VNIVERSITAT DE VALÈNCIA

Course Guide
43988 Mathematical foundations of quantum mechanics

COURSE DATA

Data Subject	
Code	43988
Name	Mathematical foundations of quantum mechanics
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2021 - 2022

Study (s)

Degree	Center	Acad. year	Period
2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1	Faculty of Chemistry	1	Annual
3156 - Theoretical Chemistry and Computational Modelling	Doctoral School	0	First term

Subject-matter

Degree	Subject-matter	Character
2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1	1 - Principles	Obligatory
3156 - Theoretical Chemistry and Computational Modelling	1 - Complementos de Formación	Optional

Coordination

Name	Department
SANCHEZ MARIN, JOSE	315 - Physical Chemistry
TUÑON GARCIA DE VICUÑA, IGNACIO NILO	315 - Physical Chemistry

SUMMARY

English version is not available

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

There are no previous prerequisites

OUTCOMES

2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- Students are able to foster, in academic and professional contexts, technological and scientific progress within a society based on knowledge and respect for: a) fundamental rights and equal opportunities between men and women, b) The principles of equal opportunities and universal accessibility for persons with disabilities, and c) the values of a culture of peace and democratic values.
- El estudiante es capaz de adaptarse a diferentes entornos culturales.
- El estudiante es capaz de resolver problemas y tomar decisiones.
- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- Comprender los fundamentos teóricos y prácticos de técnicas con las que puede analizar la estructura electrónica, morfológica y estructural de un compuesto.

LEARNING OUTCOMES

To introduce the most usual progamming techniques in physics and chemistry. The student will learn the essential computational tools and will learn to create efficient programas using the Fortran programming language.

DESCRIPTION OF CONTENTS

1. Part I

1 - Introduction. Solution of Schrödinger equation in simple systems
2 - Basic algebra
3 - Functional Spaces
4 - Approximate Methods in Quantum Chemistry: Variational Principle and Time-independent Perturbation Theory
5 - Independent and Identical Particles
6 - Angular momentum, spin.
7 - Main theorems in Quantum Mechanics
8 - Composition of Angular Momenta.

2. Part II

9- Pure states and mixed states
10- Postulates of Quantum Mechanics
11- Compatible and incompatible observables
12- Density operators
13- Time evolution pictures
14- Time dependent perturbation theory
15- Compound systems. Correlation and entanglement
16- Discrete representations. Basis changes
17- Position and momentum representations
18- Second quantization formalism
19- Reduced density operators and matrices. Natural spinorbitals

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	30,00	100
Seminars	12,00	100
Development of individual work	30,00	0
Study and independent work	33,00	0
Preparation of practical classes and problem	20,00	0
TOTAL	**125,00**	

TEACHING METHODOLOGY

Lecture: The Professor will deliver lectures about the theoretical contents of the course during two-hour sessions. The presentations will be based on the different materials available at the Moodle platform.

Network teaching: All the tools available at the Moodle website (http://www.uam.es/moodle) will be used (uploading of teaching materials, utilization of work team strategies, wiki, blogs, e-mail, etc.).

Online Seminars: After the lecturing period, online seminars between the Professor and the students will be arranged at the *virtual classroom* in order to discuss the results being obtained, the potential problems and difficulties in using the various methodologies as well as to supervise the preparation of the required reports.

Tutoring sessions: The professor can organize either individual or group tutoring sessions about particular topics and questions raised by students.

EVALUATION

Ordinary assessment

The knowledge acquired by the student will be evaluated along the course. The educational model to follow will emphasize a continuous effort and advance in training and learning.

The final student mark will be based on exercises that must be done during the course. The next criteria will be followed for assessment of student exercises:

- 60% from a set of proposed exercises.

- 40% from the student reports, discussions between the student and professor in tutoring session and seminars.

Extraordinary assessment

The student will have to repeat those exercises not presented during the course and repeat those incorrectly done. The student will also do a final exam. The student mark will be obtained from:

- 100% from the student exercises presented and discussions between the student and the teachers.

REFERENCES

Basic

- a) Nivel básico / Very basic level

  Quantum Chemistry (6th edition 2008)
  Ira N Levine
  Prentice Hall

Student Solutions Manual for Quantum Chemistry
Ira N Levine

Molecular Quantum Mechanics (5th Edition 2010)
Peter W. Atkins , Ronald S. Friedman
Oxford University Press

Quantum Chemistry (2nd edition 2008)
Donald A. McQuarrie
University Science Books

Problems and Solutions for Mcquarrie's Quantum Chemistry
Helen O. Leung , Mark Marshall

b) Nivel Recomendado / Recommended level

Quantum Mechanics, Volume 1 and 2
Claude Cohen-Tannoudji , Bernard Diu , Frank Laloe
Wiley-Interscience (2005)

Quantum Mechanics (2nd Edition, 2000)
B.H. Bransden, C.J. Joachain
Benjamin Cummings

Problems and Solutions in Quantum Chemistry and Physics
Charles S. Johnson Jr. , Lee G. Pedersen
Dover Publications (1987)

Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory
Attila Szabo , Neil S. Ostlund
Dover Publications (1996)

c) Nivel avanzado / Advanced level

Quantum Mechanics Non-Relativistic Theory, Third Edition: Volume 3
L. D. Landau , L. M. Lifshitz

Quantum Mechanics (2 Volumes in 1)
Albert Messiah

Quantum Mechanics (2 volumes)
Alberto Galindo, Pedro Pascual
Springer (1991)

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

English version is not available