VNIVERSITAT DE VALÈNCIA

Course Guide
44970 Mathematical foundations of quantum mechanics

COURSE DATA

Data Subject	
Code	44970
Name	Mathematical foundations of quantum mechanics
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	1 - Fundamentos	Obligatory

Coordination

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

SUMMARY

To understand the mathematical tools needed to develop the main methods in Quantum Mechanics and to understand the main concepts and applications.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

OUTCOMES

2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus

- 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.
- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- Students are familiar with the fundamental postulates of Quantum Mechanics necessary for a good understanding of the most common methods used in quantum chemistry
- Students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.
- Students are able to work as a team both at multidisciplinary level and with their own peers respecting the principle of equality of men and women.
- Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
- Students are organized at work demonstrating that they know how to manage their time and resources.
- Students understand the theoretical and practical bases of computational techniques with which they can analyze the electronic, morphological and structural structure of a compound and interpret the results adequately.
- Students understand and manage the mathematical tools required for the development of theoretical chemistry both in fundamental aspects and applications.

LEARNING OUTCOMES

To understand the mathematical tools needed to develop the main methods in Quantum Mechanics and to understand the main concepts and applications.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	31,00	100
Seminars	12,00	100
TOTAL	43,00	

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 (https://posgrado.uam.es) 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

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

Resit

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

- 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.

Additional

- 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).

  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).