Universitat Autònoma de Barcelona

2023/2024

Quantum Phenomena I

Code: 103287
ECTS Credits: 6

Degree	Type	Year	Semester
2501922 Nanoscience and Nanotechnology	OB	3	1

Contact

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Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject. Please note that this information is provisional until 30 November 2023.

Prerequisites

It is recommended to have passed the subjects "Chemical Bonding and Structure of Matter", "Mechanics and Waves" and "Classical Physics"

Objectives and Contextualisation

Acquisition of basic knowledge of Quantum Mechanics and its application to simulate and analyze the properties

of matter at the nanoscopic scale.

The course is organized into three units. The first one introduces the foundations of the quantum description of th

A second unit develops these foundations to turn them, by introducing approximations, into a

powerful tool for the calculation of real systems.The third part is devoted to the application of quantum-based me

for the simulation of nanoscopic systems.

Competences

- Apply the concepts, principles, theories and fundamental facts of nanoscience and nanotechnology to solve problems of a quantitative or qualitative nature in the field of nanoscience and nanotechnology.
- Communicate orally and in writing in one's own language.
- Demonstrate knowledge of the concepts, principles, theories and fundamental facts related with nanoscience and nanotechnology.
- Interpret the data obtained by means of experimental measures, including the use of computer tools, identify and understand their meanings in relation to appropriate chemical, physical or biological theories.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse physical, chemical and biological problems in the field of nanoscience and nanotechnology and propose answers or suitable studies for their resolution, including when necessary the use of bibliographic sources.
- Recognise the terms used in the fields of physics, chemistry, biology, nanoscience and nanotechnology in the English language and use English effectively in writing and orally in all areas of work.
- Resolve problems and make decisions.

Learning Outcomes

1. Analyse situations and problems in the field of physics and propose answers or studies of an experimental nature using bibliographic sources.
2. Apply Schroedinger's equation to one-dimensional quantum systems like potential wells and/or oscillators and to three-dimensional ones like molecules.
3. Apply the acquired theoretical contents to the explanation of experimental phenomena.
4. Communicate orally and in writing in one's own language.
5. Correctly use computer tools to calculate, graphically represent and interpret the data obtained, as well as its quality.
6. Critically evaluate experimental results and deduce their meaning.
7. Draft reports on the subject in English.
8. Employ information and communication technology in the documentation of cases and problems.
9. Indicate the physical bases of quantum mechanics and relate them with experimental facts.
10. Interpret basic texts and bibliographies in English on physics and materials.
11. Learn autonomously.
12. Manage the organisation and planning of tasks.
13. Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
14. Perform bibliographic searches for scientific documents.
15. Present brief reports on the subject in English.
16. Propose creative ideas and solutions.
17. Reason in a critical manner
18. Recognise in physical and chemical processes the phenomena of energy exchange and the laws that govern them.
19. Recognise the terms for processes and devices for the generation, storage and transport of energy, as well as the applications and impact of nanomaterials on the environment.
20. Recognise wave-particle duality.

21. Resolve Schrödinger's equation for one-dimensional problems and be able to calculate the tunnel effect in different physical systems.
22. Resolve problems and make decisions.
23. Resolve problems with the help of the provided complementary bibliography.
24. Understand the properties of atoms and molecules with quantum mechanics.
25. Use data processors to produce reports.

Content

Unit 1: Laying the foundations

Historical background

1.1 The Bohr model

1.2 Wave-particle duality

1.3 Mathematical tools

1.4 The postulates of Quantum Mechanics

1.5 The uncertainty principle

Some analytically soluble problems

1.6 Particle in a box

1.7 Harmonic oscillator

1.8 Rigid rotor

1.9 Hydrogen atom

1.10 Angular momentum

1.11 Atomic orbitals

1.12 Spin

Unit 2: The machinery

2.1 Many-electron atoms (the hellium atom)

2.2 Antisymmetry: the Pauli Principle

2.3 Slater determinants

2.4 Approximation methods: variation theory and perturbation theory

2.5 Molecular electronic structure

2.6 The Born-Oppenheimer approximation

2.7 Molecular orbital approximation (MO)

2.8 The Hartree-Fock Self-Consistent Field Method (HF-SCF)

2.9 The selection of basis set

2.10 Electron correlation

2.11 Beyond the Hartree-Fock approximation: post-HF methods

2.12 Density Functional Theory (DFT)

2.13 Exchange-correlation functionals

2.14 Errors and accuracy in computational chemistry

Unit 3: Applications

3.1 Molecular modeling

3.2 Models and approximations

3.3 Atomistic simulations

3.4 What can be computed?

3.5 A chemical reaction in the computer: the Potential Energy Surface (PES).

3.6 Simulation of complex systems. Hybrid QM/MM methods.

3.7 What we get from calculations: real examples.

Practical classes: Computational Lab

Practice 1. Molecular electronic structure. Hartree-Fock Method. Basis set. Thermochemistry.

Practice 2. Supramolecular interactions. DFT methods. Optimization of geometry. Correlation and dispersion effe

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

Methodology

Lectures

In the lectures the teacher will explain the content of the program with au

Students will have a pdf version of the course slides in the Virtual Campus of the UAB.

Practice classes

Practice classes will serve to consolidate and put into practice the knowle

These classes conceived to solve specific exercises, will be interspersed with the lectures to reinforce certain

aspects or will be given at the end of the thematic units.
The approach / resolution of the exercises

will be carried out in the practice sessions under the direction of the teacher.

The students will have the statements of the exercises that they must solve throughout the course,

as well as the solved exercises, once the resolution has been made in class.

Computational Lab

Computational Lab sessions will take place in the computer classroom. Support material will be supplied

to the students through the UAB Virtual Campus.
The students will use calculation programs

that apply the methodology of Quantum Mechanics to study the structure and evolution of nanoscopic systems.

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	12	0.48	3, 11, 6, 8, 17, 22, 25
Lectures	28	1.12	2, 9, 18, 20, 24, 21

Practice classes	10	0.4	1, 2, 9, 18, 20, 24, 21, 23, 22
Type: Supervised			
Oral presentation	4	0.16	1, 3, 6, 8, 15, 14, 12, 10, 13, 17, 19, 7, 23
Type: Autonomous			
Study	68	2.72	2, 11, 9, 16, 17, 18, 20, 24, 21, 23

Assessment

Written exams

They constitute 70% of the grade. There will be two partial exams throug

The two partial exams have the same weight (35%). A mark equal to or greater than 4 (out of 10) in each partial

need to pass the subject without going to the second-chance exam.

In case of not having reached a grade of 4 in one or both partial exams the student will have to retake the exam

(second-chance exam). This second-chance exam is only for those that

haven't passed the course yet and covers all the subjects of the course. In order to take part in the second-chan

it will be compulsory to have done at least one of the two partial exams,

in addition to the computational lab and the oral presentation. It will be necessary to reach a grade of 4 (out of 1(

the second-chance exam in order to pass the course.

A grade equal to or higher than 8 in the two partial exams is required to qualify for a "Distinction with Honours" r

Practical classes: Computational Lab

They constitute 15% of the grade. The students will have to answer the questions formulated in the scripts of the

The students must fill out a lab report for each one of the practices.

Attendance at practice sessions and presentation of

reports are mandatory.

Oral presentation of an article

It constitutes 15% of the grade. In the last weeks of the course the stude

searching, in the highest impact-factor journals of the field of Nanosciences,

a recent article in which quantum calculations are an important part of the results, and expose publicly,

to the entire class, the article.

Each group will have a time for the presentation and there will

also be a question time. The oral presentation is mandatory.

Single assessment

The attendance to the practical sessions and the presentation of the repo

obligatory for all the students.

More than these two assessment activities, the students who have joined the single assessment modality

will have to carry out a Final test that will consist of an exam of all the theoretical topics and problems of the subj

This test is carried out on the day in which the students of continuous assessment take the second partial exam.

The qualification of the student will be:

Course grade= (Final test grade 70% + Practice grade 15% + Oral prese
If the final grade does not reach 5, the student will have another opportur

exam that will be held on the date set by

the coordination of the degree. In this test you will be able to recover 70% of the note corresponding to the theor

and problems part. The other two evaluative activities are

not recoverable.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Lab reports	15%	10	0.4	3, 2, 11, 6, 4, 8, 14, 12, 9, 13, 18, 20, 24, 21, 23, 22, 5, 25
Oral presentation of a paper	15%	10	0.4	1, 3, 2, 11, 6, 8, 15, 14, 9, 10, 13, 16, 17, 19, 18, 20, 7, 24, 21, 23, 22
Written exam (parcial or second-chance exams)	70%	8	0.32	3, 2, 6, 4, 9, 17, 18, 20, 24, 21, 23, 22

Bibliography

"Quantum Chemistry" sixth edition, Ira N. Levine, Prentice Hall, 2009. ISBN: 978-0136131069.

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

"Essentials of Computational Chemistry: Theories and Models", second edition, Christopher J. Cramer, Wiley, 2004. ISBN: 0 470 09181 9.

"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.

"Electronic Structure: Basic Theory and Practical Methods", Richard M. Martin, Cambridge University Press, 2004. ISBN: 0 521 78285 6

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

Software

Practice classes of the Computational Lab will be performed using Gaussian 16 program

for the calculations and Gausview 6 for building and visualization of molecules.