Teaching Guide				
Identifying Data				2016/17
Subject (*)	Profundización en Química Física		Code	610509002
Study programme	Mestrado en Investigación Química e Química Industrial (plan 2016)			
Descriptors				
Cycle	Period	Year	Type	Credits
Official Master's Degree	Yearly	First	Obligatoria	3
Language	SpanishEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química Física e Enxeñaría Química 1			
Coordinador	Penedo Blanco, Francisco Jose	E-mail	francisco.penedo.blanco@udc.es	
Lecturers	Penedo Blanco, Francisco Jose Santaballa Lopez, Juan Arturo	E-mail	francisco.penedo.blanco@udc.es arturo.santaballa@udc.es	
Web	miiquimica.webnode.es/			
General description	This subject is aimed to cover concepts, and theoretical and experimental tools, which weren't included in the previous step of Chemistry Degree. They are essential for the adequate comprehension of another Master subjects. Specifically, concepts and characteristics of intermolecular forces, intermolecular energies, radial distribution functions in gases and condensed phases, interface interactions, interface behaviour and reactivity modeling will be shown. All the information related to subjects in this Master is centralized on the webpage shown above. This webpage is the reference for all students, regardless of the center where they study.			

Study programme competences	
Code	Study programme competences
A1	Define concepts, principles, theories and specialized facts of different areas of chemistry.
A2	Suggest alternatives for solving complex chemical problems related to the different areas of chemistry.
A4	Innovate in the methods of synthesis and chemical analysis related to the different areas of chemistry
B1	Possess knowledge and understanding to provide a basis or opportunity for originality in developing and / or applying ideas, often within a research context
B2	Students should apply their knowledge and ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study.
B4	Students should be able to communicate their conclusions, and the knowledge and the reasons that support them to specialists and non-specialists in a clear and unambiguous manner
B5	Students must possess learning skills to allow them to continue studying in a way that will have to be largely self-directed or autonomous.
B7	Identify information from scientific literature by using appropriate channels and integrate such information to raise and contextualize a research topic
B10	Use of scientific terminology in English to explain the experimental results in the context of the chemical profession
B11	Apply correctly the new technologies to gather and organize the information to solve problems in the professional activity.

Learning outcomes			
Learning outcomes	Study programme competences		
To comprehend concepts and characteristics of intermolecular forces. To understand the different terms that comprise the total interaction energy between molecules.	AC1	BC1 BC4 BC5 BC7 BC10	
To understand the related concepts and the structural information provided by the radial distribution function in gas and condensed phases.	AC2	BC1 BC2 BC11	

To understand the thermodynamic and structural properties of the interactions between phases in contact. To comprehend the different approaches to modeling the behavior and reactivity of the interfaces.	AC1 AC2 AC4	BC1 BC2 BC4 BC5	

Contents	
Topic	**Sub-topic**
ITEM 1. Electrical properties of molecules.	Electric dipole moments. Polarizabilities. Relative permittivities.
ITEM 2. Intermolecular forces.	Dipole-dipole attractions . Dispersion forces. Hydrogen bonds. Hydrophobic interaction. Total interaction: intermolecular potentials.
ITEM 3. Intermolecular interactions in liquids: radial distribution function.	Radial distribution function and its calculation.
ITEM 4. General concepts on interfaces.	Interfaces: a frontier between systems. Unbalanced energy. Excess Gibbs free energy. Special features of the interfaces liquid-fluid phase and solid-fluid phase. Molecular mobility in solids. Environmental variables affecting the excess surface free energy.
ITEM 5. Thermodynamics of interactions at the interface.	Differences in the study of liquid-fluid phase and solid-fluid phase interfaces. Classification based on the intermolecular forces and the energy involved in the interaction: physisorption and chemisorption. Monolayers and multilayers of adsorbate. Isotherms, types I to V. Determination of surface areas on solids, BET method. Hysteresis phenomena on adsorption-desorption cycles.
ITEM 6. Structural study of interfaces. Theoretical developments.	Basic concepts. The electrical double layer at the interface. Charge transfer. Application to the study of colloidal aggregates and electrical charge transfers.
ITEM 7. Experimental techniques of study and characterization of interfaces.	Photoelectron spectroscopy. Microscopies.

Planning				
Methodologies / tests	**Competencies / Results**	**Teaching hours (in-person & virtual)**	**Student?s personal work hours**	**Total hours**
Guest lecture / keynote speech	A1 B1 B2 B10	16	16	32
Seminar	A4 B4 B7 B11	4	6	10
Supervised projects	A2 B1 B2 B5	4	14	18
Mixed objective/subjective test	A2 A1 B4 B1	4	8	12
Personalized attention		3	0	3
(*)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	The teacher presents and explains the fundamental concepts of each topic, and the related theoretical developments.
Seminar	They are interactive small group sessions in which the teacher provides concrete examples related to the keynote speech. Case studies and discussion will take place between students and the handling of diverse scientific documentation is encouraged.
Supervised projects	In small group sessions, students will have to resolve, individually or in groups, the problems posed by the teacher. The student will submit a hard copy of the results, for further evaluation.
Mixed objective/subjective test	Final exam in which multiple choice questions and practical exercises are included. It is intended to assess the knowledge acquired by students and their skills on reasoning, synthesis and critical thinking.

Personalized attention

Methodologies	Description
Supervised projects Seminar	Throughout all sessions of the small group classes, the tutoring of students will be enhanced, helping to raise doubts and to solve them. Personal attention will be scheduled throughout the class period, via interactive tests which intend to assess the progress of the student achieving the learning aims of the subject. The students may apply for individual tutorials in the teacher's office in the appropriate schedule. In the specific case of part-time students, or exemption of assistance, seminars and supervised work will be led through interactive online support, email or moodle, with a timing similar to that of small group classes scheduled.

Assessment			
Methodologies	Competencies / Results	Description	**Qualification**
Supervised projects	A2 B1 B2 B5	The submitted paper (practical exercises) will be graded according to the methodology applied, the optimization of the resolution and the accuracy of the results.	20
Mixed objective/subjective test	A2 A1 B4 B1	Each student will perform a mixed test, aimed to demonstrate the abilities to solve problems and to answer multiple choice conceptual questions. The assessment will check the acquired knowledge and the accuracy of the results.	75
Seminar	A4 B4 B7 B11	Student assessment in these sessions is based upon student participation in the discussions and issues raised in the classroom, and their skills in problem solving.	5

Assessment comments
To pass the course there are two basic requirements: 1) Regular attendance to all evaluable activities, except for students with part-time or waiver of assistance, as indicated below. 2) To achieve a minimum score of 4 (out of 10) in every evaluable activities. Such minimum score not be achieved in any one of these activities, the final grade will be Fail (4.0). To pass the subject, the overall rating may not be less than 5 (out of 10). "Not attended" assessment mark will be applied when the conducted activities add up to less than 25% of the total score. In the context of continuous assessment, marks obtained in seminars and supervised work can be retained for the second chance, provided they score above the minimum of 4 previously cited. The rating of the mixed test achieved in this second chance will replace that the first one. Students evaluated in the second chance may only qualify for honors if the maximum number of licenses for the course were not exhausted at the first opportunity. In the following academic courses, the teaching-learning process, including assessment, would start over, which means that the students must complete all scheduled activities for the new course. In the case of students with part-time, or exemption from assistance, all assessed activities can be conducted online, and ranked as if they were in attendance, so the design of a specific protocol it is not necessary.

Sources of information	
Basic	- P. Atkins, J. de Paula (2014). Physical Chemistry, 10th ed.. Oxford University Press - I. N. Levine (2004). Fisicoquímica, 5th ed.. McGraw-Hill - F. MacRitchie (1990). Chemistry at Interfaces. Academic Press - D. Myers (1999). Surfaces, Interfaces and Colloids: Principles and Applications. VCH Publishers
Complementary	- J.M. Hollas (2004). Modern Spectroscopy, 4th ed.. John Wiley&Sons - S.R. Morrison (1990). The Chemical Physics of Surfaces, 2nd ed.. Plenum Press

Recommendations
Subjects that it is recommended to have taken before
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
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.