Drawing Modes

Drawing modes: The software is capable of displaying simulation results as natural tiles, spheres and atoms / bonds (for net structures). Drawing modes can be switched at will by the user.

Additional drawing modes are available within the visualiser for each of the operating modes discussed in the previous section. These methods are accessed through the “Drawing” menu on the visualiser toolbar.

Tiles mode either displays tiles as polygons (the default method discussed in the previous section), as spheres with radii defined as the root mean square of a tile’s vertex coordinates, as spheres with a radius equal to the average of all root mean square radii across all tiles, or as points (3, Top).

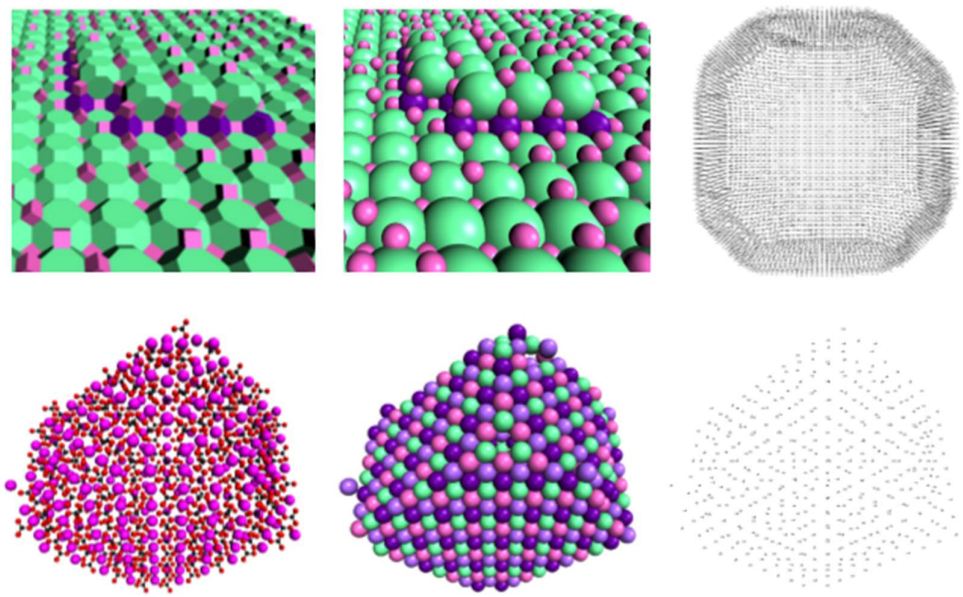

***Figure 3, Top**: Three different drawing modes for a crystal of the zeolite LTA, all using the tiles operating mode. **From Left to Right**: Natural tiles, spheres with radii calculated by the root mean square of all a tile’s vertices, and points at the centre of each tile. **Bottom**: Three different drawing modes for a small calcite crystal, all using the molecular (atoms and bonds) operating mode. **From Left to Right**: Molecules with atoms and bonds displayed, average spheres at molecule centres, and points.*

Net (average spheres) mode is only capable of displaying species as average spheres or points, whereas net (atoms and bonds) mode displays molecules as atoms and bonds, as average spheres or as points (Figure 3, Bottom). All options related to drawing modes are found in the “Drawing” drop-down menu on the visualiser toolbar. Options are enabled or disabled depending on which structures type is loaded. All options available for tile structures come under the “Tile Crystals” submenu under the “Drawing” menu, while all options available for net crystals are shown under the “Net Crystals” submenu.