Biochar.ipynb

Final modified clusters from Step 13

LAMMPS

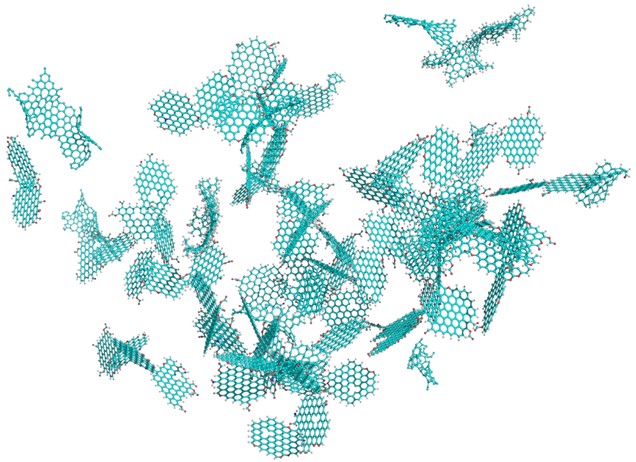
Helium density and d-distance between clusters

ESR: Functional groups

MALDI FTICR-MS: Molecular weight distribution

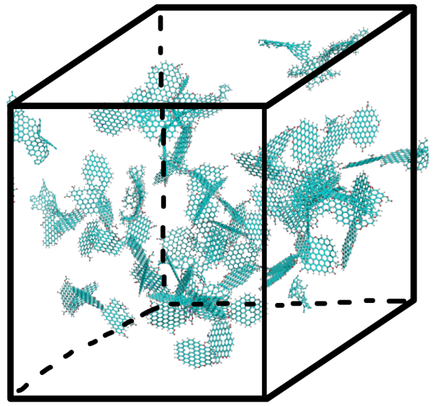
Step 14:

Convert PDB file to LAMMPS data using VMD or OVITO



Step 15:

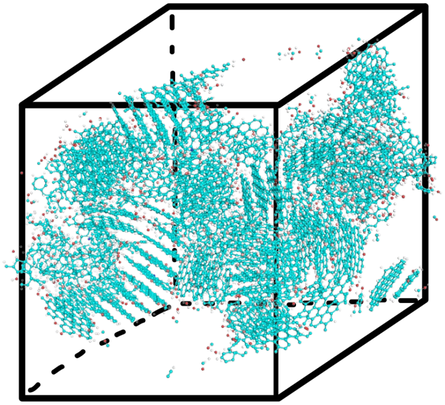
Simulation box



x, y, and z are defined based on the helium density and the MW of the system

Step 16:

Fix the helium density

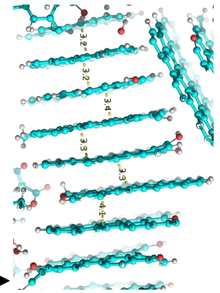


Obtain the 3D representation

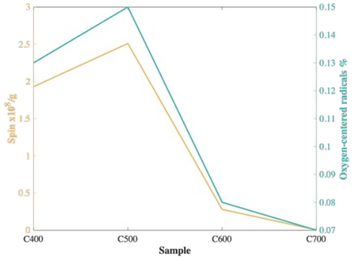
Step 17:

Validate the atomistic model

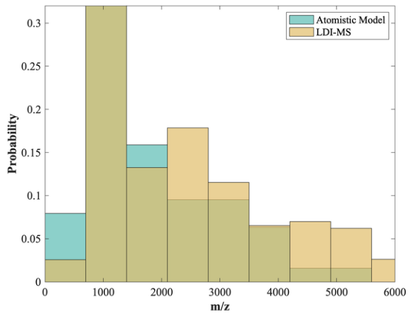
d-distance



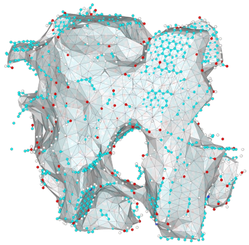
ESR



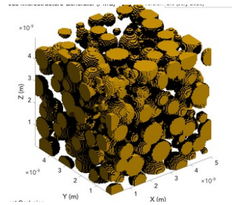
LDI-FTICR-MS



Surface Area



Porosity



Input data