- **Sort the atoms into bins**
    - Collect all data into a structured array and then slice along each of the 3 cell vectors using positions which are scaled relative to the unit cell in order to get the correct bin shapes.
    - Pad the bins array with one layer of bins to satisfy periodic boundary conditions.
    - Vectorise the data in each bin.

- **Search for nearest neighbours**
    - Loop through all unique pairs of bins by considering mostly forward pairs instead of all neighbouring pairs.
    - Use a cutoff to find all the atom pairs which are considered bonded.
    - Add these pairs to a bond dictionary containing the bonding information for the whole crystal.