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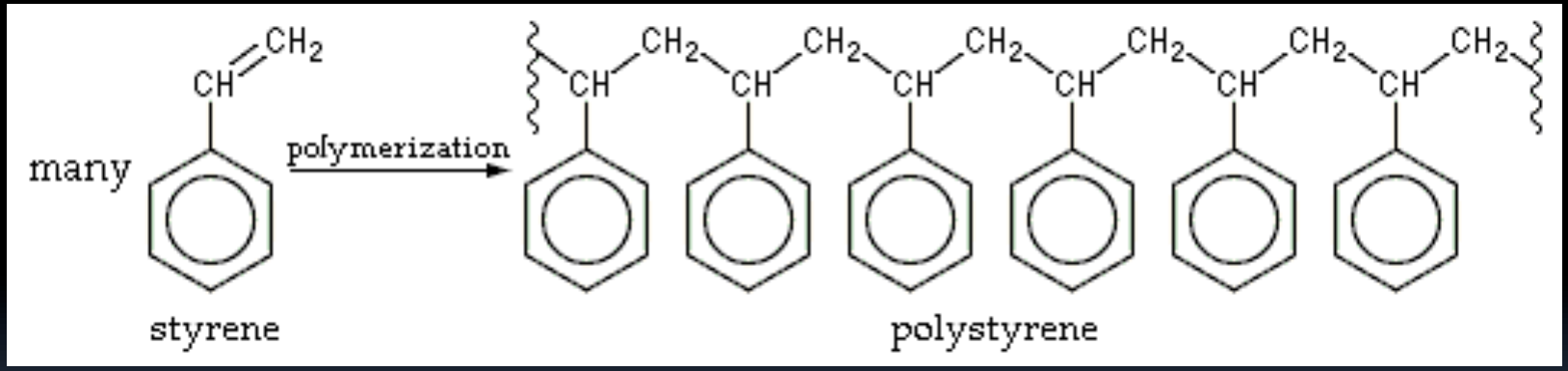
MODELING DIFFUSION IN POLYSTYRENE

Project Overview

- Long-term goal: Understanding diffusion in glassy polystyrene
  - Diffusion constant
  - Polymer/flame retardant mixture
- Short-term goal: Polystyrene dimer, 2,4Diphenylpentane

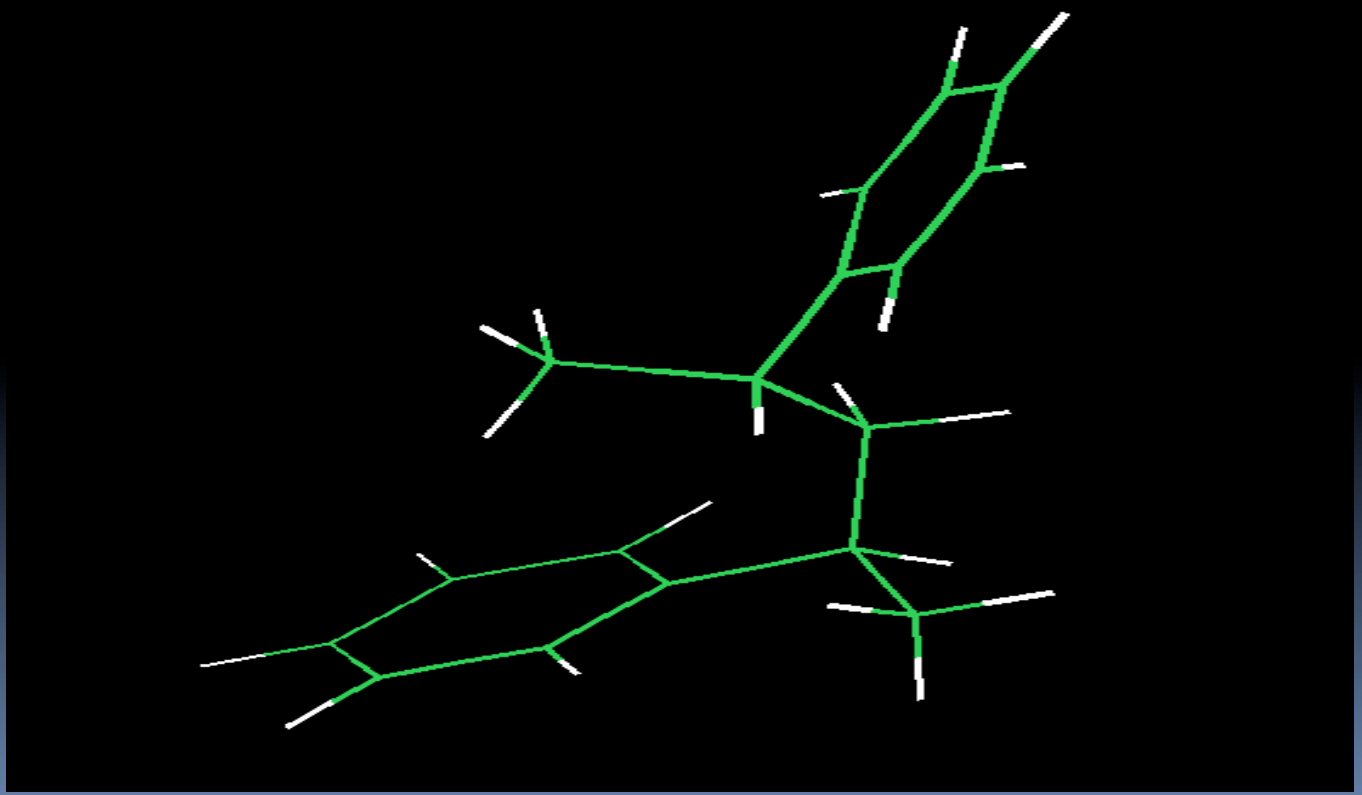
Polystyrene

$(C_8H_8)_n$: Alkane backbone with phenyl group on every other C



Dimer

- 2,4-Diphenylpentane = pentane with 2 phenyl groups on the 2 and 4 carbons



TraPPE-UA Model

- Simplifies multiple atoms in pseudo-atom
- Gives force field parameters
  - Lennard-Jones parameters- used for Van der Waal's interactions
  - Bond length and force constant
  - Bend angle and force constant
  - Torsional potential parameters

PINY MD

- Molecular Dynamics simulations
- Parameter files:
  - Dimer.init : initial configuration
  - Dimer.bond : bond length, force
  - Dimer.bend : bend angle, force
  - Dimer.tors : torsional parameters
  - Dimer.vdw : van der waal's

The simulation

- Initial config: group of 256 atoms in a box
- Millions of time steps, each 2 fs
- Step uses inter-/intra-molecular forces to move atoms
  - Verlet algorithm used to integrate Newtonian eq's of motion
- Distance from center divided into bins
- Each write: # atoms in each bin
- Range of temperatures, down to T_g

The diffusion constant

- PINY MD gives distribution of particles with time
- Width of distribution = C * D * t
  - D = diffusion constant
  - C = 2 for 1D, 6 for 3D
- Plot width vs t: linear, slope = C * D

Project steps

- Determine D for pure dimer
- Determine D for dimer/flame retardant mixture
  - Remove slab or sphere from center of equil. dimer , replace with slab/sphere of flame retardant
  - Brominated aromatic, probably estimated using benzene
- Repeat for trimer, and further depending on time
  - End goal: to work our way up to full polystyrene

Personal goals

- Learn Linux, Fortran
- Learn more about computer science and HPC in general
- Better understand the math and relationships behind MD simulations
  - Verlet algorithm, Newtonian mechanics, vector/ matrix operations, Monte Carlo simulation