32527 - METHODS IN THEORETICAL CHEMISTRY I

Syllabus Information

Code - Course title: 32527 - METHODS IN THEORETICAL CHEMISTRY I

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

Theoretical Chemistry Methods I

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: Alfredo Sánchez
- Email: sanchez@uv.es
- Institution: University of Valencia
- Department: Physical Chemistry
- Phone: +34 963544712

b. Lecturer:
- Name and surname: Olalla Nieto Faza
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- Institution: University of Vigo
- Department: Organic Chemistry
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c. Master's coordinators:
- Manuel Alcamí. manuel.alcami@uam.es
- Sergio Díaz-Tendero. sergio.diaztendero@uam.es

1.12.Competences and learning outcomes

1.12.1.Competences

BASIC AND GENERAL COMPETENCES

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.

CROSS-COMPREHENSIVE COMPETENCES

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

SPECIFIC COMPETENCES

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.

CE15 – Students understand the basic principles of "ab initio" methodologies and Density Functional Theory.

CE16 - Students are able to discern between the different existing methods and know how to select the most appropriate method for each problem

1.12.2.Learning outcomes

As a result of participating in this course, students will be able to:

- Understand the theoretical and practical bases of computational techniques used in the electronic, structural and morphological analysis of a compound and interpret the results adequately.
- Understand the basic principles of "ab initio" methods, and Density Functional Theory.
- Shed light on what method is the most appropriate for each problem, considering the differences between them.
- Demonstrate knowledge and comprehension of the facts, applying concepts, principles and theories associated with Theorical Chemistry and Computational Modelling.

1.13.Course contents

1. Ab initio Methods:

- Hartree-Fock methods: RHF y UHF
- Basis functions, pseudopotentials and effective potential.
- Variational savefunction-based Electron Correlation Methods: Configuration Interaction and multiconfigurationals methods
- Moller-Plesset Perturbation Theory
- Introduction to Coupled Cluster methods

2. Density Functional Theory:

- Preliminary concepts. Hohenberg-Kohn Theorems.
- Kohn-Sham Method.
- Density Functional Approximations (DFAs; approximations to exchange-correlation functionals)

In the part of Quantum Chemical Methods we will formulate the main theorems in which the different methodologies are based and the most important "ab initio" methods will be studied. In the Functional Density Theory section the students should understand the basis ideas in which the theory is based. The student should understand how the different correlation-exchange functionals are developed and their main features. The student should know how to select the most adequate method for a fixed problem.

1.14.Course bibliography

- Helgaker, T., Jørgensen, P., Olsen, J.; Molecular Electronic-Structure Theory. John Wiley & Sons Ltd, 2000
- Szabo, A., Ostlund, N. S.; Modern Quantum Chemistry. Introduction to Advanced Electronic Structure Theory. McGraw-Hill, 1989
- Roos, B. Editor; Lecture notes in quantum chemistry: European summer school in quantum chemistry. Springer-Verlag 1994. Chapters on CC, CI, MCSCF, calibration
- Linear-Scaling Techniques in Computational Chemistry and Physics. Zaleśny, R.; Papadopoulos, M.G.; Mezey, P.G.; Leszczynski, J. (Eds.). Springer (Berlin) 2011
- A Chemist's Guide to Density Functional Theory. W. Koch and M.C. Holthausen, Wiley-VCH, 2001
- Density-Functional Theory of Atoms and Molecules. R.G. Parr and W. Yang, Oxford University Press, New York, 1989
- Electronic Structure. R.M. Martin, Cambridge University Press, Cambridge, 2004

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	35
Independent study time	90

2.2.List of training activities

Activity	# hours
Lectures	20
Seminars	15
Practical sessions	
Clinical sessions	

Computer lab	
Laboratory	
Work placement	
Supervised study	
Tutorials	
Assessment activities	
Other	

Lecture: The Professor will deliver face-to-face, or, online video 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.).

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

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.

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:

- 70% from the student report,
- 30% from discussions between the student and professor in tutoring sessions and seminar.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	70
Continuous assessment	30

3.2.Resit

The student will have to face a final exam, including both theory and practical exercises. The student mark will be obtained from:

- 70% from the final exam,
- 30% from the individual work.

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	70
Continuous assessment	30

4.Proposed workplan

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