COURSE DESCRIPTION

COURSE DETAILS

Title (of the course): **QUÍMICA COMPUTACIONAL APLICADA**
Code: 100477
Degree/Master: **GRADO DE QUÍMICA** Year: 4
Name of the module to which it belongs: APLICADO
Field: QUÍMICA (OPTATIVA 3)
Character: OPTATIVA Duration: SECOND TERM
ECTS Credits: 3.0 Classroom hours: 30
Face-to-face classroom percentage: 40.0% Study hours: 45
Online platform: http://www3.uco.es/amoodle

LECTURER INFORMATION

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PREREQUISITES AND RECOMMENDATIONS

Prerequisites established in the study plan

The student must have approved the block of 60 credits corresponding to the basic subjects and at least 30 credits of compulsory subjects.

Recommendations

None specified

COURSE DESCRIPTION

INTENDED LEARNING OUTCOMES

CB3	written and oral communication in the native language
CB5	The capacity for data management and to generate information / understanding
CB10	Ability to study independently for continued professional development.
CE6	Principles of quantum mechanics and its place in the description of the structure and properties of atoms and molecules.
CE21	The ability to show knowledge and understanding of the essential facts, concepts, principles, and theories relating to chemistry
CE22	The ability to apply knowledge to solve qualitative and quantitative problems according to previously developed models
CE26	To gain skills in managing and processing chemical data and information.
CE31	interpretation of data from previous observations and measurements in the laboratory in terms of their significance and the theories that support them
CU2	To understand and improve basic IT skills

OBJECTIVES

To get knowledge about the main principles of Computational Chemistry and the different calculation methods and its applications in the prediction of the physico-chemical properties of the molecules plus the design of new compounds with predefined properties.

CONTENT

1. Theory contents

1. Theory contents Lesson 1. An Outline of What Computational Chemistry Is All About. 1.1 What You Can Do with Computational Chemistry. 1.2 The Tools of Computational Chemistry. 1.3 Putting It All Together. 1.4 The Philosophy of Computational Chemistry. 1.5. The Development of Quantum Mechanics. The Schrödinger Equation. 1.5.1 The Origins of Quantum Theory: Blackbody Radiation and the Photoelectric Effect. 1.5.2 Radioactivity. 1.5.3 Relativity. 1.5.4 The Nuclear Atom. 1.5.5 The Bohr Atom.

Lesson 2. Molecular Mechanics. 2.1. Perspective. 2.2 The Basic Principles of Molecular Mechanics. 2.2.1 Developing a Forcefield. 2.2.2 Parameterizing a Forcefield. 2.2.3 A Calculation Using Our Forcefield. 2.3 Examples of the Use of Molecular Mechanics

Lesson 3. Introduction to Quantum Mechanics in Computational Chemistry. 3.1 The Simple Hückel Method – Theory. 3.2 The Simple Hückel Method – Applications. 3.3 Strengths and Weaknesses of the Simple Hückel Method. 3.4 The Extended Hückel Method – Theory. 3.5 An Illustration of the EHM: the Protonated Helium Molecule. 3.6 The Extended Hückel Method – Applications. 3.7 Strengths and Weaknesses of the Extended Hückel Method

Lesson 4. Ab initio Calculations. 4.1 The Basic Principles of the Ab initio Method. 4.1.1 Preliminaries. 4.1.2 The Hartree SCF Method. 4.1.3 The Hartree–Fock Equations. 4.2 Basis Sets. 4.2.1 Introduction. 4.2.2 Gaussian Functions; Basis Set Preliminaries; Direct SCF. 4.2.3 Types of Basis Sets and Their Uses

Lesson 5. Semiempirical Calculations. 5.1 Perspective. 5.2 The Basic Principles of SCF Semiempirical Methods. 5.2.1 Preliminaries. 5.2.2 The Pariser-Parr-Pople (PPP) Method. 5.2.3 The Complete Neglect of Differential Overlap (CNDO) Method. 5.2.4 The Intermediate Neglect of Differential Overlap (INDO) Method. 5.2.5 The Neglect of Diatomic Differential Overlap (NDDO) Methods.

Lesson 6. Density Functional Calculations. 6.1 Perspective. 6.2 The Basic Principles of Density Functional Theory. 6.2.1 Preliminaries. 6.2.2 Forerunners to Current DFT Methods. 6.2.3 Current DFT Methods: The Kohn– Sham Approach

COURSE DESCRIPTION

2. Practical contents

Molecular mechanics calculations. Semi-empirical calculations. Ab initio calculations. Geometric optimization calculations. Molecular dynamics calculations. Quantitative structure-activity relationships. Determination of QSAR parameters

SUSTAINABLE DEVELOPMENT GOALS RELATED TO THE CONTENT

Quality education

METHODOLOGY

General clarifications on the methodology (optional)

Seminars will take place at the computers classroom. Attendance to lectures and seminars is mandatory

Methodological adaptations for part-time students and students with disabilities and special educational needs

Part-time students will be interviewed in each individual case. The modifications in the methodology will be designed to better match each situation.

Face-to-face activities

Activity	Large group	Medium group	Total
Assessment activities	3	-	3
Lectures	14	-	14
Seminar	-	13	13
Total hours:	***17***	***13***	***30***

Off-site activities

Activity	Total
Exercises	10
Self-study	35
Total hours	***45***

WORK MATERIALS FOR STUDENTS

Exercises and activities - *http://moodle.uco.es/moodlemap/*
Lessons summary - *http://moodle.uco.es/moodlemap/*
Placement booklet - *http://moodle.uco.es/moodlemap/*

COURSE DESCRIPTION

EVALUATION

Intended learning	Case study/clinical case discussion/scientific work discussion	Problem solving	Real and/or simulated tasks
CB10	X	X	X
CB3		X	X
CB5	X	X	X
CE21	X		
CE22	X	X	X
CE26	X	X	
CE31	X	X	
CE6	X	X	X
CU2	X	X	X
Total (100%)	***30%***	***40%***	***30%***
Minimum grade	***4***	***4***	***4***

(*)Minimum mark (out of 10) needed for the assessment tool to be weighted in the course final mark. In any case, final mark must be 5,0 or higher to pass the course.

Method of assessment of attendance:

Attendance to the lecture is mandatory

General clarifications on instruments for evaluation:

Software will be provided by the person in charge. The final exam represents 30% of the final grade. During the seminars the students will have to solve different exercises related to the computer lab, which represents 40% of the grade, they must also complete questionnaires about each theoretical lesson, which represents another 30% of the final grade.

Clarifications on the methodology for part-time students and students with disabilities and special educational needs:

The adaptations of the didactic methodology for part-time students, students with disabilities and special educational needs, will be specified once the cause of this group is known.

Clarifications on the evaluation of the first extraordinary call and extra-ordinary call for completion studies:

Depending on each case, the same criteria will be applied as those applied during the last ordinary call taken by the student, maintaining the percentages of each evaluation criterion: Real and/or simulated tasks (30%), computer exercises (40%) and questions (30%)

COURSE DESCRIPTION

Qualifying criteria for obtaining honors:

Average qualification equal to or greater than 9. The MH number will depend on the students numbers, in accordance with the UCO regulations

BIBLIOGRAPHY

1. Basic Bibliography

Computational Chemistry. E. G. Lewars. Ed: Springer. 2011, 2ª ed.
Computational Medical Chemistry for Drug Discovery. P. Bultink (Ed.) Ed: Marcel Dekker. 2004
Theoretical and Computational Chemsitry. Juan Andrés y Juan Beltran. Editorial: Universitat Jaume I. 2000
Physical Chemistry. Atkins y de Paula. Ed. Panamericana, 2008. 8ª Edición
Physical Chemistry. Thomas Engel y Philip Reid. Ed. Pearson Addison Wesley. 2006.
Physical Chemistry. J. Bertrán, J. Núñez, Ed. Ariel Ciencia, 2002

2. Further reading

None

COORDINATION CRITERIA

Tasks deadlines
Tasks performance

SCHEDULE

Period	Assessment activities	Lectures	Seminar
1# Fortnight	0,0	4,0	0,0
2# Fortnight	0,0	4,0	4,0
3# Fortnight	0,0	4,0	6,0
4# Fortnight	0,0	2,0	3,0
5# Fortnight	3,0	0,0	0,0
Total hours:	***3,0***	***14,0***	***13,0***

The methodological strategies and the evaluation system contemplated in this Course Description will be adapted according to the needs presented by students with disabilities and special educational needs in the cases that are required.

CONTINGENCY PLAN: CASE SCENARIO A

Case scenario A will correspond to a diminished on-site academic activity due to social distancing measures affecting the permitted capacity of classrooms.

COURSE DESCRIPTION

METHODOLOGY

General clarifications on the methodology on case scenario A

A multimodal (hybrid) teaching system will be adopted, combining both on-site and remote classes via videoconference (synchronous) that will be held in the timetable approved by the corresponding Faculty or School. The time distribution of teaching activities (both on-site and remote) will be decided by the aforementioned Faculties and Schools bearing in mind the permitted capacity of classrooms and social distancing measures as established at that time.

Seminars will take place at the computers classroom. Attendance to lectures and seminars is mandatory

EVALUATION

Intended learnig	Case study/clinical case discussion/scientific work discussion	Problem solving	Real and/or simulated tasks
CB10	X	X	X
CB3		X	X
CB5	X	X	X
CE21	X	X	X
CE22	X		X
CE26	X	X	
CE31	X	X	
CE6	X	X	X
CU2	X	X	X
Total (100%)	***30%***	***40%***	***30%***
Minimum grade	***4***	***4***	***4***

(*)Minimum mark (out of 10) needed for the assessment tool to be weighted in the course final mark. In any case, final mark must be 5,0 or higher to pass the course.

Method of assessment of attendance (Scenario A):

Attendance to the lecture is mandatory

General clarifications on instruments for evaluation (Scenario A):

Software will be provided by the person in charge. The final exam represents 30% of the final grade. During the seminars the students will have to solve different exercises related to the computer lab, which represents 40% of the grade, they must also complete questionnaires about each theoretical lesson, which represents another 30% of the final grade.

COURSE DESCRIPTION

Clarifications on the methodology for part-time students and students with disabilities and special educational needs (Scenario A):

The adaptations of the didactic methodology for part-time students, students with disabilities and special educational needs, will be specified once the cause of this group is known.

CONTINGENCY PLAN: CASE SCENARIO B

Case scenario B will bring about a suspension of all on-site academic activities as a consequence of health measures.

METHODOLOGY

General clarifications on the methodology on case scenario B

On-site teaching activities will be held via videoconference (synchronous) in the timetable approved by the corresponding Faculty or School. Alternative activities will be proposed for reduced groups in order to guarantee the acquisition of course competences.

Seminars will take place at the computers classroom. Attendance to lectures and seminars is mandatory

EVALUATION

Intended learnig	Case study/clinical case discussion/scientific work discussion	Problem solving	Real and/or simulated tasks
CB10	X	X	X
CB3		X	X
CB5	X	X	X
CE21	X	X	
CE22	X		X
CE26	X	X	
CE31	X	X	X
CE6	X	X	X
CU2	X	X	X
Total (100%)	***30%***	***40%***	***30%***
Minimum grade	***4***	***4***	***4***

(*)Minimum mark (out of 10) needed for the assessment tool to be weighted in the course final mark. In any case, final mark must be 5,0 or higher to pass the course.

COURSE DESCRIPTION

Moodle Tools	Case study/clinical case discussion/scientific work discussion	Problem solving	Real and/or simulated tasks
Attendance	X	X	X
Forum	X	X	X
Workshops	X	X	X

Method of assessment of attendance (Scenario B):

Attendance to the lecture is mandatory

General clarifications on instruments for evaluation (Scenario B):

Software will be provided by the person in charge. The final exam represents 30% of the final grade. During the seminars the students will have to solve different exercises related to the computer lab, which represents 40% of the grade, they must also complete questionnaires about each theoretical lesson, which represents another 30% of the final grade.

Clarifications on the methodology for part-time students and students with disabilities and special educational needs (Scenario B):

The adaptations of the didactic methodology for part-time students, students with disabilities and special educational needs, will be specified once the cause of this group is known.