SI2710 Molecular Modelling 7.5 credits

Molekylär modellering

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

Establishment

Course syllabus for SI2710 valid from Autumn 2007

Grading scale

A, B, C, D, E, FX, F

Education cycle

Second cycle

Main field of study

Physics

Specific prerequisites

Recommended 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

This is an advanced level course given in collaboration between Stockholm University and KTH, and provides a research-focused introduction to modern theoretical methods of biophysical chemistry. After completing the coursework, students are expected to:

- 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.
- Be able to 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

- TEN1 - Examination, 4.5 credits, grading scale: A, B, C, D, E, FX, F
- LAB1 - Laboratory Work, 3.0 credits, grading scale: A, B, C, D, E, FX, F

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.

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

Other requirements for final grade

Computer laborations (LAB1, 3 ECTS credits) and written exam (TEN1, ECTS 4,5 credits).

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.