FBB3570 Multiscale Modelling in Chemistry and Biology 10.0 credits

Flerskalig modellering i kemi och biologi

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 FBB3570 valid from Spring 2020

Grading scale

P, F

Education cycle

Third cycle

Specific prerequisites

PhD students who have the fundamental knowledge of molecular modeling, in particular quantum chemistry.

Language of instruction

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

Intended learning outcomes

This course aims at providing students with fundamental concepts, principles, and methods in multiscale modelling. You will learn how to use multiscale modelling methods to study large molecular systems.

For whom: PhD students

Course contents

1. Introduction to multiscale modelling
2. Review of electronic structure calculation methods
3. Modelling of interatomic interactions
4. Methods for atomistic scale simulations
5. Meso-scale simulation methods
6. Computer exercises
7. Projects

Examination

• DEL1 - Participation, 4.0 credits, grading scale: P, F

• INL1 - Hand in exercise, 2.0 credits, grading scale: P, F

• PRO1 - Proect work, 4.0 credits, grading scale: P, 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.

Other requirements for final grade

Attendance on at least 80% of the lectures, finish all the exercises and projects and present the results.

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.