

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_{AB}, Coefficient_2_{AB})

End input file reading

Build the 26 unit cells surrounding the central cell

Begin defects screening

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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  $BO_{AB} = 10^{(Coefficient_{1AB} * Distance_{AB} + Coefficient_{2AB})}$ 
      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
```