DEPARTMENT OF CHEMISTRY AND MOLECULAR BIOLOGY

KEM321 Applied Quantum Chemistry, 10 credits

Tillämpad kvantkemi, 10 högskolepoäng

Second Cycle

Confirmation

This course syllabus was confirmed by Department of Chemistry and Molecular Biology on 2013-07-05 and was last revised on 2017-10-04 to be valid from 2017-10-04, autumn semester of 2017.

Field of education: Science 100%

Department: Department of Chemistry and Molecular Biology

Position in the educational system

The course is classified at the level 90-120 credits for Degree of Bachelor. Alternatively it can be read as a course at second cycle level for Degree of Master (120 credits) and also as a freestanding course. This course replaces the earlier courses KEM320 and KEN320 and may not be included together with one of these in the same degree.

The course can be part of the following programmes: 1) Master's Programme in Chemistry (N2KEM), 2) Bachelor of Science Programme in Medicinal Chemistry (N1LMK) and 3) Bachelor of Science Programme in Chemistry (N1KEM)

Main field of studies	*Specialization*
Chemistry	A1N, Second cycle, has only first-cycle course/s as entry requirements

Entry requirements

For admission to the course, passed courses in science comprising 90 credits (or, alternatively, passed courses in pharmacy/medicine comprising 120 credits) are required, which must include course KEM040 Physical chemistry (15 credits), alternatively course FYP203, Quantum Physics A, or equivalent knowledge. Knowledge in mathematics corresponding to course MMGK11, Mathematics for Science (15 credits) is recommended.

Learning outcomes

On successful completion of the course the student will be able to:

Knowledge and understanding

- **explain** the role of the quantum chemistry in chemistry and its potential to solve chemical problems,
- **describe** the idea behind the independent-electron approximation, self-consistent field and Hartree-Fock method,
- **explain** the electron correlation and its the effect on chemical systems and processes,
- **explain** the principle behind density functional theory (DFT) and the Kohn-Sham (KS) formalism, **describe** the approximations that are used in practical DFT calculations,
- **describe** methods to determine equilibrium geometries, their advantages and disadvantages,
- **explain** the stages that lead from computational results to measurable thermochemical quantities,
- **explain** in general how electric and magnetic properties are calculated.

Competence and skills

- **set up** a calculation for a given problem and **choose** appropriate calculation methods and basic set as well as **justify** the choice,
- **use** quantum chemical calculations to examine the thermochemistry and reaction mechanisms of a simple reaction,
- **present** the results of a calculation in oral and written form.

Judgement and approach

- **interpret** the results of quantum chemical calculations and **put them in connection** with experimental results,
- **notice** and **account for** potential problems for the calculation on certain types of molecules or processes,

- **critically assess** the reliability of the achieved results.

Course content
The course treats quantum chemical calculation methods with a clear focus on their application to solve chemical problems. The following subjects will be treated:

1. Quantum Mechanics and chemistry
2. The foundations of the quantum mechanical description: Wave function, Schrödinger equation, the Born-Oppenheimer approximation
3. Independent electrons: Orbitals, self-consistent fields (SCF), the Hartree-Fock method
4. Mathematical description of the orbitals: Basis functions–idea, Slater and Gauss functions, split-valence functions, diffuse and polarisation functions, classification of basic sets
5. Electron correlation: Description and consequences for the behaviour of the molecules
6. The standard method of today's quantum chemistry: Density functional theory (DFT)–basic ideas, Kohn-Sham (KS) formalism as path to a useful computational scheme, necessary approximations for exchange/correlation (XC), various types of XC functionals (LDA, GGA, mGGA, hybrid-GGA)
7. Determining equilibrium geometries for molecules and complexes: Geometry optimisation
8. To calculate and interpret molecular vibrations: IR and Raman spectra
9. Study of reaction mechanisms, thermochemistry
10. Treatment of solvent effects
11. Analysis of orbitals and elektron density
12. Calculation of electronic properties: polarisability, NMR properties, susceptibility
13. Semiempirical methods
14. Current trends in the quantum chemistry: Linear scaling, local orbital methods, multi-scale modelling

The teaching sessions are complemented by computer-based laboratory sessions, where important points of the theory are demonstrated and are trained based on modern quantum chemical program packages.

Sub-courses

1. **Theory part** *(Teoretiska delen),* 6 higher education credits
   Grading scale: Pass with Distinction (VG), Pass (G) and Fail (U)

2. **Computer exercises** *(Datalaborationer),* 4 higher education credits
   Grading scale: Pass (G) and Fail (U)

Form of teaching

Module 1: Teaching is conducted in the form of lectures and exercises.

Module 2: Teaching is conducted in the form of computer-based laboratory sessions including presentations.

Language of instruction: Swedish and English
As principal rule, the course is given in Swedish but can be given completely or partly in English if the circumstances require it.

Assessment

Module 1: Examination takes place based on a written examination.

Module 2: Examination takes place based on active participation in laboratory sessions and presentations.

If a student who has failed the same part of the examination twice wishes to change examiner before the next examination a written application shall be sent to the department responsible for the course and shall be granted unless there are special reasons to decline it (Chapter 6, Section 22 of Higher Education Ordinance).

In cases where a course has been discontinued or has undergone major changes, the student shall normally be guaranteed at least three examination occasions (including the ordinary examination) during a period of at least one year from the last time the course was given.

Grades

The grading scale comprises: Pass with Distinction (VG), Pass (G) and Fail (U).
Module 1: Grade Pass with distinction, Pass or Fail will be awarded.

Module 2: Grade Pass or Fail will be awarded.

Final grade: For grade of Pass on the whole course, grades of Pass on module 1 and Pass on module 2 are required. For grade of Pass with distinction on the whole course, grade of Pass with distinction on module 1 and Pass on module 2 are required.

Course evaluation

Students who participate in or have completed a course should be given the possibility to anonymously express experiences of and views on the course in a course evaluation.

The results of and possible changes to the course will be communicated to students who participated in the evaluation and students who are starting the course.

Additional information