Department of Physics

Stockholm University

Syllabus

for course at advanced level

Quantum Chemistry
Kvantkemi

15.0 Higher Education Credits
15.0 ECTS credits

Course code:	FK7059
Valid from:	Autumn 2019
Date of approval:	2017-01-16
Changed:	2017-01-16
Department	Department of Physics
Main field:	Physics
Specialisation:	A1N - Second cycle, has only first-cycle course/s as entry requirements

Decision

This course plan was established by the Board of Science at Stockholm University on 2017-01-16. A technical revision was made on 2019-04-30.

Prerequisites and special admittance requirements

Admission to the course requires knowledge equivalent to passed courses (excluding introductory courses) of 45 credits in mathematics and 60 credits in physics, where the courses Quantum Mechanics, 7.5 credits (FK5020) and Atomic and Molecular Physics, 7.5 credits (FK5023) should be included; or a bachelor degree in chemistry where the course Physical Chemistry, 9 credits (KZ4009) should be included. Additionally, admission to the course requires knowledge equivalent to upper secondary school English B/English 6.

Course structure

Examination code	Name	Higher Education Credits
HELA	Quantum Chemistry	15

Course content

In the course, methods for solving the molecular Schrödinger equation, formulated within the Born-Oppenheimer approximation, are presented. Computational methods, based on the variational principle and on perturbation theory, are introduced. A strong focus is given to Hartree-Fock theory and the basics of density functional theory, but also semi-empirical methods and more exact approximations in modern quantum chemistry, including efficient algorithms, are described.

In relation to the computations, fundamental concepts are treated, such as correlation energy, electron spin, molecular orbitals, potential energy surfaces, chemical reactions, transition state theory, molecular mechanics and effects of the surroundings. An introduction to the use of quantum chemical programs is given.

Learning outcomes

Upon completion of the course, students are expected to be able to:
• have an understanding of the basic approximations used to solve the molecular Schrödinger equation
• describe different molecular computational methods, quantum mechanical and others
• plan, perform, describe and evaluate simple computational projects within quantum chemistry

Education

The education consists of lectures and computer exercises.

Participation in the computer exercises is compulsory. In the event of special circumstances, the examiner may, after consultation with the teacher concerned, grant a student exemption from the obligation to participate in certain compulsory instruction.

The course will be given in English if requested by any student enrolled.

Forms of examination

a. The course is examined as follows: knowledge assessment takes the form of written and oral exams and written and oral presentations of computer exercises. If the instruction is in English, the examination may also be conducted in English.

b. Grades will be set according to a seven-point scale related to the learning objectives of the course:
A = Excellent
B= Very good
C = Good
D = Satisfactory
E = Adequate
Fx = Fail, some additional work required
F = Fail, much additional work required

c. The grading criteria will be distributed at the beginning of the course.

d. In order to pass the course, a minimum grade of E is required.

e. Students who receive a failing grade on a regular examination are allowed to retake the examination as long as the course is still provided. The number of examination opportunities is not limited. Other mandatory course elements are equated with examinations. A student who has received a passing grade on an examination may not retake the examination to attain a higher grade. A student who has failed the same examination twice is entitled to have another examiner appointed, unless there are special reasons to the contrary. Such requests should be made to the department board.

The course includes at least two examination opportunities per year when the course is given. At least one examination opportunity will be offered during a year when the course is not given.

f. Students awarded the grade Fx are given the opportunity to improve their grade to E. The examiner decides the supplementary assignments to be performed and the pass mark criteria. The supplementary assignments will take place before the next examination session.

Interim

SStudents may request that the examination be conducted in accordance with this course plan even after it has ceased to be valid. However, this may not take place more than three times over a two year period after course instruction has ended. Requests must be made to the departmental board. The provision also applies in the case of revisions to the course plan (and the revisions of the course literature).

Limitations

The course may not be included in examinations in combination with course Quantum Chemistry, 15 credits (FK7009) or equivalent.

Misc

The course can be included as part of the master's programs offered at the Physics department, but is also offered as a separate course.

Required reading

The course literature is decided by the department board and published on the Department of Physics’s website at least two months before the start of the course.