FACULTY OF CHEMISTRY

**SUBJECT CARD**

Name of subject in English: **Theoretical Chemistry**
Main field of study (if applicable): Biotechnology
Specialization (if applicable): Bioinformatics
Profile: academic
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code: CHC024061
Group of courses: NO

| | Lecture | Classes | Laboratory | Project | Seminar |
|---|---|---|---|---|---|
| Number of hours of organized classes in University (ZZU) | 30 | | 30 | | |
| Number of hours of total student workload (CNPS) | 120 | | 60 | | |
| Form of crediting | Exam | | crediting with grade | | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 4 | | 2 | | |
| including number of ECTS points for practical (P) classes | | | 2 | | |
| including number of ECTS points for direct teacher-student contact (BK) classes | 1 | | 1 | | |

**PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES**

1. General Chemistry, Physics I and II
2. Algebra, Mathematical Analysis
3. Physical Chemistry, Introduction to Quantum-Chemistry

C1. Introduction to basic concepts of atoms and molecules.

C2.The skills for predicting structure of molecular systems basing on quantum-chemical methods.

C3.The theoretical interpretation of thermodynamical and electronic properties of molecules and ions.

C4.The ability to make molecular modeling.

## SUBJECT EDUCATIONAL EFFECTS

**related to knowledge:**

PEK_W01 – the understanding of problems and shortcomings of classical physics in the microscopic description,
PEK_W02 – the knowledge of quantum mechanical postulates and elements of operator mathematics,
PEK_W03 – the ability to construct of Schrödinger equation (SE) for selected physical problems and for any molecular system,
PEK_W04 – the understanding of SE for hydrogen atom and the interpretation of equation solution,
PEK_W05 – the understanding of atomic structure,
PEK_W06 – the basic knowledge of molecular orbital theory,
PEK_W07 – the understanding of the theory of hybrid orbitals, mesomeric concept, and the idea of multi-center bonds,
PEK_W08 – the knowledge of procedures to solve Hartree-Fock equations and the correlation energy,
PEK_W09 – the understanding of molecular interactions.

**related to skills:**

**Relating to skills:**

PEK_U01 – is able to practical apply data from periodic system of elements,
PEK_U02 – knows the interpretation of electronic spectra of hydrogen atom and heavy atoms,
PEK_U03 – the ability to predict molecular structure of organic and inorganic molecules,
PEK_U04 – the ability to interpret of spectroscopic data with regard to quantum-chemical calculations,
PEK_UO5 – the ability to study chemical reaction mechanisms.

**related to social competences:**

PEK_K01 student is ready to critically evaluate his/her knowledge and received content

## PROGRAMME CONTENT

| Lectures | | Number of hours |
|---|---|---|
| Lec 1 | **Classical and quantum mechanics**. Mathematical bases of probability theory. Experimental base for wave-corpuscular dualism. The development of quantum concept with elements of Bohr theory and reasons for its collapse. | 2 |
| Lec 2 | **The foundations of quantum mechanics**. Postulates of quantum mechanics. The definition of wavefunction and its probabilistic interpretation. The definition of operators representing observables. | |
| Lec 3 | **The foundations of quantum mechanics II**. Schrödinger equation. Eigenvalues and eigenfunctions of Schrödinger equation. Mean values of observables. Properties of eigenfunctions in the case of Schrödinger equation without time. | 2 |
| Lec 4 | **Hydrogen atom**. Schrödinger equation for hydrogen and hydrogen-like cations. The solution with regard energies and wavefunction. Geometric properties of hydrogen-like orbitals. Quantum numbers. Energy levels and emission spectra of hydrogen. | |
| Lec 5 | **Pauli exclusion.** Electron spin. Multiplicity of many-electron system. Electronic states of atoms (atomic terms). Fermions and bosons. The concept of spinorbital. Pauli exclusion principle. Slater determinant. Electronic configuration. The structure of periodic system of elements. Hundt's rules. | 2 |

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|---|---|---|
| Lec 6 | **Many-electron atom.** Hamiltonian and Schrödinger equation for many-electron atom. Slater determinant. Wavefunctions for many electron atoms. Single-electron approximation – spinorbitals and orbitals. Pauli exclusion principle as an antysymmetric function. | 2 |
| Lec 7 | **Hartree-Fock equations.** The energy expression in single electron approximation. The derivation of Hartree-Fock equations. One and two electron integrals. Exchange energy. Closed and open-shell electronic configuration. The selection rules for optical transition. | 2 |
| Lec 8 | **Molecule.** Born-Oppenheimer approximation. Schrödinger equation for molecules. Molecular orbital theory. Linear combination of molecular orbitals concept. Hartree-Fock-Roothaan-Hall equations. Thae atomic basis set. Slater and Gaussian functions. | 2 |
| Lec 9 | **Chemical bond.** Electrostatic and covalent character of chemical bonds. Type of bonds. Orbitals $\sigma$ and $\pi$. Bonding, antybonding, and nonbonding orbitals – energies and geometrical representation. The electronic structure of diatomic molecules. The bond order. | 2 |
| Lec 10 | **Localized orbitals.** Hybridization $sp^3$, $sp^2$ and sp. The representation of electronic density in molecules. Localized orbitals as a tool for the structure prediction. The molecular structure of moieties including phosphorous. The concept of mesomeric representation. Multicenter bonds. | 2 |
| Lec 11 | **Molecular spectroscopy I.** The rotation and vibration separation. Rotational spectra of diatomic molecules and elements of microwave spectroscopy. The selection rules. | 2 |
| Lec 12 | **Molecular spectroscopy II.** Vibarational spectra of diatomic and many-atoms molecules. IR and Raman spectra. The selection rules. | 2 |
| Lec 13 | **Molecular properties based on energy.** Ionization energy, electron affinity. Thermodynamics of chemical processes. Mass spectrometry. The transition state theory. Reaction mechanism. | 2 |
| Lec 14 | **Properties of molecules based on wavefunction.** Electronic density in the molecule. The bond order. Charge distribution in molecules. Dipole and higher moments in molecules. | 2 |
| Lec 15 | **Molecular interactions.** The theory of molecular interactions. Electrostatic, exchange, induction, dispersion interactions. Charge-transfer complexes. Hydrogen bond. The second order structure of molecular complexes. Conformational analysis. | 2 |
| | | 30 |
| **Laboratory** | | **Number of hours** |
| Proj 1 | The local lab and the computing center organization. Accounts distribution and basic information about systems. | 2 |
| Proj 2 | Elements of UNIX (commends). | 2 |
| Proj 3 | Elements of UNIX (editors). | 2 |
| Proj 4 | Gaussian-90 program structure. Execution of the program. | 2 |

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|---|---|---|
| Proj 5 | The structure representation, matrix-Z. | 2 |
| Proj 6 | The Hartree-Fock calculations. The output file structure. | 2 |
| Proj 7 | Molecular graphics program – Molden. | 2 |
| Proj 8 | Structure optimizations. | 2 |
| Proj 9 | Frequencies, thermochemistry, and vibrational spectra. | 2 |
| Proj 10 | Project I – structure and properties of molecule. | 2 |
| Proj 11 | Energetics of chemical reaction. | 2 |
| Proj 12 | Project II – frequency calculations, spectra simulation. | 2 |
| Proj 13 | Heat of reaction, synthesis reaction, atomic charge distribution. | 2 |
| Proj 14 | Project III – the reaction mechanism. | 2 |
| Proj 15 | Transition state. Molecular interactions. | 2 |
| | | 30 |

**TEACHING TOOLS USED**

N1.
N2.
N3.

**EVALUATION OF SUBJECT EDUCATIONAL EFFECTS ACHIEVEMENT**

| **Evaluation** (F – forming (during semester), P – concluding (at semester end) | Educational effect number | Way of evaluating educational effect achievement |
|---|---|---|
| P | PEK_Lec01-PEK_Lec15 | Final exam |
| F3 | PEK_La1-PEK_La15 | Projects |

**PRIMARY AND SECONDARY LITERATURE**

**PRIMARY LITERATURE**

[1] M. A. Ratner, G. C. Schatz, Introduction to Quantum Mechanics in Chemistry. Prentice Hall, Upper Saddle River, 2001.
[2] L. Piela, Ideas of Quantum Mechanics
[3] Gaussian-90 electronic manual

**SECONDARY LITERATURE:**

[1] Quantum Mechanics for Chemists, D. O. Hayward, PWN, Warszawa, 2007.
[2] P. W. Atkins, Physical Chemistry, PWN Warszawa, 2003

**SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)**

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Zał. nr 5 do ZW 25/2019

Załącznik nr 4 do programu studiów