Universitat Autònoma de Barcelona

2018/2019

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

Prerequisites

It is compulsory to have passed the first-year subject "Fonaments de Química" (Foundations of Chemistry). It is advisable to have passed the first-year subjects of "Matemàtiques" (Math) and "Física" (Physics).

Objectives and Contextualisation

The main goal of the course is to acquire basic knowledge of quantum chemistry. Because quantum chemistry deals with atomic and molecular systems and the physics that describes their behavior and properties is not intuitive, an important goal of the course is that the students learn how to reason using quantum concepts and to work out their implications at a macroscopical level. Learning to use the mathematics and IT tools to solve atomic and molecular exercises is also an important goal of the course, as is that the student becomes familiar with computational chemistry software.

Skills

- Adapt to new situations.
- Be ethically committed.
- Communicate orally and in writing in ones 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 ones 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

Foundations of Quantum Mechanics

Historical Background

Mathematical Foundations

Postulates of Quantum Mechanics

Heisenberg's Uncertainty Principle

Particle in a Box

Harmonic Oscillator

Atomic Structure

Angular Momentum

Hydrogen Atom

Spin. Antisymmetry Principle

Many-electron Atoms

Molecular Structure

Born-Oppenheimer Approximation

H_2^+ Molecule

MO-LCAO Approximation

H_2 Molecule

Hartree-Fock Method

Electron Correlation

DFT Methods

Practical Sessions

Session 1. Electronic Structure. Hartree-Fock Method

Session 2. Potential energy surfaces I. Molecular structure. Reaction energy.

Session 3. Potential energy surfaces II. Chemical reactivity.

Session 4. Project on chemical reactivity.

Methodology

The teaching methodology consists of four educational activities: master classes, problem solving sessions, seminars and practical sessions.

Master Classes

The lecturer will explain the syllabus content with visual support media which will be made available through the Moodle classroom.

Problem Solving Sessions

During the course the description of the problems that the students should solve will be handed over. During the practical sessions and under supervision of the lecturer, some representative problems will be fully solved or guidance on how to approach their sollution will be provided.

Seminars

In order to reinforce the understanding of the subject, the lecturer will provide different texts, exercises and other materials to be discussed/worked in a team out of the lecture room. In these sessions the different results obtained will be shared among all attendants and discussed.

Practical Sessions

In the practical sessions the students will get acquainted with computational chemistry software. The sessions take place in the computer room and will be done in pairs. The students will apply the methods of quantum chemistry to study the structure and reactivity of chemical systems. In the last session and under the supervision of a lecturer, the knowledge gained will be applied to tackle a specific chemical problem. The results of this project will be collected in a report and will be presented and discussed in the seminars.

Activities

Title	Hours	ECTS	Learning outcomes

Type: Directed			
Master classes	32	1.28	1, 7, 16, 9, 2, 10, 13
Practical sessions	16	0.64	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
Type: Supervised			
Personal project	8	0.32	3, 15, 16, 8, 9, 2, 10, 12, 13, 14, 17, 5, 18
Type: Autonomous			
Personal Study	47	1.88	8, 10, 14

Evaluation

Exams: three exams will be scheduled, two of them partial and one final. A student that passes both partial exams DOES NOT have to take the final exam. A student failing the first partial cannot take the second partial and MUST go straight to the final exam to pass the subject. The FINAL exam will evaluatie the full syllabus taught during the semester. Students that have scored less than 5 points out of 10 in any of the two partial exams must take the final exam. The score in this final exam will be the final score of the course for students finding themselves in this situation, and it will be necessary to score at least 4 out of 10 points in order to be able to average the grade of the exam with the grades coming from lab and evidence work. Students wanting to increase their grade can also take the final exam. Be advised, however, that turning in the final exam for correction implies that the grade of this exam substitutes any grade coming from the partial exams. To take part in the final exam it is necessary that the student has taken at least one partial exam, has taken the lab work and turned in at least one of the evidences.

Lab work: both attendance of the lab sessions and turning in the reports is compulsory. The last practical session is conceived as an open project different for each group of students. Results obtained in this session will be presented and discussed in a written report (open format) and presented in public orally.

Evidences: thorughout the course students are required to turn in a minimum of two complementary exercises on the subjects dealt with in the lecture room.

Evaluation activities

Title	Weighting	Hours	ECTS	Learning outcomes
Evidences	5%	2	0.08	16, 4, 9, 6, 2, 13, 14, 5
Exams (partials and final)	60%	8	0.32	3, 13, 14, 5
Lab work	35%	25	1	1, 7, 3, 15, 16, 8, 9, 10, 11, 12, 13, 14, 17, 5, 18

Bibliography

BASIC BIBLIOGRAPHY

"*Química Cuántica*" J. Bertran, V. Branchadell, M. Moreno, M. Sodupe, Ed. Síntesis. ISBN:84-7738-742-7 (electronic version in: www.sintesis.com)

OTHER BIBLIOGRAPHY

"Química Cuántica" I.N. Levine, Ed. Prentice Hall. ISBN: 84-205-3096-4

"Absolutely Small" M. D. Fayer, Ed. McGraw-Hill. ISBN: 978-0814414880

"Elementary Quantum Chemistry" F.L. Pilar, Ed. McGraw-Hill. ISBN: 0-07-100857-8

"Molecular Quantum Mechanics" P.W. Atkins, Ed. Oxford, ISBN: 0-19-855170-3