Name: ***Theoretical chemistry (C-PS.II2-TeorCH)***
Name in Polish:
Name in English: ***Theoretical chemistry***

Information on course:

Course offered by department: Faculty of Chemistry
Course for department: Faculty of Chemistry

Default type of course examination report:

Examination

Language:

English

Description:

LECTURES:
STATISTICAL THERMODYNAMICS
1. Classical and quantum mechanical foundations.
2. Ensembles and postulates.
3. Maxwell¬Boltzmann distribution.
4. Microcanonical, canonical and grandcanonical ensembles and thermodynamics.
5. Ideal monoatomic and diatomic gases. Statistical interpretation of heat capacity.
6. Monoatomic crystal. The Einstein model.
7. Chemical equilibrium in ideal gas mixtures.
8. Statistical derivation of Langmuir and BET isotherms.
QUANTUM CHEMISTRY
9. Time-dependent and time-independent Schrodinger equation. Wave function and probability density for stationary states.
10. The many-electron systems. The Hamiltonian operator. Issue of solving the Schrodinger equation for molecules
11. Two basic approximations leading to the Hartree-Fock method
12. The Roothaan aproximation, basis sets and the Hartree-Fock-Roothaan (HFR) method.
13. Numerical aspects of the HFR method.
14. The HFR method in calculations of molecular properties. Dipole moments, charge density and population analysis.
15. Electron correlation. The CI and MP2 methods.
16. Calculating the nuclear magnetic shielding conatants (NMR), forces constants (Hessian and IR spectroscopy) and simulation of the AFM experiments.

LABORATORIES:
1. An intro to quantum chemistry including postulates of quantum mechanics, consideration of basic systems (particle in the box, harmonic oscillator, rotator and hydrogen-like atom), variational and perturbational approximation methods, Schrödinger equation, Born-Oppenheimer approximation.
2. One-electron approximation and the Hartree-Fock method: principles and applications. Roothaan approximation and types of basis sets. Electron correlation and post-HF methods: configuration interaction (CI) and coupled cluster (CC), Möller-Plesset perturbational theory (MP2, MP3, MP4)
3. Potential Energy Surfaces, Transition State Theory, Density Functional Theory, semiempirical methods, relativistic effects.
4. The basics of running PQS software: creation and analysis of input file.
5. Geometry optimization of selected systems (mainly simple molecules), analysis of an output file vs. its graphical presentation using PQSMol programme. The iterative SCF process, Hartree-Fock vs. DFT and semiempirical methods.
6. Calculations concerning transition states for some of the following problems: inversion of ammonia, keton-enol tautomery, Walden inversion, SN1 reaction, etc.
7. Simulation of the IR and NMR spectra of simple organic molecules. Thermodynamic properties.
8. Introduction to quantitative structure-activity relationship (QSAR), computer aimed drug design (CADD), ONIOM computational approach – group project.

Bibliography:

1. T.L. Hill, An Introduction to Statistical Thermodynamics.
2. A. Szabo, N.S. Ostlund, Modern quantum chemistry, introduction to advanced electronic structure theory.
3. D.B. Cook, Handbook of computational chemistry.
4. M.H. Everdell, Statistical Mechanics and its Chemical Applications.

Learning outcomes:

KNOWLEDGE
W1. Students know the basics of statistical mechanics. K_W02

W2. Students know the foundations of ensemble method of Gibbs and are able to formulate the statistical thermodynamics postulates. K_W09
W3. Students are familiar with the basic assumptions of Maxwell-Boltzmann distribution. K_W09
W4. Students know the basic relations between cannonical sum of states and thermodynamics functions K_W09
W5. Students know the statistical theory of heat capacity of mono and di-atomic gases. K_W09, K_W11
W6. Students know the statistical theory of crystals and are familiar with Einstein model of monoatomic crystal. K_W09, K_W11
W7. Students know the statistical derivation of equilibrium constant of chemical reaction. K_W09
W8. Students know the assumptions of the Langmuir and BET model of adsorption and understand the relationship between adsorbate pressure and amount adsorbed in each model K_W09, K_W10, K_W11
W9. A student should know three basic approximatins which have to be introduced in order to able to practically solve the Schroedinger equation for many-electron systems K_W09
W10. A student should know what the electron correlation is and how big is their contribution to the total energy K_W09
W11. A student should be able to describe the Configuration interaction (CI)method and Moller-Plaset (MP) perturbation theory. K_W09
W12. A student should be familiar with theoretical description of Nuclear Magnetic Resonance (NMR) spectroscopy. K_W09, K_W15

SKILLS
U1. Students are able to explain the basic assumptions of statistical thermodynamics K_U16
U2. Students can derive the Maxwell-Boltzmann distribution and calculate mean values of mechanical variables. K_U04, K_U16
U3. Students can calculate translational, vibrational and rotational sum of states for ideal, diatomic gas. K_U04, K_U05
U4. Students can derive the ideal gas law formula.K_U05, K_U16
U5. Students are able to discuss the relation between temperature and heat capacity of ideal gas and Einstein crystal K_U05, K_U16
U6. Students can write the equilibrium constant of ideal gas chemical reaction by using molecular partition functions of reaction components. K_U05, K_U16
U7. Should be able to use knowladge from theoretical chemistry courses to interprete thermodynamics functions for selected chemical systems at the molecular level K_U16, K_U23
U8. A student is able to solve selected problems using PQS software.

ATTITUDES
K1. Is able to formulate new problems which can be solved theoretically K_K03
K2. Students understand the need for continuous broadening of theoretical knowledge of theoretical chemistry K_K01

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Contact hours (with academic teacher) 60 h
Lectures: 30h
Laboratories: 30h
ECTS - 2,0
Non-contact hours (student's own work) 120 h
Preparation for laboratories and reports from exercises - 60 h
Literature reading - 30h
Preparation for exam - 30 h
ECTS - 4,0
Total number of ECTS points - 6,0
Consultations - 2 h

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Written reports from exercises W8-W12, U8
Written exam W1-W12, U1-U7
Activity K1, K2

Requirements

Basic knowledge of mathematics, physics and fenomenological thermodynamics

Course credits in various terms:

<without a specific program>

Type of credits	Number	First term	Last term
European Credit Transfer System (ECTS)	6	14/15L	