Formularz opisu przedmiotu (formularz sylabusa) na studiach wyższych, doktoranckich, podyplomowych i kursach dokształcających

A. The basis of Quantum Chemistry

Nazwa pola	Komentarz
Name of the subject (in Polish and English)	***Podstawy Chemii Kwantowej*** ***Introductory Quantum Chemistry***
Unit offering the subject	Faculty of Chemistry
Unit for which the subject is offered	Faculty of Chemistry
Subject code	**06001-S1-O-PCK**
ERASMUS code	
Number of ECTS credits	*5*
Method of assessment	lecture – examination Tutorial – graded credit Laboratory – graded credit
Language of instruction	English
Designation whether a subject may be credited more than once	**No**
Allocation of the subject to subject groups	Obligatory subject
Total student workload	***Contact hours with teacher:*** – participation in lectures - 25 hrs – participation in tutorials – 25 hrs – participation in laboratory – 10 hrs – consultations – 20 hrs ***Self-study hours:*** - preparation for lectures – 15 hrs - writing projects 5 hrs - reading literature- 5 hrs - preparation for test/ examination- 20 hrs Altogether 125 hrs: 25hrs/ECTS = 5 ECTS
Learning outcomes - knowledge	W1: Student learns: the basis of quantum chemistry and simply models of quantum chemistry, principles of spectroscopy, base of application of software package Maxima for linear algebra (K-W04, K-W05, K_W14)
Learning outcomes - skills	U1: Student understands the importance of quantization in physics and chemistry: is able to build and solve simple models of quantum chemistry, is able to use the mathematical package Maxima for solving quantum-chemical models and problems (K_U03, K_U04).
Learning outcomes - social competencies	K1: Student works independently and efficiently with a lot of information, recognizes the dependence between the phenomena and

	correctly pulls conclusions using the principles of logic. K2: Student thinks creatively in order to improve existing or develop new solutions. K3: Student is focused on continuous acquisition of knowledge , skills and experience, sees the need for continuous improvement and to raise the professional competence; knows the limit of their own knowledge and understand the need for further education. K4: Student is working steadily and has a positive approach to the difficulties arising out on the way to achieving the final goal, keeps his deadlines and understand the necessity of systematic work on all projects. K5: Student understand the importance of computer science and quantum chemistry in chemical science and in practice, independently performs the agreed targets , undertakes independent and sometimes difficult decisions, can independently search for information in the literature. (K_K01, K_K02, K_K03, K_K05, K_K06, K_K07)
Teaching methods	*Expository teaching methods:* lecture – conventional lecture tutorials – description, discussion laboratory -- description *Exploratory teaching methods:* tutorials – classic problem-solving, case study laboratory – project work, practical
Prerequisites	1. Basic physics 2. Basic mathematics
Brief description of the subject	The Quantum Chemistry course is meant to be an introductory course of the electronic theory of atoms and molecules explaining fundamental concepts rather than going deeply into formal details. Particular attention is paid to building theoretical models for chemistry, their origin, validity and limitations. The main purpose of the course is to promote the understanding of chemistry in terms of basic physics. The course gives an introduction to the vibrational, rotational and electronic spectroscopy of atoms and molecules.
Complete description of the subject	**Lectures:** 1.From Classical to Quantum Mechanics. 2.Blackbody radiation. The photoelectron effect. Particles exhibit wave-like behaviour. Atomic spectra and the Bohr model of the hydrogen atom. The Heisenberg uncertainty principle. 3.The quantum mechanical postulates. The Schrödinger equation. The physical meaning associated with the wave function. Probability. 4.Using quantum mechanics on simple system: the free particle, the particle in a box, the harmonic oscillator, angular motion and the rigid rotator. 5.The hydrogen atom. Eigenvalues and eigenfunctions for the total energy. The hydrogen atom orbitals. The radial probability distribution function.

	6.The variational method and perturbation theory. 7.Many electron atoms. Helium. Introducing electron spin. Indistinguishability of electrons. The Slater determinants. 8.Quantum states for many-electron atoms and atomic spectroscopy. Good quantum numbers. Terms, levels, and states. 9.The electronic Hamiltonian. The H2+ molecules. The ground and excited states. LCAO MO wave function. 10.The Born-Oppenheimer approximation. The vibrational and rotational spectroscopy of diatomic molecules. Electronic spectroscopy. 11. MO configurations of homonuclear and heteronuclear diatomic molecules. 12.Semiempirical MO treatments of planar conjugated molecules. The Hückel MO methods. **Tutorials:** 1.Classical mechanics. The Newton's equations: free particle and harmonic oscillator. 2.Observables, operators, eigenfunctions and eigenvalues. Normalisation and orthogonality. Spherical and cartesian coordinates. 3.Operators and their formulation. Hermitian and Linear operators. Commuting and noncomuting operators. Eigenfunctions, eigenvalues and experimental measurements. 4.Operators and quantum mechanics: the free particle, the particle in a box, the two-particle rigid rotator, the harmonic oscillator, and electronic Hamiltonians. 5.The expectation value. 6.Using quantum mechanics on simple systems. the free particle, the paricle in a box, the two-particle rigid rotator, the harmonic oscillator, 7.The hydrogen atom. Solving the Schrödinger equation for the hydrogen atom. 8.The vibrational, rotational, and electronic spectroscopy of diatomic molecules. Examples. 9.The independent electron approximation. Symmetric/antisymmetric wave function, Slater's determinants. 10. Many-electron atoms Good quantum numbers. Terms, levels, and states. Examples. 11.MO configurations of homonuclear diatomic molecules from lithium to fluorine. Heteronuclear diatomic molecules. Stable and unstable molecules and ions. Examples. 12.The Hückel theory. Determinantion of HMO energies and AO coefficients. Applications of HMO energies and coefficients.

	Laboratory: 1.**Arithmetic in Maxima:** introduction, arithmetic, addition, subtraction, scalar multiplication, division, powers. or exponentation, matrix multiplication, square root of x, **float** function, big numbers, precision, functions **sin**, **cos**, **tg,** , **ctg**, **ln**, linear and nonlinear equations, derivatives, integrals, Taylor series, matrix calculations, plots of one or more functions. 2.**Maxima and Quantum Chemistry:** normalization, operators and commutators, expectation values, plots of functions and energies; the particle in a box, the harmonic oscillator, the rigid rotator, the hydrogen like ions, radial and angular functions (Legendre polynomials, spherical harmonics, associated Legendre polynomials, Hermite polynomials, Laguerre polynomials).
Literature	**The course will be based on lectures notes. As references, we will use:** 1. Lucjan Piela, Ideas of Quantum Chemistry, Elsevier, London, 2007. 2. IRA N. Levine, Quantum Chemistry, Prentice Hall 2008. 3. Frank Jensen, Introduction to Computational Chemistry, Wiley, Germany, 2008. *4. R. Grinter, The Quantum in Chemistry. An Experimentalist's View, John Wiley & Sons, Ltd, 2005.*
Assessment methods & criteria	**Assessment methods:** **Lecture:** - written examination- . W1 **Tutorials:** - test – activity **Laboratory:** – own project **Assessment criteria:** Final evaluation will be a combination of the final marks of two module components: written exam – 60 % and tutorials 40 % fail- 49 % satisfactory- 50-60 % satisfactory plus- 61-65 % good - 66—75 % good plus- 76—80 % very good- 81-100 %
Work placement	not applicable

B) Opis przedmiotu cyklu : Basic of quantum Chemistry

Nazwa pola	Komentarz

Didactic cycle	2014/2015 W (winter)
Method of assessment of the subject in the cycle	lecture- examination tutorial- graded credit laboratory – graded credit
Type of classes, number of hours of classes and methods of assessment	lecture- 25 hrs; examination tutorial- 25 hrs; written tests, graded credit laboratory – 10 hrs, practical project, graded credit
Subject coordinator	Prof. dr hab. Maria Barysz
Subject teachers	prof. dr hab. Maria Barysz, dr hab. Piotr Jankowski
Nature of the subject	obligatory
Limit of places available in each group	Lecture – one group, no limit tutorials :group(s)- 22 students laboratory: groups 8 students
Time and place	Faculty of Chemistry , date will be specified later
Learning outcomes	As in part A
Assessment methods & criteria	As in part A
List of topics	As in part A
Teaching methods	As in part A
Literature	As in part A