

**COURSE DATA****Data Subject**

<b>Code</b>	44990
<b>Name</b>	Modelling electronic structure
<b>Cycle</b>	Master's degree
<b>ECTS Credits</b>	6.0
<b>Academic year</b>	2022 - 2023

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. year</b>	<b>Period</b>
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	Faculty of Chemistry	2	Annual

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	4 - Optativas de segundo	Optional

**Coordination**

<b>Name</b>	<b>Department</b>
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

## 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 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.

## LEARNING OUTCOMES

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
<b>TOTAL</b>	<b>45,00</b>	

**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, 5<sup>a</sup> Ed., Prentice Hall, 2000.

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