UNIVERSIDAD AUTÓNOMA DE MADRID

31239 - MASTER THESIS

Syllabus Information

Code - Course title: 31239 - MASTER THESIS

Degree: 616 - Máster en Química Teórica y Modelización Computacional (2013)
621 -
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional

Faculty: 104 - Facultad de Ciencias

Academic year: 2019/20

1.Course details

1.1.Content area

Master Thesis

1.2.Course nature

651 - Master Final Project
616 - Compulsory
621 - Master Final Project

1.3.Course level

651 - Máster (MECES 3)
616 - Máster (MECES 3)
621 - Máster

1.4.Year of study

616 - Máster en Química Teórica y Modelización Computacional (2013): 2
621 - : 1
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional: 2

1.5.Semester

Annual

1.6.ECTS Credit allotment

30.0

1.7.Language of instruction

English

1.8.Prerequisites

There are no prerequisites.

1.9.Recommendations

There are no recommendations.

1.10.Minimum attendance requirement

Attendance is mandatory.

1.11.Faculty data

Student's Tutor.

a. Master's Coordinators:
Sergio Díaz-Tendero: sergio.diaztendero@uam.es
Manuel Alcamí: manuel.alcami@uam.es

1.12.Competences and learning outcomes

1.12.1.Competences

BASIC AND GENERAL SKILLS
CB6 – Students possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a research context.
CB7 - Students know how to apply the acquired knowledge and their problem solving capacity in new or little known environments within broader (or multidisciplinary) contexts related to their area of study.
CB8 - Students are able to integrate knowledge and face the complexity of making judgments from information that, incomplete or limited, includes reflections on social and ethical responsibilities linked to the application of their knowledge and judgments.
CB9 - Students know how to communicate their conclusions and the knowledge and reasons that support them to specialized and non-specialized audiences in a clear and unambiguous way.
CB10 - Students possess the learning skills that allow them to continue studying in a way that will be self-directed or autonomous.
CG01 - 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.
CG02 - Students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.
CG03 - 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.
CG04 - 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.

CROSS-COMPREHENSIVE SKILLS
CT01 - Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
CT02 - Students are organized at work demonstrating that they know how to manage their time and resources.
CT03 - 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.
CT04 - Students are able to generate new ideas based on their own decisions.

SPECIFIC SKILLS
CE01- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
CE02 – Students broaden and/or acquire knowledge of the basic methods of Quantum Chemistry and evaluate its applicability in a critical way.
CE03 – 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.
CE04 - 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.
CE05 – 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.
CE06 – Students are able to make a contribution through an original research that extends the frontiers of knowledge in Chemical simulation, developing a substantial corpus that deserves, at least in part, the publication referenced at national level.
CE09 - Students understand the basis of Statistical Mechanics formulated from the collectivities.
CE10 - Students know how to calculate partition functions and apply quantum and classical statistics to the ideal systems of interest in Chemistry.
CE11 - Students possess the necessary mathematical basis for the correct treatment of the symmetry in atoms, molecules and solids, with emphasis in the possible applications.
CE12 – Students are familiar with the fundamental postulates of Quantum Mechanics necessary for a good understanding of the most common methods used in quantum chemistry.
CE13 - Students handle the most common programming techniques in physics and chemistry and are familiar with the essential computational tools in these areas.
CE14 – Students are able to develop efficient programs in FORTRAN in order to use such tools in their daily work.
CE15 – Students understand the basic principles of "ab initio" methodologies and Density Functional Theory.
CE16 - Students are able to discern between the different existing methods and know how to select the most appropriate method for each problem.
CE17 - Students understand and manage the mathematical tools required for the development of theoretical chemistry both in fundamental aspects and applications.
CE18 – Students know theories and methods of calculation associated with kinetic processes and evaluate its applicability to the calculation of speed constants.
CE19 - 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.
CE20 - 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).
CE21 – 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.
CE22 – Students know the existence of advanced computational techniques such as instruction and data channeling, superscalar and multiscalar processors, chain operations, parallel platforms, etc.
Specific skills from CE23 to CE28 are related to the optional courses module as follows:
CE23 - Students have both user-level and administrator-level knowledge of complex UNIX / Linux based computing systems. This includes day-to-day operations, security, and also scheduling Shell scripts to automate tasks with the goal of maintaining an operating system complexity calculation system with high availability.
CE24 - Students know the fundamentals of lasers and are familiar with the resolution of time-dependent problems and the treatment of states of the continuum.
CE25 - Students acquire the practical knowledge necessary to carry out studies in biochemical systems using computer simulations.
CE26 - Students are able to relate macroscopic observations carried out within the field of Chemical Kinetics with individual collisions taking place at the molecular level.
CE27 - Students are familiar with the fundamentals of the methods used to treat excited states and are able to handle the most frequently used programs for the treatment of excited states.
CE28 - Provide basic methodology for the treatment of periodic systems, crystals and polymers.

1.13.Course contents

Design, planning and development of an original research project.

1.14.Course bibliography

Lectures suggested by tutor.

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	#horas
Contact hours (minimum 33%)	300
Independent study time	450

2.2.List of training activities

Activity	# hours

Lectures	
Seminars	46
Practical sessions	
Clinical sessions	
Computer lab	
Laboratory	
Work placement	
Supervised study	4
Tutorials	20
Assessment activities	
Other	230

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.

3.Evaluation procedures and weight of components in the final grade

3.1.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.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

4.Proposed workplan