# COURSE DATA

| Data Subject | |
|---|---|
| **Code** | 44990 |
| **Name** | Modelling electronic structure |
| **Cycle** | Master's degree |
| **ECTS Credits** | 6.0 |
| **Academic year** | 2021 - 2022 |

**Study (s)**

| Degree | Center | Acad. year | Period |
|---|---|---|---|
| 2245 - Master's Degree Erasmus Mundus in Theoretical Chemistry and Computational M | Faculty of Chemistry | 2 | Annual |

**Subject-matter**

| Degree | Subject-matter | Character |
|---|---|---|
| 2245 - Master's Degree Erasmus Mundus in Theoretical Chemistry and Computational M | 4 - Optativas de segundo | Optional |

**Coordination**

| Name | Department |
|---|---|
| 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

### 2245 - Master's Degree Erasmus Mundus in Theoretical Chemistry and Computational M

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- 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 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 organized at work demonstrating that they know how to manage their time and resources.
- Students have the ability of analyze and synthesize in such a way that they can understand, interpret and evaluate the relevant information by assuming with responsibility their own learning or, in the future, the identification of professional exits and employment fields.
- Students are able to discern between the different existing methods and know how to select the most appropriate method for each problem.
- Students understand and manage the mathematical tools required for the development of theoretical chemistry both in fundamental aspects and applications.

This course will be held at the Sorbonne University of Paris, an Erasmus Mundus partner, and will introduce the study of different models, from micro to meso-scale, to deal with complex biological systems.

## WORKLOAD

| ACTIVITY | Hours | % To be attended |
|---|---|---|
| Computer classroom practice | 20,00 | 100 |
| Theory classes | 20,00 | 100 |
| Tutorials | 5,00 | 100 |
| TOTAL | 45,00 | |

## TEACHING METHODOLOGY

## English version is not available

## EVALUATION

### Regular assessment

The final mark for the course will be based on: 20% final exam of the course and 80% corresponding to the delivery of a report of exercises proposed by the professor.

### Resit

The grade will be based on the report of the proposed exercises.

## REFERENCES

### Basic

- Engel, T. y Reid, P., Quantum Chemistry and Spectroscopy, Prentice Hall, 2006.

  Levine, I., Quantum Chemistry, 5ª Ed., Prentice Hall, 2000.

  Foresman, J.B. y Frisch, A., Exploring chemistry with electronic structure methods, 2ª Ed., Gaussian, 1996.

## 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