High-Throughput Processing

High-Throughput: A number of functions are built into the visualiser to assist with the processing of a large number of coordinate files. These operations can be used to automatically process large volumes of data while users perform other tasks.

Due to the vast quantities of simulations conducted when studying various combinations of energy values during crystal studies, the visualiser was designed to contain a method for high-throughput screening of results. After conducting the data file loading stage of visualisation, users can select "File > Process a Directory > Single Images" to engage high throughput mode. Selecting this option will open the usual file explorer window seen when loading simulation (.XYZ) data files. Once a file is selected however, the visualiser will automatically scan through every simulation data file within the specified folder and take a single image with the same simulation parameters for each file. For this to occur automatically, all simulation files within the folder must have identical data (.vis) files – the same rules apply as for sharing state files. As the visualiser takes an image with the same parameters for each simulation file, it is generally recommended for users to open a single simulation file first and tune all parameters to their desired values before selecting the "Process a Directory" option. Simulations files with multiple frames will execute the "Save All Frames" command when loaded into the visualiser using this method.

Users can also specify for a short movie of the crystal rotating around the X, Y or Z axes to be recorded in place of a single image by selecting the "Process + Rotate Movie" option in the "File" drop-down menu. Rotation movies generated through this method will only be
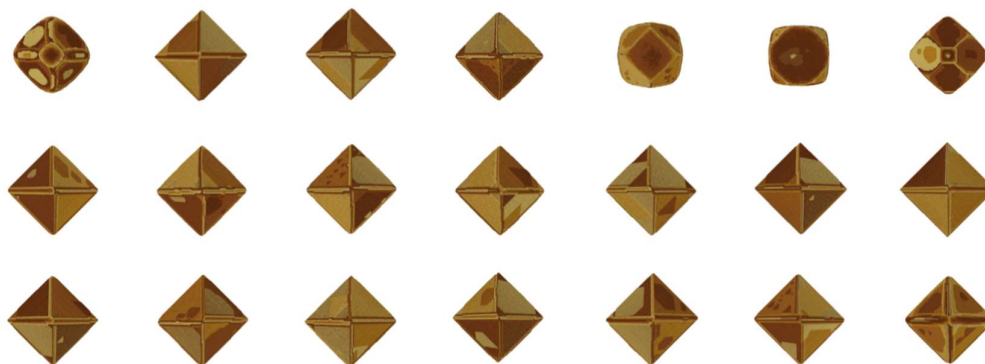

Figure 15: Images taken using the high-throughput processing mode within the visualiser. All images are separate simulations of FAU with varying energies for tile condensation, resulting in differences in crystal morphologies and surface structures.

constructed of 9 frames, due to file space constraints when managing a large number of separate simulations. For multi-frame simulations, these images will only be collected for the final simulation frame to limit the amount of data produced (e.g. a 50 frame simulation capturing 9 images per file would create 450 images if this did not occur).

A further option for users to select for high throughput processing is found under "File > Process a Directory > Cycle Species Types". This option performs similarly to the high throughput function for taking single images of simulations, but will cycle between displaying single species types (tile types, molecule types or atom types) sequentially, recording an image for each. This function is useful for locating internal defects such as the hourglass zoning seen in MFI in Figure 9. The same thing will occur for multi-frame simulations as for the rotation movies, the visualiser will skip to the final frame then take the series of images.

Images taken using high throughput processing of a large set of FAU crystal simulations are shown in Figure 15.