FCK3001 Computational Chemistry 7.5 credits

Beräkningskemi

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

Establishment

Course syllabus for FCK3001 valid from Spring 2019

Grading scale

P, F

Education cycle

Third cycle

Specific prerequisites

Eligible for studies at the third-cycle level and prior knowledge from quantum mechanics at the second cycle.

Language of instruction

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

Intended learning outcomes

After completion of the course the student should have the knowledge and ability to

- demonstrate for the level of the course adequate acquired knowledge in the specialized topics of the course.
- design, plan and carry out a project to address a scientific problem by computer-aided modelling applied within the specialized scope of the course.
- present and motivate orally own project results, and critically evaluate own and others' presented project results.
- reflect on the selected scientific problem with respect to environmental, human or societal aspects.

Course contents

The course consists of two parts that in total comprises approximately 200 hours. The first part includes 24 hours of teacher-led lectures, 12 hours of student-led seminars, and individual self-studies corresponding to a work load of roughly a week of full-time studies. Topics include second quantization for electronic structure theory, group theory applications to electronic and vibrational wavefunctions, density functional theory for molecular systems, correlated approaches in electronic structure theory: perturbation theory methods, configuration-interaction methods, coupled cluster, and geminal methods.

The second part consists of a compulsory project assignment for four weeks that corresponds to a work load of about three weeks of full-time studies. The students work in small groups where each group selects a scientific research problem in computational chemistry. The project involves autonomous and independent work where the students are expected to read and review the relevant scientific literature, design a modeling strategy, carry out computations on high-performance computer systems using modern quantum chemistry software, and disseminate the strategy, obtained results and critical analysis in form of a written report and an oral presentation that takes the form of a seminar.

Course literature

Molecular Electronic-Structure Theory, Wiley, 2000, ISBN: 978-0-471-96755-2; Density-Functional Theory of Atoms and Molecules, Oxford University Press, 1994, ISBN: 978-0-19-509276-9.

Examination

- DEL1 - Attendance, 3.0 credits, grading scale: P, F
- PRO1 - Project, 4.5 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.

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

Examination takes the form of active course participation at 80% during the lectures in the first part of the course, and for the second part, the project assignment is examined based on a passed project report and an oral seminar. Grading criteria are specified in the course PM.

Other requirements for final grade

Passed attendance of 80% on lectures.
Passed project report.
Passed project seminar.

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.