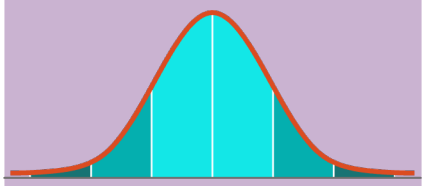
Input data

BPCA.ipynb



From BPCA yields obtain the aromatic cluster size distribution

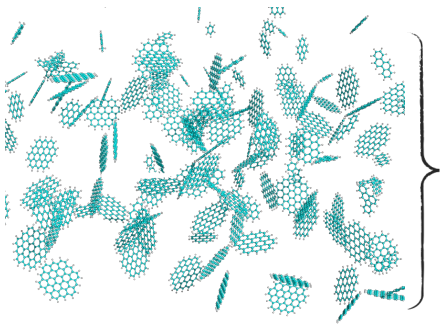
Biochar.ipynb

multi-CP ^{13}C NMR: Ether, aliphatic chains, carbonyl, carboxyl, non-hexagonal rings + Ultimate Analysis: C, H, O, N H/C, O/C, xb

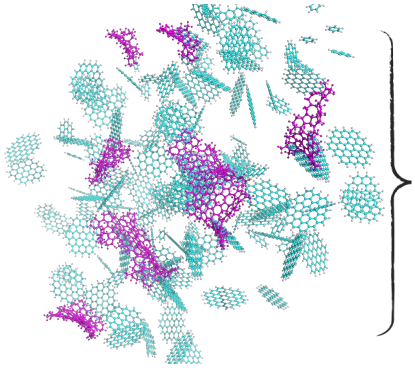
Find the number (n) of functional groups needed to fit the characterization data

Steps 4 to 11

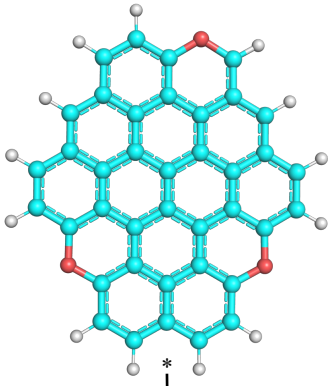
Step 1:
100% Aromatic Carbon
100% Aromatic Hydrogen



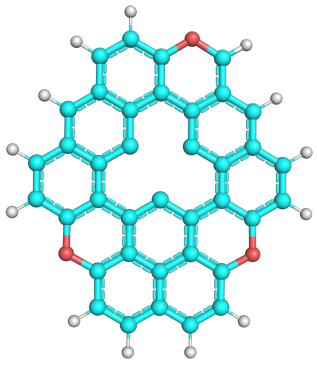
Step 2:
Include amorphous clusters: non-hexagonal rings



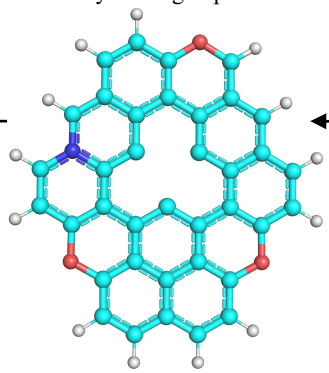
Step 3:
Ether groups



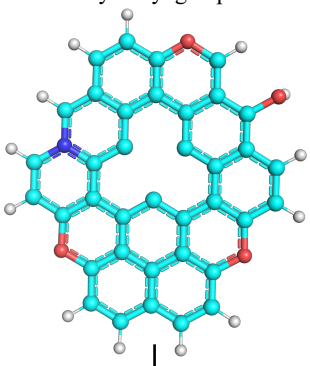
Step 4:
Holes within the structure



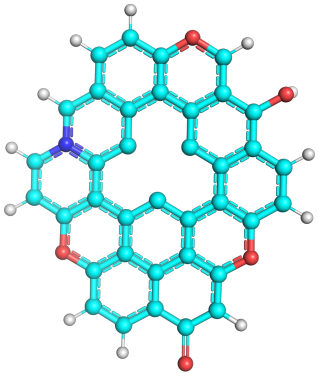
Step 5:
Pyridinic groups



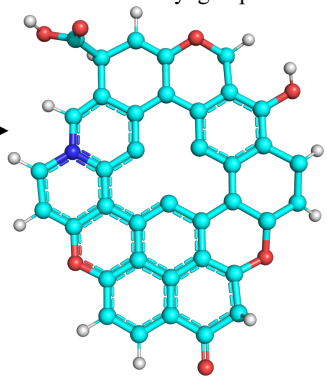
Step 6:
Hydroxyl groups



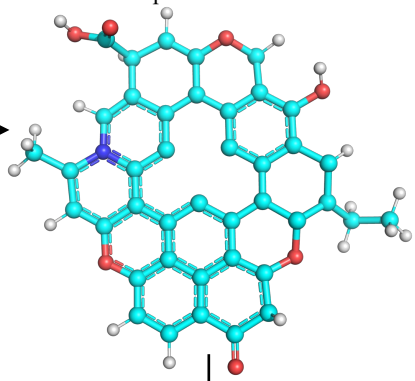
Step 7:
Carbonyl groups



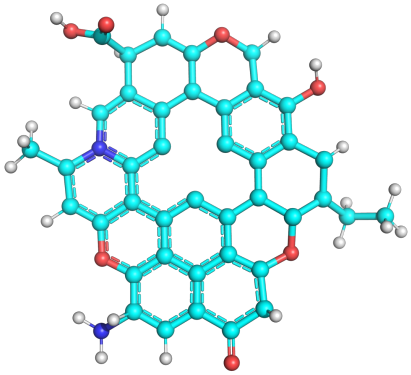
Step 8:
Carboxyl groups



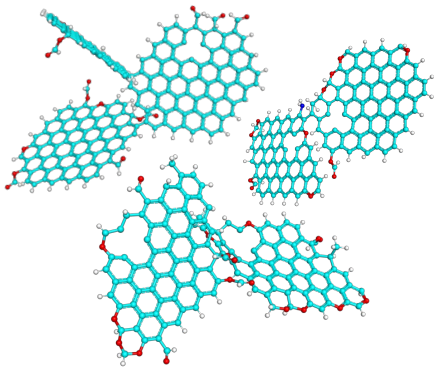
Step 9:
Aliphatic chains



Step 10:
Amines and quaternary nitrogen



Step 11:
Fit the H/C ratio by creating a cross-linked network between clusters



Step 12:
Check NMR data and elemental analysis after all the modifications

Step 13:
If the error is below 10%, save the PDB file and proceed to step 14; if it is above 10%, restart from step 1 and adjust chemical constraints.