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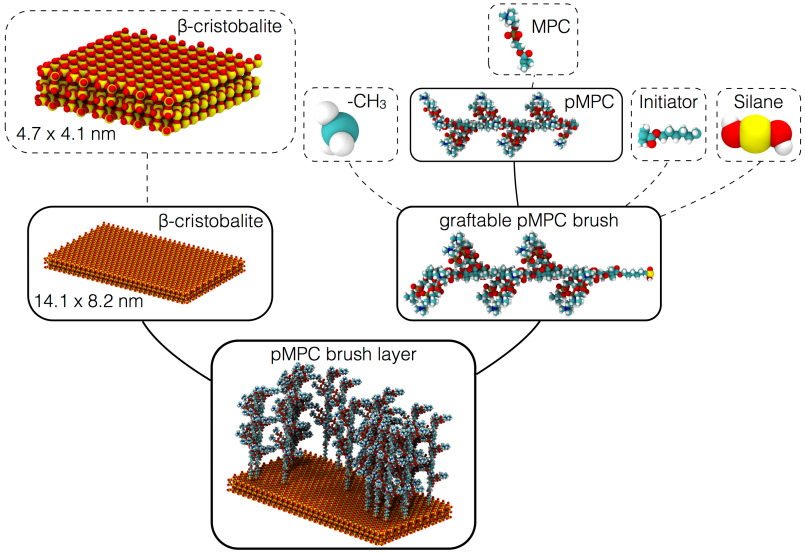
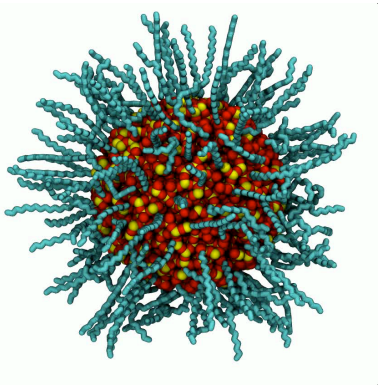
MoSDeF

A Molecular Simulation and Design Framework





ChBE 4830

September 7, 2017

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Plan for this week

- Tuesday, 9/5
  - Introduction to MoSDeF
  - Installing mBuild, Foyer, and HOOMD
  - Homework
    - Lennard-Jones simulations in HOOMD
    - mBuild tutorials
- Today (9/7)
  - Interactive MoSDeF tutorial
  - Homework
    - Setting up a complex molecular system using mBuild and Foyer

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Interactive tutorial (Instructions)

- ❑ Pull the latest changes from the class git repo
  - o Navigate to the directory where the repository was cloned (likely your home directory)
    - >> cd chbe4830
    - >> git pull
  - o If you still need the link:
    - https://github.com/summeraz/chbe4830
- ❑ Navigate to the `MoSDeF` directory
  - o >> cd MoSDeF
  - o Launch the Jupyter notebook application
    - >> jupyter notebook
  - o Select the `Tutorial.ipynb` file

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mBuild Interactive Tutorial

- Building an alkane
  - Creating structure files for small molecules using Avogadro
    - https://avogadro.cc/
  - Constructing a hexane molecule piece by piece
  - Constructing a hexane molecule using the `Polymer` recipe
  - Obtaining an energy minimized structure
  - Adding and removing particles from Compounds
    - e.g. attach a hydroxyl to the hexane
  - Filling a box with molecules
  - Functionalizing surfaces

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Homework Assignment

- Using mBuild, construct a system featuring 100 molecules of (3,3,4,4,5,5,6,6,6-Nonafluorohexyl)benzene (NFHB) in a simulation box with dimensions of 3nm x 3nm x 3nm
  - Fill in the class definitions in the Jupyter notebook that is located in the `Assignment4` directory of the git repo (titled `Assignment.ipynb`)
  - Use the PDB structure files provided for benzene, CF_3, CF_2, and CH_2 to first create a prototype for a single molecule, then use this class to help in defining a class for the full system
  - Instantiate your system class and save **an atom-typed system** to .top file format