Chem 442: Homework for lecture 3

(only need to turn in **BOLD** assignment; do all assignments by due date)

Note on running applets: some browsers have strong restrictions on running Java applets or HTML5 applets. If you have no luck with your computer, a library computer (chem library) may do better, or do it with a friend from class.

1. Turn in Go again to the Lennard-Jones potential MD simulation online (the link is in the "L2" row of the Course Schedule). Start the simulation as-is by hitting the green "Start" button. Now the Verlet algorithm starts moving the atoms. Select "Preset" "Two atoms."

a. Does a diatomic molecule form or not? What type of motion does this molecule undergo?

b. Now make sure that "Mouse/touch" is set to "drag," and use the mouse to drag one of the atoms just a little. Now what motions does the molecule undergo (name all three types)?

c. Keep things running, and increase the box size to 15. (You can "Pause" the simulation, then move the "Box size" slider, the click "Resume." It will look like the molecule shrinks and slows down; that's just because it plots the bigger box in the same amount of space). Now hit "Faster" several time carefully. What happens to the amplitude of the vibration? As you keep hitting "Faster," the molecule will eventually dissociate. What happens to the frequency of the vibration just before it dissociates (slower or faster than before)?

2. Now run Preset "Hot and Cold." A hot drop (red balls) will hit a cold drop (blue balls). What happens to the temperature of the two drops after they merge? Look carefully: does the back end of the blue droplet instantly turn more red? You could use the simulation to calculate the thermal conductivity of the droplets!

3. Now run "Friction:" A large molecule will slide down an inclined plane. What happens to the temperature of the molecule as it slides down? Eventually, the molecule comes to a rest at the bottom. So first, potential energy was converted into kinetic energy when the particle slid down. After it's all over, where did the energy go? (Remember, overall energy is conserved.)