

This pseudo code is for screening the following artifacts: 1) isolated atoms, 2) overlapping atoms, 3) misplaced hydrogens, 4) under-bonded carbons and 5) over-bonded carbons.

**Begin input file reading**

Read the unit cell vectors, element symbols and atom coordinates from the geometry file  
Read the atom typing radii (AT\_radii) for all elements  
Read list of metal elements  
Read the list of elements involved in the bond order screening (H, B, C, N, O, Cl, Br)  
Read the coefficients for Pauling bond order equation (Coefficient\_1<sub>AB</sub>, Coefficient\_2<sub>AB</sub>)

**End input file reading**

**Build the 26 unit cells surrounding the central cell**

**Begin defects screening**

Loop over atoms in the central unit cell (atom\_A)  
  Loop over other atoms in the central unit cell (atom\_B)  
    Loop over all 27 unit cell images of atom\_B  
      Calculate distance (D) between atom\_A and current image of atom\_B  
      IF atom\_A is hydrogen  
        IF  $D \leq AT\_radii_A + AT\_radii_B + 0.3 \text{ \AA}$   
          Label A and B are “hydrogen connected”  
        End IF  
      End IF  
      IF  $D_{\min} < 0.5 * (AT\_radii_A + AT\_radii_B)$   
        Label the structure with overlapping atoms  
      End IF  
      IF  $D \leq AT\_radii_A + AT\_radii_B$   
        Add this image of atom\_B to first neighbor list of atom\_A  
      End IF  
    End loop  
  End loop  
  IF atom\_A is carbon  
    Loop over atoms (atom\_B) in first neighbor list of atom\_A  
      Calculate  $BO_{AB} = 10^{(Coefficient\_1_{AB} * Distance_{AB} + Coefficient\_2_{AB})}$   
      IF atom\_B is hydrogen  
        IF  $BO_{AB} > 1.25$   
          Set  $BO_{AB} = 1.25$   
        End IF  
      End IF  
    End loop  
    Calculate  $SBO_A = \sum_B BO_{AB}$   
    IF  $SBO_A < 3.3$   
      Label the structure with under-bonded carbon  
    End IF  
    IF  $SBO_A \geq 5.5$   
      Label the structure with over-bonded carbon  
    End IF  
  End IF  
  IF first neighbor list of atom\_A is empty  
    Label the structure with isolated atom  
  End IF  
  IF atom\_A is hydrogen  
    IF atom\_A is “hydrogen connected” to nitrogen or oxygen plus a metal  
      Label the structure with misplaced hydrogen  
    End IF  
  End IF  
End loop

**End defects screening**