FSI3400 Molecular Modelling 7.5 credits

Molekylär modellering

This is a translation of the Swedish, legally binding, course syllabus.

If the course is discontinued, students may request to be examined during the following two academic years

Establishment

Course syllabus for FSI3400 valid from Spring 2009

Grading scale

Education cycle

Third cycle

Specific prerequisites

Differential equations, fourier transforms, thermodynamics, electrostatics, basic quantum mechanics and chemistry.

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

After completed course, the PhD student should be able to:

- explain atomic interactions from quantum chemistry and use quantum chemistry programs.
- master molecular mechanics force fields, parameterization, and their limitations. They should further be able to carry out energy minimization and molecular dynamics simulations of simple systems.
- critically choose between methods and modeling levels for water and protein applications.
- have a basic understanding of bioinformatics, chemoinformatics, structure prediction and folding.
- describe advanced molecular modeling methods such as free energy calculation and solvation energies. for small molecules, docking, and modern drug design applications.

Course contents

Quantum chemistry: Single- and multiple electron systems. Ab initio-methods, Hartree-Fock equations, gaussian basis sets. Orbitals, calculation of partial charges, practical program usage.

Molecular force fields: Bonds, angles, torsions. Electrostatics and van der Waal forces, parameterisation from experiments or quantum chemistry. Effective pair potentials, hydrogen bonds. Computation of molecular properties and limitations, examples of commonly used force fields.

Energy landscapes: Minimizations, algorithms, normal modes, transition states and reaction pathways.

Simulation methods: Molecular dynamics, equilibration, thermodynamical properties from simulations, stochastic dynamics, energy conservation. Monte Carlo methods and conformational analysis.

Bioinformatics: Sequence analysis, protein structure, homology modeling, 3D structure prediction from sequence, chemoinformatics, combinatorial databases.

Advanced applications: Free energy calculations from simulations, free energy of solvation, chemical reactions, molecular docking, modern drug design with simulations and quantum chemistry.

Course literature

Leach, A. R. Molecular modelling - principles and applications, 2nd ed., ISBN 0-582-38210-6

Examination

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

Other requirements for final grade

Computer laborations and written exam.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.