

PH: 322 Molecular Simulation Homework 4 Due date: 15th April

1. Partial atomic charge calculation: Take isobutene and water molecule. Compute the Mulliken charge as well ESP charge. If you have access to Cerius2 (SERC has this) compute the Qeq charges also.

2. Write a Monte Carlo code to simulate LJ fluid. Use the spline switching function with a cut-off of $r_c = 2.5\sigma$. Calculate the equation of state (ρ^* vs P^*) at $T^* = 1$. Do the calculation with and without long-range corrections and report the values in table for $\rho^* = 0.05, 0.4, 0.65, 0.7, 0.8, 0.85$ and $0.9, 1.1$

3. Using the Monte Carlo code (supplied) compute the equation of state (P^* vs η) for a system of 400 hard spherocylinder with $L/D = 3$. Give equation of state for $P^* = 1$ to $P^* = 9$

Note that the volume of a spherocylinder with an aspect ratio L/D is

$$v_{hsc} = \pi D^3 / 6 + \pi LD^2 / 4$$

The reduced density (packing fraction) $\eta = \rho v_{hsc}$

Also identify various phases like Isotropic, Nematic and Smectic

4. Einstein diffusion and Green Kubo formalism

Show that the mean square displacement is given by (D is the diffusion constant, d is the dimension)

$$\langle r^2(t) \rangle = 2dDt = 2t \int_0^t d\tau \langle \mathbf{v}(0) \cdot \mathbf{v}(\tau) \rangle$$