2020/2021

Quantum Phenomena I

Code: 103287
ECTS Credits: 6

Degree	Type	Year	Semester
2501922 Nanoscience and Nanotechnology	OB	3	1

The proposed teaching and assessment methodology that appear in the guide may be subject to changes as a result of the restrictions to face-to-face class attendance imposed by the health authorities.

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

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

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

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

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 ones 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 Schroedingers 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 ones 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

1.1 Historical background

1.2 The Bohr model

1.3 Wave-particle duality

1.4 Mathematical tools

1.5 The postulates of Quantum Mechanics

1.6 The uncertainty principle

1.7 Some analytically soluble problems

1.8 Particle in a box

1.9 Harmonic oscillator

1.10 Rigid rotor

1.11 Hydrogen atom

1.12 Angular momentum

1.13 Atomic orbitals

1.14 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 Applications of Quantum Mechanics.- Hierarchy of theoretical methods.

3.2 Simulations as computational experiments. - Theories and models.- Calculation levels.

3.3 Structures and reactions: Potential energy surfaces.- Geometry optimizations.- Calculation of molecular properties.

3.4 Complex systems

Practical classes: Computational Lab

Session 1. Electronic structure. Hartree-Fock Method. Electronic correlation. DFT methods.
Session 2. Optimization of geometry. Determination of molecular propert
Session 3. Potential energy surfaces. Minima. Binding, assembly and rea
Session 4. Potential energy surfaces. Transition States. Simulation of ch

Methodology

Lectures

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

Practice classes

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

aspects or will be given at the end of the thematic units. Students will have the statements of the exercises that v

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

Lab

Computational Lab sessions will take place in the computer classroom. Support material will be supplied to the s
The students will use calculation programs

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

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

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

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

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

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

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

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

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

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"Molecular Quantum Mechanics" fourth edition, Peter Atkins, Ronald Friedman, Oxford University Press, 2005. ISBN 019-927498-3.

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

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

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