UNIVERSITY OF GOTHENBURG

DEPARTMENT OF CHEMISTRY AND MOLECULAR BIOLOGY

KED321 Applied quantum chemistry for master and PhD students, 15 higher education credits

Tillämpad kvantkemi för master- och forskarstuderande, 15 högskolepoäng

Second Cycle

Confirmation

This course syllabus was confirmed by Department of Chemistry and Molecular Biology on 2014-10-28 and was last revised on 2016-09-01 to be valid from 2016-09-01, autumn semester of 2016.

Field of education: Science 100%
Department: Department of Chemistry and Molecular Biology

Position in the educational system

The course is classified as a graduate course. Alternatively it can be read as a freestanding course at the level 120-150 credits and is then counted as a course at second cycle level for Degree of Master (120 credits).

The course can be part of the following programme: 1) Master's Programme in Chemistry (N2KEM)

Main field of studies	*Specialization*
Chemistry	A1F, Second cycle, has second-cycle course/s as entry requirements

Entry requirements

For admission to the course, a Degree of Bachelor or the equivalent in a scientific field is required. Within the scope of the course requirements, passed course KEM040, physical chemistry (15 credits) or the equivalent knowledge and passed course MMGK11, Mathematics for natural scientists A1 (15 credits) or the equivalent knowledge are 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 and **at a general level describe** calculation methods that include correlation effects in the wave function explicitly,
- **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,
- **explain** the limitations of non-relativistic quantum chemistry and **at a general level describe** methods to include relativistic effects in quantum chemical methods.

Skills and abilities

- **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,
- **plan** and **carry out** a smaller project where a chemical problem is treated with quantum chemical calculations,
- **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. Advanced calculation methods to describe electron correlation: Configuration interaction (CI), Coupled Cluster (CC), Møller-Plesset perturbation theory (MP), multi-reference SCF (MCSCF)
7. 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)
8. Determining equilibrium geometries for molecules and complexes: Geometry optimisation
9. To calculate and interpret molecular vibrations: IR and Raman spectra
10. Study of reaction mechanisms, thermochemistry
11. Relativistic effects in the quantum chemistry?consequences of relativistic effects, calculation methods
12. Beyond the ground state?time-dependent density functional theory to describe excited state and dynamic processes
13. Treatment of solvent effects
14. Analysis of orbitals and elektron density
15. Calculation of electronic properties: polarisability, NMR properties, susceptibility
16. Semiempirical methods
17. Current trends in the quantum chemistry: Linear scaling, local orbital methods, multi-scale modelling

In the course, a project work is included, where the student applies quantum chemical calculation methods on a self-chosen problem.

Sub-courses

1. **Theory part** *(Teoretiska delen),* 10 higher education credits
   Grading scale: Pass with Distinction (VG), Pass (G) and Fail (U)
2. **Computer exercises** *(Datalaborationer),* 5 higher education credits
   Grading scale: Pass (G) and Fail (U)

Form of teaching

Module 1: Teaching is conducted in the form of lectures, exercises and a project work.

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 project work.

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