# Tile vs. Net

Is this a tile or net simulation?: "net" means that the structure is built of single units that are linked together (suitable for molecular and ionic crystals, MOFs and metals). In this case a new tab [Net Options] appears. "tile" means that the system is built from 3-dimensional tiles (suitable for zeolites and framework materials). In this case a new tab [Tile Options] will appear where information about the energies of the tiles can be entered.

"net" and "tile" are the two procedures within *CrystalGrower* used to assemble partitioned crystal structures when simulating crystal growth. Both refer to the methodology used to partition crystal structures using the *ToposPro* software.
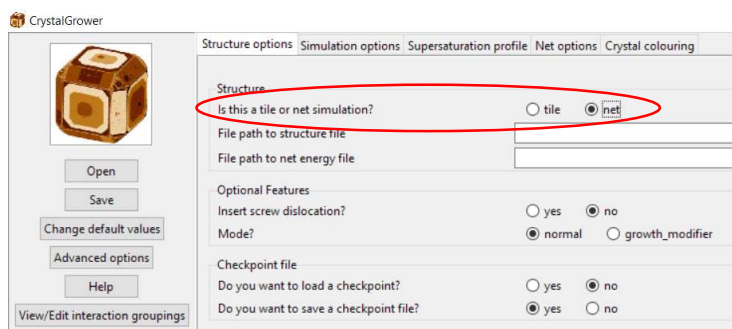
"net" refers to the use of a simplified net, where each species in the system (e.g. a molecule or ion) is simplified to be represented as a single centroid (the node of the simplified net). Interactions between neighbouring molecules are recorded from each centroid to centroid (the edges of the simplified net). *ToposPro* retains the connectivity of the original net, which is also reproduced in the structure file, allowing users to investigate the local connectivity (i.e. atom to atom connections) which form the neighbour to neighbour interactions. "net" structures require the use of an additional file (the net energy file or net.txt, discussed later) to assign energies to the neighbour to neighbour interactions. This methodology is suited for the majority of structures aside from the exceptions mentioned for use with "tile" structures.
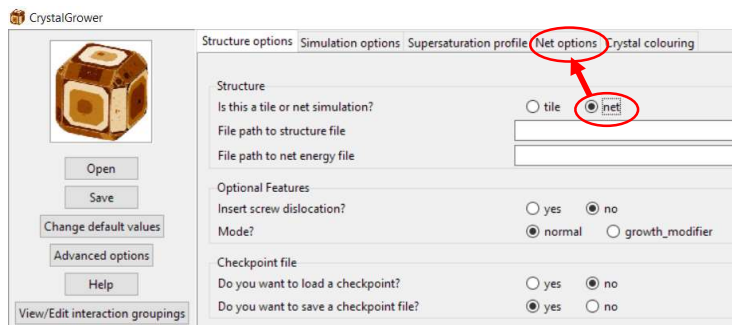
"tile" refers to the use of natural tiles (or in some cases modified natural tiles) to partition structures. Natural tiles are space-filling three-dimensional polyhedra that follow a set of mathematical rules. These are also calculated using *ToposPro,* although a different procedure is used in place of the simplified net calculation. This methodology is best used for zeolites and framework materials (e.g. SAPOs, AlPOs and MeAPOs) due to their assembly from cage structures.
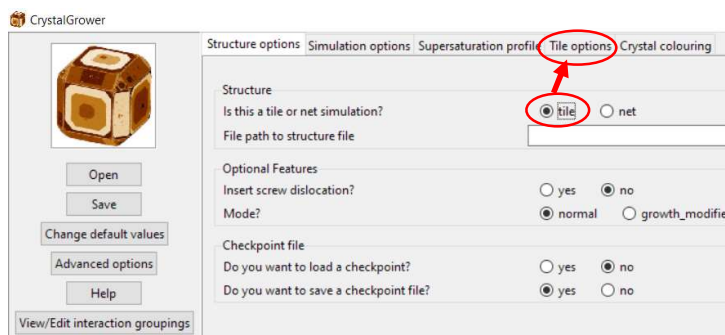
See the detailed manual sections on input files and *ToposPro* for more information.