

## KEMM28, Chemistry: Molecular Quantum Mechanics, 7.5 credits

*Kemi: Molekylär kvantmekanik, 7,5 högskolepoäng*  
Second Cycle / Avancerad nivå

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### Details of approval

The syllabus was approved by Study programmes board, Faculty of Science on 2008-04-29 and was last revised on 2008-04-29. The revised syllabus applies from 2008-04-30, autumn semester 2008.

### General Information

The course is an optional second-cycle course for a degree of Master of Science in Chemistry and is a compulsory course for a degree of Master of Science in Organizing Molecular Matter.

*Language of instruction:* English and Swedish  
When necessary, the course in full is given in English.

#### *Main field of studies*

Chemistry

Organizing Molecular Matter

#### *Depth of study relative to the degree requirements*

A1N, Second cycle, has only first-cycle course/s as entry requirements

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### Learning outcomes

The course aims to provide good knowledge of the basic theories about chemical bonds and intermolecular interaction and how they control the behaviour of matter.

The aim of the course is that on its completion students will have acquired the following skills and knowledge:

- the ability to understand and apply the principles of quantum mechanics to molecular systems
- thorough understanding of chemical bonds
- the ability to use quantum mechanical computer programmes to calculate the properties of molecular systems, interpret results and assess sources of errors

## Course content

*Lectures:* The course covers two areas, quantum mechanics and quantum chemistry. The quantum mechanics section takes up the basic equations that control the behaviour of microscopic particles. The quantum chemical section takes up how these basic equations control the behaviour of atoms and molecules.

*Project:* A small project will be carried out, with a focus on quantum chemistry.

## Course design

Teaching comprises lectures and exercises in which theoretical aspects are treated. During the course there is one compulsory project that is presented orally.

## Assessment

The course is assessed with a written or oral examination. Re-sit examinations are offered soon after the examination to students who do not pass.

*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.

To be awarded Pass on the whole course, students must pass the examination and pass the project.

The examination grades are: Pass with Distinction, Pass or Fail. Grades for the compulsory components are: Pass or Fail.

The final grade for the course is determined by the result of the examination.

## Entry requirements

To be eligible for this course students must have basic eligibility and 90 higher education credits in completed Science courses, including passes in courses equivalent to:

- KEMA00 General and Analytical Chemistry 7.5 credits, KEMA01 Organic Chemistry – Basic Course 7.5 credits, KEMA02 Inorganic Chemistry – Basic Course 7.5 credits and KEMA03 Biochemistry – Basic Course 7.5 credits, or KEM101 General Chemistry 1 15 credits and KEM102 General Chemistry 2 15 credits, or KEM111 Chemistry for Environmental and Biological Sciences – General Course 1 15 credits and KEM122 Chemistry for Environmental and Biological Sciences – General Course 2 15 credits

and

- KEMB09 Physical Chemistry – Basic Course 15 credits or KEM103 General Chemistry 3 15 credits,

- KEMB08 Molecular Interactions and Structure 15 credits, or KEM016 Physical Chemistry 15 credits/KEMB19 Physical Chemistry 15 credits and
- one of the courses MATA01 Mathematics for Scientists 1 15 credits, MATA11 Mathematics 1 Alpha 15 credits, MAT015 Mathematics for Scientists 1 15 credits or MAT131 Mathematics 1 Alpha 15 credits.

Admission requirements are also fulfilled for those with basic eligibility and passes in courses equivalent to:

- 90 credits in Physics including Physics 3: Modern Physics 30 credits or FYS023 Physics 3: General Course 30 credits and
- 30 credits in Mathematics

or

- 60 credits in Chemistry, 60 credits in Physics and 60 credits in Mathematics

Equivalent knowledge that has been gained in another way also provides eligibility for the course.

### **Further information**

The course cannot be credited as part of a degree programme that also includes KEM063 Theoretical Chemistry 15 credits or KEMM08 Theoretical Chemistry 15 credits.

## Subcourses in KEMM28, Chemistry: Molecular Quantum Mechanics

Applies from H13

0711 Molecular Quantum Mechanics, 6,0 hp

Grading scale: Fail, Pass, Pass with distinction

0712 Molecular Quantum Mechanics, Compulsory Elements, 1,5 hp

Grading scale: Fail, Pass

Applies from H07

0701 Molecular Quantum Mechanics, 7,5 hp

Grading scale: Fail, Pass, Pass with distinction

0702 Molecular Quantum Mechanics, Compulsory Elements, 0,0 hp

Grading scale: Fail, Pass