



| Teaching Guide | | | | |
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| Identifying Data | | | | 2015/16 |
| Subject (*) | Química Física 1 | Code | 610G01016 | |
| Study programme | Grao en Química | | | |
| Descriptors | | | | |
| Cycle | Period | Year | Type | Credits |
| Graduate | 1st four-month period | Second | Obligatoria | 6 |
| Language | SpanishEnglish | | | |
| Teaching method | Face-to-face | | | |
| Prerequisites | | | | |
| Department | Química Física e Enxeñaría Química 1 | | | |
| Coordinador | Rodriguez Barro, Pilar | E-mail | pilar.rbarro@udc.es | |
| Lecturers | Garcia Dopico, Maria Victoria Rodriguez Barro, Pilar Vilariño Barreiro, Maria Teresa | E-mail | victoria.gdopico@udc.es pilar.rbarro@udc.es teresa.vilarino@udc.es | |
| Web | | | | |
| General description | <p>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.</p> <p>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.</p> <p>(English lecturer: Teresa Vilariño)</p> | | | |

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



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|---|--------------------------------|----------|----------|
| 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 | |
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| Topic | Sub-topic |
| QUANTUM CHEMISTRY | |
| 1. Postulates of quantum mechanics | <ul style="list-style-type: none"> - 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. | <ul style="list-style-type: none"> - 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. | <ul style="list-style-type: none"> - 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. | <ul style="list-style-type: none"> - Motion of a particle in a ring. - Wave functions. Spherical harmonics. - Rotational energy: energy levels. - The quantization of angular momentum. |
| 5. Hydrogenic atoms. | <ul style="list-style-type: none"> - 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. | <ul style="list-style-type: none"> - Perturbation theory. - Variational method. - Lineal variational trial functions: secular determinant. |
| 7. Many-electron atoms. | <ul style="list-style-type: none"> - Helium atom. - Spin angular moment. - Pauli exclusion principle. - Periodic Table. |
| 8. Atomic spectroscopy. | <ul style="list-style-type: none"> - Electron configuration of atoms. - Total orbital angular moment: Russell-Saunders coupling and jj coupling. - Term symbols. Hund's rules. Selection rules. |



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| 9. The chemical bond: the hydrogen molecule-ion. | <ul style="list-style-type: none"> - The Born-Oppenheimer approximation. - Molecular orbital theory and valence-bond theory. - Molecular orbital treatment of hydrogen molecule-ion. |
| 10. Diatomic molecules. | <ul style="list-style-type: none"> - General considerations for bond formation. - Homonuclear diatomic molecules. - Heteronuclear diatomic molecules. Polar bonds and electronegativity. |
| 11. Conjugated and aromatic molecules. | <ul style="list-style-type: none"> - Semi-empirical methods. - Pi-electron approximation. - Free electron molecular orbital theory. - The Hückel approximation. |
| STATISTICAL THERMODYNAMICS | |
| 12. Foundations of statistical thermodynamics. | <ul style="list-style-type: none"> - 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 | 29 | 58 | 87 |
| Seminar | A14 A15 B2 B3 | 10 | 25 | 35 |
| Laboratory practice | A1 A8 A21 C1 C3 | 10 | 3 | 13 |
| Supervised projects | A1 A8 A16 B2 B3 B5 C1 C3 | 0 | 10 | 10 |
| Objective test | A1 A8 A14 | 1 | 0 | 1 |
| 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 | <p>Activity to be developed in small groups.</p> <p>In-depth study of the contents introduced in the keynote lectures.</p> <p>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.</p> <p>The activities to be carried out before and during each session are indicated prior to-face session.</p> |
| Laboratory practice | <p>Computer practices developed at the informatic labs.</p> <p>Practical problems related to the contents of Quantum Chemistry are solved by using computer software commonly used in scientific calculations.</p> |



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| Supervised projects | <p>Supervised homework to be performed in groups of 2-3 students.</p> <p>Students should carry out two activities related to some of the contents of the subject.</p> <p>The activities will be proposed by the lecturers through the e-learning platform along the semester. The activities will have a submission deadline, a written report will have to be handed and it will have to be explained to the instructor in a to-face session.</p> <p>All homework will be submitted and graded as a group.</p> <p>Supervised learning process aimed at helping students to work independently, under the guidance of the lecturer.</p> |
| Objective test | <p>Written in-class exam to be held at mid-semester.</p> <p>The test can combine multiple-choice questions and short answer questions.</p> <p>The basic principles and the formulation of quantum theory and their applications to simple systems are evaluated.</p> <p>The test is solved and discussed in a subsequent session.</p> <p>It will serve as feed-back to both students and instructors to assess the progress of the teaching-learning process.</p> |
| Mixed objective/subjective test | <p>Final written exam to be held at the end of semester, and in second chance in July.</p> <p>Knowledge, understanding, reasoning and critical thinking are assessed.</p> <p>It will consist on a combination of different types of questions: multiple choice and/or short answer combined with problem solving.</p> <p>It will be held on the dates approved by the Faculty Board.</p> |

Personalized attention

| Methodologies | Description |
|---------------------|--|
| Supervised projects | <p>Homework done by each group of 2-3 students should be presented to the instructor in a tutoring session.</p> <p>In addition, students are encouraged to make use of the tutoring sessions to solve any doubt.</p> <p>Tutoring schedule will be decided at lecturers and students convenience.</p> |

Assessment

| Methodologies | Competencies | Description | Qualification |
|---------------------------------|--------------------------------|--|---------------|
| Objective test | A1 A8 A14 | <p>Written in-class exam at mid-semester.</p> <p>The basic principles and the formulation of quantum theory and their applications to simple systems are assessed as short answer questions and/or multiple-choice questions.</p> | 10 |
| Mixed objective/subjective test | A1 A8 A12 A14 A15 A21 B2 B3 | <p>Final written exam at the end of semester.</p> <p>All contents of the subject are assessed.</p> <p>It has two different types of questions: short answer questions (50%) combined with problem solving (50%).</p> | 70 |
| Laboratory practice | A1 A8 A21 C1 C3 | <p>Assessment of skills in solving problems of Quantum Chemistry by using computer software commonly used in scientific calculations.</p> <p>Attendance to all scheduled computer lab. sessions is mandatory to pass the course.</p> <p>The final written report is also assessed.</p> | 10 |



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| 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 subject. Apart from the solution of the problem, the submitted written task and the oral presentation also contribute to the assessment. All members of a group get the same mark. | 10 |
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Assessment comments

Requirements to pass the course:

- Attendance to all scheduled computer lab sessions is mandatory to pass the course.

- It is compulsory both taking the mid-term test and the regular attendance to the keynotes and seminar sessions to attend computer practical sessions.

- It is mandatory to obtain a minimum mark of 1.5 (out of a possible 5) in each of the parts of the final written exam and a minimum mark of 4 (out of a possible 10) to pass the course.

- To pass the course, the final grade has to be equal to or greater than 5 (out of a possible 10) and the minimum score on the final written exam. If the average is equal to or greater than 5 (out of 10) but the threshold marks were not met, the final mark will be 4.5 (fail).

- Any student who has attended the practical sessions or the final exam will be assessed.

Second opportunity of July- According to the rules contained in "Probas de Avaliación e Actas de Cualificación de Grao e Mestrado", the so-called "second opportunity of July" is understood as a second opportunity to retake the final written exam. The mark of this second exam will be considered together with the others obtained during the course, corresponding to the other activities. The percentages of the different contributions will be the same as those of the former "first opportunity".

-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.

Successive academic years:

- The teaching-learning process, including assessment, refers to an academic course and, therefore, will restart as new with every new academic year, including all activities and assessment procedures scheduled for that course.

Mixed objective/subjective test dates:

Final written exam for the two opportunities will be held on the official dates approved by the Faculty Board.

Sources of information

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| Basic | <ul style="list-style-type: none">- 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 |
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| Complementary | <ul style="list-style-type: none">- Science Direct (). http://www.sciencedirect.com.- Publicaciones de la American Chemical Society (). http://pubs.acs.org/about.html.- http://www.m-w.com (). DICCIONARIO DE INGLÉS ONLINE (Merriam Webster).- 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/.- Página Web de ISI Web of Knowledge (). http://isi02.isiknowledge.com/.- 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). QUÍMICA CUÁNTICA 5ª ed. Prentice Hall- DÍAZ PEÑA, M. ROIG MUNTANER, A. (1988). QUÍMICA FÍSICA. Alhambra- LEVINE, I.N. (2004). FISICOQUÍMICA 5ª edición. McGraw-Hill <p> </p> |
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Recommendations

Subjects that it is recommended to have taken before

Matemáticas 1/610G01001

Matemáticas 2/610G01002

Física 1/610G01003

Física 2/610G01004

Química 1/610G01007

Química 2/610G01008

Subjects that are recommended to be taken simultaneously

Subjects that continue the syllabus

Química Física 2/610G01017

Other comments

(*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.