

Module Name		Modul Code		
Physical Chemistry 5: Statistical Thermodynamics		chem2003		
Module Coordinator				
Prof. Dr. Jürgen Grotemeyer				
Organizer				
Section Chemistry				
Faculty				
Faculty of Mathematics and Natural Science				
Examination Office				
Examination Office Chemistry				
ECTS Credits		5		
Evaluation		Graded		
Duration		One Semester		
Frequency		Annually Summer Term		
Workload per ECTS Credit		30 h		
Total Workload		150 h		
Contact Time		42 h		
Independent Study		108 h		
Teaching Language		English		
Module Courses				
Course Type	Course Name	Compulsory/Optional	SWS	
Lecture	Statistical Thermodynamics	Compulsory	2	
Exercise	Statistical Thermodynamics	Compulsory	1	
Examination(s)				
Examination Name	Type of Examination	Evaluation	Compulsory/Optional	Weighting
Mixed Examination: Statistical Thermodynamics	Other	Graded	Compulsory	100

Further Information on the Examination(s)

Exams:

- Solution of homework assignments (H),
- Short questions (T, 10 min every 2 weeks),
- Written exam at end of lecture period (K).

Module grade:

- The module marks are calculated according to the following formula:

$$P = 0,3 \times (\%H) + 0,3 \times (\%T) + 0,4 \times (\%K)$$

or

$$P \geq 0,6 \times (\%K)$$

whichever is better.

The minimum number of points to pass is 60 %.

Scheduled time for written exam: End of lecture period,

1st repetition: Before start of lecture period of the following semester,

2nd repetition: After lecture period of the following semester.

Exam language: German

Relevance for final grade M.Sc. Chemistry, M.Sc. Business Chemistry:

- Module grade weighted with CP number enters into M.Sc. grade.

Relevance for final grade M.Ed. Chemistry 2-Subject:

- Module grade enters not M.Ed. grade.

Course Content

- Basic postulates of statistical thermodynamics: Boltzmann's definition of the entropy, elements of probability theory and combinatorics, binomial distribution, thermodynamics of a system of elements with two energy states,
- Systems of independent particles: Polynomial distribution, Lagrange multipliers, Boltzmann-distribution, molecular partition function of the electron in a box, ideal gas, partition function of the harmonic oscillator, Einstein's model of solids, semiclassical approximation, state integrals of translation, rotation, and vibration, equipartitioning law,
- Systems of interacting particles: The Gibbs ensemble (microcanonical, macrocanonical), relation to the chemical potential, canonical state integrals and partition function, ideal gas and van-der-Waals gas, cluster expansion of the molecular partition function,
- Multi-component systems: Entropy of mixing, Gibbs paradox, partition function of mixtures, van-der-Waals theory of mixtures, Bragg-Williams model, phase transitions, Landau theory,
- Systems of reacting particles: Variational calculation of the equilibrium composition, statistical expression for the equilibrium constant, transition state theory,
- Quantum statistics: Analysis of the partition function for fermions and bosons, ideal Bose gas, Bose-condensation, ideal Fermi gas, theory of metals.

Learning Outcome

The students learn the foundations, concepts and methodology of statistical thermodynamics. Next to the basic concepts, the module focuses on the application of these concepts on practical examples. The students develop an understanding, how statistical thermodynamics forms a bridge from the molecular properties to the macroscopic properties of gases, liquids and solids.

Reading List

- Lehrbücher der Physikalischen Chemie,
- B. N. Roy, Fundamentals of Classical and Statistical Thermodynamics,
- W. Göpel, H.-D. Wiemhöfer, Statistische Thermodynamik, Spektrum Akademischer Verlag,
- Lecture Notes.

Use	Compulsory/ Optional	Semester
Master, 1-Subject, Chemistry, (Version 2007)	Compulsory	1 or 2
Master, 1-Subject, Chemistry, (Version 2016)	Compulsory	1 or 2
Master, 1-Subject, Business Chemistry, (Version 2008)	Optional	1 or 2
Master, 1-Subject, Business Chemistry, (Version 2014)	Optional	1 or 2
Master, 1-Subject, Business Chemistry, (Version 2017)	Optional	1 or 2
Master, 2-Subject, Studies in Secondary Education, Chemie, (Version 2007)	Optional	1 - 4
Master, 2-Subject, Studies in Secondary Education, Chemie, (Version 2017)	Optional	1 - 4