Universitat Autònoma de Barcelona

2022/2023

Quantum Chemistry

Code: 102503
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OB	2	1

Contact

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Use of Languages

Principal working language: catalan (cat)

Some groups entirely in English: No

Some groups entirely in Catalan: Yes

Some groups entirely in Spanish: No

Teachers

Ricard Gelabert Peiri

Miquel Moreno Ferrer

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) might run into difficulties that 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.

(Depending on the actual lab schedule Parts 4 and 5 might be exchanged in the sequence)

Lab Sessions

- Session 1. Model Systems. Particle in a box, harmonic oscillator.
- 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.

Methodology

The 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 wherever 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 some fundamental aspects of quantum mechanics using model systems. 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.

Activities

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

Assessment

Assessment of the performance of the student in the subject will be done through three contributions: written exams, lab reports, 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 written exams part and the lab reports part. Students not meeting these requirements will fail the subject.

- Written Exams. 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 at least 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 both partial exams does not have to write the supplemental exam. Otherwise, the supplemental exam must be taken. The final score of the written exams part will be the average of the partial exams for those students that get a pass on both, or the marks of the supplemental exam for the rest of students. In this context, a "pass" means to obtain 4,0 marks out of 10,0 in the corresponding exam. Those students that, having passed both 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 Reports. Attending practical sessions, performing fully the task and turning in the lab reports is compulsory. During the lab work of each session a model report will be published using the Campus Virtual platform. Lab reports shall be turned in on an individual basis and must be within the deadline. The final marks for the Lab Reports part will be a weighted average of the marks of the four reports, as the complexity of each session is not uniform. At the lecturer's discretion individual students might be required for a viva session to discuss their findings and conclusions.

- Evidences (Take-home Exercises). 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 must be within the deadline. The final score for the Evidences part will be a weighted average, taking into account the complexity of each proposed 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 on the final score of the subject, and their contribution will be additive to those of the compulsory items: in particular it is noted that this could bring the final score of some students over 10,0, in which case the final score will be decreased to this figure. In no case will the marks of the "Challenges" waive the requirement of getting a minimum of 4,0 over 10,0marks in both the written exams and lab reports section for any student.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Evidences	15%	6	0.24	16, 4, 9, 6, 2, 13, 14, 5
Lab Reports	30%	21	0.84	1, 7, 3, 15, 16, 8, 9, 10, 11, 12, 13, 14, 17, 5, 18
Written Exams (Partials and Supplemental)	55%	7	0.28	3, 13, 14, 5

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 Windows OSes 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.