UNIVERSIDADE DA CORUÑA

Teaching Guide				
Identifying Data				2022/23
Subject (*)	Physical Chemistry 1		Code	610G01016
Study programme	Grao en Química			
Descriptors				
Cycle	Period	Year	Type	Credits
Graduate	1st four-month period	Second	Obligatory	6
Language	SpanishEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química			
Coordinador	Rodriguez Barro, Pilar	E-mail	pilar.rbarro@udc.es	
Lecturers	Rodriguez Barro, Pilar Vilariño Barreiro, Maria Teresa	E-mail	pilar.rbarro@udc.es teresa.vilarino@udc.es	
Web				
General description	This course deals with the microscopic behavior of matter. It presents an introduction to quantum mechanics and statistical thermodynamics. The course begins with an examination of the key concepts, the basic principles and the formulation of quantum theory and applications to simple systems ? the particle in a box, the harmonic oscillator, the rigid rotor and the hydrogen atom. It continues with a discussion of atomic structure and atomic spectra. The final lectures on quantum chemistry cover applications to chemical bonding including valence bond and molecular orbital theory and molecular structure. The last part of the course covers elementary statistical mechanics that allows one to study the methodology to calculate macroscopic properties of equilibrium systems from molecular properties. (English lecturer: Teresa Vilariño)			

Study programme competences	
Code	Study programme competences
A1	Ability to use chemistry terminology, nomenclature, conventions and units
A8	Knowledge of principles of quantum mechanics and atomic and molecular structure
A12	Ability to relate macroscopic properties of matter to its microscopic structure
A14	Ability to demonstrate knowledge and understanding of concepts, principles and theories in chemistry
A15	Ability to recognise and analyse new problems and develop solution strategies
A16	Ability to source, assess and apply technical bibliographical information and data relating to chemistry
A21	Understanding of qualitative and quantitative aspects of chemical problems
B2	Effective problem solving
B3	Application of logical, critical, creative thinking
B5	Teamwork and collaboration
C1	Ability to express oneself accurately in the official languages of Galicia (oral and in written)
C3	Ability to use basic information and communications technology (ICT) tools for professional purposes and learning throughout life

Learning outcomes			
Learning outcomes	Study programme competences		
To know the principles of quantum chemistry.	A1 A8 A14 A15 A16	B2 B5	C3

To know the principles of statistical thermodynamics.	A1 A12 A14 A16	B2 B5	C3
To be able to perform calculations independently, even when a computer is needed.	A1 A14 A15 A16 A21	B2 B5	C1 C3
To acquire literature search skills to be able to search for and use scientific literature.	A14 A15 A16 A21	B3	C1 C3
To acquire skills in the use of computer tools to solve problems.	A8 A15	B2 B3	C3

Contents	
Topic	**Sub-topic**
QUANTUM CHEMISTRY	
1. Postulates of quantum mechanics	- Postulate 1: the state of a quantum-mechanical system is completely specified by its wave function. - Postulate 2: quantum-mechanical operators represent classical mechanical variables. - Postulate 3: eigenvalue equation. - Postulate 4: average value. - Postulate 5: time-dependent Schrödinger equation.
2. Translational motion: a particle in a box.	- A particle in a one-dimensional box: wave functions and energy levels. - A particle in two and more dimensions:separation of variables and degeneracy.
3. Vibrational motion: the harmonic oscillator.	- Quantum mechanical model: wave functions and energy levels. - The harmonic oscillator as a model for a vibrating diatomic molecule. - Anharmonicity.
4. Rotational motion: rigid rotator.	- Motion of a particle in a ring. - Wave functions. Spherical harmonics. - Rotational energy: energy levels. - The quantization of angular momentum.
5. Hydrogenic atoms.	- Formulation of the Schrödinger equation. - Atomic orbitals and their energies. - The radial probability distribution function. - The lineal combination of degenerate wavefunctions. - Zeeman effect.
6. Aproximation methods.	- Perturbation theory. - Variational method. - Lineal variational trial functions: secular determinant.
7. Many-electron atoms.	- Helium atom. - Spin angular moment. - Pauli exclusion principle. - Periodic Table.
8. Atomic spectroscopy.	- Electron configuration of atoms. - Total orbital angular moment: Russell-Saunders coupling and jj coupling. - Term symbols. Hund´s rules. Selection rules.

9. The chemical bond: the hydrogen molecule-ion.	- The Born-Oppenheimer approximation. - Molecular orbital theory and valence-bond theory. - Molecular orbital treatment of hydrogen molecule-ion.
10. Diatomic molecules.	- General considerations for bond formation. - Homonuclear diatomic molecules. - Heteronuclear diatomic molecules. Polar bonds and electronegativity.
11. Conjugated and aromatic molecules.	- Semi-empirical methods. - Pi-electron approximation. - Free electron molecular orbital theory. - The Hückel approximation.
STATISTICAL THERMODYNAMICS	
12. Foundations of statistical thermodynamics.	- Fundamentals of statistical mechanics. - Basis of statistical thermodynamics. - Statistical thermodynamics of ideal gases. - Statistical interpretation of the thermodynamic properties of solids.

Planning				
Methodologies / tests	Competencies	Ordinary class hours	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A1 A8 A12 A21	28	56	84
Seminar	A14 A15 B2 B3	10	25	35
Laboratory practice	A1 A8 A21 C1 C3	10	5	15
Supervised projects	A1 A8 A16 B2 B3 B5 C1 C3	0	10	10
Objective test	A1 A8 A14	2	0	2
Mixed objective/subjective test	A1 A8 A12 A14 A15 A21 B2 B3	3	0	3
Personalized attention		1	0	1
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	Description
Guest lecture / keynote speech	Oral presentation, complemented by the use of audiovisual material and the interaction with the students, to introduce the basic contents of the subject to transmit knowledge and facilitate learning.
Seminar	Activity to be developed in mid-size groups. In-depth study of the contents introduced in the keynote lectures. Questions and problems related to the contents of the subject are discussed and/or are solved in group, with support and direct supervision of the lecturer. The activity to be carried out before and during each session are indicated prior to a face-to-face session.
Laboratory practice	Computer practices developed at the informatic labs. Practical problems related to the contents of Quantum Chemistry are solved by using computer software commonly used in scientific calculations. Students must solve and hand-in a questionnaire concerning the practical sessions.
Supervised projects	Homework performed in groups aimed at helping students to work independently, under the guidance of the lecturer. Activities related to the contents of the seminars are proposed. They must be solved in group and, subsequently, must be explained to the instructor in a face-to-face session. This activity is open exclusively to students attending the seminars on a regular basis (80%).

Objective test	Two tests to be held during the semester. The tests can combine multiple-choice questions and short answer questions. - First test at mid-semester. The formulation and the basic principles of quantum theory and its application to simple systems are assessed. - Second test at the end of semester. The application of quantum chemistry to atoms and molecules is assessed. The tests are solved and discussed in a subsequent session. They will serve as feed-back to both students and instructors to assess the progress of the teaching-learning process.
Mixed objective/subjective test	Final written exam to be held at the end of semester, and in second chance in July. Knowledge, understanding, reasoning and critical thinking are assessed. It will consist on a combination of different types of questions: multiple choice and/or short answer combined with problem solving. It will be held on the dates approved by the Faculty Board.

Personalized attention	
Methodologies	**Description**
Seminar Supervised projects	Homework of supervised projects done by each group should be presented to the instructor in a tutoring session. In addition, students are encouraged to make use of the tutoring sessions to solve any doubt. Tutoring schedule will be decided at lecturers and students convenience. Part-time students and those with special academic leave permission could ask for presential or email tutorials when necessary.

Assessment			
Methodologies	**Competencies**	**Description**	**Qualification**
Objective test	A1 A8 A14	Two tests during the semester. The tests will consist of short short answer questions and/or multiple-choice questions. - First test at mid-semester. The basic principles and the formulation of quantum theory and their application to simple systems are assessed. It contributes 10% to the final mark. - Second test at the end of semester. The application of quantum chemistry to atoms and molecules is assessed. It contributes 10% to the final mark.	20
Mixed objective/subjective test	A1 A8 A12 A14 A15 A21 B2 B3	Final written exam at the end of semester. It will be held on the official dates approved by the Faculty Board. All contents of the subject are assessed. It has two different types of questions: short answer questions (50%) combined with problem solving (50%).	60
Laboratory practice	A1 A8 A21 C1 C3	Assessment of skills in solving problems of Quantum Chemistry by using computer software commonly used in scientific calculations. Attendance to all scheduled computer lab. sessions is mandatory to pass the course. The final written report is also assessed.	10
Supervised projects	A1 A8 A16 B2 B3 B5 C1 C3	Assesment of teamwork skills in resolution of problems or questions related to the contents of the seminars. Apart from the solution of the proposed activities, the active paticipation in the face-to-face session also contribute to the assessment. Only students who attend the seminars on a regular basis (80%) can participate and be evaluated in this activity.	10

Assessment comments

Requirements to pass the course:
- Attendance to all scheduled computer lab sessions is mandatory to pass the course.
- It is compulsory the regular attendance to
the keynotes and seminar sessions to attend computer practical sessions.
- To pass the course, the final average grade has to be equal to or greater than 5 (out of a
possible 10) and the minimum score on the final written exam must have been 4.5 (out of 10). If the average grade is equal to or greater than 5 (out of 10) but the threshold
mark on the final examn was not met, the final grade will be 4.5 (fail).
- Students who has attended the practical sessions or the final exam will be assessed.
Second opportunity of July- In the second opportunity, the student should retake the final written test, whose grade will replace the one obtained in the written final test in the first opportunity. The grades of the rest of the activities corresponding to the continuous assessmente will be kept when the mark would be equal to or greater than 5.0 out of 10. The supervised projects and objetive tests graded below 5.0 out of 10 may be resit in the written test (adding the percentage of their contribution to the percentage of the grade of the final mixed test). The grade of the laboratory practices cannot be resit.
- In the second opportunity, a final mixed test will be carried out, whose grade will replace the one obtained in the mixed test of the first opportunity, maintaining the grades of the rest of the activities carried out in the continuous evaluation with a grade equal to or greater than 5.0 out of 10. Tutored works and objective tests with a grade lower than 5.0 (out of 10) may be recovered in the final mixed test (adding the percentage corresponding to the weight of the final mixed test grade). The qualification of the laboratory practices will not be able to recover.
-Mark Honors: priority is given in the first opportunity (January). Honors may only be granted in July if their number have not be exhausted in January final qualifications.
Early examination call of December
- To pass the course, it is compulsory for students to have attended all the practical sessions at least once.
- The examination will consist on a mixed objective/subjective test that will represent the 100% of the final grade. To pass the course, the score of the test must be equal to or greater than 5.0 (out of 10).
- If the grade of the written test is equal to or greater than 5,0 (out of 10) but the student didn´t attend all the practical sessions, the final grade will be 4.5 (fail).
Part-time students (according to the rules of the UDC):
The same evaluation criteria listed above are applied.
Students with special academic permission (according to the rules of the UDC):
It is not mandatory to attend classroom lectures, to hand-in the supervised projects and to attend the objective tests.
It is compulsory to attend computer practical sessions. It will be tried to fit the dates to the student's availability.
The final grade will be the sum of 10% of the mark obtained in the practical sessions and 90% of the mark obtained in the mixed test. The same criteria will be applied to both opportunities.
Students who has not attended the final exam will be assessed as "non attendance".
Any fraudulent performance in any evaluation activity, once verified, will directly involve the qualificaction of Fail (0.0) in the corresponding call, thus invalidating any mark obtained in the continuous assessment for any resit.

Sources of information

Basic	- ENGEL, T; REID, P. (2006). QUÍMICA FÍSICA. Pearson Addison Wesley - ENGEL,T REID,P. (2013). PHYSICAL CHEMISTRY. Pearson Education - ATKINS, P.W. (2008). QUÍMICA FÍSICA. Panamericana - ATKINS, P.W. (2014). PHYSICAL CHEMISTRY. Oxford University Press - McQUARRIE (1997). PHYSICAL CHEMISTRY. University Science Books - ENGEL,T REID,P. (2013). PHYSICAL CHEMISTRY. https://eur02.safelinks.protection.outlook.com/?url=https%3A%2F%2Fresolver.vitalsource.com%2F9781292 - ENGEL,T REID,P. (2006). QUÍMICA FÍSICA. https://bookshelf.vitalsource.com/#/search?q=9788483226995&request_token=eyJhbGciOiJkaXIiLCJlbmM - ATKINS, P.W. (2008). QUÍMICA FÍSICA. https://sfx.bugalicia.org/aco?url_ver=Z39.88-2004&url_ctx_fmt=info:ofi/fmt:kev:mtx:ctx&ctx_e
Complementary	- Science Direct (). http://www.sciencedirect.com. - Publicaciones de la American Chemical Society (). http://pubs.acs.org/about.html. - Página Web de ISI Web of Knowledge (). http://isi02.isiknowledge.com/. - Página Web del Curso de Química Cuántica del Instituto Tecnológico de Massachusetts MIT (en inglés) (). http://ocw.mit.edu/courses/chemistry/5-61-physical-chemistry-fall-2013/lecture-notes/. - http://www.m-w.com (). DICCIONARIO DE INGLÉS ONLINE (Merriam Webster). - LOWE (2006). QUANTUM CHEMISTRY 3ª Ed.. Elsevier - RAFF, L.M. (2001). PRINCIPLES OF PHYSICAL CHEMISTRY. Prentice Hall - HERNANDO, J. M. (1974). PROBLEMAS DE QUÍMICA FÍSICA. Gráficas Andrés Martín - McQUARRIE (2008). QUANTUM CHEMISTRY. University Science Books - LEVINE, I.N. (2001). QUIMICA CUÁNTICA 5ª ed. Prentice Hall - DÍAZ PEÑA,M. ROIG MUNTANER, A. (1988). QUÍMICA FÍSICA. Alhambra - LEVINE, I.N. (2004). FISICOQUÍIMICA 5ª edición. McGraw-Hill

Recommendations
Subjects that it is recommended to have taken before
Mathematics 1/610G01001 Mathematics 2/610G01002 Physics 1/610G01003 Physics 2/610G01004 General Chemistry 1/610G01007 General Chemistry 2/610G01008
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
Physical Chemistry 2/610G01017
Other comments
Green Campus Faculty of Sciences ProgramTo achieve an immediate sustainable environment and comply with point 6 of the "Environmental Declaration of the Faculty of Sciences (2020)",the documentary works carried out in this subject: a) They will be requested mainly in virtual format and computer support. b) If done on paper: - Plastics will not be used. - Double-sided prints will be made. - Recycled paper will be used. - Drafts will be avoided.