FKF3410 Molecular Modeling for Materials Design 7.5 credits

Molekylär modellering för materialdesign

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 FKF3410 valid from Autumn 2016

Grading scale

Education cycle

Third cycle

Specific prerequisites

Basic course in thermodynamics, statistical mechanics or equivalent, and familiarity with computers.

Language of instruction

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

Intended learning outcomes

Course aims:

As the relevant length scales in man-made materials become smaller and smaller, processes on the molecular and atomistic level become increasingly important for its final properties. These processes can in many cases be understood within the framework of classical thermodynamics and statistical mechanics, but are, due to the great komplexity of the systems, difficult to grasp without the help of computer simulations.

One method to simulate processes on this scale is classical molecular dynamics (MD), which, due to the rapid development of both hardware and software, in recent years has become an important tool within materials science, with applications in, e.g., solid materials, polymers, soliutions and suspensions, and composites.

The aims of this course is that the student will:

· Be familiar with the theoretical foundation for simulations of classical particles

· Be able to set up, run, and analyze MD simulations of simple systems

· Be able to adapt the simulations to the problem at hand (w.r.t. force fields, simulation parameters, analysis method, etc.)

· Be able to relate the simulations to experimental methods

· Be able to visualize and present the results in the form of graphs and molecular graphics

· Understand the limitations of MD as a method

For whom:

Graduate student in chemistry with an interest in molecular mechanisms

Course contents

The lectures will treat:

- The MD method
- Force fields
- Ensembles
- Mass distribution functions, corellation functions, fluctuations
- Carbohydrate models (cellulose, hemicellulose, water models, etc.)
- Free energy methods (solubility, ligand-substrate binding, chemical modification)
- Methods for enhanced sampling (Replica exchange, steered MD)
- Simulating mechanical properties
- Advanced analysis (normal modes, quantum corrections, simulated vibrational spectroscopy)

Introduction to HPC environments (High Performance Computing)

Disposition

The main stuff is presented in 10 two-hour lectures, which also include practical elements. The most central parts are exemplified in two computer exercises. The course ends with a project assignment in wich the student will perform and analyze a larger simulation and present the results in the form of a written report. This assignment is planned together with the teacher and should be connected to the student's own PhD project.

Course literature

Handouts

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

At least 80% attendance to the lectures. Approved reports for the computer exercises and an approved project assignment.

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.