Faculty of Science

KEMM48, Chemistry: Statistical Thermodynamics and Molecular Simulation, 7.5 credits

Kemi: Statistisk termodynamik och molekylsimulering, 7,5 högskolepoäng

Second Cycle / Avancerad nivå

Details of approval

The syllabus was approved by Study programmes board, Faculty of Science on 2019-01-22 to be valid from 2019-01-22, 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 of Science (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	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 objective of the course is to enable students to acquire basic knowledge of statistical mechanics. An important objective is to enable students to acquire specialised understanding of the concept of entropy and thereby bridge the opposition between a microscopic approach (statistical mechanics) and a macroscopic one (thermodynamics).

Knowledge and understanding

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

- account for and apply principles of statistical mechanics to ensembles of molecules
- describe the link between statistical mechanics and thermodynamics
- describe approximate theories of statistical mechanics for liquids and solutions

Competence and skills

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

- apply numerical methods such as Molecular Dynamics and Metropolis Monte Carlo
- use tools of statistical mechanics to calculate properties of macroscopic systems both with and without software

Judgement and approach

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

- evaluate results of numerical calculations and assess sources of error
- assess and judge approximations and their limitations

Course content

Lectures and calculation exercises (6 credits): The course starts with an introduction of basic concepts of statistical mechanics. Thermodynamic transformations are compared with equivalent ensembles within statistical mechanics. Approximate theories of liquids and solutions. Simulation methods. Calculation exercises are used to practise the different tools and arguments of statistical mechanics.

Laboratory sessions and written assignments (1.5 credits).

Course design

The teaching consists of lectures, calculation exercises, laboratory sessions and written assignments. Compulsory participation is required in laboratory sessions, written assignments 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,
- MATA02 Mathematics for Scientists 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 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
- 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 KEMM38 Statistical Thermodynamics and Molecular Simulation 7.5 credits.

Subcourses in KEMM48, Chemistry: Statistical Thermodynamics and Molecular Simulation

Applies from H19

1901 Statistical Thermodynamics and Molecular Simulation, 6,0 hp
Grading scale: Fail, Pass, Pass with distinction
1902 Statistical Thermodyn. and Mol. Simulation, Comp. Elements, 1,5 hp
Grading scale: Fail, Pass