Ordered Structure Energy Penalty

Energy penalty associated with ordered structure [kcal/mol]: this option will only appear if an "ordered" structure is selected in the previous question (currently under development). The value entered relates to the difference in energy of crystallisation for different components in a tile simulation – for example Al vs Si insertion in a zeolite structure.

This location is where the energy penalty is implemented for a specific element type within an ordered tile structure. The energy input here is a scaling factor which is multiplied by the condensation energy for a tile vertex occupied by the chosen atom type. The condensation energy for tile vertices is specified in the Tile options tab in the user interface.