CHM 695: Sample Exam Paper

1. In GROMOS force–field, torsional potential is defined by

$$K_\phi \left[1 + \cos\delta \ \cos m\phi\right] \ .$$

Write the values of the following parameters for an ethane molecule, if the barrier for the torsional rotation is 5 kcal/mol.

K_ϕ	m	δ

2. In TIP3P rigid water model, potential is given by

$$\sum_i \sum_j k_{\rm C} \frac{q_i q_j}{r_{ij}} + \frac{A}{r_{\rm OO}^{12}} - \frac{B}{r_{\rm OO}^{6}}$$

where $k_{\rm C}$ is the electrostatic constant, $\{q_i\}$ are the charges, A and B are the Lennard-ones parameters.

   (a) If by mistake, one uses two times larger value of B, but every other parameters the same as in the standard parameter set of TIP3P water model, interpret how equilibrium density of water computed from an NPT run using such modified potential will be different to that computed using the correct TIP3P parameters - i.e. interpret if it will be increased or decreased or no change will occur.

   (b) Qualitatively sketch the behaviour of velocity autocorrelation function with the correct TIP3P parameters and with the wrong TIP3P parameters (as given above) in an NVT simulation.

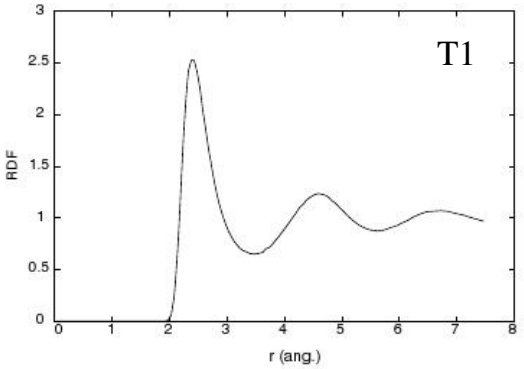
3. Explain briefly, the issues in computing long-range electrostatics in periodic systems and how these problems are solved by performing Ewald summation.

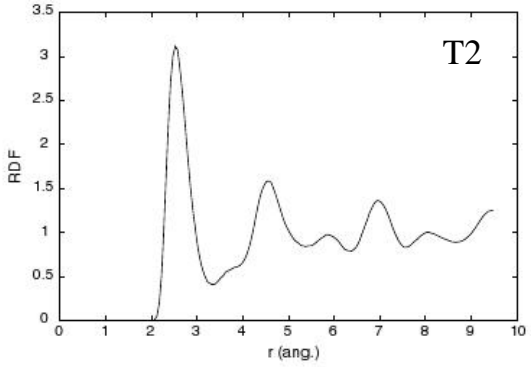
4. Sketch kinetic energy and potential energy curves as a function of time during a molecular dynamics simulation in NVE ensemble for the following cases, where the initial temperature is 0 K:

   (a) Starting configurations atoms are at equilibrium.

   (b) Starting configurations of atoms are far from equilibrium.

5. (3 marks) Radial radial distribution functions for Ni from two independent molecular dynamics simulation of bulk Ni at two different temperatures T1 and T2 are given below. In (only) one case melting of Ni is observed. Identify which and justify your choice.





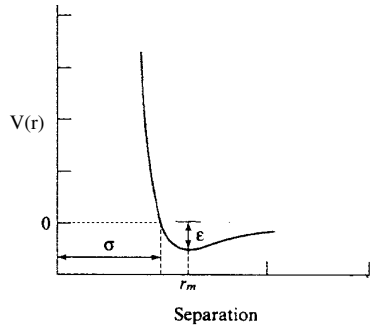
6. (2 marks) Derive equations of motion on atoms if the Langrangian of the system is defined as

$$\mathcal{L}(\mathbf{R}, \dot{\mathbf{R}}) = \sum_I M_I \dot{\mathbf{R}}_I^2 - U(\mathbf{R}) - \frac{1}{2}\kappa \left[S(\mathbf{R}) - \alpha\right]^2$$

7. (4 marks) Show that the marked (in the figure below) distance and height of the Lennard–Jones potential

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

are σ and ϵ, respectively.



8. Using your program written for one–dimensional simple harmonic oscillator with Andersen thermostat, perform the following computer experiments. From MD trajectory at NVT ensemble:

   (a) Compute $\langle x \rangle$

   (b) Compute $\langle \dot{x} \rangle$

   (c) Make probability distributions of x

   (d) Make probability distribution of $m\dot{x}$

   (e) Make a plot of phase-space

   Based on these results, interpret if Anderson thermostat gives correct canonical distribution. (Note: you may choose a suitable value of mass, potential parameters and time steps).