Course: FYS-7306 2014-01 Molecular Modeling of Bio- and Nanosystems

Exam: 15.12.2014 at 09.00-12.00

Calculator: Not allowed

1) Discuss the strengths and limitations of all commonly used molecular simulation techniques: quantum-mechanical simulations, atomistic (classical) methods, and coarse-grained (classical) techniques.

Assume that you should use simulations to consider the binding of an enzyme with a receptor, and then study the chemical reaction induced by the enzyme on the receptor. How would you use molecular simulation techniques to consider these processes?

2) Please answer the points below:

a) How are valence angles described in a classical potential?

b) What types of interactions are present between the following atom pairs of the cholesterol molecule shown in Figure 1: O3-C5; O3-C10; C13-C16

c) Consider that you need to describe the cholesterol molecule in a united atom force field. How many atom types would you proposed to describe the molecule and why?

Figure 1. Structure of the cholesterol molecule with atom numbering. The chemical symbol for the carbon atom 'C' is omitted.

3) What is time step in MD simulations? Propose two different methods to increase the time step in MD simulations.

4) Answer questions (a) to (c).

a) Define local minimum, global minimum and saddle point and explain how to differentiate between a minimum and a saddle point.

b) When do we need to use an unrestricted calculation? Give an example of a compound which requires the use of an unrestricted calculation?

c) Which are the shortcomings of Gaussian type orbitals? Which is the major advantage in using Gaussian type orbitals as compared to Slater type orbitals?

5) Describe minimal basis sets: definition, performance, notations and limitations.