COURSE DATA

DATA SUBJECT

Code: 36463
Name: Computational Chemistry
Cycle: Undergraduate Studies
ECTS Credits: 6
Academic year: 2025-26

STUDY (S)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Facultat de Química	4	First quarter

SUBJECT-MATTER

Degree	Subject-matter	Character
1110 - Degree in Chemistry	Physical Chemistry Applied	ELECTIVES

COORDINATION

TUÑON GARCIA DE VICUÑA IGNACIO NILO

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 / LEARNING OUTCOMES

1110 - Degree in Chemistry

Apply metrology in chemical processes, including quality management.

At the end of the course, the student will interpret the data from observations and measurements in the laboratory in terms of their significance and the theories that support them.

At the end of the subject, the student will evaluate, interpret and synthesize the chemical data and information correctly.

Collaborate effectively in work teams, assume responsibilities and leadership roles, and contribute to collective improvement and development.

Communicate effectively both orally and in writing, adapting to the context and audience.

Comprender la empresa como una realidad sistémica e inherentemente compleja, reconociendo e identificando las dimensiones consustanciales a los sistemas de gestión empresarial y los condicionantes, externos e internos, que inciden sobre su gestión.
Ser capaces de categorizar y jerarquizar las decisiones organizativas, e interpretar los procesos de adopción de decisiones en el ámbito de los modelos teóricos. Discriminar y manejar los principales métodos y técnicas disponibles para la elaboración del diagnóstico estratégico. Poder elaborar un diagnóstico estratégico básico.

Comprender las particularidades contables que presenta la regulación jurídico-mercantil de las empresas, relacionando la legislación mercantil aplicable a los distintos tipos operaciones societarias con la contabilidad de los hechos económicos que se regulan. Aprender a relacionar las leyes mercantiles que se ocupan de los concursos de acreedores con la contabilidad, adquiriendo práctica en el manejo de determinados textos legales vigentes.

Contribute to the design, development and implementation of solutions that respond to social demands, using the Sustainable Development Goals as a reference.

Demonstrate both inductive and deductive reasoning skills.

Demonstrate critical and self-critical thinking, considering professional ethics, moral values and social implications of the different activities carried out throughout the degree.

Demonstrate the ability to analyse, synthesise and reason critically.

Describe the characteristics and behaviour of the different states of matter and the theories used to explain them.

Distinguish between the qualitative and quantitative aspects of chemical problems.

Evaluate the risks involved in the use of chemical substances and laboratory procedures.

Express ideas correctly, both orally and in writing, in any of the official languages of the Valencian Community.

Handle the instrumentation used in the different areas of chemistry.

Identify chemical processes in everyday life.

Identify the main types of chemical reactions and their associated key characteristics.

Identify the structure and reactivity of the main classes of biomolecules and the chemistry of key biological processes.

Implement sustainable and environmentally friendly methodologies.

List the principles of quantum mechanics and apply them to the description of the structure and properties of atoms and molecules.

Relate chemistry to other disciplines.

Relate theory to experimentation.

Ser capaces de analizar la influencia que sobre el diseño del sistema de información de costes, ejercen, tanto la actividad concreta desarrollada por la entidad como la tecnología utilizada, la estructura organizativa y el estilo de dirección. Calcular costes preestablecidos y relacionarlos con la planificación y el control de la actividad interna. Seleccionar aquellos indicadores de gestión que faciliten el desempeño personal, estableciendo la frecuencia y el formato en función del usuario de destino.

Ser capaces de configurar y manejar un sistema integrado para la gestión contable de la empresa. Utilizar la hoja de cálculo como herramienta de análisis de la información económica de la empresa. Saber aplicar programas de apoyo a tareas específicas de gestión.

Solve problems effectively.

Understand and analyse, from the perspective of the degree programme, social inequalities based on sex and gender; integrate gender-sensitive approaches into problem-solving and solution design.

Use chemical terminology, nomenclature, conventions and units correctly.

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
- Koopman¿s 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

PRESENCIAL ACTIVITIES

Activity	Hours
Tutorials	12,00
Computer classroom practice	48,00
Total hours	**60,00**

NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	0,00
Individual or group project	20,00
Independent study and work	35,00
Preparation of lessons	25,00
Preparation for assessment activities	10,00
Resolution of case studies	0,00
Total hours	**90,00**

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%)

Final warning

Copying or plagiarism of any assignment that is part of the evaluation will make it impossible to pass the course, and the student will be subject to the appropriate disciplinary procedures.

Please note that, according to Article 13 d) of the University Student Statute (RD 1791/2010, December 30), "*it is the duty of a student to refrain from using or cooperating in fraudulent procedures in evaluation tests, in the work performed or in official University documents*".

REFERENCES

- 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.
- 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