Course: FYS-7306 Molecular Modeling of Bio- and Nanosystems

Exam: 22.01.2013

Calculator: Not allowed

1) Consider the following questions:

a) Assume you should simulate the chemical reaction between a sphingomyelinase (an enzyme) and sphingomyelin (SM), where the enzyme cuts the lipid SM into two pieces. Which would be the most appropriate classical force field to consider for this reaction and why?

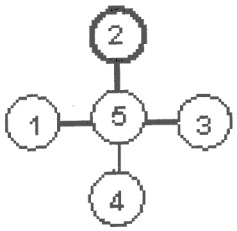
b) If you used a quantum-mechanical technique for the same purpose overall, what would you gain, and what would you lose (advantages and disadvantages)?

c) Assume that you described a lipid (whose size was given by a radius of about 1 nm) with a spherical particle, and here the spherical particle description would be the coarse-grained model you would use in further studies. Now, if you employed this coarse-grained model in large-scale studies of lipid systems, what would be the smallest length and time scales that you could trust with your coarse-grained description?

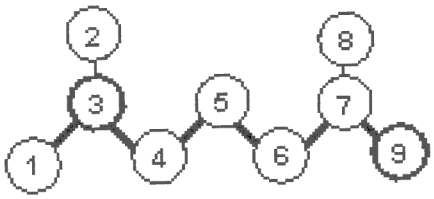
2) (a) What are nonbonding interactions? What types of nonbonding interactions are considered in Classical MD, how are they described by potential functions?

(b) List all pairs of atoms interacting via non bonded interactions in these two molecules:

(A) methane all atom



(B) 2,6 methylheptane



3) What are periodic boundary conditions? What type of PBC can be used in simulations, explain why they are used.

4) Answer questions (a)-(c) with no more than 4-5 lines.

a) Describe three simplifications used in semiempirical methods.

b) What are contracted GTOs and why were they introduced?

c) What is a minimal basis set? Describe the minimal basis set of the carbon atom.

5) Characterize briefly and give examples of LDA; GGA and hybrid xc-functionals. Describe and compare their performance in calculations of molecular structures of covalently bound main group elements.