10.491 Integrated Chemical Engineering Materials Design Module

Assignment #1: Introduction to Molecular Modeling Software (to be completed by Wed, 4/14/99)

For this module we will make extensive use of the MSI molecular simulation software available on Athena (Biosym v4.0.0, runs on any Silicon Graphics workstation) to perform structure-property calculations and to simulate the behavior of materials. Simulations are useful for at least two purposes: (1) observation of a simulation can often provide qualitative insights about what is going on at the molecular level; (2) by invoking rules of statistical mechanics, simulations can provide quantitative estimates of many properties of a material that would otherwise have to be measured in the lab or looked up in a book (assuming either of these options were available - in most product design cases, they are not.)

To start up the MSI software, refer to the "How to" section of the Materials Design Module (MDM) web site (http://heavenly.mit.edu/~eprof).

For this first assignment, you will set up your account, become familiar with the course web site, and work through a few tutorials of the Biosym software. There is nothing to hand in.

1. If you have not already done so, start Netscape and make sure that you can access the MDM web site. You should check this site daily for reading and assigments. All the reading material is also organized in the Course Notes section of the MDM site.

2. You have been given a user account with additional disk space on the Chemical Engineering File Server ("chefs"). See the "How to" section of the MDM site for how to access this disk space. Create a subdirectory for ICE on chefs. From there, start up the MSI software as described in the "How to" section of the MDM site.

3. Step though the InsightII General Modeling Tutorials shown below to become familiar with the Biosym software. Click on the blue arrow in the Pilot window to execute each command in order. Toggle on the "Show Menus" option, in order to familiarize yourself with the menu names (like "Molecule Get") and the parameter boxes. All of the windows you will see can be brought up by clicking on the menus at the top of the Insight window. In general, all default values should be filled in for you on these tutorials, so that you need only click on "Execute" to continue. Don't click through the steps too quickly - some steps may involve a short energy optimization or molecular dynamics simulation. Be sure to wait for these to finish (the message "Discover job finished" will appear in information area at the bottom of the window) before continuing.

a. Basics/Lesson 1 "Basic Tools"
b. Building/Lesson 1 "Building in 3D"
c. Building/Lesson 3 "Defining Repeat Units"

d. Analysis/Lesson 1 “Analyzing Results of a Molecular Dynamics Simulation”

After you have worked through the tutorials, exit insightII (using the ”Session Quit” menu option) and look at the list of files in your directory. You should see a file called insight.log. This is the default name given to the log of all the commands that were executed in your most recent insightII session. Every time you run insightII, this file will be overwritten. For this homework, the file may only contain instructions to run the tutorials, but in future homeworks these files can be very useful for the professor or TA to see what you have done and to help you solve problems, so be sure to rename the .log files from any sessions that you want to save before you start insightII again.