COURSE DATA

Data Subject	
Code	44990
Name	Modelling electronic structure
Cycle	Master's degree
ECTS Credits	6.0
Academic year	2022 - 2023

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

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

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.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

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.