VNIVERSITAT DE VALÈNCIA

Course Guide
44993 Master's final project

COURSE DATA

Data Subject	
Code	44993
Name	Master's final project
Cycle	Master's degree
ECTS Credits	30.0
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	6 - Master's final project	End Labour Studies

SUMMARY

Design, planning and development of an original research project.

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 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 broaden and/or acquire knowledge of the basic methods of Quantum Chemistry and evaluate its applicability in a critical way.
- Students acquire an overview of the different applications of the Theoretical Chemistry and modeling in the fields of Chemistry, Biochemistry, Materials Sciences, Astrophysics and Catalysis.
- Ser capaz de realizar una contribución a través de una investigación original que amplíe las fronteras del conocimiento en simulación Química, desarrollando un corpus sustancial, que merezca, al menos en parte, la publicación referenciada a nivel nacional.
- Students are familiar with the fundamental postulates of Quantum Mechanics necessary for a good understanding of the most common methods used in quantum chemistry
- Students handle the most common programming techniques in physics and chemistry and are familiar with the essential computational tools in these areas.
- Students are able to develop efficient programs in FORTRAN in order to use such tools in their daily work.
- Students understand the basic principles of "ab initio" methodologies and Density Functional Theory
- Students know theories and methods of calculation associated with kinetic processes and evaluate its applicability to the calculation of speed constants.

- Student are familiar with computational techniques which, based on mechanics and molecular dynamics, are the basis for designing molecules of interest in fields such as pharmacology, petrochemistry, etc.
- Students know and critically evaluate the applicability of advanced methods of quantum chemistry to quasi-generated systems, such as systems with transition metals or excited states (their spectroscopy and reactivity).
- Students know the theories and calculation methods for the study of solids and surfaces. Critical evaluation of its applicability to problems of catalysis, magnetism, conductivity, etc.
- Students know the existence of advanced computational techniques such as instruction and data channeling, superscalar and multiscalar processors, chain operations, parallel platforms, etc.
- 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 work as a team both at multidisciplinary level and with their own peers respecting the principle of equality of men and women.
- Students develop a critical thinking and reasoning and know how to communicate them in an egalitarian and non-sexist way both in oral and written form, in their own language and in a foreign language.
- Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
- 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 generate new ideas based on their own decisions.
- Students have the ability to handle the main sources of scientific information related to Theoretical Chemistry and Computational Modeling. They are able to search for relevant information in web pages of structural data, physical chemical experimental data, databases of molecular calculations, databases of scientific bibliography and scientific works.
- 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 know how to calculate partition functions and apply quantum and classical statistics to the ideal systems of interest in Chemistry.
- Students possess the necessary mathematical basis for the correct treatment of the symmetry in atoms, molecules and solids, with emphasis in the possible applications.
- 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)

English version is not available

WORKLOAD

ACTIVITY	Hours	% To be attended
Graduation project		100
*Realización del Trabajo Fin de Máster	450,00	0
Seguimiento i tutorización del Trabajo Fin de Máster	295,00	0
Presentación y defensa del Trabajo Fin de Máster	5,00	0
TOTAL	**750,00**	

TEACHING METHODOLOGY

Seminars: The Professor and the students will 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.

Oral presentations of pre-prepared topics, including discussions with other students and professors.

Guidance and supervision in the preparation of reports.

Monitoring Master Thesis.

Active participation in tasks that allow the development of communication skills.

EVALUATION

Regular assessment

100% Making of a written report about an original research work done by the student and public and oral defence of it before a court evaluator.

Resit

100% Making of a written report about an original research work done by the student and public and oral defence of it before a court evaluator.

REFERENCES

Basic

- Lectures suggested by tutor.