COURSE DATA

Data Subject	
Code	36463
Name	Computational Chemistry
Cycle	Grade
ECTS Credits	6.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Faculty of Chemistry	4	First term

Subject-matter

Degree	Subject-matter	Character
1110 - Degree in Chemistry	15 - Physical Chemistry Applied	Optional

Coordination

Name	Department
TUÑON GARCIA DE VICUÑA, IGNACIO NILO	315 - Physical Chemistry

SUMMARY

DESCRIPTORS: Theoretical models and computational simulation. Molecular mechanics. Molecular dynamics. Quantum chemistry. Calculation of properties. Applications.

Together with the Theory and the Experiment, the Simulation (modelling) is the third pillar of the scientific knowledge. Since the decade of the 90, the evolution of computing has allowed the useful and effective incorporation of the modelling in the Chemical surroundings: The Computational Chemistry.

Computational Chemistry is an area of multidisciplinary knowledge, where different areas such as computer and documentation, mathematics (optimisation, algebra of operators, calculation, differential equations, etc.) physics and chemical-physical, quantum chemistry, biochemistry, organic, inorganic and analytical chemistry, and even engineering, converge. It pretends, then, to give a global vision of the Chemistry from the perspective of modelling as the backbone of all the knowledge acquired during the studies.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

General Chemistry I & III, Mathematics I & II, Computational Tools in Chemistry, Physical Chemistry I & II, Inorganic Chemistry III, Biochemistry, Organic Chemistry III.
Those given in the prerequisite matters, especially those obtained such as foundations of mathematics, statistics, optimisation, quantum mechanics and spectroscopy.

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

1110 - Degree in Chemistry

- Develop capacity for analysis, synthesis and critical thinking.
- Show inductive and deductive reasoning ability.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.
- Demonstrate knowledge of the characteristics and behaviour of the different states of matter and the theories used to describe them.
- Demonstrate knowledge of the principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules.
- Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry.
- Solve qualitative and quantitative problems following previously developed models.
- Interpret data from observations and measurements in the laboratory in terms of their significance and the theories that underpin them.
- Relate theory and experimentation.
- Recognise and evaluate chemical processes in daily life.
- Understand the qualitative and quantitative aspects of chemical problems.
- Relate chemistry with other disciplines.

- Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration.
- Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences.
- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.
- Have basic skills in the use of information and communication technology and properly manage the information obtained.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

The previous section includes the competences contained in the document VERIFICA. This subject addresses part of the learning results of the matter Computational Chemistry that allow to acquire specific knowledge of chemistry, cognitive skills and general skills recommended by the EUROPEAN CHEMISTRY THEMATIC NETWORK (ECTN) for the Chemistry Eurobachelor® Label. The following table lists the learning outcomes acquired in the subject Computational Chemistry related to the competences of the degree in Chemistry.

SPECIFIC KNOWLEDGE OF CHEMISTRY	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Computational Chemistry **that contemplate the learning outcomes EUROBACHELOR®**
The characteristics of the different states of matter and the theories used to describe them.	Demonstrate knowledge of the characteristics and behaviour of the different states of matter and the theories used to describe them..(CE3).
The principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules	Demonstrate knowledge of the principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules..(CE5).

COMPETENCES AND COGNITIVE SKILLS	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Computational Chemistry **that contemplate the learning outcomes EUROBACHELOR®**
Ability to demonstrate knowledge and understanding of the facts, concepts, principles and fundamental theories related to the topics mentioned above.	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry..(CE13).
Ability to apply this knowledge and understanding to the solution of common qualitative and quantitative problems.	Solve qualitative and quantitative problems following previously developed models..(CE14). Recognise and analyse new problems and plan strategies to solve them..(CE15). Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Competences to present and argue scientific issues orally and in writing to a specialized audience.	Relate chemistry with other disciplines.(CE26). Prepare reports, surveys and industrial and environmental projects in the field of chemistry..(CE27). Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate. (CG6). Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences..(CB4).
Ability to calculate and process data, related to information and chemistry data.	Solve qualitative and quantitative problems following previously developed models..(CE14). Recognise and analyse new problems and plan strategies to solve them..(CE15).

COMPETENCES AND COGNITIVE SKILLS RELATED TO THE PRACTICE OF CHEMISTRY	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Computational Chemistry **that contemplate the learning outcomes EUROBACHELOR®**
Ability to interpret data derived from observations and laboratory measurements in terms of their relevance, and relate them to the appropriate theory.	Interpret data from observations and measurements in the laboratory in terms of their significance and the theories that underpin them..(CE20). Relate theory and experimentation..(CE22). Recognise and evaluate chemical processes in daily life..(CE23). Understand the qualitative and quantitative aspects of chemical problems..(CE24). Relate chemistry with other disciplines.(CE26).
GENERAL COMPETENCES	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Computational Chemistry **that contemplate the learning outcomes EUROBACHELOR®**
Ability to apply practical knowledge to solve problems related to qualitative and quantitative information.	Solve problems effectively..(CG4). Solve qualitative and quantitative problems following previously developed models..(CE14). Relate theory and experimentation..(CE22). Recognise and evaluate chemical processes in daily life..(CE23). Understand the qualitative and quantitative aspects of

	chemical problems..(CE24).
Calculation and arithmetic capabilities, including aspects such as analysis error, estimates of orders of magnitude, and correct use of the units.	Develop capacity for analysis, synthesis and critical thinking.. (CG1). Show inductive and deductive reasoning ability..(CG2). Solve problems effectively..CG4).
Competences in information management, in relation to primary and secondary sources, including information retrieval through on-line searches.	Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate..(CG6). Have basic skills in the use of information and communication technology and properly manage the information obtained.(CT2).
Ability to analyse materials and synthesize concepts.	Develop capacity for analysis, synthesis and critical thinking.. (CG1). Show inductive and deductive reasoning ability..(CG2). Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration..(CB3).
Ability to adapt to new situations and make decisions.	Demonstrate the ability to adapt to new situations..(CG9). Recognise and analyse new problems and plan strategies to solve them..(CE15). Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration..(CB3).
Skills related to information technology such as word processing, spreadsheet, recording and storage of data, internet use related to the subjects.	Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate..(CG6). Have basic skills in the use of information and

	communication technology and properly manage the information obtained.(CT2).
Competences in oral and written communication, in one of the main European languages, in addition to the language of the country of origin.	Demonstrate ability to work in teams both in interdisciplinary teams and in an international context..(CG5). Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional. (CG7). Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community. (CT1). Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences..(CB4). Have basic skills in the use of information and communication technology and properly manage the information obtained.(CT2).
Study skills necessary for professional development. These will include the ability to work autonomously.	Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation..(CG3). Demonstrate ability to work in teams both in interdisciplinary teams and in an international context..(CG5). Learn autonomously.(CG8). Demonstrate the ability to adapt to new situations..(CG9). Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.(CB5).

These learning outcomes, once the subject Computational Chemistry has been completed, should allow the student to:

1. - Demonstrate the ability to distinguish the domains of application of the various theories, methods and models of Chemistry.

2. - Demonstrate the ability to select the appropriate method to the type of chemical problem and know the expected errors.

3. - Demonstrate ability to recognize chemical-physical effects that are taken into account and are required in the calculations and simulations of chemical compounds and reactions.

4. - Demonstrate current knowledge of the status of applications (Software) for the calculation and simulation of wide use in Computational Chemistry and its main "target problems”.

5. - Demonstrate ability to generate computational information (input, common formats in Computational Chemistry applications…) from chemical data (empirical, molecular or structural formulas, molecular symmetry…).

6. - Demonstrate ability to perform basic computer simulations of molecular structures, molecular properties and chemical reactions in the gas phase.

7. - Demonstrate ability to perform basic computer simulations of infinite systems, condensed media or biological environments.

8. - Demonstrate ability to analyse and assess the results of the computer simulations.

DESCRIPTION OF CONTENTS

1. Hands-on calculation environment

4,5 hours of explanation and practical work

Computational Chemistry
- Computer work environment: Linux
- Molecular Potential Energy
- Molecular geometry specification: Z- matrix
- Gaussian input
- Gaussview & ChemOffice

2. Seminar on Hartree-Fock (I)

1 Seminar session of 1,5 hours

Hartree-Fock (HF) Equations
- Molecular Hamiltonian
- Poly-electron and mono-electron functions
- Molecular energy: Core Integrals, Coulomb Integrals and exchange Integrals
- Slater rules
- Coulomb and exchange operators
- Optimal spin-orbitals: Brillouin Theorem

Fock operator: HF ecuations
Canonical HF equations

3. Seminar on Hartree-Fock (II)

1 Seminar session of 1,5 hours

Physical interpretation of the solutions of the HF equations
Core integrals, Coulomb integrals and exchange integrals
Occupied and virtual orbitals
Orbital energy and molecular energy
Koopmans theorem

4. Seminar on Hartree-Fock (III)

1 Seminar session of 1,5 hours

Restricted HF for closed shell systems: Roothaan equations
Closed shell HF: Restricted Spin-Orbitals
Introducing a basis set: Roothaan Equations
Charge density
Fock matrix expression
Basis set orthogonalization
SCF procedure
Expectation Values and population analysis

5. Seminar on Hartree-Fock (IV)

1 Seminar session of 1,5 hours

Unrestricted HF for open shell systems: Pople-Nesbet equations
Open shell HF: Unrestricted Spin-Orbitals
Basis set introduction: Pople-Nesbet equations
Unrestricted density matrices
Expression of the Fock matrices
Solution of the unrestricted SCF equations
The dissociation problem and its unrestricted solution: H2 molecule as an example

6. Seminar on optimization of molecular geometries

1 Seminar session of 1,5 hours

Molecular optimization
Minimum energy structures
Optimizing a function: methods
Stationary structures

7. Seminar on density functional theory

1 Seminar session of 1,5 hours

Density functional theory
Basic principles of the density functional theory (DFT)
Kohn-Sham approximation
DFT applications
DFT strengths and weaknesses

8. Fundamentals of Reactivity

1 Seminar session of 1,5 hours

Chemical reactivity
Potential Energy Surfaces
Stationary Structures
Minimum Energy Path
Transition State Theory

9. Semempirical methods

1 Seminar session of 1 hour

Semiempirical Molecular Orbital Methods
Aproximation of the Hartree-Fock integrals
Classification Extended Hückel, Zero Differential Overlap (ZDO) and Neglect of Differential Diatomic Overlap (NDDO)
Theory and use of the parametrizations Austin Model (AM1) and the Parametric Models number 3 (PM3) and number 6 (PM6)

10. Post-HF methods (I)

1 Seminar session of 1,5 hours

Electron correlation
Electron correlation
Formal properties of the methods:
- o Extensivity
- o Size-consistency
- o N-dependency

The role of the double and singly excited configurations in the wavefunction
Rayleigh-Schrodinger perturbation theory
Many body perturbation theory (MBPT)

11. Post-HF methods (II)

1 Seminar session of 1,5 hours

Calculation methods of the electron correlation
MP2 and MP4 Moller-Plesset methods
Excitation degree and perturbation order
Configuration interaction. The size-consistency problem
Coupled Cluster theory

12. Molecular Mechanics and continuum models

1 Seminar session of 1,5 hours

Molecular Mechanics
Justification of the molecular mechanics (MM)
Energy terms
Force field parameterization and examples
Continuum models: energetic terms and calculation

13. Molecular Dynamics

1 Seminar session of 1,5 hours

Molecular Dynamics
Justification of the simulation methods
System definition: boundary conditions
Molecular Dynamics

14. Energy and electron structure

Practical work in the computer lab of 4,5 hours

Ionization Energies and electron affinities of atoms
Dissociation curves: HCl and HH
Visualization of the electron density and molecular orbitals
Concepts: HF calculation and basis functions

15. Molecular structure optimization

Practical work in the computer lab of 6 hours

Function optimization: methods
Stationary structures. Classification
HF structure optimization. Basis set effect
Density functional methods
Optimization with DFT methods
Potential energy curves
Stationary structures

16. Chemical reactivity

Practical work in the computer lab of 3 hours

Potential Energy Surface (PES)
Transition state
Minimum energy path
Transition State Theory
PES Calculation for the F- + CH3Cl chemical reaction
Calculation of the rate constant
Direct localization of transition states

17. Semiempirical calculations

Practical work in the computer lab of 2 hours

Semiempirical methods vs Hartree-Fock/post-Hartree-Fock
Comparison of geometries and stability of molecules of increasing size
Conceptes: accuracy criteria of quantum chemistry methods

18. Spectroscopic calculations

Practical work in the computer lab of 3 hours

Rotational, vibrational and electron spectroscopy
Normal modes
Thermochemistry

Concepts: transitions between energy levels. Partition functions, thermodynamic properties

19. Solvent effects on chemical processes

Practical work in the computer lab of 4,5 hours

Discrete and continuous models
Effect of the solvent on the tautomer equilibrium
Effect of the solvent on the conformational equilibrium
Effect of the solvent on the chemical reactivity

Concepts: intermolecular interactions

20. Molecular Dynamics Calculations

Practical work in the computer lab of 4,5 hours

Introduction to the description of large systems
Force fields. The water case
Molecular Dynamics of the liquid water. Radial distribution function and coordination number
MD of aqueous solutions. Diffusion coefficient
MD of biomolecules. Protein folding

Concepts: configuration space

21. Applications

2 sessions in the computer lab of 2 hours each

Development of two small projects where the students apply the concepts and methods that have been explained in the course contents as a whole.

WORKLOAD

ACTIVITY	Hours	% To be attended
Computer classroom practice	48,00	100
Tutorials	12,00	100
Development of individual work	20,00	0
Study and independent work	35,00	0
Preparation of evaluation activities	10,00	0
Preparing lectures	15,00	0
Preparation of practical classes and problem	10,00	0
TOTAL	**150,00**	

TEACHING METHODOLOGY

Practical sessions in the computer room: Includes seven practical sessions of 3-6 hour long each. They consist of a first part, in which the teacher summarizes the fundamentals and techniques necessary for the implementation of the practice. In a second part, the student carries out the practice development using appropriate software packages. They correspond to thematic units from UT14 to UT20.

The conclusion of the practice is to finish the calculations and write a brief report of the results that must be delivered within a maximum of one week. The average dedication by the student is approximately 2 hours of autonomous work, per session.

In order that the students have, for independent work, exactly the same set of programs used in the computer room, the exercises will be made using a virtual disk that contains the operating system and all necessary calculation programs in the course, and the students will have a copy of that.

Seminars: They consist of 13 sessions of 1 or 1.5 hours, as a seminar, where the fundamental concepts of Computational Chemistry will be presented, emphasizing the most important aspects for the application of the methods of calculation. They correspond to thematic units UT1 to UT13.

Personalized Practical work: In the last two practice sessions in the computer lab, students will have to develop one small calculation project using all the course concepts and methods. It is expected that the student will end independently the practical work of each session, using about 4 hours, the remaining being autonomous work. The conclusion of the project is to finish the calculations and draft a report of the results that must be defended orally. They correspond to the thematic unity UT21.

EVALUATION

For assessment of the Computational Chemistry course it will be taken into account:

- Final exam: test based in the completion of a project: a written report must be handled in and defended orally (60%)

- Assessment of the participation in oral presentations (10%)

- Assessment of the reports corresponding to the practical sessions (20%)

Continuous assessment of each student, based on regular attendance at school and classroom activities, participation and degree of involvement in the teaching-learning process (10%)

REFERENCES

Basic

- CRAMER, C.J. Essentials of Computational Chemistry. Theories and Models. Wiley, 2004.
- LEWARS, E.G. Computational Chemistry. Introduction to Theory and Applications of Molecular and Quantum Mechanics. 2ª Ed. Springer, 2011
- JENSEN, F. Introduction to Computational Chemistry. Wiley, 1999.

Additional

- BERTRÁN RUSCA, J., BRACHANDELL GALLO, V., MORENO FERRER, M., SODUPE FERRER, M. Química Cuántica: fundamentos y aplicaciones computacionales. Síntesis. Madrid, 2000
- LEVINE, I.N. Química Cuántica. 5a ed. Prentice Hall, 2001.
- SZABO, A., OSTLUND, N.S. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory. Dover, 1996