

# Syllabus

## for course in education at postgraduate level

### Quantum chemical methods in chemical physics

**15 Höskolepoäng**  
**15 ECTS credits**

<b>Course code:</b>	FK40002
<b>Valid from:</b>	VT 2018
<b>Established:</b>	2017-12-14
<b>Department:</b>	Department of Physics
<b>Subject:</b>	Chemical Physics

#### Decision

This course plan has been adopted by Fysikum's board on 12/14/2017.

#### Prerequisites and special admittance requirements

Admitted to graduate level education

#### Course objectives

The course aims to broaden the doctoral student's knowledge of the research area (chemical physics)

#### Content

The course deals with methods for solving the molecular Schrödinger equation within the framework of the Born-Oppenheimer approximation.

Calculation methods based on the variational method and perturbation theory are introduced. A focus is on The Hartree-Fock method and the basics of density functional theory but also semi-empirical methods and more exact approximations in modern quantum chemistry, as well as efficient algorithms, are described.

In relation to the calculations, the course treats basic concepts such as electron correlation, electron spin, molecular orbitals, potential surfaces, chemical reactions, transition-state theory, molecular mechanics and environmental effects. Introduction to the use of quantum chemical computer programs.

#### Learning outcome

After completing the course, the student is expected to be able to:

- describe the basic approximations that lie behind the solution of the molecular Schrödinger equation
- give an account of various molecular calculation methods in quantum chemistry
- plan, implement, describe and evaluate simple quantum chemical calculation projects.
- assimilate and to some extent evaluate studies with modern calculation methods.

### **Form of instruction**

The teaching consists of lectures and computer exercises.

A project work in chemical physics around a current research question, where different calculation methods can be evaluated and discussed is included. The project includes simple calculations and a short literature study which is reported orally and in writing.

Participation in the computer exercises and the group teaching integrated with them is mandatory. If there are special reasons the examiner can, after consultation with the relevant teacher, grant the student exemption from the obligation to participate in certain compulsory activities.

The course is taken together with FK7059.

The course is taught in English.

Undervisningen består av föreläsningar och datorövningar.

### **Forms of examination**

The course is examined in the following way:

- a) Knowledge is checked through assignments and a written test.  
If the teaching takes place in English, the examination may also be conducted in English.
- b) Grading according to a two-point grading scale: Pass or Fail.
- c) The course's grading criteria are distributed at the start of the course.
- d) Students who fail the regular exam have the right to undergo additional exams as long as the course is given.

The number of examination occasions is not limited. Other compulsory course parts are equated with exams.

### **Transitional provisions**

Students can request that the examination be carried out according to this syllabus even after it has ceased to apply, however, no more than three times during a two-year period after teaching on the course has ended. This should be requested to the institution's board. The provision also applies when revising the syllabus.

### **Restrictions**

The course cannot be included in the degree together with the course Quantum Chemistry, 15 credits (FK7009), (FK7059) or corresponding course.

### **Course literature**

Course literature is announced well in advance of the start of the course.