



LUND UNIVERSITY
Faculty of Science

SYLLABUS

Date
25 October 2017

Reg. Nr.
U 2017/362

Syllabus for the course Advanced Statistical Thermodynamics and Molecular Simulation, NAKE016 *Swedish title: Avancerad statistisk termodynamik and molekylsimulering*

The course syllabus was confirmed by the Faculty board for graduate studies 25 October 2017. The course is in the third cycle and amounts to 7.5 credits.
The course syllabus is formally approved in Swedish. This is a translation.

Learning outcomes

The course aims to provide a deeper understanding of Statistical Mechanics theories, methods, and tools. The course also aims to bridge the microscopic properties of single particles (Statistical Mechanics) and macroscopic properties (Thermodynamics). A sub-goal is to build an understanding of the link between interactions and dynamics. The students should also get an update on recent advances in the field. On completion of the course, participants shall be able to:

Knowledge and understanding

- Describe and apply or utilize various Statistical Mechanical ensembles, and describe relations between these ensembles.
- Account for the connection between Statistical Mechanics and Thermodynamics.
- Account for the connection between interactions and dynamics.

Skills and abilities

- Account for numerical methods, such as Integral equations and theories, Density Functional equations and theories, Molecular Dynamics, Metropolis Monte Carlo simulations, and Brownian Dynamics simulations.
- Use advanced Statistical Mechanical tools, with as well as without the aid of computer programs, to calculate various static and dynamic properties of macroscopic systems.

Judgement and approach

- Interpret results from numerical calculations, and analyse sources of error.
- Describe Statistical Mechanical theories for liquids and solutions, and also account for approximations and limitations

Course content

The course starts with a repetition of basic statistical-mechanical concepts, methods, and tools. It then continues with more advanced theories for liquids and solutions, simulation methods as well as transport properties and dynamics for liquids and solutions. The course is given in a thematic form with lectures and tutorials (self studies) as well as laboratory work and laboratory report hand-ins which all highlight the different themes.

Teaching

The teaching entails lectures, tutorials, laboratory work and report writing. Mandatory laborative components occur throughout the course, which include written reports.

Assessment

Assessment is based on the written reports from the laborative components.

Grading scale

Possible grades are Pass and Fail. To pass the course, the student must pass all laborations and reports.

Language of instruction

If there is at least one participant who doesn't speak Swedish, the course is given in English. Otherwise, the course is given in Swedish or English.

Entry requirements

Admitted to PhD studies in Chemistry, Physics, or corresponding subject, with prior knowledge corresponding to the second cycle course "Statistical Thermodynamics and Molecular Simulation" (KEMM38).

Additional information

The course cannot be credited together with the following courses given at the University of Gothenburg: "Statistical Thermodynamics (15 credits)" or "Statistical Mechanics with focus on Liquids, Solutions and Colloidal Systems" (15 credits).