Quantum Phenomena I

Code: 106816
ECTS Credits: 6

2024/2025

Degree	Type	Year
2504602 Nanoscience and Nanotechnology	OB	2

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Teachers

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Teaching groups languages

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Prerequisites

No explicit prerequisites apply. However, it is highly recommended that students attending the Fenomens quàntics I course have already passed the Enllaç Químic i Estructura de la Matèria", "Física General: Mecànica i Ones" and "Fonaments de matemàtiques" courses.

Objectives and Contextualisation

Acquisition of basic knowledge of Quantum Mechanics and its application to simulate and analyze the properties of matter at the nanometric scale. The course is organized in three units. In the first, the fundamentals of the quantum description of matter are introduced. A second unit develops, introducing approximations, these foundations to turn them into a powerful machinery for calculation. The third part shows its applications in the simulation of nanoscopic systems.

Learning Outcomes

1. CM16 (Competence) Use knowledge of physics to solve problems on the nanoscale.
2. KM29 (Knowledge) Understand the principles of quantum mechanics and how they can be used to describe the structure and properties of matter on an atomic and molecular scale.
3. KM29 (Knowledge) Understand the principles of quantum mechanics and how they can be used to describe the structure and properties of matter on an atomic and molecular scale.
4. SM27 (Skill) Apply the tools used in quantum physics and computational calculus to simple systems.
5. SM28 (Skill) Gather, summarise and present results and conclusions of scientific publications.

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Content

1. Fundamentals

1.1. Postulates of quantum mechanics

Historical introduction. Elements of mathematics. Postulates of Quantum Mechanics. Heisenberg's Uncertainty Principle.

1.2. Application to systems with analytical solution:

Particle in a Box, Harmonic Oscillator, Rigid Rotor

1.3. Atomic structure.

Hydrogen atom. angular momentum. Atomic orbitals. Spin. Polyelectronic atoms (the helium atom). Antisymmetry: Pauli principle. Slater's determinants. Approximate methods: Theory of Variations and Theory of Disturbances

2. Machinery

2.1 Molecular electronic structure

Born-Oppenheimer approximation. Approximation of Molecular Orbitals (OM). The self-consistent Hartree-Fock (HF-SCF) method. Bases of atomic orbitals. Beyond the Hartree-Fock method: post-HF methods.

2.2 Density Functional Theory (DFT)

Theorems of Hohenberg and Kohn. Kohn-Sham approximation. Exchange-correlation functionals. Known limitations of DFT methods. Errors and precision in computational chemistry

3. Applications

3.1 Application of Quantum Mechanics to molecular simulation.

Models and approximations. Atomistic simulations. Structures and reactions: Potential Energy Surfaces. Geometry optimization. Calculation of molecular properties

3.2 Simulation of complex systems.

Molecular mechanics. Hybrid QM/MM methods. Simulation of materials.

Practical classes (Computational laboratory)

Practice 1. Molecular electronic structure. Hartree-Fock method. Base sets. thermochemistry

Practice 2. Supramolecular interactions. DFT methods. Influence of electronic correlation and dispersion.

Practice 3. Simulation of chemical reactions: potential energy surfaces. Minima and transition states.

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes

Type: Directed			
Computational lab	8	0.32	SM27, SM28, SM27
Excersise sessions	15	0.6	CM16, SM27, CM16
Lectures	30	1.2	KM29, KM29
Type: Autonomous			
Study	75	3	CM16, KM29, SM27, CM16

The teaching methodology is based on three types of activities: theory classes, excersices classes and lab sessions.

• Theory classes. It is a course with a high theoretical content. The theory of the course will be presented by the teaching staff in the classroom, using support materials where necessary. This material will be available to students in advance through the Campus Virtual platform. Additionally, additional material will be provided to facilitate the students' study

• Exercise Classes. Exercise solving is one of the main objectives of the course. At the beginning of the course, a comprehensive collection of exercises for the entire course, together with a form and their solution, will be distributed on the Campus Virtual platform. In regular sessions, some of these exercises will be solved in detail.

• Lab sessions. All the lab sessions of this course correspond to computer simulations and are carried out on a computer labs. Three practices have been scheduled. Students will use licensed software to perform quantum mechanical calculations of the electronic structure of small and medium-sized molecules. The molecular structure, the reactivity at the thermodynamic level and the reaction dynamics in some simple reactions will be studied.

Note: 15 minutes of a class will be set aside, within the calendar established by the center/degree, for students to fill in the teacher performance and subject evaluation surveys /module.

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
Daily work evaluation	15%	5	0.2	CM16, KM29
Exams	70%	8	0.32	CM16, KM29, SM27
Lab reports	15%	9	0.36	CM16, SM27, SM28

The evaluation of "Fenomens Quàntics I" will be based on three contributions: written exams, practice reports and daily work. Of these three, it is a requirement to pass "Fenòmens Quàntics I" to have obtained a minimum grade of 4.5 out of 10.0 in the written exams and a 5.0 for the overall grade of the subject. Those who do not achieve these minimum grades do not pass Fenòmens quàntics I. The overall grade of the subject is calculated as:

grade= (Partials · 7.0 + Practices · 1.5 + Daily ·1.5)/100

• Theoretical Content: Partial exams (70% of the final grade)

Two written partial exams will be scheduled. Each partial exam will have the same weight in the final grade (35%). The grade of these exams aims to reflect the theoretical knowledge of the subject achieved by the students and their ability to apply it to problem solving.

Students who obtain more than a 4.5 in the two partial tests and thereby achieve a 5.0 overall grade for the course, do not have to take the final exam. Otherwise, it will be compulsory to take the final exam. Even so, in order to take part in the final exam test, the student must, at least, have taken a partial exam, completed the lab session and submitted at least one of the daily work excercises.

The final exam will be unique and will include the content of the two partial exams. You will not be able to attend this final test to raise your grade. In addition, students who have obtained a grade equal to or higher than 8 in the two partial exams may be qualified with a "Matrícula de honor" qualification.

• Lab sessions. Practice reports (15% of the final grade).

Attendance at the lab sessions is mandatory. The lab sessions grade is determined by the correctness of the practical reports. The final mark of the practice reports will be a weighted average of the reports.

• Daily work. (15% of the final mark).

Throughout the course, it will be proposed to solve additional exercises related to the content of the course that has been covered. These will be more elaborate exercises than those solved in class and may require the use of knowledge from different topics already studied in the syllabus. The final grade for daily work will be a weighted average of the associated grades.

Unique Assessment

Attendance at practice sessions and the presentation of reports is mandatory for all students, regardless of the assessment modality they are enrolled in. In addition, students who have taken the single assessment modality will have to take a final test which will consist of an examination of the entire theoretical content, exercises and daily work of the course. This test will be carried out on the day that continuous assessment students take the second part exam. The student's grade will be:

Subject grade= (Exam · 8.5 + Practices · 1.5)/100

If the exam grade does not reach 4.5 or the overall grade does not reach 5, the student has another opportunity to pass the subject through a second final exam. This will be held on the date set by the coordination of the qualification. In this test students can recover 70% of the grade corresponding to the theory and problems part. The other assessment activities are not recoverable.

Bibliography

"Molecular Quantum Mechanics" fifth edition, Peter Atkins, Ronald Friedman, Oxford University Press, 2010. ISBN 019-927498-3.

"Química Cuántica", Joan Bertran, Vicenç Branchadell, Miquel Moreno, Mariona Sodupe, Editorial Síntesis, 2000. ISBN: 84 7738 742 7.

"Introduction to Quantum Mechanics" third edition, David J. Griffiths, Darrell F. Schroeter, Cambridge University Press, 2018. ISBN: 9781107189638.

"Computational Chemistry", Jeremy Harvey,Oxford University Press, 2018, ISBN: 9780198755500

Software

Gaussian16 and Gaussview

Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	1	Catalan	first semester	afternoon
(PLAB) Practical laboratories	1	Spanish	first semester	morning-mixed
(PLAB) Practical laboratories	2	Spanish	first semester	morning-mixed
(TE) Theory	1	Catalan	first semester	afternoon