UAB
Universitat Autònoma de Barcelona

Quantum Chemistry

Code: 102503
ECTS Credits: 6

2024/2025

Degree	Type	Year
2502444 Chemistry	OB	2

Contact

Name: Ricard Gelabert Peiri

Email: ricard.gelabert@uab.cat

Teachers

Ricard Gelabert Peiri

Miquel Moreno Ferrer

Teaching groups languages

You can view this information at the end of this document.

Prerequisites

It is compulsory to have passed the first-year subject "Fonaments de Química" (Foundations of Chemistry). It is highly advisable that students taking this subject have also passed the first-year subjects "Matemàtiques" (Math) and "Física" (Physics). Students who have failed these subjects and take "Química Quàntica" (Quantum Chemistry) will run into difficulties that can hinder their progress through this subject.

Objectives and Contextualisation

Chemistry studies matter, its properties, transformations and its interaction with electromagnetic radiation. Because the basic building blocks of matter (electrons and atomic nuclei) do not obey classical mechanics but the less intuitive quantum mechanics, it is a must to apply rigorously its principles to derive the laws governing matter, its structure, the bond types and its transformations, and see its consequences at macroscopic level. This is the aim of quantum chemistry as a discipline within a modern concept of chemistry.

As a subject, its primary goal is that students develop the habit of thinking about chemistry using quantum mechanics concepts in a correct manner and to draw consequences. A second goal is that students develop a rigorous explanation of the basic principles of chemistry, which they have often been using in a mechanical way in introductory courses of chemistry (especially those related to chemical bond). Third, students have to develop abilities to use mathematical tools to solve problems related to atomic and molecular structure. Related to the latter, it is important to familiarize the student with the use of computer tools in the field of quantum chemistry, such that it is adopted as yet another tool in the study of matter and its properties.

Competences

- Adapt to new situations.
- Be ethically committed.
- Communicate orally and in writing in one's own language.
- Have numerical calculation skills.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Manage, analyse and synthesise information.
- Obtain information, including by digital means.
- Operate with a certain degree of autonomy and integrate quickly in the work setting.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse chemical problems and propose suitable answers or studies to resolve them.
- Resolve problems and make decisions.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.
- Show initiative and an enterprising spirit.
- Show motivation for quality.
- Use IT to treat and present information.
- Use the English language properly in the field of chemistry.

Learning Outcomes

1. Adapt to new situations.
2. Be ethically committed.
3. Communicate orally and in writing in one's own language.
4. Describe the principles of quantum mechanics and recognise their application to the description of the structure and properties of atoms and molecules.
5. Have numerical calculation skills.
6. Identify and analyse problems related with the structure of molecules.
7. Learn autonomously.
8. Manage the organisation and planning of tasks.
9. Manage, analyse and synthesise information.
10. Obtain information, including by digital means.
11. Operate with a certain degree of autonomy and integrate quickly in the work setting.
12. Propose creative ideas and solutions.
13. Reason in a critical manner
14. Resolve problems and make decisions.
15. Show initiative and an enterprising spirit.
16. Show motivation for quality.
17. Summarise a scientific text related with the subject in the English language
18. Use IT to treat and present information.

Content

Theory Lectures

- Part 1: Foundations of Quantum Mechanics. History background. Mathematical basis. Postulates of quantum mechanics. Heisenberg's uncertainty principle. Model systems: particle in a box, harmonic oscillator.

- Part 2: Atomic Structure. Angular momentum. Hydrogen atom. Spin. Many-electron atoms. Antisymmetry principle. Slater determinants. Exclusion principle. Approximate methods: variational method. Aufbau principle. Periodic table.

- Part 3: Molecular Structure. The molecular Hamiltonian. The Born-Oppenheimer approximation. The H_2^+ molecule. The MO-LCAO approximation. The H_2 molecule. Qualitative studies: diatomic and poliatomic molecules.

- Part 4: Theoretical and Computational Chemistry. Determination of Electronic Structure. The Hartree-Fock method. Basis sets. Electron correlation. The configuration interaction method. Density functional methods.

- Part 5: Theoretical and Computational Chemistry. Potential Energy Surfaces. Potential energy hypersurfaces. Stationary points: minima and saddle points. Significance of stationary points. Finding stationary points. Applications: molecular structure, thermodynamics and dynamics of chemical reactions, spectroscopy.

Lab Sessions

- Session 1. Model Systems: Particle in a box, harmonic oscillator. Hydrogenic Atom: Orbitals.
- Session 2. Electronic Structure I: Hartree-Fock method. Basis sets.
- Session 3. Electronic Structure II: Optimization of molecular geometries. Chemical Reactivity I: Chemical thermodynamics.
- Session 4: Chemical Reactivity II: Reaction kinetics.

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Lab Sessions	20	0.8	1, 7, 3, 8, 9, 2, 10, 11, 13, 14, 17, 5, 18
Problem Solving Sessions	10	0.4	1, 7, 15, 9, 10, 12, 13, 14, 5
Seminars	2	0.08	3, 9, 13, 18
Theory Lectures	32	1.28	1, 7, 16, 9, 2, 10, 13
Type: Supervised			
Practical Case	8	0.32	3, 15, 16, 8, 9, 2, 10, 12, 13, 14, 17, 5, 18
Type: Autonomous			
Personal Study	44	1.76	8, 10, 14

Lecturing is based on four different activities: theory lectures, problem-solving sessions, seminars and lab sessions.

- Theory Lectures. This subject has a substantial theoretical content. The theory content will be developed by the lecturer in the classroom, using supporting materials where appropriate. This material will be made available to students in advance in the Campus Virtual platform. Besides, a certain number of materials is available for streaming in asynchronous manner, and could be used if the lecturer so decides either to support the theory lectures or to replace them.

- Problem Solving Sessions. Problem solving is one of the main goals of the subject. At the beginning of the term an extensive collecion of exercises will be made available to the students, along with a formula selection and a solution set. As the syllabus coverage advances the lecturer will inform the students of which exercises in this collection can be attempted. In periodic sessions a selection of these exercises will be solved in depth.

- Seminars. A total of two seminars will be scheduled to take place: one before each partial exam. At the lecturer's discretion or based on the interests of the students, these sessions can be used to solve doubts, provide deeper insights in some aspects of the syllabus, do group discussions on selected texts, quotations or other results, such that the discussion can be meaningfully connected to the syllabus content.

- Lab Sessions. All lab sessions are simulation sessions and are carried out on computers. A total of four lab sessions are scheduled. The first of these will take place shortly before the first partial exam, and the rest before the second partial exam. In the first practical session students will use software developed by the lecturing staff to simulate somefundamental aspects of quantum mechanics using model systems along with a part focusing on the hydrogenic atom. In the remaining practical sessions licensed software will beused to perform quantum mechanical studies of the electronic structure of small- to medium-sized molecules. In this last batch of sessions students will study molecular structure, reactivity at thermodynamic and dynamical levels for simple reactions. A part of these sessions will be devoted to the study of an individualized reaction for each student.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Evidences	10%	6	0.24	16, 4, 9, 6, 2, 13, 14, 5
Lab Contents	30%	21	0.84	1, 7, 3, 15, 16, 8, 9, 10, 11, 12, 13, 14, 17, 5, 18
Written Exams (Partials and Supplemental)	60%	7	0.28	3, 13, 14, 5

Continuous Evaluation

Assessment of the performance of the student in the subject will be done through three contributions: Theory Contents, Lab Contents, and Evidences (take-home exercises). To pass the subject it is a requisite that the student has achieved a global mark of 4.0 over 10.0 on both the Theory Contents and the Lab Contents. Students not meeting these requirements will fail the subject.

- Theory Contents. These count 60% towards the final grade. The grade in this section indicates the student's knowledge of the theoretical aspects of the subject and his/her capacity to apply them to solve problems. A total of three written exams are scheduled along the semester: two partial exams and a supplemental exam. Each partial exam will include the part of the syllabus covered during the corresponding part of the term, while the supplemental exam will cover the full syllabus. To be allowed to take part in the supplemental exam a student must, at least: have written one partial exam, have attended the practical sessions and have turned in at least one evidence (take-home exercise). A student that gets a pass on the Theory Contents via partial exams does not have to write the supplemental exam. Otherwise, the supplemental exam must be taken. The final score of the part of Theory Contents will be the weighted average of the partial exams (the first partial exam has a weight of 60% and the second of 40%) if this grade is at least of 4.0 out of 10.0, or the grade of the supplemental examotherwise Students that, having passed the Theory Contents part via partial exams are willing to try and increase their marks can request to write the supplemental exam in written form (E-Mail) to the lecturer, who will ackowledge receipt. These students can write the supplemental exam, with the understanding that if they turn in the exam to the lecturer/invigilators, the score of the supplemental exam substitutes completely the score of both partial exams (i.e. it is possible to reduce their score).

- Lab Contents. Lab Contents contribute 30% to the final grade of the subject. Attending practical sessions is compulsory. The grade of the Lab Contents consists of two parts, both contributing 50% of the grade: One is the grade obtained from the corrected lab reports, and the other is the grade of an exam on the lab.

    - During the lab work of each session a model report will be published using the Campus Virtual platform. Lab reports shall be turned in using the channel and before the deadline that will be made public to the students during the lab session. The final marks for the lab reports part will be a weighted average of the marks of all reports, as the complexity of each session is not uniform. At the lecturer's discretion individual students might be required to discuss their lab work.

    - Alongside the 2nd partial exam students will also get an exam based on the lab work done.

  To be able to pass the subject it is necessary to obtain a grade of at least 4.0 out of 10.0 in the Lab Contents grade, computed as the mean with equal weighting of the lab reports grade and the lab exam. This grade is final and cannot be recovered.

- Evidences (Take-home Exercises). These contribute 10% to the final grade of the subject. Over the term a number of exercises will be proposed, related to the extent of syllabus already covered. These will be exercises more ellaborate than those solved in the classroom, and might require use of knowledge of other parts of the theory syllabus already studied. Evidences shall be turned in on an individual basis and before the deadline. The final score for the Evidences part will be a weighted average, taking into account the complexityof eachproposed task.

- Challenges. Additionally, at the lecturer's discretion a reduced set of voluntary advanced exercises could be proposed. These advanced exercises try to stimulate students willing to improve their grasp of the subject and deepen their knowledge. These will be exercises of larger complexity and might require the use of concepts in the syllabus, concepts from other subjects, checking with bibliographical sources and even to use specialized software to carry out simulations. Overall, the full contribution of these "challenges" will be a maximum of 1.0 mark over 10.0 on the final score of the subject depending on the total number of Challenges proposed, and their contribution will be additive to those of the compulsory items: in particular it is noted that this could bring the final score over 10.0, in which case the final score will be decreased to this figure. In no case will the grade of the "Challenges" waive the requirement of getting a minimum grade of 4.0 over 10.0 in both the Theory Contents and Lab Contents section for any student.

Single Evaluation

Attending lab sessions, turning in the lab reports and writing the practical exam are compulsory requirements of the subject, as they are for students taking the continuous evaluation.

Srudents who have chosen to take the Single Evaluation itinerary will have to write two exams on the same day the rest of students take the second partial exam:

- The first exam will cover the complete syllabus of the subject (theory and exercises). The grade obtained in this paper is the student's grade in Theory Contents.

- The second exam is a short paper related to the lab activity. The Lab Contents grade of the student is computed in the same way as for the rest of students: 50% of the grade comes from the lab reports and 50% from this exam.

To have a possibility to pass the subject the student needs to reach a minimal grade of 4.0 out of 10.0 in both the Theory Contents and the Lab Contents. If this is the case, the final grade of the subject is computed as follows:

$$\text{Final Grade} = (70\times\text{Theory Contents} + 30\times\text{Lab Contents})/100$$

If the final grade computed with the above formula does not reach 5.0 out of 10.0 or the grade of the Theory Contents does not reach 4.0 out of 10.0 the student has a second chance to pass the subject by taking a supplemental exam on a date to be determined by the Degree Coordinator. In this supplemental exam the student can only recover the grade on Theory Contents. The grade of Lab Contents cannot be recovered: A student not achieving a grade of 4.0 out of 10.0 on his/her Lab Contents cannot pass the subject.

"Non-Evaluable" Status

The status "Non-Evaluable" will be assumed for students having no grade for Theory Contents or Lab Contents. To this end, and depending on the kind of evaluation (continuous or single), it must be borne in mind that:

- Students following the Continuous Evaluation model will not have a grade for Theory Contents if they have only written one partial exam but no supllemental exam, or have no exam grades altogether. Students following the Single Evaluation model will not have a grade for Theory Contents if they have not written at least one of the two written exams they are entitled to.
- Irrespective of the evaluation model followed by the student: no grade for Lab Contents will be given to a student if any of the following circumstances applies: (1) s/he has not attended the lab sessions, (2) s/he has not turned in at least one lab report, (3) s/he has not taken the written lab exam.

Bibliography

Basic Reference Texts

- J. Bertran, V. Branchadell, M. Moreno, M. Sodupe, *Química Cuántica,* Síntesis, 2000, ISBN: 978-8477387427 (electronic version at: www.sintesis.com)

Additional Literature

- I. N. Levine, *Química Cuántica*, 5ª Ed, Prentice Hall, 2001, ISBN: 978-8420530964.

- F. L. Pilar, *Elementary Quantum Chemistry*, 2nd Ed., Dover, 2003. ISBN: 978-04864114645.

- P. W. Atkins, R. Friedman, *Molecular Quantum Mechanics*, 5th Ed., Oxford, 2010. ISBN: 978-0199541423.

Software

Lab session 1 uses software developed by the lecturing staff using Python and standard open source libraries. Executable images for Linux and/or Windows OS will be distributed to execute them in the students' personal computers. No installation of python or libraries will be required.

Lab sessions 2, 3 and 4 require the use of GaussView and Gaussian 16, of Gaussian, Inc. This software is used under license and is installed in the computers of the SIDCiB of the UAB, where it runs under Linux.

Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	1	Catalan	first semester	morning-mixed
(PAUL) Classroom practices	2	Catalan	first semester	morning-mixed
(PLAB) Practical laboratories	1	Catalan	first semester	afternoon
(PLAB) Practical laboratories	2	Catalan	first semester	afternoon
(PLAB) Practical laboratories	3	Catalan	first semester	afternoon
(PLAB) Practical laboratories	4	Catalan	first semester	afternoon
(PLAB) Practical laboratories	5	Catalan	first semester	afternoon
(PLAB) Practical laboratories	6	Catalan	first semester	morning-mixed
(PLAB) Practical laboratories	7	Catalan	first semester	morning-mixed
(PLAB) Practical laboratories	8	Catalan	first semester	morning-mixed
(SEM) Seminars	1	Catalan	first semester	morning-mixed
(SEM) Seminars	2	Catalan	first semester	afternoon
(TE) Theory	1	Catalan	first semester	morning-mixed
(TE) Theory	2	Catalan	first semester	afternoon