

Naturvetenskapliga fakulteten

Statistical Thermodynamics and Molecular Simulation, NAKE009 (7.5 credits) and NAKE010 (without lab work, 6 credits)

*Statistisk termodynamik och molekylsimulering,
7,5 hp eller (utan laborieriedel) 6 hp*

Third Cycle / Forskarnivå

Details of approval

The syllabus was approved by the Research education board, Faculty of Science 2017-04-04. The syllabus applies from 2017-04-04.

General Information

The course is an optional third-cycle course at the Department of Chemistry. Language of instruction: Swedish and English. When necessary, the course in full is given in English.

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.

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 (NAKE010).

Laboratory work and hand-ins correspond to 1.5 hp. (Cannot be accredited separate from the lecture part)

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

Possible grades are Pass and Fail. To be awarded a passing grade on the whole course (7.5 credits NAKE009), students must pass the written exam and pass the compulsory components (laborations and hand-in assignments). Passing the exam, without passing the laborations and hand-in assignments, renders 6 credits (NAKE010).

Entry requirements

Admitted to research studies at the Faculty of Science or Technology, and at least 15 credits in Mathematics and 30 credits in Physics or Physical/Theoretical Chemistry. Or corresponding knowledge.

Further information

The course is given also in the second cycle, under the course code KEMM38. Students who have been awarded credits for KEMM38 cannot also get credits for the corresponding parts of NAKE009, and vice versa.