LatticeMaker Bond Building.

This version of LatticeMaker will optionally create bonds between atoms in the lattice. The methods used by LatticeMaker to create bonds are flexible enough to cope with most bonding situations. For a lattice which contains only one atom type (for example Si) the simplest bonding scheme is to use nearest neighbour bonding, with a suitable distance selected. The bond distance is limited to 10Å (as no real bonds would ever be this long). The maximum coordination number of each atom is currently fixed at 8 bonds. If the number of bonds exceeds 8 then any extra bonds are ignored. If you wish to build a lattice which contains more than one atom type and only hetro-nuclear bonds are allowed then using the atom filters option allows the user to selected allowed bonding combinations. Select the atoms which you wish to make bond to from the left hand list. Then select from the right hand list (shift-clicking if necessary) the atoms you want to bond to. After you have made you selection press Save to remember your selection. Repeat this for all of your atoms. The final option which allows more control over bond formation is to use the ionic radii as a bond distance parameter. When this option is chosen the value in the bond length text box is ignored, and a value equal to the sum of the radii of the two atoms to be bonded is used as the bond distance. The radii of atoms can be changed by using the Ball and Stick colour picker   or by editing the Preferences file with ResEdit. This is described on the next page.