Course: FYS-7306 **Molecular Modeling of Bio- and Nanosystems** / OANA CRAMARIUC

Exam: 07.05.2015 at 17.00-20.00

Calculator: Not allowed

1) Consider the following questions:

a) Assume you should simulate the chemical reaction between the enzyme sphingomyelinase and a lipid called sphingomyelin (SM), where the enzyme cuts the lipid SM into two pieces. What would be the most appropriate classical force field to consider in 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 is given by a radius of about 1 nm) by using 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) Please answer the points below:

(a) How are torsion angles described in a classical potential?

(b) List all torsion angles in which Nitrogen is involved (molecule shown in Figure 1).

(c) How many atom types should be used to describe the molecule in Figure 1 in an all atoms force field?

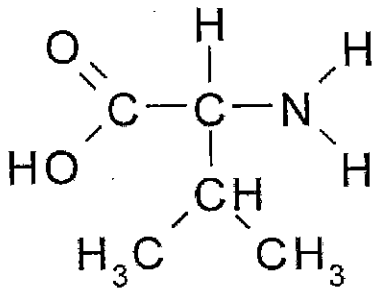

Figure 1. *Molecular structure for problem 2.*

3) Please answer the points below:

(a) What are periodic boundary conditions?

(b) Explain the minimum image convention.

(c) How are velocities initiated in molecular dynamics simulations?

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

a) List four properties or phenomena that are accessible only by electronic structure calculation methods (HF, DFT, SE, etc) and explain which is the main problem when using electronic structure calculations as compared to classical ones.

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

c) How do you address SCF convergence problems in quantum mechanical calculations?

5) Describe split basis sets and extended basis sets (with polarization, diffuse and Rydberg functions). Explain in each case the advantages of the additional basis functions, give some examples of when the basis sets are needed and also some examples of notations in the Pople and Dunning notation forms.