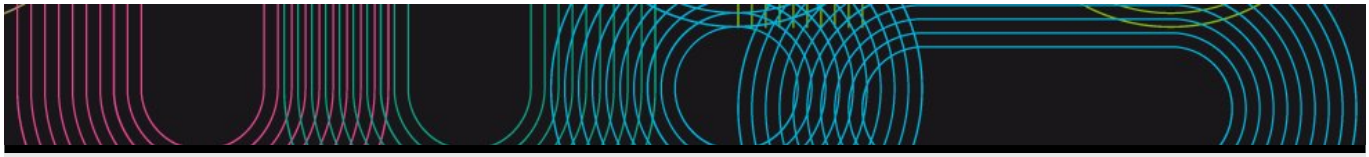

IDENTIFYING DATA				
Physics 3				
Subject	Physics 3			
Code	V11G200V01301			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	1st
Teaching language	Spanish			
Department				
Coordinator	Martínez Piñeiro, Manuel Hermida Ramón, José Manuel			
Lecturers	Hermida Ramón, José Manuel Martínez Piñeiro, Manuel Peña Gallego, María de los Ángeles			
E-mail	mmpineiro@uvigo.es jose_hermida@uvigo.es			
Web				
General description	The matter intends to be an introduction to Quantum Mechanics and Statistical mechanics, oriented to theirs applications in Chemistry.			

Competencies	
Code	
C3	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories in: principles of quantum mechanics and its application in the description of the structure and properties of atoms and molecules
C14	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: relationship between macroscopic properties and properties of individual atoms and molecules, including macromolecules
C19	Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature
C20	Evaluate, interpret and synthesize data and chemical information
C22	Process and perform computational calculations with chemical information and chemical data
C23	Present oral and written scientific material and scientific arguments to a specialized audience
D1	Communicate orally and in writing in at least one of the official languages of the University
D3	Learn independently
D4	Search and manage information from different sources
D5	Use information and communication technologies and manage basic computer tools
D6	Use mathematics, including error analysis, estimates of orders of magnitude, correct use of units and data representations
D7	Apply theoretical knowledge in practice
D8	Teamwork
D9	Work independently
D12	Plan and manage time properly
D13	Make decisions
D14	Analyze and synthesize information and draw conclusions
D15	Evaluate critically and constructively the environment and oneself

Learning outcomes		
Expected results from this subject		Training and Learning Results
To describe in an unified way the electromagnetic field by means of Maxwell's laws. Apply the basic boundary conditions in the vacuum or in materials.	C3	D1 D12 D14
To derive the equation of propagation of an electromagnetic wave, and describe its main characteristics. Relate this concept with the electromagnetic spectrum.	C3	D12 D14

To explain the empirical phenomena related with the interaction of radiation with matter which cannot be explained by the Classical Theory, and the solutions proposed (wave-corpuscle duality, quantization of the radiation).	C3	D12 D14 D15
To know the postulates of Quantum Mechanics and their consequences in the reformulation of the microscopic theory of the Classical Physics.	C3	D1 D12 D14 D15
To explain the essentials of the theory of mathematical operators, including the concepts of eigenfunction and eigenvalue, spectrum, linearity and hermiticity, complete sets of eigenfunctions, etc.	C3	D1 D9 D12 D14
To write the fundamental operators of Quantum Mechanics (position, linear and angular moment, Hamiltonian of simple systems).	C3 C19	D1 D9 D12 D14
To apply the previous concepts to the quantum- mechanical study of simple systems, like a particle in a square well potential, or to a harmonic oscilator potential, by resolving the time-independent Schrödinger equation.	C3 C19	D1 D3 D6 D8 D12 D13 D14
To calculate the eigenfunctions and eigenvalues of the angular momentum operator.	C3 C19	D6 D12 D14
To resolve the wave equation of the hydrogen atom, and calculate its eigenfunctions (orbitals).	C3 C19	D6 D8 D12 D14
To resolve the Schrödinger equation for many-electron atoms by means of approximate methods.	C3 C19 C20	D1 D5 D6 D9 D12 D13 D14
To explain in a simple way the transitions between states and the absorption and emission spectra.	C3 C19 C20 C22 C23	D1 D6 D8 D9 D12 D14 D15
To know the laws of Statistical Mechanics, which govern the behaviour of many-particle systems, in particular the Maxwell-Boltzmann statistics. Derive the partition function of a system and know in detail its physical meaning.	C14 C20 C22 C23	D1 D4 D5 D6 D7 D8 D12 D13
To apply the Maxwell-Boltzmann statistics to the case of the ideal gases of atoms and polyatomic particles to estimate thermodynamic properties, using microscopic properties like the mass, the molecular geometry and the vibrational frequencies.	C14 C19	D1 D4 D5 D6 D7 D8 D12 D13

Contents

Topic	
Electromagnetic field: equations of Maxwell.	Displacement current. Maxwell equations. Energy. Waves equations.

Quantización Of radiation. Wave-corpuscle duality	Ultraviolet catastrophe photoelectric Effect X-rays. Bragg condition. Braking radiation. Compton effect Wave-corpuscle duality
Principles of Quantum Mechanics	Limitations of Classical Physics and origin of Quantum Mechanics De Broglie Hypothesis Uncertainty Relationship Quantum Mechanics Postulates Virial Theorem
Quantum-mechanical Study of model systems	Introduction. Particle in a box of potential. Harmonic oscillator. Angular moment and rigid rotor.
Approximate methods	Introduction. Method of variations. Method of perturbations.
Hydrogen-like Atoms	Introduction. Resolution of the radial part of the equation of Schrödinger. Hydrogen-like Orbitals. Angular and magnetic moments electronic. Electronic spin. Spin-orbit coupling. Hyperfine structure. Spectra of Hydrogen-like atoms
Polielectronic atoms	Approximation of independent electrons. Antisymmetry Principle. Slater orbitals and basic functions. SCF-HF Method Terms and electronic levels. Spectra of polielectronic atoms
Statistical mechanics	Nomenclature and postulates. Canonical ensemble. Canonical partition function. Systems of non-interacting particles. Molecular partition function. Canonical partition function for a pure ideal gas. Boltzmann distribution law for non-interacting molecules. Statistical thermodynamics for ideal gases. Introduction to the study of real systems.

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	25	50	75
Problem solving	26	39	65
Introductory activities	1	1	2
Problem and/or exercise solving	4	0	4
Essay questions exam	4	0	4

*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

Methodologies

	Description
Lecturing	Discussion of the fundamental points of each subject and presentation of those which are going to be tackled in the seminars
Problem solving	Resolution of numerical problems, theoretical questions and development of the theoretical points proposed in the masterclasses with the participation of the student.
Introductory activities	Presentation of the subject with a brief desription of: sections, contents, distribution of the sections in the short tests and in the final exam general norms of evaluation,etc.

Personalized assistance

Methodologies	Description
Lecturing	Discussion of the main points of the subject. Answers to the questions related with the points raised by the students not only in the master session but also in the seminars. The students will know before the beginning of the course the schedules of the the tutorial sessions offered by the professors of the subject. In those tutorials the student will be able to review his/her examinations

Problem solving	Answers to the questions related with the points the students may have raised in the classes devoted to problem resolution and in the tutorial sessions. The students will know before the beginning of the course, the schedules of the the tutorial sessions offered by the professors of the subject. In those tutorials the student will be able to review his/her examinations

Assessment

	Description	Qualification	Training and Learning Results	
Problem solving	It will consist on the resolution of exercises and tests in the classroom. Nevertheless, the teacher will be able too to ask the student to deliver the solution to previously proposed exercises, that he/she has resolved in an autonomous way. In this case the teacher may ask the student tho explain to him indivdually how he/she has resolved the exercise.	25	C19 C20 C22 C23	D1 D3 D4 D5 D6 D7 D8 D9 D12 D13 D14 D15
Problem and/or exercise solving	During the course two short written tests will take place. They will correspond, respectively, to the contents of the sections 1 to 3 and 4 to 8 respectively. If any of those written tests is not passed the student must take on the corresponding part of the final exam (December/January). The student must take on the whole subject in the second-opportunity exam (June/July).	37.5	C3 C14 C19 C20	D6 D7 D9 D12 D13 D14
Essay questions exam	At the end of the course a full written test will take place in which the students can take on those aspects that they did not pass in the short written tets or improve in those they did pass.	37.5	C3 C14 C19 C20	D6 D7 D9 D12 D13 D14

Other comments on the Evaluation

During the course two short written tests will take place corresponding to sections 1-3, the first one, and to sections 4-8, the second. Both will contain problems and questions and, if they are passed, the student, is not obliged to take on the corresponding part of the subject in the (first-call) final exam (December/January), although he/she can do so in order to improve his/her mark. On a voluntary basis the student may participate in the seminars by solving exercises on the board. Also voluntarily the student may solve at home some proposed exercises and deliver them to the teacher. The final exam will include the whole subject but is divided into two parts corresponding to the two tests so the student can take on any or both of them, even if they have passed the short written test of that part.

The student though, must reachin the written tests a global minimum mark of 3.5/10 in order to accumulate the points obtained by resolving exercises independently or in the classroom.

In the second-opportunity evaluation (July) the student should do a full written test; the points obtained by exercise resolution (troubleshooting section) will be mantained.

On a voluntary basis, the students will be able to participate in the resolution of exercises in the seminars or deliver the answer to the written exercises proposed in the classroom.

It will be understood that any student who has not taken any written test (short or the final exam) has not really followed the subject and will not be given a mark (his/her qualification will be "no presentado").

Sources of information

Basic Bibliography

Complementary Bibliography

R. Eisberg, y R. Resnick, **Fisica Cuantica**, 1983,

M. Alonso y E.J. Finn, **Física**, 2000,

I. N. Levine, **Fisicoquímica**, 2004,

P.W. Atkins y J. de Paula, **Atkin's Physical Chemistry**, 2014,

J. Bertrán y otros, **Química Cuántica**, 2000,

I.N. Levine, **Química Cuántica**, 2001,

Recommendations
Subjects that continue the syllabus
Physical chemistry II/V11G200V01403