FCK3325 Quantum Chemistry with Applications in Physical Chemistry 12.0 credits

Kvantkemi med tillämpningar i fysikalisk kemi

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

Establishment

Course syllabus for FCK3325 valid from Autumn 2022

Grading scale

P, F

Education cycle

Third cycle

Specific prerequisites

Eligible for studies at the third-cycle level.

To be able to profit from the course the graduate student should have taken basic courses in physical chemistry or corresponding topics.

Language of instruction

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

Intended learning outcomes

Upon completion of the course the doctoral student should have the knowledge and ability to:

- Describe in detail the formalism of quantum mechanics, relate to and summarize the concepts of quantum mechanics in order to define, calculate and explain the behavior of quantum mechanical model systems.
- Describe, explain and apply basic quantum chemical theory for atomic and molecular many-electron systems to the computation of molecular properties, chemical reactivity and molecular spectroscopy.
- Apply quantum chemical calculations and modern quantum chemical software to analyse a specific research problem in physical chemistry. The research problem can, for example, be related to chemical kinetics, catalysis, spectroscopy or intermolecular interactions.

Course contents

In this course, the participants are expected to develop their proficiency in:

- Basic quantum mechanics
- Quantum chemical theory
- The application of quantum chemistry and the use of quantum chemical software for analysing a research problem in physical chemistry. The research problem is selected together with the examiner.

Examination

- TEN1 - Written exam, 6.0 credits, grading scale: P, F
- LAB1 - Compulsory attendance and written reports, 2.0 credits, grading scale: P, F
- PRO1 - Written report and oral presentation, 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.

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

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.