KD1060 Molecular Structure 7.5 credits

Molekylär struktur

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 KD1060 valid from Autumn 2011

Grading scale

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

Education cycle

First cycle

Main field of study

Chemistry and Chemical Engineering,Technology

Language of instruction

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

Intended learning outcomes

After having passed the examination, the students are expected to be able to:

- Perform quantum chemical calculations on simple model systems, such as particle-in-a-box, and from the results of such calculations analyze observable properties, such as particle position, energy and momentum,
- Relate observable properties in simple model systems to the corresponding properties for complex atomic and molecular systems, as well as estimate how these properties depend on the system size and potential energy,
- Calculate the energy of simple atomic and molecular systems from exact and approximate wavefunctions,
- Analyze the electronic probability distribution in atomic and molecular systems,
- Perform simple molecular orbital calculations on many-electron systems,
- Estimate the stability and energy level distributions of molecules based on molecular orbital calculations,
- Describe how the physical properties of materials, such as electronic conduction and magnetism, depend on the electronic structure of the building blocks,
- Give an overview of modern calculational methods of quantum chemistry and their application,
- Describe the different types of intermolecular interactions, as well as describe the consequences for the collective molecular properties relating to aggregation state, solvation and biological recognition,
- Analyze the structure of simple crystalline materials based on crystallographic data determined by X-ray or neutron diffraction, as well as to describe the function of the diffraction techniques,
- Estimate the stability of ionic materials based on the properties of the constituating ions,
- Describe fundamental spectroscopic concepts, such as absorption, stimulated emission and spontaneous emission, as well as describe how these are related to temperature and molecular properties, including energy level distribution,
- Calculate and analyze infrared and microwave spectra for diatomic molecules,
- Describe the selection rules for infrared, microwave and Raman spectra,
- Analyze infrared and Raman spectra for many-atom molecules,
- Describe different electronic spectroscopic techniques, as well as analyze electronic spectra using the Franck-Condon principle,
- Describe how a laser works and the special properties of laser radiation and application of lasers,
- Give an overview of modern spectroscopic techniques and their application,
- Give a molecular-base description of phenomena related to environmentally sustainable development of society, including the greenhouse effect and ozone-layer depletion, as well as be able to scrutinize available information regarding the effects of different chemical substances on such phenomena,
- Explain the importance of intermolecular interaction for the structure of biological macromolecules, such as DNA and proteins,
- Analyze the chemical function of enzymes based on the chemical structure and potential intermolecular interactions between functional groups of the protein active centra.

Course contents

- Elementary quantum mechanics
- Electronic structure of atoms, atomic orbitals, the basis for the periodic system
- Chemical bonding, molecular orbitals, hybridization, singlet and triplet states, applications of chemical bonding in organic, inorganic, and biological molecules
- Background to modern quantum chemical methods
- Intermolecular interactions, gases-liquids-liquid crystals-solids, supermolecular structures, e.g. biomembranes
- Spectroscopical methods such as IR, Raman, UV/VIS, NMR, MS, ESCA
- Diffraction methods
- Structural chemistry with student project (1p)

Most of the experimental methods and the computational quantum chemistry are exemplified by laboratory and/or computer exercises.

Specific prerequisites

Completed upper secondary education including documented proficiency in English corresponding to English A. For students who received/will receive their final school grades after 31 December 2009, there is an additional entry requirement for mathematics as follows: documented proficiency in mathematics corresponding to Mathematics A.

And the specific requirements of mathematics, physics and chemistry corresponding to Mathematics E, Physics B and Chemistry A.

Course literature

Atkins and de Paula
Atkins' Physical Chemistry, 9th
Oxford University Press 2010
ISBN-13: 978-0-19-954337-3

Examination

- LAB1 - Laboratory Work, 1.5 credits, grading scale: P, F
- PRO1 - Project, 1.5 credits, grading scale: P, F
- TEN1 - Examination, 4.5 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

Examination 4,5 credits
Laboratory work 1,5 credit
Project work 1,5 credit

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.