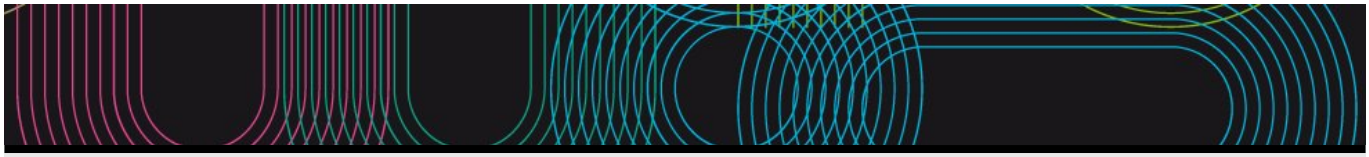

IDENTIFYING DATA

Computational Chemistry

Subject	Computational Chemistry			
Code	V11G201V01411			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Optional	4th	2nd
Teaching language	#EnglishFriendly Spanish			
Department				
Coordinator	Graña Rodríguez, Ana María			
Lecturers	Graña Rodríguez, Ana María			
E-mail	ana@uvigo.es			
Web				
General description	Computational Chemistry is a discipline using mathematical methods for the calculation of molecular properties or for the simulation of the molecular behaviour.			

Training and Learning Results

Code	
A1	Students can apply their knowledge and understanding in a manner that indicates a professional approach to their work or vocation, and have competences typically demonstrated through devising and sustaining arguments and solving problems within their field of study
B1	Ability for auronomous learning
B2	Organization and planning capacity
C36	Know the basics and be able to use different quantum mechanical methods to be applied to systems of chemical interest
D1	Ability to solve problems

Expected results from this subject

Expected results from this subject	Training and Learning Results			
Describe the main methods of calculation of the computational chemistry, knowing his applications and limitations.			C36	
Describe the elements that can contain a field of strengths of molecular mechanics.			C36	
Choose levels of quantum calculation adapted for the treatment of a chemical problem.	A1	B2	C36	
Describe fundamental algorithms employees in the calculations of computational chemistry.			C36	
Obtain properties of chemical interest doing use of computational methods (static and dynamic).		B1 B2	C36	D1

Contents

Topic	
Subject 1. Introduction: methods of calculation in Computational Chemistry.	Molecular mechanics. Hartree-Fock methods. Post Hartree-Fock methods. Density Functional Theory. Molecular Dynamics methods. Choise of method. Choise of basis set.
Subject 2. Conformational studies.	Potential energy surface. Characterization of singular points. Optimization of geometries. Optimization of transition states. Constrained optimizations. Conduction methods. Conformational sampling. IRC methods.
Subject 3. Application to spectroscopy.	Infrared spectra. Electronic excited states UV-visible spectra. NMR spectra.
Subject 4. Applications to the calculation of energy properties.	Thermodynamics properties. Basis set superposition error. Isogyric reactions. Isodesmic reactions. Homdesmotic reactions. Gn and CBS methods.
Subject 5. Applications to the chemical reactivity.	Chemical reactivity indices. Reaction dynamics. Calculation reaction rates.

Subject 6. Models of salvation.	Continuum models of salvation. Inclusion of explicit solvent molecules. Mixed methods.
Subject 7. Applications to biomolecules.	Molecular Mechanics. Molecular Dynamics. Hybrid methods QM/MM.

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	26	22	48
Practices through ICT	14	14	28
Problem solving	6	18	24
Problem and/or exercise solving	6	18	24
Essay	0	26	26

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

Methodologies

	Description
Lecturing	Exhibition by part of the professor of theoretical and practical concepts.
Practices through ICT	Computational laboratory.
Problem solving	Resolution of problems by part of the students so much in paper as with computational assistance.

Personalized assistance

Methodologies	**Description**
Lecturing	Students willing so could attend personal tutorials to solve doubts and/or uncertainties. To better optimise the procedure, the student is advised to previously contact her teacher.
Problem solving	Students willing so could attend personal tutorials to solve doubts and/or uncertainties. To better optimise the procedure, the student is advised to previously contact her teacher.
Practices through ICT	Students willing so could attend personal tutorials to solve doubts and/or uncertainties. To better optimise the procedure, the student is advised to previously contact her teacher.
Tests	**Description**
Problem and/or exercise solving	Students willing so could attend personal tutorials to solve doubts and/or uncertainties. To better optimise the procedure, the student is advised to previously contact her teacher.
Essay	Students willing so could attend personal tutorials to solve doubts and/or uncertainties. To better optimise the procedure, the student is advised to previously contact her teacher.

Assessment

	Description	Qualification	Training and Learning Results			
Problem solving	Report of exercises of the subjects 1 to 3.	30	A1	B1 B2	C36	D1
Problem and/or exercise solving	Report of exercises of the subjects 4 to 7.	40	A1	B1 B2	C36	D1
Essay	Delivery of an individual work about practical classes.	30	A1	B1 B2	C36	D1

Other comments on the Evaluation

Sources of information

Basic Bibliography

J. B. Foresman, A. Frisch, **Exploring Chemistry with Electronic Structure Methods**, 3, Gaussian Inc, 2015

Frank Jensen, **Introduction to computational chemistry**, 2, Wiley, 2006

Joan Bertran Rusca, Vicenç Branchadell Gallo, Miquel Moreno Ferrer, Mariona Sodupe Roure, **Química Cuántica**, 1, Síntesis, 2000

Complementary Bibliography

A. Szabo, N. S. Ostlund, **Modern Quantum Chemistry**, 1, Dover, 1996

Recommendations

Subjects that it is recommended to have taken before

Physics: Physics I/V11G201V01102
Physics: Physics 2/V11G201V01107
Mathematics: Mathematics 1/V11G201V01103