CH-242(b)

Statistical thermodynamics

Osterwalder Andreas, Reilly Christopher Scott

Cursus	Sem.	Type
Chemistry and chemical engineering	BA4	Obl.
HES - CGC	E	Obl.

Language of teaching	English
Credits	3
Session	Summer
Semester	Spring
Exam	Written
Workload	90h
Weeks	14
Hours	**3 weekly**
Lecture	2 weekly
Exercises	1 weekly
Number of positions	

Summary

The course covers two topics: an introduction to interfacial chemistry, and statistical thermodynamics. The second part includes concepts like the Boltzmann distribution law, partition functions, ensembles, calculations of thermodynamic properties, quantum statistics, metals, and applications.

Content

A.Interfacial Chemistry
A. 1. Surfaces and interfaces, thermodynamics of interfaces
Surface tension and thermodynamic surface functions, Young and Laplace equations, vapor pressure at curved interfaces, capillary forces, contact angle, measurement of contact angles
A.2. Thermodynamics of adsorption at interfaces, Colloids/Micelles
Gibbs adsorption equation, surfactants, hydrophobic effect, formation of micelles, monomolecular films (Langmuir-Blodgett)
A.3. Adsorption at solid/gas and solid/liquid interfaces
Langmuir isotherm, Fowler-Guggenheim, BET, adsorption in porous solids, capillary condensation in mesoporous systems

B. Statistical Thermodynamcics
B.1. The Boltzmann distribution law
Derivation, Approximation
B.2. Partition function
The translational, rotational, vibrational and electronic partition functions
B.3. Thermodynamic functions from statistical thermodynamics
U, *CV,* heat and work, Entropy, Helmholtz¿ and Gibbs¿ free energies, Chemical potential
B.4. Ensembles
The canonical ensemble, the canonical partition function, the equilibrium constant
B.5. Quantum statistics
Bose-Einstein statistics, Fermi-Dirac statistics, the grand canonical partition function
B.6. Applying partition functions and ensembles
Heat capacity of solids, Computational chemical methods
B.7. Applications of statistical thermodynamics

Keywords

Boltzmann distribution
Partition function
Ensembles
Quantum statistics

Learning Prerequisites

Required courses

Quantum Chemistry
Physics II; Thermodynamics

Important concepts to start the course

Laws of thermodynamics
Equations for quantum energy levels of particle-in-a-box, rotation and vibtration.

Learning Outcomes

By the end of the course, the student must be able to:

- Contextualise the connection between quantum mechanics and thermodynamics
- Apply the molecular partition functions
- Derive the vibrational and translational partition function
- Derive and compute thermodynamic functions from partition functions
- Describe the different ensembles
- Apply Fermi-Dirac and Bose-Einstein statistics to solids

Teaching methods

Lectures with hand outs. Exercises.

Assessment methods

Written exam

Supervision

Office hours	Yes
Assistants	Yes
Forum	No

Resources

Virtual desktop infrastructure (VDI)

No

Bibliography

Handouts of Lecture Notes and exercises, Moodle

Reference books:
Interfacial Chemistry:
Textbooks: Interfacial Science: An Introduction; G.T Barnes and I. Gentle, Oxford University Press available at Amazon.de
and/or
H. J. Butt, K. Graf, M. Kappl, Physics and chemistry of interfaces, Weinheim Wiley- VCH, 2013.

Statistical Thermodynamics:
Benjamin Widom, Statistical Mechanics: A Concise Introduction for Chemists, Cambridge University Press - 2002, ISBN-13: 978-0521009669
Donald A. McQuarrie, Statistical Mechanics, University Science Books - 2000, ISBN - 1-891389-15-7.
For introduction and as a reference for classical thermodynamics
Pierre Infelta & Michael Grätzel, Thermodynamique: Principles et Applications. BrownWalker Press - 2006. ISBN - 1-58112-995-5.

Ressources en bibliothèque

- Thermodynamique / Infelta
- Statistical mechanics / Widom
- Physics and chemistry of interfaces / Hans-Jürgen Butt, Karlheinz Graf, Michael Kappl, 4th ed., 2023
- Interfacial Science: An Introduction / G.T Barnes and I. Gentle
- Statistical mechanics / McQuarrie

Moodle Link

- https://go.epfl.ch/CH-242_b