KD2360 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 KD2360 valid from Autumn 2013

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

Admission requirements for programme students at KTH:
At least 150 credits from grades 1, 2 and 3 of which at least 110 credits from years 1 and 2, and bachelor's work must be completed, within a programme that includes:
75 university credits (hp) in chemistry or chemical engineering, 20 university credits (hp) in mathematics and 6 university credits (hp) in computer science or corresponding.

Admission requirements for independent students:
75 university credits (hp) in chemistry or chemical engineering, 20 university credits (hp) in mathematics and 6 university credits (hp) in computer science 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

After completing the course, the student should be able to:

• identify, select and explain which concepts are involved and in which way in the theoretical framework of quantum mechanics.

• identify, describe and explain the quantum mechanical behavior of simple systems, such as the harmonic oscillator and the rigid rotor.

• describe the basic properties of spin and identify the theoretical framework used to describe spin quantum mechanics.

• identify, describe and explain quantum indistinguishability for multi-particle systems and its consequences, with special emphasis on the Pauli principle.

• describe the theoretical basis of time-dependent perturbation theory and explain how it can be used to treat the interaction between electromagnetic radiation and atoms and molecules.

• describe and explain the Born-Oppenheimer approximation and the appearance of spectroscopic selection rules.

• describe the theoretical basis behind the variational method and linear variation functions, and apply these methods to simple atomic and molecular systems, such as the hydrogen atom and the hydrogen molecule ion.

• construct many-electron wavefunctions as Slater-determinants from single-electron wavefunctions within the orbital-approximation, and understand how the properties of these approximate wavefunctions compare to more exact wavefunctions.

• describe the theoretical basis and approximations behind the Hartree-Fock method, and how the these approximations affect the accuracy and the applicability of the Hartree-Fock methods for calculations on atomic and molecular systems

• describe how the Hartree-Fock method is implemented using Roothans equations in modern quantum chemical programs

• describe the theoretical basis behind post-Hartree-Fock and density functional theory methods and their implementation and use in quantum chemistry.

• calculate molecular properties and analyze chemical reactions using modern quantum chemical sofware

Course contents

The course consists of two parts. The essential quantum mechanics that is required later is covered in the first part. The basic quantum mechanical principles and their applications to model systems once mentioned in the basic course are discussed in detail. Approximative methods are introduced. The interaction between electromagnetic radiation and molecules is discussed which then leads to the basic principles of various optical (such as infrared and Raman) spectroscopies.

Methods of quantum chemical calculations and their applications in chemistry and biochemistry are treated in the second part of the course. The Hartree-Fock method, its theoretical background and implementation but also post-Hartree-Fock methods and the density functional theory are described and discussed. Their application for calculating molecular properties such as energies, molecular geometries, vibrational spectra and features of chemical reactions is introduced and illustrated. This part of the course includes quantum-chemical calculation assignments where a modern quantum chemical software package is used for computing molecular properties and chemical reactions.

Course literature

De följande böcker rekommenderas:

D. J. Griffiths: Introduction to Quantum Mechanics, 2nd ed

A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover, 1995

Examination

- LAB1 - Laborations, 3.0 credits, grading scale: P, F
- TEN1 - Written exam, 6.0 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

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.