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

Exam: 05.03.2015 at 17.00-20.00 / OANA CRAMARIUC

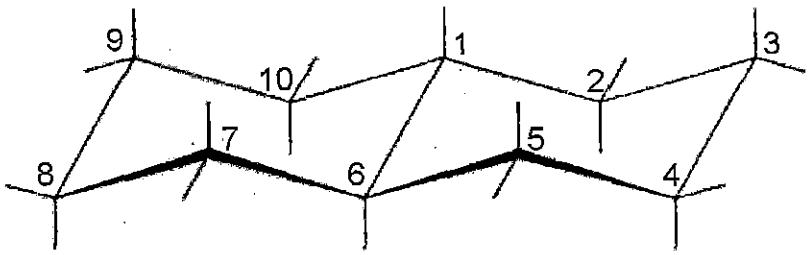
Calculator: Not allowed

1) Assume that one would like to consider a biological process where the time scales of a given process would extend from nanoseconds to seconds. Discuss how the process could be considered through different simulation techniques and discuss also how the simulation results over a given time scale could be compared with experimental data. Finally, provide examples of biological processes which cover several distinctly different time scales (for instance, from nanoseconds to seconds).

2) What type of non-bonding interactions are considered in Clasical MD simulations. Provide definitions (with formulas).

What type of interactions are present between the atoms in the structure below (atoms marked with numbers are carbon and remaining ones are hydrogen):

a) 9-10
b) 9-1
c) 9-2
d) 9-3
e) What type of united atom would be used in united atom force field for atom 1 and 2?



3) How can preasure and temperature be controled in MD simulations? Choose and explain one of these algorithm used in MD.

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.)

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

c) Describe the Born-Oppenheimer approximation (BOA) and its consequences. Do we use the BOA in geometry optimizations? Give two examples for the breakdown of the BOA.

5) Describe STO and GTO type of basis functions and compare their advantages and disadvantages. What are contracted GTOs and why do we need them?