UNIVERSIDAD AUTÓNOMA DE MADRID

32523 - MATHEMATICAL FUNDATIONS OF QUANTUM MECHANICS

Syllabus Information

Code - Course title: 32523 - MATHEMATICAL FUNDATIONS OF QUANTUM MECHANICS

Degree: 616 - Máster en Química Teórica y Modelización Computacional (2013)
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional
666 -

Faculty: 104 - Facultad de Ciencias

Academic year: 2019/20

1.Course details

1.1.Content area

Mathematical Foundations of Quantum Mechanics

1.2.Course nature

651 - Compulsory
666 - Training Supplement
616 - Compulsory

1.3.Course level

666 - Doctorado (MECES 4)
651 - Máster (MECES 3)
616 - Máster (MECES 3)

1.4.Year of study

616 - Máster en Química Teórica y Modelización Computacional (2013): 1
666 - : 99
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional: 1

1.5.Semester

Annual

1.6.ECTS Credit allotment

5.0

1.7.Language of instruction

English

1.8.Prerequisites

There are no previous prerequisites.

1.9.Recommendations

There are no recommendations.

1.10.Minimum attendance requirement

Attendance is mandatory.

1.11.Faculty data

a. Subject's coordinator:
- Name and surname: Jesús González Vázquez
- Email: jesus.gonzalezv@uam.es
- Institution: Universidad Autónoma de Madrid
- Department: Chemistry
- Room: Module 13-308
- Phone: +34 914973008

b. Lecturer:
- Name and surname: Fernando Martín García
- Email: fernando.martin@uam.es
- Institution: Universidad Autónoma de Madrid
- Department: Chemistry
- Room: Module 13-304
- Phone: +34 914974019

c. Master's coordinators:
- Sergio Diaz-Tendero: sergio.diaztendero@uam.es
- Manuel Alcami: manuel.alcami@uam.es

1.12.Competences and learning outcomes

1.12.1.Competences

BASIC AND GENERAL

CB6 – Students possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a research context.

CB7 - Students know how to apply the acquired knowledge and their problem solving capacity in new or little known environments within broader (or multidisciplinary) contexts related to their area of study.

CB8 - Students are able to integrate knowledge and face the complexity of making judgments from information that, incomplete or limited, includes reflections on social and ethical responsibilities linked to the application of their knowledge and judgments.

CB9 - Students know how to communicate their conclusions and the knowledge and reasons that support them to specialized and non-specialized audiences in a clear and unambiguous way.

CB10 - Students possess the learning skills that allow them to continue studying in a way that will be self-directed or autonomous.

CG01 - 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.

CG02 - Students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.

CG03 - 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.

CROSS-COMPREHENSIVE

CT01 - Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.

CT02 - Students are organized at work demonstrating that they know how to manage their time and resources.

SPECIFIC

CE01- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.

CE04 - 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.

CE12 – Students are familiar with the fundamental postulates of Quantum Mechanics necessary for a good understanding of the most common methods used in quantum chemistry.

CE17 - Students understand and manage the mathematical tools required for the development of theoretical chemistry both in fundamental aspects and applications.

1.12.2.Learning outcomes

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

1.13.Course contents

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.

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

1.14.Course bibliography

a) 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) 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) 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).

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	43
Independent study time	82

2.2.List of training activities

Activity	Nº hours
Lectures	31
Seminars	12
Practical sessions	
Clinical sessions	
Computer lab	
Laboratory	
Work placement	
Supervised study	
Tutorials	
Assessment activities	
Other	

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.

3.Evaluation procedures and weight of components in the final grade

3.1.Regular 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

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	60
Continuous assessment	40

3.2.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.

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	100
Continuous assessment	

4.Proposed workplan

Please, check the official schedule posted on the master website.