BB2300 Computational Chemistry 7.5 credits

Beräkningskemi

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 BB2300 valid from Autumn 2016

Grading scale

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

Education cycle

Second cycle

Main field of study

Biotechnology

Specific prerequisites

Admission requirements for programme students at KTH:
At least 150 credits from grades 1, 2 and 3 of which at least 100 credits from years 1 and 2, and bachelor's work must be completed. The 150 credits should include a minimum of 20 credits within the fields of Mathematics, Numerical Analysis and Computer Sciences, 5 of these must be within the fields of Numerical Analysis and Computer Sciences, 20 credits of Chemistry, possibly including courses in Chemical Measuring Techniques and 20 credits of Biotechnology or Molecular Biology.

Admission requirements for independent students:
A total of 20 university credits (hp) in biochemistry, microbiology and gene technology/molecular biology. 30 university credits (hp) chemistry, as well as 20 university credits (hp) in mathematics and computer science as well as bioinformatics 3,5 university credits (hp) and statistics 3,5 university credits (hp) or corresponding. Documented proficiency in English corresponding to English B.

Language of instruction

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

Intended learning outcomes

The goal with this course is to acquire knowledge in Computational Chemistry and some basic skills in carrying out calculations on problems of chemical interest. Except for learning some basic theoretical models, the emphasis is to actually carry out the calculations, and to learn about possible applications and limitations. The course contains a number of theoretical problems and descriptions how to solve these problems.

Course contents

Born-Oppenheimer-approximation, Self-Consistent-Field approach, electron correlation. Modeling of reactions. Optical, electric and magnetic properties. Solvent effects, Molecular Dynamics simulations. Presentation and analysis of characteristic examples.

Disposition

Organisation:

12 double-hours of lectures. During the course a number of exercises will be presented. These should be solved individually using the theoretical tools given.

Course literature

Laborationsbeskrivningar innehållande teori, datorinstruktioner, uppgifter och frågor. Grundläggande kursböcker är Szabo-Östlund ”Modern Quantum Chemistry” (Dover Publications), och Helgaker m fl. ”Electronic Structure Theory” (John Wiley).

Examination

- ÖVN1 - Exercises, 7.5 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.

Other requirements for final grade

A written exam, report for computer assignments and answers for questions (ÖVN1, 7,5 credits, grading scale A-F).

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.