FCK3313 Quantum Chemistry 9.0 credits

Kvantkemi

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 FCK3313 valid from Spring 2020

Grading scale

P, F

Education cycle

Third cycle

Specific prerequisites

Eligible for studies at the third-cycle level.

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:

- Describe in detail the formalism of quantum mechanics, relate to, reflect over, and summarize the concepts of quantum mechanics in order to define, calculate and explain the behavior of quantum mechanical model systems.
- Describe, reflect upon, 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 theoretical basis and framework of quantum mechanics
- quantum mechanical behavior of simple systems such as harmonic oscillator and rigid rotor
- the basic properties of the spin and the framework that can be applied in spin quantum mechanics
- explanation of the indistinguishability of quantum mechanical objects and the consequences of this with emphasis on the Pauli principle
- the theoretical basis for time-dependent perturbation theory and how it can be used to consider the interaction between electromagnetic radiation, atoms and molecules
- Born-Oppenheimer approximation and emergence of spectroscopic selection rules
- the theoretical basis behind the variational method and linear variation functions and application of these methods to simple atomic and molecular systems, such as the hydrogen atom, the hydrogen molecule and molecule ions
- construction of many-electron wavefunctions as Slater-determinants based on single-electron wavefunctions within the orbital-approximation, and how the properties of these approximate wavefunctions compare to more exact wavefunctions
- the theoretical basis and approximations behind the Hartree-Fock method, and how these approximations affect the accuracy and the applicability of the Hartree-Fock methods for calculations on atomic and molecular systems
- how the Hartree-Fock method is implemented using Roothans equations in modern quantum chemical programs
- the theoretical basis behind post-Hartree-Fock and density functional theory methods and their implementation and use in quantum chemistry
- calculation of molecular properties and analyzing chemical reactions using modern quantum chemical software

Examination

- LAB1 - Laboratory work, 3.0 credits, grading scale: P, F
- TEN1 - Written exam, 6.0 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.

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.