LEARNING MODULE DESCRIPTION (SYLLABUS)

THEORETICAL CHEMISTRY

I. General information

1. Module title

   Theoretical chemistry

2. Module code

   QC

3. Module type – compulsory or optional

   Compulsory

4. Programm title

   Chemistry

5. Cycle of studiem (1st or 2nd cycle of studiem or full master's programme

   second cycle of studies

6. Year of studies

   First year

7. Term In chich taught (summer/winter term)

   winter

8. Type of classes and the number of contact hours (e.g. lectures: 15 hours; practical courses: 30 hours)

   Lecture: 15 h, Laboratory: 45 h

9. Number of ECTS credits

   5

10. Name, surname, academic degree/title of the module lecturer/Rother teaching Staff/e-mail

    Marek Kręglewski, Professor, prof. dr. hab**., mkreg@amu.edu.pl ;**

    Iwona Gulaczyk, PhD, **gulai@amu.edu.pl;**

11. Language of classes

    English

II. Detailed information

1. Module aim (aims)

   - **Introduction to basic concepts, calculation methods and modeling techniques of quantum chemistry,**
   - **Development of skills in interpretation of quantum chemistry calculations**
   - **Development of skills in numerical and graphical modification of input and output data in the ab initio calculation**

2. Pre-requisites in terms of knowledge, skills and social competences (if relevant)

   Basic knowledge in mathematical analysis (in particular basic skills in differential and integral calculus) and basic concept of physics (in particular of classical mechanics).

3. Module learning outcomes in terms of knowledge, skills and social competences and their reference to programme learning outcomes

Learning outcomes symbol*	Upon completion of the course, the student will:	Reference to programme learning outcomes#
QC_1	Understands and explains the postulates of quantum mechanics	CHE2_W01, CHE2_W02, CHE2_W06, CHE2_U01, CHE2_U05
QC_2	Explains how to solve exactly the basic models of quantum mechanics, how to characterize the solutions, indicates the applications of models	CHE2_W01, CHE2_W02, CHE2_W06, CHE2_U01, CHE2_U02, CHE2_U05, CHE2_U08
QC_3	Understands the interactions on atomic and molecular level and describes the resulting chemical properties	CHE2_U02, CHE2_U05, CHE2_U08
QC_4	Applies the basic approximate quantum calculations to complex atomic and molecular systems	CHE2_U02, CHE2_U05, CHE2_U08, CHE2_U09
QC_5	Knows how to extract, modify and present the results of quantum mechanical calculations	CHE2_W01, CHE2_W02, CHE2_W09, CHE2_U01, CHE2_U05, CHE2_U07, CHE2_U08, CHE2_U09, CHE2_U10, CHE2_U12, CHE2_K01, CHE2_K02
QC_6	Is able to present in graphical form the results of ab initio calculations, also those referring to the reaction path	CHE2_W01, CHE2_W02, CHE2_W07, CHE2_U01, CHE2_U05, CHE2_U07, CHE2_U08, CHE2_U10, CHE2_U14, CHE2_U15, CHE2_K01, CHE2_K02
QC_7	Knows how to use the bibliographic sources	CHE2_W01, CHE2_W08, CHE2_U09, CHE2_U10, CHE2_U11, CHE2_U13, CHE2_K02
QC_8	Applies the safety and ergonomics rules in the computer laboratory	CH2_U15, CHE2_K03, CHE2_K04

4. Learning content

Module title : Theoretical chemistry		
Learning content symbol*	Learning content description	Reference to module learning outcomes #
TK_01	Industrial safety In the computer laboratory	QC_8
TK_02	Introduction to quantum mechanics (black body radiation, photoelectric effect, wave-particle duality). Postulates of the quantum mechanics	QC_1
TK_03	Exact solution of the Schrödinger equation: tunnelling effect, particle in a box. Analysis and visualization of the solutions for a hydrogen atom	QC_2, QC_3
TK_04	Approximate variational method of solving the Schrödinger equation. One-electron approximation. Hartree-Fock method. Electron correlation. Molecular orbitals, functional basis.	QC_4
TK_05	The Gaussian package: possible applications, graphical interface GaussView. Practical quantum mechanical calculations using the Gaussian package. Multielectron atom,	QC_4, QC_5, QC_6

	Mendeleev periodic table	
TK_06	Separation of electrons and nuclei in molecules. Chemical Bond. Potential energy surface. Force constants. Force field. Energy levels in molecules. Molecular geometry optimization. Excited states, the CI method.	QC_4, QC_5, QC_6
TK_07	Graphical presentation of the ab initio calculation.	QC_4, QC_5, QC_6
TK_08	Calculation of the two-dimensional potential function for a molecule.	QC_3, QC_4, QC_5, QC_6, QC_7
TK_09	Modelling the reaction energy path, activation energy for a complex molecular system.	QC_4, QC_5, QC_6

** e.g. TK_01, TK_02, … (TK stands for "treści kształcenia" /learning content/ in Polish)*

 # e.g. KHT_01 – module code as in Table in II.3

5. Reading list

1) Levine, Ira N., Quantum Chemistry; 7th Edition; Pearson/Prentice Hall; 2013.

2) Atkins, Peter W., and Friedman, Ronald S., Molecular Quantum Mechanics; 4th Edition; Oxford University Press; 2005

3) Piela, Lucjan, Ideas of quantum chemistry, 2nd Edition, Elsevier, 2013

6. Information on the use of blended-learning (if relevant)

B-learning will be used In homeworks, test, individual projects

7. Information on where to find course materials

Home page Zakład Chemii Teoretycznej, Wydział Chemii UAM
http://www.staff.amu.edu.pl/~zcht/dydaktyka.htm

III. Additional information

1. Reference of learning outcomes and learning content to teaching and learning methods and assessment methods

Module title: Theoretical chemistry			
Symbol of module learning outcome*	Symbol of module learning content#	Methods of teaching and learning	Assessment methods of LO achievement&
QC_1	TK_02	Lecture, laboratory	F-checking skills during laboratory work S-test: knowledge and skills assessment
QC_2	TK_03	Lecture, laboratory	F-checking skills during laboratory work S-test: knowledge and skills assessment
QC_3	TK_03, TK_08	Lecture, laboratory	F-checking skills during laboratory work S-test: knowledge and skills assessment
QC_4	TK_04, TK_05, TK_06, TK_07, TK_08, TK_09	Lecture, laboratory	F-checking skills during laboratory work S-test: knowledge and skills assessment

QC_5	TK_05, TK_06, TK_07, TK_08, TK_09	Lecture, laboratory	F-checking skills during laboratory work S-test: knowledge and skills assessment
QC_6	TK_05, TK_06, TK_07, TK_08, TK_09	Laboratory	F-checking skills during laboratory work S-test: knowledge and skills assessment
QC_7	TK_08	Laboratory	F-checking skills during laboratory work S-test: knowledge and skills assessment
QC_8	TK_01	Laboratory	F-checking skills during laboratory work S-test: knowledge and skills assessment

** e.g. KHT_01 – module code as in Table in II.3 and II.4*
 # e.g. TK_01 – learning content symbol as in II.4
& Please include both formative (F) and summative (S) assessment

2. Student workload (ECTS credits)

Module title: Theoretical chemistry	
Activity types	Mean number of hours* spent on each activity type
Contact hours with the teacher as specified in the programme	60
Independent study 1-preparation for laboratory	15
Independent study 2-library-based work	5
Independent study 3-Description of the laboratory results	25
Independent study 4-Time for b-learning and consultations	5
Independent study 5-exam preparation	30
TOTAL HOURS	140
TOTAL NUMBER OF THE ECTS POINTS (THE COURSE)	5

** Class hours – 1 hour means 45 minutes*
#Independent study – examples of activity types: (1) preparation for classes, (2) data analysis, (3) library-based work, (4)writing a class report, (5) exam preparation, etc.

3. Assessment criteria

Laboratories

Before starting the laboratory student should be familiar with the principles of occupational health and safety in the laboratory. This knowledge will be checked before first laboratory (formative assessment).

Before each laboratory the knowledge and skills concerning the current topic will be checked. To start the experiments a student should obtain at least 2 points (the scale is from 0 to 3). Additional 1 point can be obtained for excellent performance of experiment (mainly assessment of student's skills) and 1 point for correctness of report, including esthetics.

At the last laboratory, beside of weekly test of knowledge and skills, students will solve the test, which cover the main topics raised on laboratories. The questions will be given in the form of problems to be solved. The maximum points that can be obtained is 8.

According to collected points students will receive:

5.0 47-50 pts **4.5** 43-46 pts **4.0** 37-42 pts **3.5** 31-36 pts **3.0** 25-30 pts

Lecture

The exam will be in written form. Minimum 25 points must be obtained to pass the exam (maximum is 50). The final mark will base on points obtained on a written exam as well as on points collected on laboratories. Students will receive the final mark:

5.0 91-100 pkt.

4.5 81-90 pkt.

4.0 71-80 pkt.

3.5 61-70 pkt.

3.0 51-60 pkt.