# COURSE DATA

| Data Subject | |
|---|---|
| **Code** | 44974 |
| **Name** | Methods of theoretical chemistry I |
| **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 | 2 - Métodos | Obligatory |

**Coordination**

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

# SUMMARY

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.

# 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 understand the basic principles of "ab initio" methodologies and Density Functional Theory
- 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 adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
- 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 are able to discern between the different existing methods and know how to select the most appropriate method for each problem.

## 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.

## DESCRIPTION OF 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)

## WORKLOAD

| ACTIVITY | Hours | % To be attended |
|---|---|---|
| Theory classes | 20,00 | 100 |
| Seminars | 15,00 | 100 |
| **TOTAL** | **35,00** | |

## TEACHING METHODOLOGY

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.

## 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:

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

### 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.
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## REFERENCES

### Basic

- 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. Zaleny, 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