KD2360 Quantum Chemistry 9.0 credits

Kvantkemi

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

Establishment

Course syllabus for KD2360 valid from Autumn 2023

Grading scale

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

Education cycle

Second cycle

Main field of study

Chemical Science and Engineering, Chemistry and Chemical Engineering

Specific prerequisites

Bachelor's degree in engineering or in sciences including 75 credits in chemistry or chemical engineering, 20 credits mathematics and/or programming. English B/6.

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 will be able 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.

Course contents

The course introduces basic concepts and methods of quantum chemistry.

Examination

- TEN1 - Written exam, 6.0 credits, grading scale: A, B, C, D, E, FX, F
- LAB1 - Laborations, 3.0 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.

Other requirements for final grade

Examination (TEN1; 6 credits)
Laboratory work (LAB1; 3 credits)

Final grade will be the same than the grade from the written/oral examination

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.