Zachodniopomorski Uniwersytet Technologiczny w Szczecinie

Faculty of Chemical Technology and Engineering

Field of study	Chemical Engineering		
Mode of study	stationary	*Level*	first cycle
Graduate's qualification	inżynier		
Area(s) of study	nauki techniczne		
Educational profile	general academic		
Module			
Course unit	**Statistical Thermodynamics**		
Code	ChEn_1A_S_C17b		
Field of specialisation			
Administering faculty	Institute of Chemical Engineering and Environmental Protection Processes		
ECTS	5,0	*ECTS (forms)*	5,0
Form of course credit	credits	*Language*	english
Electives	6	*Elective group*	

Form of instruction	*Code*	*Semester*	*Hours*	*ECTS*	*Weight*	*Credit*
lecture	W	5	30	2,0	0,50	credits
laboratory course	L	5	45	3,0	0,50	credits

Leading teacher	Story Anna (Anna.Story@zut.edu.pl)
Other teachers	Story Anna (Anna.Story@zut.edu.pl)

Prerequisites

W-1	Principles of Thermodynamics and Chemical Bonding

Module/course unit objectives

C-1	The aim of the course is to provide fundamental knowledge of Statistical Thermodynamics. An important aim of the course is to provide in-depth understanding of the concept of entropy and thus bridge the opposition between a microscopic approach (statistical mechanics) and a macroscopic one (thermodynamics). An important aim of the course is to understand how intermolecular interaction affects the properties of matter. After completing the course, student knows: (1) the principles of statistical mechanics on ensembles of molecules, (2) the association between statistical mechanics and thermodynamics, (3) how intermolecular interaction affects the properties of matter. Student is also able to use statistical mechanical software to calculate the properties of macroscopic systems and proper interpretation of the results.

Course content divided into various forms of instruction		*Number of hours*
T-W-1	Introduction to the Statistical Thermodynamics. General remarks	2
T-W-2	Review of classical Thermodynamics. Energy and the First Law of thermodynamics. Entropy and the Second Law of thermodynamics. Thermodynamic functions and equilibrium conditions. Change of phase and phase equilibrium	4
T-W-3	Fundamentals assumptions of Statistical Thermodynamics. Phase space. Statistical Mechanics Based on Postulates	4
T-W-4	Discrete theory of probability	4
T-W-5	Continuous theory of probability	4
T-W-6	Entropy and ensembles in statistical mechanics. Classical Ensembles (statistical, microcanonical, canonical and grand canonical). Quantum Ensembles (Quantum Canonical Ensemble, Quantum and Classical Statistics, Simple Quantum Systems)	4
T-W-7	Introduction to Monte Carlo Method. Using Monte Carlo Simulations to Compute Ensemble Averages	4
T-W-8	Molecular Simulation. Monte Carlo Simulations. Introduction to Molecular Dynamics. Examples of software used in simulations of Statistical Thermodynamics issues	4
T-L-1	During the laboratory course selected open-source software will be used to simulate issues of statistical thermodynamics. Modelling will be carried out on the basis of the Monte Carlo methods, as well as the molecular dynamics method, with using selected open-source software, e.g. GROMACS, CP2K, HOOMD-blue, LAMMPS, MOIL, RedMD	45

Student workload - forms of activity		*Number of hours*
A-W-1	Lecture participation	30
A-W-2	Individual literature studies	20
A-W-3	Repetition of the lecture content to the written test	8
A-W-4	One-on-On Teaching Consultation	2
A-L-1	Classroom participation	45
A-L-2	Preparation of reports	30
A-L-3	Literature studies	10

Student workload - forms of activity		*Number of hours*
A-L-4	One-on-One Teaching Consultations	5

Teaching methods / tools	
M-1	Activating methods – lecture and didactic discussion, multimedia presentation
M-2	Practical methods – simulations of thermodynamics problems using molecular dynamics and Monte Carlo methods

Evaluation methods (F - progressive, P - final)		
S-1	P	Written final exam based on the lecture contents
S-2	P	Written reports

Designed learning outcomes	Reference to the learning outcomes designed for the fields of study	Reference to the learning outcomes defined for the particular areas of education	Reference to learning outcomes leading to the degree of "inżynier"	Course objectives	Course content	Teaching methods	Evaluation methods
Knowledge							
ChEn_1A_C17b_W01 Student possesses a general knowledge about the fundamental principles of statistical mechanics,as well as the association between statistical mechanics and thermodynamics. Student knows how intermolecular interaction affects the properties of matter. Student knows different methods of simulations of issues related to statistical thermodynamics	ChEn_1A_W10 ChEn_1A_W15	P6S_WG_TA11	P6S_WG_IA11	C-1	T-W-1 T-W-5 T-W-2 T-W-6 T-W-3 T-W-7 T-W-4 T-W-8	M-1	S-1
Skills							
ChEn_1A_C17b_U01 Student possesses an ability to use specialized software in a way to simulate different issues related to statistical thermodynamics. Student is able to proper interpretation of the obtained results	ChEn_1A_U01 ChEn_1A_U03 ChEn_1A_U05 ChEn_1A_U07 ChEn_1A_U08 ChEn_1A_U16	P6S_UO P6S_UU P6S_UW_TA11 P6S_UW_TA14	P6S_UW_IA11 P6S_UW_IA14	C-1	T-L-1	M-2	S-2
Other social / personal competences							
ChEn_1A_C17b_K01 Student understands the importance of statistical thermodynamics in different applications. Student has an ability independently or in group to use specialized software as a modeling tool. Student understands the need to train and improve his/her professional and personal competences.	ChEn_1A_K01 ChEn_1A_K03 ChEn_1A_K04 ChEn_1A_K05	P6S_KK P6S_KO P6S_KR		C-1	T-L-1 T-W-7 T-W-1 T-W-8 T-W-3	M-1 M-2	S-1 S-2

Required reading
1. Keith Stowe, An Introduction to Thermodynamics and Statistical Mechanics, Cambridge University Press, Cambridge, 2007
2. Gunnar Jeschke, Advanced Physical Chemistry: Statistical Thermodynamics, Swiss Federal Insitute of Technology Zurich, 2015
3. Normand M. Laurendeau, Statistical Thermodynamics Fundamentals and Applications, Cambridge University Press, Cambridge, 2005

Supplementary reading
1. Yung-Kuo Lim, Problems and Solutions on Thermodynamics and Statistical Mechanics, World Scientific Publishing Co. Pte. Ltd., Singapore, 1990