KD2340 Molecular Thermodynamics 7.5 credits

Molekylär termodynamik

This is a translation of the Swedish, legally binding, course syllabus.

If the course is discontinued, students may request to be examined during the following two academic years

Establishment

Course syllabus for KD2340 valid from Autumn 2013

Grading scale

A, B, C, D, E, FX, F

Education cycle

Second cycle

Main field of study

Chemical Science and Engineering,Chemistry and Chemical Engineering

Specific prerequisites

Admission requirements for programme students at KTH:
At least 150 credits from grades 1, 2 and 3 of which at least 110 credits from years 1 and 2, and bachelor's work must be completed, within a programme that includes: 75 university credits (hp) in chemistry or chemical engineering, 20 university credits (hp) in mathematics and 6 university credits (hp) in computer science or corresponding.

Admission requirements for independent students:
75 university credits (hp) in chemistry or chemical engineering, 20 university credits (hp) in mathematics and 6 university credits (hp) in computer science or corresponding. Documented proficiency in English corresponding to English B

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

The power of thermodynamics, which remains one of the founding blocks of chemistry, is it generality. In most thermodynamic courses, however, the microscopic and molecular origin of the mechanisms on which it is based on are usually avoided. In this course we address this gap, developing a basic knowledge in statistical thermodynamics to understand the forces that drive molecules and be able to predict their combined behavior in physical, chemical, and biological systems.

After completion of the course, assuming attendance to every lecture and active participation in tutorials, the students should be able to:
• describe and apply the principles of probability to predict molecular behavior.
• describe and explain the concept of the Boltzmann distribution law, molecular partition function and partition function of a system.
• predict some macroscopic properties from atomic and molecular structures using statistical mechanics.
• describe the molecular interpretation of macroscopic properties such as energy, entropy, temperature and heat capacity.
• predict gas-phase chemical reaction equilibria from atomic structures.
• describe and explain phase equilibria based on the concept of chemical potential.
• describe the molecular properties of regular mixtures and predict phase separation in liquid mixtures.
• analyze physical kinetics phenomena in terms of non-equilibrium statistical mechanics.
• predict, using a statistical thermodynamic approach, how the rate of a chemical reaction depends on the molecular structures involved.
• combine the laws of electrostatics and thermodynamic equilibrium (i.e. Poisson-Boltzmann equation) to predict equilibria in solutions containing charged species.
• describe the intermolecular interactions that hold liquids and solids together.
• interpret phase transition diagrams in statistical thermodynamic terms.
• describe the processes of binding and adsorption to a surface.
• describe the anomalous thermodynamic properties of water and describe the origin of the hydrophobic effect.
• explain the molecular thermodynamic properties of simple macromolecules in solution.

Course contents

- Principles of probability.
- The Boltzmann distribution law.
- The statistical mechanics of simple gases & solids and the molecular interpretation of

temperature and heat capacity.
- Chemical and phase equilibria.
- Solutions, mixtures and transfer of molecules between phases.
- Physical (i.e. diffusion, permeation and flow) and Chemical Kinetics.
- Electrostatics: Coulomb's Law, electrostatic potential and electrochemical equilibria.
- Intermolecular interactions and phase transitions.
- Adsorption, binding and catalysis.
- Thermodynamic properties of water.
- Introduction to the thermodynamics of polymer solutions.

Disposition

The course will be given by lectures and tutorials. Handouts of the lectures will be provided regularly covering the topics discussed in the class. Tutorials will supplement the lectures and a significant amount of time will be spent on working problem and answering questions. The structure of the lectures will closely follow the content found in the book we recommend for this course.

Course literature

Ken A. Dill and Sarina Bromberg, Molecular Driving Forces, 2nd Edition, Garland Science. ISBN 978-0-8153-4430-8. Additional material will be provided during the course.

Examination

- LAB1 - Laborations, 1.0 credits, grading scale: P, F
- TEN1 - Examination, 6.5 credits, grading scale: A, B, C, D, E, FX, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

Other requirements for final grade

The final grade is based on the grade of the examination.

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.