UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course: MOLECULAR MODELLING
Code: 311122
Type: CORE COURSE
ECTS credits: 6
Degree: 2366 - MASTER DEGREE PROGRAMME IN CHEMICAL
Academic year: 2023-24
Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY
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: **BERNABE BALLESTEROS RUIZ** - Group(s): **20**

Building/Office	Department	Phone number	Email	Office hours
Marie Curie, primera planta	QUÍMICA FÍSICA	926052049	bernabe.ballesteros@uclm.es	L,M: 9-11h J: 17-19h

Lecturer: **MARIA REYES LOPEZ ALAÑON** - Group(s): **20**

Building/Office	Department	Phone number	Email	Office hours
Marie Curie (segunda planta))	QUÍMICA FÍSICA	926052779	reyes.lopez@uclm.es	Tuesday and Wednesday: 10-12 h Thursday: 17-19 h

Lecturer: **MARIA DEL PILAR PRIETO NUÑEZ-POLO** - Group(s): **20**

Building/Office	Department	Phone number	Email	Office hours
San Alberto Magno	QUÍMICA INORG., ORG., Y BIOQ.	+34926052615	mariapilar.prieto@uclm.es	

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	

2. Pre-Requisites

Basic knowledge of Quantum and Computational Chemistry is recommended.

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

The aim of the course is for students to deepen their knowledge of Quantum and Computational Chemistry previously acquired in the course of Chemical Sciences.
The course is designed for students who are studying chemistry.
Along with theory and experiment, simulation (modelling) is the third pillar of scientific knowledge. Since the 90s of the last century,
the development of powerful and low-cost computers, as well as the development of software with simple user interfaces, has allowed the use of computational tools to become more widespread.
It has allowed the use of computational tools not to be limited to the specialised chemist, but to become a common tool for the entire chemical environment.
chemist.
The aim, therefore, is to provide a global vision of chemistry from the perspective of modelling as the backbone of all the knowledge acquired in undergraduate studies.
in undergraduate studies.

4. Degree competences achieved in this course

Course competences

Code	Description
CB06	Possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a research context
CB07	Students are able to apply their acquired knowledge and problem-solving skills in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study.
CB08	Students are able to integrate knowledge and deal with the complexity of making judgements on the basis of incomplete or limited information, including reflections on the social and ethical responsibilities linked to the application of their knowledge and judgements.
CB09	Students are able to communicate their conclusions and the ultimate knowledge and rationale behind them to specialist and non-specialist audiences in a clear and unambiguous way.
CB10	Students possess the learning skills that will enable them to continue studying in a largely self-directed or autonomous way.
CE02	Integrate quantum mechanics into the determination of the structure and properties of atoms and molecules of interest in research and development laboratories.
CE03	To know the usefulness of the molecular design, simulation and calculation methods that characterise computational chemistry, as well as to be proficient in the use of these methods.
CE08	Design a sustainable development of chemistry in its application at research level as in any professional activity, through advanced knowledge of synthesis and analysis methodologies.

CE09	To develop experiments that serve as a basis for R+D+I activities in the field of chemistry, facilitating their transfer to the productive world by means of new standardised work procedures validated for routine and/or control laboratories.
CG01	Transfer the concepts and fundamentals of chemistry in the context of scientific research and/or in the specialised profession of the chemist.

5. Objectives or Learning Outcomes

Course learning outcomes

Description

Acquire knowledge of the theoretical basis, limitations and fields of application of the main methods of computational chemistry.

Analyse chemical phenomena and processes through simulation both individually and as part of a team.

Apply computer tools to work with remote workstations, perform calculations on remote workstations and transfer files to/from remote workstations.

Combine the advanced modelling techniques of chemistry with the appropriate computational support, as well as develop simulations that facilitate the understanding of theoretical and experimental concepts.

Establish structure-reactivity relationships through empirical correlations.

Interpret the results of a kinetic or computational study and present them appropriately, complementing them with the information obtained from the bibliographic search carried out previously.

Solve problems of structure, spectroscopy or reactivity by theoretical methods.

6. Units / Contents

Unit 1: Molecular Orbital Theory. Born-Oppenheimer approximation. Electronic wave function. Slater's determinant. Variational method. CLOA approximation. Basic functions

Unit 2: Computational methods: Semiempirical methods and Hartree-Fock method.

Unit 2.1 Practical 1: Introduction and use of computational chemistry programs including graphical displays

Unit 3: Post-Hartree-Fock methods. Electronic correlation. Interaction of configurations. Multiconfigurational self-consistent method (MCSCF). Moller-Plesset perturbation method. Coupled-cluster methods (practices 2 and 3).

Unit 3.1 Practice 2 :Optimization of geometries. Absolute and relative energies. Base superposition error (BSSE).

Unit 3.2 Practice 3: Electronic connection methods. Dissociation of the hydrogen molecule.

Unit 4: Density functional methods. Hohenberg and Kohn theorems. Koh-Sham method. Local density approximation. Generalized gradient approximation. Hybrid functionals (practices 6 and 7).

Unit 5: Potential energy surfaces. Potential energy surface (PES) analysis. Stationary points. Transition states. Intrinsic reaction coordinate (IRC). Thermodynamics and chemical kinetics (practice 4 and 5).

Unit 5.1 Practice 4: SEP analysis. Localization of transition states of unimolecular and bimolecular reactions.

Unit 5.2 Practice 5: Chemical reactivity (Kinetic control and thermodynamic control. Isotopic effect)

Unit 5.3 Practice 6:Optimization of organometallic compounds. Study of molecular properties: Mulliken charges and NBOs. Binding orders. Dipole moments. Topology of frontier molecular orbitals.

Unit 5.4 Practice 7:Photophysical properties. Absorption and emission spectra. RAMAN spectra. NMR spectra

Unit 5.5 Practice 8: Study of ionic hydration. Effect of the solvent.

Unit 6: Molecular Mechanics. Force fields. Bond stress. Angular deformation.torsion. Electrostatic interactions. Van der Waals interaction. Parametrization. Available force fields. Solvent modeling. Molecular Dynamics simulation.

Unit 7: Hybrid QM/MM methods. Coupling of QM/MM regions. Multilayer methods. Cavities. (Practice 8)

7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Practicum and practical activities report writing or preparation [OFF-SITE]	Self-study	CB08 CB09 CE03	1.6	40	Y	Y	
Class Attendance (theory) [ON-SITE]	Lectures	CB06 CB08	1.16	29	Y	N	
Study and Exam Preparation [OFF-SITE]	Problem solving and exercises	CB07 CB08 CB10	2.4	60	Y	N	
Analysis of articles and reviews [OFF-SITE]	Case Studies	CB07 CE03	0.24	6	Y	Y	
Final test [ON-SITE]	Work with simulators	CB07 CB09 CE02 CE03	0.2	5	Y	Y	
Group tutoring sessions [ON-SITE]	Group tutoring sessions	CB09	0.08	2	Y	Y	
Class Attendance (practical) [ON-SITE]	Practical or hands-on activities		0.32	8	Y	Y	
		Total:	**6**	**150**			
		Total credits of in-class work: 1.76					**Total class time hours: 44**
		Total credits of out of class work: 4.24					**Total hours of out of class work: 106**

As: Assessable training activity

Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System

Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Test	45.00%	60.00%	
Practicum and practical activities reports assessment	50.00%	40.00%	
Assessment of active participation	5.00%	0.00%	

Total:	**100.00%**	**100.00%**	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject , an ordinary and an extraordinary one (evaluating 100% of the competences).

9. Assignments, course calendar and important dates

Not related to the syllabus/contents

Hours	**hours**

Unit 1 (de 7): Molecular Orbital Theory. Born-Oppenheimer approximation. Electronic wave function. Slater's determinant. Variational method. CLOA approximation. Basic functions

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Study and Exam Preparation [AUTÓNOMA][Problem solving and exercises]	2
Final test [PRESENCIAL][Work with simulators]	.5
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.2

Unit 2 (de 7): Computational methods: Semiempirical methods and Hartree-Fock method.

Activities	**Hours**
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	4
Class Attendance (theory) [PRESENCIAL][Lectures]	4
Study and Exam Preparation [AUTÓNOMA][Problem solving and exercises]	10
Final test [PRESENCIAL][Work with simulators]	.8
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.2
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	1

Unit 3 (de 7): Post-Hartree-Fock methods. Electronic correlation. Interaction of configurations. Multiconfigurational self-consistent method (MCSCF). Moller-Plesset perturbation method. Coupled-cluster methods (practices 2 and 3).

Activities	**Hours**
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	10
Class Attendance (theory) [PRESENCIAL][Lectures]	5
Study and Exam Preparation [AUTÓNOMA][Problem solving and exercises]	10
Analysis of articles and reviews [AUTÓNOMA][Case Studies]	2
Final test [PRESENCIAL][Work with simulators]	.8
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.2
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	2

Unit 4 (de 7): Density functional methods. Hohenberg and Kohn theorems. Koh-Sham method. Local density approximation. Generalized gradient approximation. Hybrid functionals (practices 6 and 7).

Activities	**Hours**
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	15
Class Attendance (theory) [PRESENCIAL][Lectures]	6
Study and Exam Preparation [AUTÓNOMA][Problem solving and exercises]	15
Analysis of articles and reviews [AUTÓNOMA][Case Studies]	2
Final test [PRESENCIAL][Work with simulators]	.8
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	2

Unit 5 (de 7): Potential energy surfaces. Potential energy surface (PES) analysis. Stationary points. Transition states. Intrinsic reaction coordinate (IRC). Thermodynamics and chemical kinetics (practice 4 and 5).

Activities	**Hours**
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	6
Class Attendance (theory) [PRESENCIAL][Lectures]	5
Study and Exam Preparation [AUTÓNOMA][Problem solving and exercises]	15
Final test [PRESENCIAL][Work with simulators]	.9
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	1
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	2

Unit 6 (de 7): Molecular Mechanics. Force fields. Bond stress. Angular deformation.torsion. Electrostatic interactions. Van der Waals interaction. Parametrization. Available force fields. Solvent modeling. Molecular Dynamics simulation.

Activities	**Hours**
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Study and Exam Preparation [AUTÓNOMA][Problem solving and exercises]	4
Analysis of articles and reviews [AUTÓNOMA][Case Studies]	1
Final test [PRESENCIAL][Work with simulators]	.4
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.2

Unit 7 (de 7): Hybrid QM/MM methods. Coupling of QM/MM regions. Multilayer methods. Cavities. (Practice 8)

Activities	**Hours**
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	5
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Study and Exam Preparation [AUTÓNOMA][Problem solving and exercises]	4
Analysis of articles and reviews [AUTÓNOMA][Case Studies]	1
Final test [PRESENCIAL][Work with simulators]	.8
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	.2
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	1

Global activity

Activities	**hours**

Analysis of articles and reviews [AUTÓNOMA][Case Studies]	6
Practicum and practical activities report writing or preparation [AUTÓNOMA][Self-study]	40
Class Attendance (theory) [PRESENCIAL][Lectures]	29
Final test [PRESENCIAL][Work with simulators]	5
Study and Exam Preparation [AUTÓNOMA][Problem solving and exercises]	60
Group tutoring sessions [PRESENCIAL][Group tutoring sessions]	8.4
Total horas:	148.4

10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
J.L Calais	Quantum Chemistry Workbook: Basic Concepts and Procedures in the Theory of the Electronic Structure of Matter	John wiley$Sons	INC	978-0471594352	1994	The QuantumChemistry Workbook is a step-by-step study guide to the innerworkings of nature's fundamental systems: free atoms, smallmolecules, polymers, and crystals.
J.B. Foresman and A. Frisch	Exploring Chemistry With Electronic Structure Methods: A Guide to Using Gaussian	Gaussian Inc	Pittsburgh	978-1935522034	2014	This book will teach you how to use electronic structure calculations to investigate chemical problems. It uses the Gaussian software
Christopher Cramer	Essential of Computational Chemistry	John wiley$Sons	NY	ISBN: 978-0-470-0918	2004	This book provides a balanced introduction to this dynamic subject. Suitable for both experimentalists and theoreticians, a wide range of samples and applications drawn from all key areas are included. The book carefully guides the reader through the necessary equations, providing explanations of information and reasoning where necessary and firmly placing each equation in context.
	https://www.wiley.com/en-us/Essentials+of+Computational+Chemistry%3A+Theories+and+Models%2C+2nd+Edition-p-9780470091821#:~:text=Essentials%20of%20Computational%20Chemistry%20provides,drawn%20from%20all%20key%20areas.					
F. Jensen	Introduction to Computational Chemistry	John wiley$Sons	NY	978-1118825990	2017	Introduction to Computational Chemistry 3rd Edition provides a comprehensive account of the fundamental principles underlying different computational methods. Fully revised and updated throughout to reflect important method developments and improvements since publication of the previous edition, this timely update includes the following significant revisions and new topics: * Polarizable force fields * Tight-binding DFT * More extensive DFT functionals, excited states and time dependent molecular properties * Accelerated Molecular Dynamics methods * Tensor decomposition methods * Cluster analysis * Reduced scaling and reduced prefactor methods
	https://www.wiley.com/en-us/Introduction+to+Computational+Chemistry%2C+3rd+Edition-p-9781118825990					
I.N Levine	Química Cuántica	Prentice Hall		84-205-3096-4	2001	Clear and precise concepts of the computational methods.
S. M. Bachrach,	Computational Organic Chemistry. 2nd ed.;	John Wiley & Sons	Weinheim, Germany	978-1-118-29192-4	2014	
J. Bertrán et al.	Química Cuántica	Síntesis	Madrid	8477387427 / 9788477	2002	This book represents an effort to integrate the fundamentals of Quantum Mechanics, its chemical applications and computational practice, in a balanced, concise and didactic way. Special emphasis is placed on the axiomatic development of Quantum Mechanics and on the necessary simplifications to be able to apply it to real chemical systems.