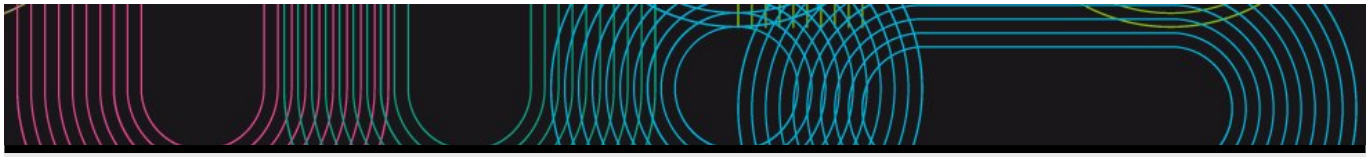

IDENTIFYING DATA				
Physics III				
Subject	Physics III			
Code	V11G200V01301			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	1st
Teaching language	Spanish			
Department				
Coordinator	Flores Rodríguez, Jesús Ramón			
Lecturers	Flores Rodríguez, Jesús Ramón Martínez Piñeiro, Manuel			
E-mail	flores@uvigo.es			
Web				
General description	The matter pretends 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
Describe *unificadamente the electromagnetic field by means of the laws of Maxwell. Apply the basic conditions of border in the empty or in presence of material means.	C3	D1 D12 D14
Derive the equation of propagation of an electromagnetic wave, characterised through his main characteristic. Relate this concept with the electromagnetic spectrum.	C3	D12 D14
Explain the empirical phenomena related with the interaction radiation matter no explained by the Classical Theory, and the solutions proposed for his resolution (duality wave corpuscle, *cuantización of the radiation).	C3	D12 D14 D15

Bill the postulates of the Quantum Mechanics and his consequences in the reformulation of the microscopic theory of the Classical Physics.	C3	D1 D12 D14 D15
Explain the foundations of the theory of mathematical operators, including the concepts of function and own value, spectrum, *linealidad and *hermiticidad, space of functions, etc.	C3	D1 D9 D12 D14
Write the fundamental operators of the Quantum Mechanics (position, linear and angular moment, Hamiltonian of simple systems).	C3 C19	D1 D9 D12 D14
Apply the previous concepts to the mechanical study-quantum of simple systems, like a particle subjected to a potential of *pozo square infinite, or to a harmonic potential, resolving the equation of Schrödinger independent of the time.	C3 C19	D1 D3 D6 D8 D12 D13 D14
Calculate the functions and own values of the for the moment angular operator.	C3 C19	D6 D12 D14
Resolve the equations of wave of the atom of hydrogen, calculating his orbital.	C3 C19	D6 D8 D12 D14
Resolve the equation of Schrödinger for atoms *polielectrónicos by means of approximate methods.	C3 C19 C20	D1 D5 D6 D9 D12 D13 D14
Explain of simple form the transitions between states and the spectrums of broadcast or resultant absorption.	C3 C19 C20 C22 C23	D1 D6 D8 D9 D12 D14 D15
Bill the laws of the Statistical mechanics that govern the behaviour of systems of particles, *particularizado to the statistics of Maxwell *Boltzmann. Derive the function of partition of a system and know in detail his physical meaning.	C14 C20 C22 C23	D1 D4 D5 D6 D7 D8 D12 D13
Apply the statistics of Maxwell *Boltzmann to the case of the ideal gases monkey and polyatomic to estimate thermodynamic properties from microscopic properties like mass, molecular geometry and frequencies of vibration.	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
Master Session	26	49.4	75.4
Troubleshooting and / or exercises	26	39	65
Introductory activities	1	0.6	1.6
Short answer tests	4	0	4
Long answer tests and development	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
Master Session	*Expoisición Of the fundamental appearances of each subject and approach of those that go to tackle in the seminars
Troubleshooting and / or exercises	Resolution of numerical problems, theoretical questions and development of the theoretical appearances posed in the Masterclasses with the participation of the student.
Introductory activities	Class of presentation of the *asignatura with exhibition: of parts of the *temario, contents, distribution in short proofs and final examination, general norms of evaluation, etc.

Personalized attention

Methodologies	Description
Master Session	Answers to the questions related with the matter that pose the students in the classes of resolution of problems and in *tutorías. The students will know from principle of course the schedules of *tutorías of the professors of the matter. In the *tutorías the students will be able to review his examinations
Troubleshooting and / or exercises	Answers to the questions related with the matter that pose the students in the classes of resolution of problems and in *tutorías. The students will know from principle of course the schedules of *tutorías of the professors of the matter. In the *tutorías the students will be able to review his examinations

Assessment

	Description	Qualification	Training and Learning Results
Troubleshooting and / or exercises	Basically it will centre in the resolution of exercises in the classroom. Nevertheless, it will be able to *tambien ask to the student that deliver exercises proposed and that the resolve of autonomous way. In this case the professor will be able to ask to the student that explain him *indivdualmente as it has resolved the exercise.	15	
Short answer tests	They will celebrate 2 proofs of short answer. They will refer , respectively, to the matter of the subjects 1 to 3 and 4 to 8. The *superación of each one of them will allow that the students can not going back to examine of this matter in the final examination of the *cuatrimestre, but no like this in the examination of second opportunity (June-July).	42.5	
Long answer tests and development	When finishing the course will celebrate a complete proof in which the students that wish it will be able to repeat those appearances that did not surpass in the short proofs realised.	42.5	

Other comments on the Evaluation

During the course will realise two short proofs referred to the subjects
1-3, the first, and to the subjects 4-8, the second. Both will contain
problems and questions and his *superación will free to the students of this
part of the *asignatura. Of voluntary way, the students will be able to participate in the resolution of exercises in the seminars or deliver exercises proposed.Also will be able to present to a final examination, that will include all the matter, that will allow them increase the punctuation reached in
the partial.All student will have to reach at least a qualification of 3.5 on 10
in the global of his proofs written to be able to accumulate the corresponding
punctuation to resolution of exercises.
In the second announcement will keep the punctuation reached
by means of the resolution of exercises. This examination will value of
similar way to the final examination.
The student that do not present to any proof during the course will be described in first announcement as no presented.

Sources of information

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

Subjects that it is recommended to have taken before

Physics: Physics I/V11G200V01102
Physics: Physics II/V11G200V01201
Mathematics: Mathematics I/V11G200V01104
Mathematics: Mathematics II/V11G200V01203