

UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course: CO	MPUTATIONAL CHEMISTRY			Code: 310584				
Type: CO	RE COURSE		ECTS credits: 6					
Degree: 232	6 - MASTER DEGREE PROGF	AMME IN CHEM	Academic year: 2019-20					
Center: 1 - F	ACULTY OF SCIENCE AND C	HEMICAL TECH	NOLOGY Group(s):20					
Year: 1			Duration: First semester					
Main language: Spanish Second language:								
Use of additional languages:			English Friendly: Y					
Web site:			Bilingual: N					
Lecturer: MARIA REYES	LOPEZ ALAÑON - Group(s): 2	20						
Building/Office	Department	Phone number	Email	Office hours				
Marie Curie (segunda planta))	QUÍMICA FÍSICA	926052779	reyes.lopez@uclm.es	Lunes y Martes: 11-13 h Miércoles de 16:30h a 18:30h.				
Lecturer: LUCIA SANTOS PEINADO - Group(s): 20								
Building/Office Department Phone number Email Office hours								
Edifico Marie Curie/2.05	QUÍMICA FÍSICA	926052480	lucia.santos@uclm.es	Lunes v jueves 10.00h-12.00h miércoles 18h-20h				

2. Pre-Requisites

Not established

3. Justification in the curriculum, relation to other subjects and to the profession

Not established

4. Degree competences achieved in this course

Course competences	
Code	Description
E02	Relating the macroscopic and supramolecular properties with those of atoms, molecules and non-molecular chemical compounds.
E03	Knowing the principles of quantum mechanics and their application to the determination of the structure and properties of atoms and molecules.
E04	Knowing the usefulness of the methods of design, simulation and molecular calculations, as well as having skills in the handling of these methods.
G01	Knowing the precision of the experimental data and its use for the planning of experimental research work.
T02	Ability to work in a team and to exercise leadership functions, fostering the entrepreneurial character
T04	Ability to use specific software for research in chemistry.
Т05	Ability to obtain bibliographic information at the research level, including Internet resources (databases, specialized scientific bibliography, social networks, etc), as well as carry out a selection and classification of it.

5. Objectives or Learning Outcomes

Course learning outcomes

Description

To analyze chemical phenomena and processes through simulation at individual level and as a team

To apply computer tools to work with remote work stations, to perform calculations and transfer files from or to them.

To acquire knowledge about the theoretical basis, limitations and application areas of the main methods in Computational Chemistry

To establish structure-reactivity relationships from empirical correlations

To interpret the results of a kinetic or computational study and present them properly, supported by the information obtained from previous bibliographic search To use properly the research software used in the laboratory and in the computer room

To solve structure, spectroscopy or reactivity problems using theoretical methods.

To combine advanced modeling techniques in Chemistry with the support of computational tools and to develop simulations in order to facilitate the understanding of theoretical and experimental concepts.

6. Units / Contents		
Unit 1:		
Unit 2:		
Unit 3:		
Unit 4:		
Unit 5:		
Unit 6:		
Unit 7:		

Unit 8:

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	R	Description
Class Attendance (theory) [ON- SITE]	Lectures	E02 E03 G01	1	25	Y	N	I Y	ſ
Study and Exam Preparation [OFF- SITE]	Self-study		1.5	37.5	Y	Y	Ý	
Workshops or seminars [ON-SITE]			0.4	10	Y	N	ΙY	(
Computer room practice [ON-SITE]	Work with simulators		0.9	22.5	Y	Y	Ύ	(
Practicum and practical activities report writing or preparation [OFF- SITE]	Self-study		0.88	22	Y	Y	Ύ	
Writing of reports or projects [OFF- SITE]	Guided or supervised work		1	25	Y	N	I Y	(
Final test [ON-SITE]	Self-study		0.12	3	Y	Y	Ύ	(
Other off-site activity [OFF-SITE]	Self-study		0.2	5	Y	N	ΙY	(
Total:			6	150				
Total credits of in-class work: 2.42			Total class time hours: 60.5					
Total credits of out of class work: 3.58			Total hours of out of class work: 89.5					

As: Assessable training activity Com: Training activity of compulsory overcoming R: Rescheduling training activity

8. Evaluation criteria and Grading System							
	Grading System						
Evaluation System	Face-to-Face	Self-Study Student	Description				
Assessment of activities done in the computer labs	25.00%	25.00%					
Practicum and practical activities reports assessment	10.00%	10.00%					
Assessment of problem solving and/or case studies	15.00%	15.00%					
Assessment of active participation	5.00%	5.00%					
Final test	45.00%	45.00%					
Total:	100.00%	100.00%					

9. Assignments, course calendar and important dates Not related to the syllabus/contents Hours

hours

10. Bibliography and Sources								
Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description		
C. J. Cramer	Essentials of Computational Chemistry	John Wiley&Sons, LTD	N.Y	0-471-48552-7	2002			
F. Jensen	Introduction to Computational Chemistry	John Wiley&Sons LTD	N.Y	13-978-0-470-01187-4	2007			
I.N. Levine	Química Cuántica	Prentice Hall	Madrid	84-205-3096-4	2001			
J. Bertrán, V. Branchadell; M. Moreno y M. Sodupe	Química Cuántica	Síntesis	Madrid	84-7738-742-7	2002			
J.B. Foresman and A,. Frisch	Exploring Chemistry with Electronic Structure Methods	Gaussian Inc	Pittsburgh	0-9636769-3-8	1996			
J.L Calais	Quantum Chemistry Workbook	John Wiley&Sons. INC		0-471-59435-0	1994			
Juan Andrés, J. Bertrán (eds)	Química Teórica y Computacional	P. de la Universidad Jaume I Castellón	Castellón	84-8021-312-4	2000			
L.E. Bailey, M.D.Trotiño	Q.C. La Química Cuántica en 100 problemas	UNED	Madrid	84-362-1350-5	2004			
	http://www.cup.uni-muenchen.de/	oc/zipse/computat	ionalchemi	stry1.html				
	http://www.cup.uni-muenchen.de/oc/zipse/computationalchemistry2.html							