Faculty of Science

KEMM58, Chemistry: Molecular Quantum Mechanics, 7.5 credits

Kemi: Molekylär kvantmekanik, 7,5 högskolepoäng

Second Cycle / Avancerad nivå

Details of approval

The syllabus was approved by Study programmes board, Faculty of Science on 2019-01-21 to be valid from 2019-01-21, autumn semester 2019.

General Information

The course is an elective second-cycle component of a degree of Master of Science (120 credits) in Chemistry and compulsory for a degree of Master (120 credits) in Organizing Molecular Matter.

Language of instruction: English

Main field of studies	*Depth of study relative to the degree requirements*
Organizing Molecular Matter	A1F, Second cycle, has second-cycle course/s as entry requirements
Chemistry	A1F, Second cycle, has second-cycle course/s as entry requirements

Learning outcomes

The aim of the course is to enable students to acquire good knowledge of the basic theories of chemical bonding and intermolecular interaction and how they determine the behaviour of matter. The course provides students with an advanced introduction to modern quantum chemistry.

Knowledge and understanding

On completion of the course, the students shall be able to

- account for the basics of quantum mechanics

- account for the quantum mechanical principles of atoms and molecular systems
- explain the concept of wave function
- describe in detail the electronic structure of atoms and chemical bonding
- name the symmetrical properties of molecular wave functions
- account for the most important calculation methods of modern quantum chemistry and explain their limitations

Competence and skills
On completion of the course, the students shall be able to

- use quantum mechanical software for the calculation of the properties of molecular systems
- solve specific problems of molecular quantum mechanics
- analyse the symmetry of molecules
- discuss the limitations of the calculation methods
- provide a general summary and presentation of the key methods of modern quantum chemistry and a recommendation for an appropriate method
- execute a minor individual project and present the results obtained orally and in writing

Judgement and approach
On completion of the course, the students shall be able to

- evaluate the results of calculation codes and make qualified assessments of sources of error
- critically review and discuss approximations that are used in quantum chemistry

Course content

Lectures (6 credits): The course covers two fields, quantum mechanics and quantum chemistry. The quantum mechanics component deals with the basic equations that control the behaviour of microscopic particles. The quantum chemistry component addresses how these basic equations control the behaviour of atoms and molecules.

The following topics are included in the course: the basics of quantum mechanics, linear movement, rotational motion and the hydrogen atom, angular momentum and spin, group theory and symmetry, approximations in quantum chemistry, atoms and molecules, computational chemistry, and introduction to spectroscopy.

Computer exercises and project work (1.5 credits): The course includes computer exercises covering the following elements: graphical user interfaces for quantum chemistry software, practical exercises with group theory, use of semiempirical methods and use of ab initio methods.

A minor project focusing on quantum chemistry is to be executed individually.

Course design

The teaching consists of lectures, seminars, computer exercises and project work. Compulsory participation is required in laboratory exercises, project work and associated elements.

Assessment

The assessment is based on a written exam at the end of the course and on compulsory components throughout the course.

Students who fail an assessment will be offered another opportunity for assessment soon thereafter.

The examiner, in consultation with Disability Support Services, may deviate from the regular form of examination in order to provide a permanently disabled student with a form of examination equivalent to that of a student without a disability.

Subcourses that are part of this course can be found in an appendix at the end of this document.

Grades

Marking scale: Fail, Pass, Pass with distinction.
For a grade of Pass on the whole course, the student must have passed the exam and the compulsory components.

The grades awarded for the exam are Fail, Pass and Pass with Distinction. The grades awarded for the compulsory components are Fail and Pass.

The final grade is determined by the grade for the exam.

Entry requirements

To be admitted to the course, students must meet the general entry requirements for higher education and requirements for English proficiency corresponding to English 6 from Swedish upper secondary school, and have passed 90 credits in science courses including courses equivalent to:

- KEMA20 General Chemistry 15 credits, or KEMA10 General Chemistry 7.5 credits and KEMA12 Inorganic Chemistry- Basic Course 7.5 credits, KEMA01 Organic Chemistry- Basic Course 7.5 credits and KEMA03 Biochemistry- Basic Course 7.5 credits,
- KEMB09 Physical Chemistry- Basic Course 15 credits
- KEMM30 Molecular Driving Forces and Chemical Bonding 15 credits
- MATA02 Mathematics for Scientists 15 credits, or the equivalent

The admission requirements are also met by students who satisfy the general entry requirements for higher education and requirements for English proficiency corresponding to English 6 from Swedish upper secondary school, and have passed courses equivalent to

- 75 credits in physics including FYSC11 Atomic and Molecular Physics 7.5 credits and FYSC13 Solid State Physics 7.5 credits, and
- 30 credits in mathematics

Students who have obtained the equivalent knowledge by other means may also be admitted to the course.

Further information

The course may not be included in a degree together with KEMM28 Molecular Quantum Mechanics 7.5 credits.

Subcourses in KEMM58, Chemistry: Molecular Quantum Mechanics

Applies from H19

1901 Molecular Quantum Mechanics, 6,0 hp
Grading scale: Fail, Pass, Pass with distinction
1902 Molecular Quantum Mechanics, Compulsory Elements, 1,5 hp
Grading scale: Fail, Pass