Faculty of Science

KEMM38, 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 is an old version, approved by Study programmes board, Faculty of Science on 2016-08-11 and was valid from 2017-01-01 , spring semester 2017.

General Information

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

When necessary, the course in full is given in English.

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

Learning outcomes

The course aims to provide a basic understanding of Statistical Mechanics. An important goal is to provide a deeper understanding of Entropy, thus bridging the apparent contradiction between a microscopic (Statistical Mechanics) and a macroscopic (Thermodynamics) treatment. After a completed course, the student should have gained knowledge and skills, as outlined below.

Knowledge and understanding

On completion of the course the student will be able to:

- apply and utilize various Statistical Mechanical ensembles, and describe relations between these ensembles

- account for the connection between Statistical Mechanics and Thermodynamics.

Competence and skills

On completion of the course the student will be able to:

- apply numerical methods, such as Molecular Dynamics Metropolis Monte Carlo simulations
- use Statistical Mechanical tools with, as well as without, the aid of computer programs to calculate various properties of macroscopic systems.

Judgement and approach

On completion of the course the student will be able to:

- interpret results from numerical calculations, and analyse sources of error
- describe and present Statistical Mechanical theories for liquids and solutions, and also evaluate approximations and assess limitations.

Course content

Lectures: The course starts with an introduction of basic Statistical Mechanical concepts. Thermodynamical transformations are compared with corresponding Statistical Mechanical ensembles. Approximate theories for liquids and solutions. Simulation methods.

Tutorials: Here, the student acquires skills to utilize Statistical Mechanical tools.

Lectures and tutorials correspond to 6 credits.

Laboratory work and hand-ins correspond to 1.5 hp.

Course design

The teaching entails lectures and tutorials. The course also includes compulsory hand-in exercises, as well as laboratory work, where the latter includes written reports.

Assessment

The course is assessed with a written examination, and by the compulsory components.

A re-sit examination is offered soon after the examination to students who do not pass.

Grades

Marking scale: Fail, Pass, Pass with distinction.
To be awarded a passing grade on the whole course, students must pass the examination and pass the compulsory components.

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

The final grade for the course is determined by the grade on the final examination.

Entry requirements

To be eligible for this course students must have basic eligibility, English 6 and 90 higher education credits in completed Science courses, including courses equivalent to:

- KEMA10 General Chemistry, 7.5 credits, KEMA01 Organic Chemistry – Basic Course, 7.5 credits, KEMA12 Inorganic Chemistry – Basic Course, 7.5 credits, and KEMA03 Biochemistry – Basic Course, 7.5 credits

and

- KEMB09 Physical Chemistry – Basic Course, 15 credits,
- KEMB08 Molecular Interactions and Structure, 15 credits, and
- MATA02 Mathematics for Scientists, 15 credits, or equivalent.

Admission requirements are also fulfilled for those with basic eligibility, English 6, and courses equivalent to:

- 75 credits of Physics including: FYSC11 Atomic and Molecular Physics, 7.5 credits, and FYSC13 Solid State Physics, 7.5 credits

and

- 30 credits of 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 KEMM18 Statistical Thermodynamics, 7.5 credits.