10.491 Integrated Chemical Engineering Materials Design Module

Assignment #2: Introduction to Polymer Modeling
Due Wed, 4/21/99, 10am

In preparation for this assignment, work through the following General Modeling Tutorials in InsightII, if you have not done so already (these were done in Assigment #1)

a. Building/Lesson 3 "Defining Repeat Units"
b. Analysis/Lesson 1 "Analyzing an MD simulation"

as well as the following Polymer Tutorials:

c. Building Polymer Chains/Lesson 1 "Building a Homopolymer with Specific Repeat Unit Configuration")
d. Building Polymer Chains/Lesson 4 "Building a Random Copolymer using Reaction Probability Information"

When you have completed these, exit InsightII and restart it to initiate a new .log file(s). At the end of this assignment, you will turn in the log(s) of your session(s) *by email.* Do not hand in hard copies of these .log files; email each .log file that results from your work on this assignment to the TA, nwaheed@mit.edu. Each file should be sent as a separate message or attachment, suitably labeled so that the TA knows in what order they were generated, if more than one.)

1. Construct a polymer of poly(caprolactone) [IUPAC name: poly(6-hydroxyhexanoic acid)], or PCL, with degree of polymerization (DP) of 10 (hint: chemical formula of repeat unit is $C_6H_{10}O_2$). Make sure all the backbone bonds of the repeat unit are in the *trans* orientation (torsion angle=0 degrees) before polymerizing, or else you will get a very "crumpled" chain.)

2. Define a new repeat unit which is a *constitutional isomer* of the poly(caprolactone) repeat unit (as defined by InsightII, with hydrogen "leaving groups"). Your repeat unit should be one which gives rise to a polymer different from PCL when polymerized.

3. Define a new repeat unit which is a *configurational isomer* of the repeat unit you made in Part 2. Label the two repeat units constructed in Parts 2 and 3 with their correct R and S chirality designations.

4. Polymerize an *atactic* chain of your new polymer (using either or both of the repeat units defined in Parts 2 and 3) with DP=10. Rotate the molecule on your screen and identify the R- and S-chiral carbons on the chain, to confirm that the 10-mer is indeed atactic.

5. Using the Discover_3 module, run a short optimization on each of the repeat units and polymer chains on your screen, in order to remove any unrealistic geometric features, like stretched bond lengths.

6. Using the Discover_3 module, run a short, 10000 fs (femptosecond, 10^{-15} s) T=400K molecular dynamics simulation of the atactic polymer chain you have created. This is a model of an isolated decamer molecule (i.e. a 10-mer chain in vacuum). You can use the Simple_Min_Dyn strategy for this, where steps=10000 (1 step = 1 fs) and History =100 (save a snapshot for your simulation every 100 fs, for a total of 100 snapshots in the .his file. Typically, you only need to save 100-200 snapshots per simulation, in order to keep file sizes down.) Estimated time of simulation: 20 min.

7. After the simulation is completed, you can use the Analysis module to animate the trajectory (i.e. the saved snaphots from the simulation), to visualize the molecular motion. Use Unanimate to turn this off.

8. From the simulation trajectory, generate graphs of the potential energy and of the distance measured from one end of chain to other, each as a function of time. What do these plots tell you about the *conformation* of the chain at 400 K in vacuum? Does this result seem reasonable to you? Why or why not? (Turn in your answers as part of this assignment.)

9. Print out a plot of your screen to turn in for this assignment. To do this, first arrange all the objects on your InsightII screen for best viewing, and render all molecules in ball-and-stick mode before printing out. Use the Export_Plot option under the File pulldown, with the following settings:

Printer Type	postscript
Plot to Printer	ON
Printer Name	preview
Save_Device_File	ON
output file	homework2.ps
Print Command	xpsview -skipc -igc insight_temp.eps &

After executing this command, you can use the lpr command to print out the resulting file, called homework2.ps. Turn in this plot in class.

If you do this homework over multiple sessions, it is ok to export a plot of your results at the end of each session and turn in multiple plots.