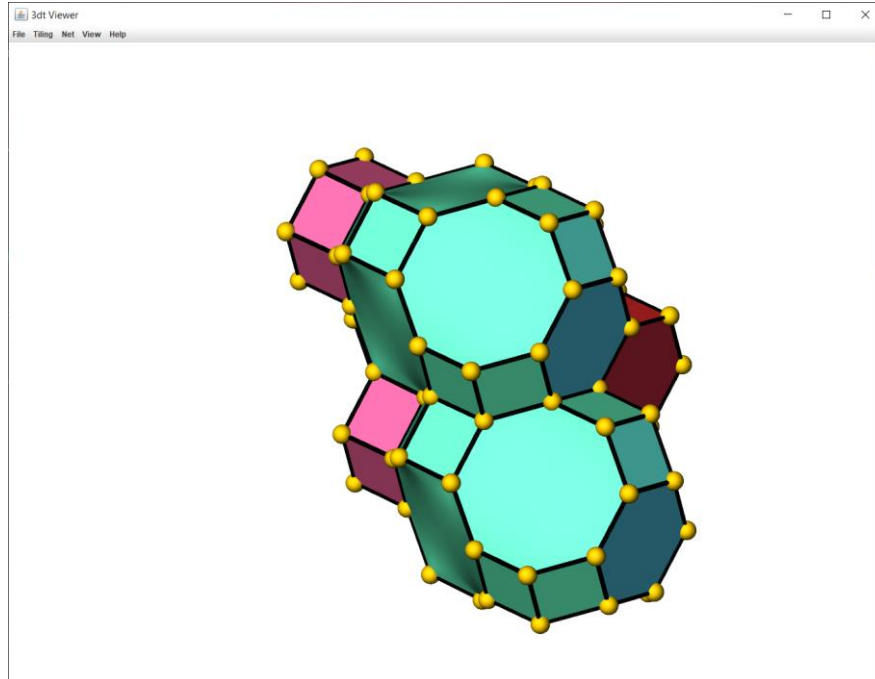


- Bear in mind the different types of light – ambient light is lighting that comes from all directions with no particular source, specular light is light that is reflected predominantly in one direction (e.g. the shiny spots on a snooker ball) and diffuse light is light that is reflected in all directions (i.e. diffused, like the colour from the rest of a snooker ball).

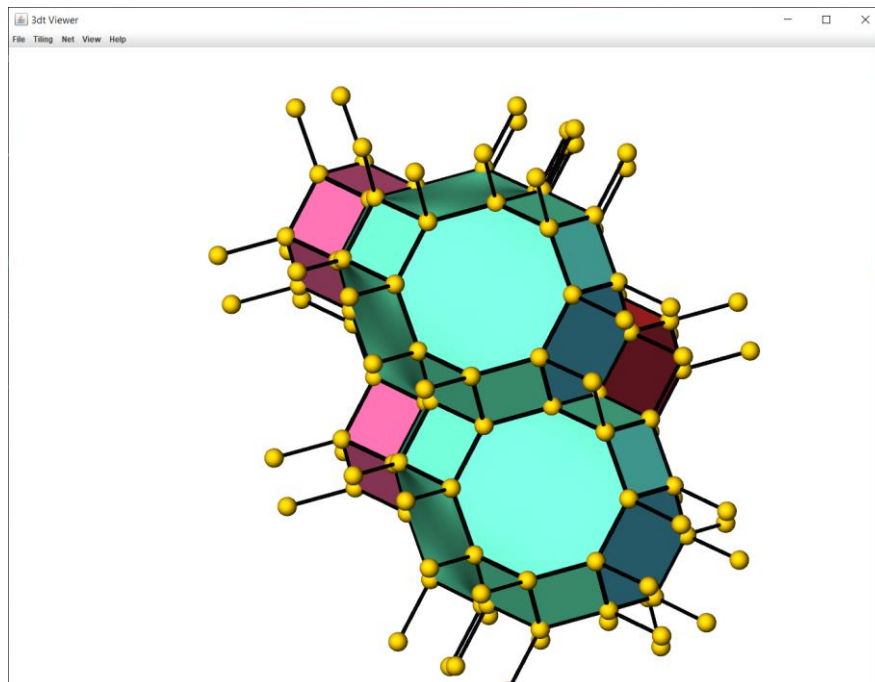
15.) Moving back to the *3dt* window, users can use the “Tiling” drop-down menu to change the structure displayed on the screen. Selecting “This” or pressing T on the keyboard will reload the current tiling, selecting “First” or pressing F on the keyboard will jump to the first structure in the *3dt* file while “Last” or L will jump to the final structure in the file. Selecting “Next” or N on the keyboard and “Previous” or P on the keyboard will skip back and forth between the structures in the file. Users can also jump to a particular structure number with “Jump To...” or J and search for a structure name with “Search...” or CTRL+F. Users can also switch to the dual net of the tiling (where centres of the tiles become vertices) with “Dualize”, or convert the tiling to its maximum symmetry with “Max. Symmetry”. Finally, “Recolor” will cycle through colour schemes for the tiling.



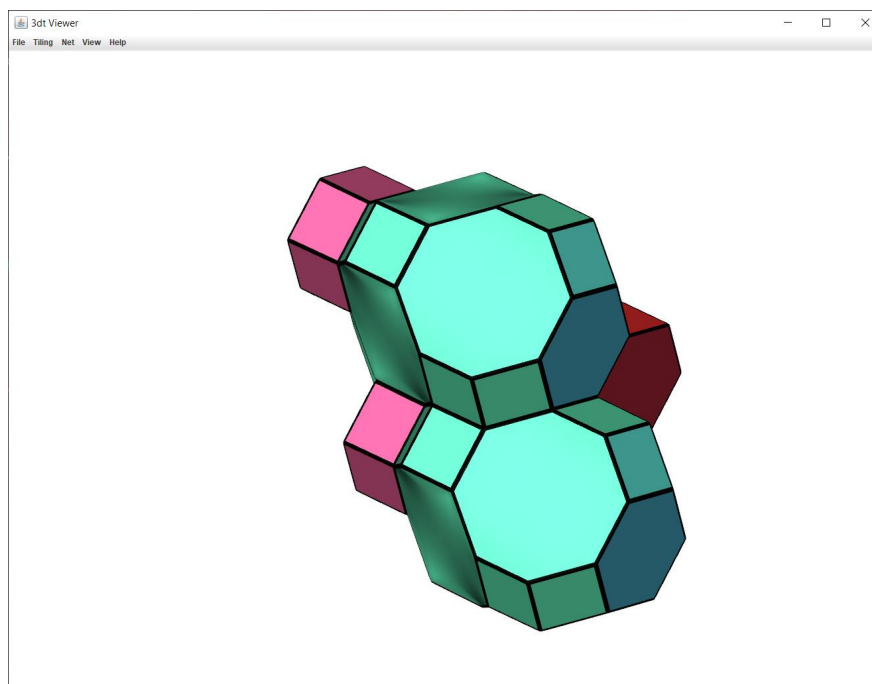
- 16.) The “Net” drop-down menu allows users to add a crystal net on top of the displayed tiling by selecting “Update Net”. Using the net options in the controls window and the right-click shortcuts make it easy to display the net exactly how it is required.



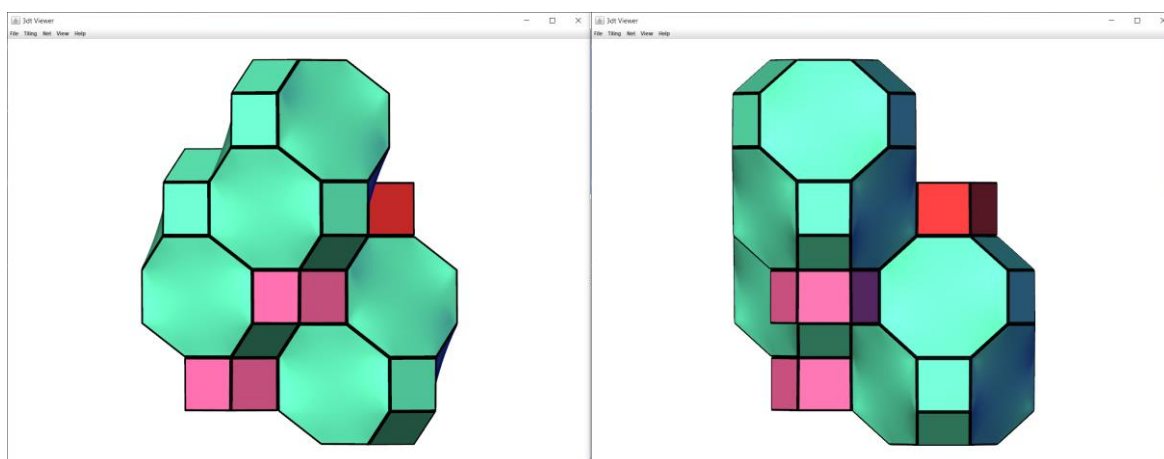
- Selecting “Grow Net” or pressing G on the keyboard will display the next connection from each of the currently displayed net nodes.



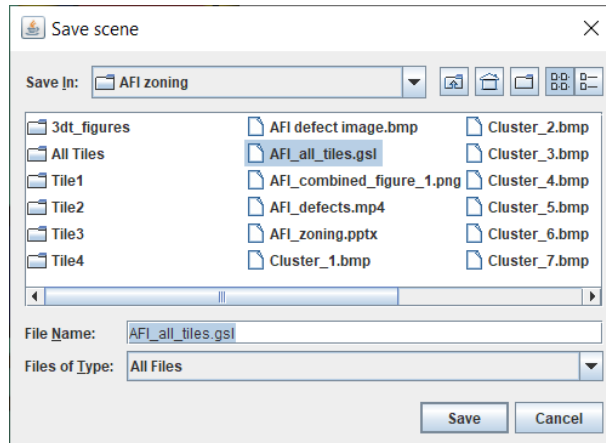
- Selecting “Clear Net” will remove the net completely.



- 17.) Selecting the view drop-down menu will display several options for setting the viewing angle of the displayed tiling. Users can select the principle XYZ directions, along with common Miller indices such as $[011]$ and $[111]$, and can choose to rotate the structure with buttons instead of using the mouse.



- 18.) Users can save all the operations they have performed on a structure in *3dt* to be used later. Selecting “Save Scene” or “Save Scene As.” will open a saving window to create a .gsl file – a Gavrog scene file which can be opened at any point in *3dt*. This will contain all the colouring, net and view options and load them immediately. Users do not need to load the tiling (.cgd) file before loading the .gsl file.



- 19.) Once the tiling is displayed in the desired way, users can save an image using *3dt*'s built-in raytracing routine. Raytraced images are very high quality images that are a great addition to any presentation or report discussing framework / tile structures. Press File and “Raytraced Image” or CTRL+R on the keyboard to start the image generation process. Specify the dimensions, format and save location desired for the image and press Save. This will then open a window showing the image being composed one segment at a time.



- 20.) Once the image is generated, it can be inserted into any report or presentation like a regular image. Note that the raytraced image can look slightly different to what is displayed in *3dt* as more complex lighting and shadow calculations are performed during raytracing, hence why the saving period can take a few seconds. The final image will look something like the following:

