Excercise 1

Assignment 1. (1/3) Install VMD or go to Linux machines in D208. Go to the course web page and dowload mystery.xyz.

- Load the file in VMD (in shell you can type vmd to run the program)
- Play the simulation through
- Feel free to play around for a while with VMD
- Choose a snapshot, depict, save and attach it to the excercise report. Your figure should depict balls with sticks of white/red for H/O. Use white background without the coordinate arrows from your choise of point of view.

VMD manual can be found at
http://www.ks.uiuc.edu/Research/vmd/current/ug.pdf
If you already have a favorite visualization program and are a true guru with it, feel free to do this assignment using it.

Assignment 2. (1/3) Why do simulations sometimes heavily fail to fulfill the ergodic hypothesis. Please give an example (a real or a model system).

Assignment 3. (1/3) Let the wavefunction of a molecular system be $\Phi(\mathbf{r}, \mathbf{R}, t)$ and

$$H_e \Psi_k(\mathbf{r}, \mathbf{R}) = E_k(\mathbf{R}) \Psi_k(\mathbf{r}, \mathbf{R}),$$

just like (1.4) in the lectures. Derive the Born-Oppenheimer approximation (1.5) starting with the general expansion

$$\Phi(\mathbf{r}, \mathbf{R}, t) = \sum_k \Psi_k(\mathbf{r}, \mathbf{R}) \chi_k(\mathbf{R}, t).$$

In your derivation you will need to estimate some matrix elements to be small. What conditions does this apply to? What happens if this assumption does not hold?

Return your solution to Ville *moleculardynamicssimulations@gmail.com*, **latest Wed 11.9.2013 10:15**. To maintain good relations with the assistant, you might want to consider sending a single PDF with all three solutions.