Faculty of Science

KEMM30, Chemistry: Molecular Driving Forces and Chemical Bonding, 15 credits

Kemi: Molekylära drivkrafter och kemisk bindning, 15 högskolepoäng

Second Cycle / Avancerad nivå

Details of approval

The syllabus was approved by Study programmes board, Faculty of Science on 2018-11-23 and was last revised on 2022-12-06. The revised syllabus applies from 2022-12-06, autumn semester 2023.

General Information

The course is an elective course in the second cycle for a degree of Master of Science in Chemistry and a compulsory second cycle course for a degree of Master of Science in Applied Computational Science with specialization in Chemistry.

Language of instruction: English

Main field of studies	*Depth of study relative to the degree requirements*
Applied Computational Science	A1N, Second cycle, has only first-cycle course/s as entry requirements
Chemistry	A1N, Second cycle, has only first-cycle course/s as entry requirements

Learning outcomes

The aim of the course is to enable students to acquire a basic framework to describe (bio)molecules and their interactions from a basic microscopy perspective. This includes quantum chemistry, statistical thermodynamics, intermolecular interaction and spectroscopy. The students are to acquire knowledge of chemical bonding, and molecular properties and how they relate to thermodynamics, temperature and interactions in solution.

The student will learn how spectroscopy and models for intermolecular interactions can be used to understand basic properties of biomolecules such as proteins, DNA and membranes. Concepts such as hydrophobic exchange, cooperative bonding, depletion interactions, hydrogen bonding and electric multilayers will be addressed.

In order to be able to manage large data sets generated through experiments, simulations or database searches, and analyse and present complex data, students will acquire basic knowledge of programming and scripts.

The fist part of the course will provide students with basic knowledge of programming and scripts that will be used throughout the course. This includes case studies involving realistic scenarios of how data sets are imported, analysed and visualised. The examples may include but are not limited to: kinetics in biochemistry and catalysis, atomic force microscopy (AFM), electrochemistry, calorimetry, optical spectroscopy, online databases and literature management.

Knowledge and understanding

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

- explain the theory and application of statistical thermodynamics
- describe how (bio)molecules, particles and ions interact
- explain temperature from a microscopy perspective
- account for the basic principles for which basic optical spectroscopy is designed, such as the transition dipole moment and selection rules
- explain and provide an advanced and qualitative description of the relationship between spectroscopic measurements and molecular properties for electronic structural properties of several important types of molecules and materials
- explain essential aspects of electronic processes in functional materials including how they relate to inherent electronic structural properties
- explain how physical properties and chemical bonds can be predicted using modern electronic structure calculations
- explain the influence of polar and non-polar solvents in partitioning, intermolecular interactions, electronic structure and solvation.

Competence and skills

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

- import, visualise and apply models to large data sets
- create interactive reports including completed publications, advanced data analysis and explanatory text
- perform electronic structure calculations of small molecules in gas phase and in solution, and interpret the results
- perform calculations using statistical thermodynamics to describe atoms and molecules, and their interactions
- use programmes of modern quantum chemistry to calculate physical properties and bonding properties of different types of molecules and materials
- use results from electronic structure calculations to discuss molecular structure and bonding, and explain chemical properties in both molecular systems and materials systems
- analyse spectroscopic data and extract relevant molecular properties such as bonding duration and molar absorption coefficient.

Judgement and approach

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

- assess and provide an informed discussion of the importance of the approximations used for intermolecular interactions and statistical thermodynamics
- use knowledge of theoretical chemical calculations to make relevant assessments of the physical properties of several common types of molecules and materials

- assess the advantages and disadvantages of different theoretical methods and argue for a choice of method to study different properties related to molecular structure, bonding and reactivity
- critically assess quantum chemical calculations with regard to precision and chemical relevance
- critically review research reports
- evaluate the limitations of molecular structure information made available by spectroscopic measurements.

Course content

The *lectures* (7.5 credits) deal with quantum chemistry and statistical thermodynamics, including statistical interpretation of entropy and ensembles. The course highlights basic contributions to interactions between atoms, (bio)molecules and surfaces. Furthermore, it includes basic programming/scripts for import and analysis of complex data, and assembly, visualisation and presentation of data. The elements of rotational, vibrational and electronic spectroscopy, both in absorption and emission phases, and basic concepts, Raman spectroscopy and circular dichroism spectroscopy will also be addressed.

The *exercises and written assignments* (4 credits) aim to illustrate and provide examples of the concepts that are introduced and discussed in the lectures. The written assignments may generate bonus points that can be added to the result of the written exam.

The *laboratory sessions* (3.5 credits) aim to illustrate and provide examples of the concepts that are introduced in the lectures and may be intended for experiments or calculation. Students will be trained in report writing and peer reviewing involving critical review and constructive feedback.

Course design

The teaching consists of lectures, possibly recorded ones, exercises, written assignments and laboratory sessions. The written assignments, laboratory sessions and associated components are compulsory.

Assessment

The assessment is based on a written exam at the end of the course and on the 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 written assignments and laboratory reports are Fail and Pass.

The final grade is determined by a weighted aggregate of the exam result and the bonus points for the written assignments.

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/b from Swedish upper secondary school, and have passed 90 credits in science courses including courses equivalent to:

- KEMA20 General Chemistry 15 credits,
- KEMA01 Organic Chemistry- Basic Course 7.5 credits,
- KEMA03 Biochemistry- Basic Course 7.5 credits,
- KEMB09 Physical Chemistry- Basic Course 15 credits, and
- MATA03 Mathematics for Scientists 1, 15 credits or the equivalent.

Students also satisfy the entry requirements if they meet the general entry requirements for higher education and requirements for English proficiency corresponding to English 6/b from Swedish upper secondary school, and have passed courses equivalent to:

- 75 credits in physics including knowledge corresponding to 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 KEMB08 Molecular Interactions and Structure 15 credits.

The course is offered at the Department of Chemistry, Lund university.

Subcourses in KEMM30, Chemistry: Molecular Driving Forces and Chemical Bonding

Applies from H19

1901 Molecular Driving Forces and Chemical Bonding, 7,5 hp
Grading scale: Fail, Pass, Pass with distinction
1902 Molecular Driving Forces and Chemical Bond., Comp. Elements, 4,0 hp
Grading scale: Fail, Pass
1903 Molecular Driving Forces and Chemical Bonding, Lab. Work, 3,5 hp
Grading scale: Fail, Pass