UNIVERSIDAD AUTÓNOMA DE MADRID

31236 - ADVANCED COMPUTATIONAL TECHNIQUES

Syllabus Information

Code - Course title: 31236 - ADVANCED COMPUTATIONAL TECHNIQUES

Degree: 616 - Máster en Química Teórica y Modelización Computacional (2013)
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

Advanced Computational Techniques

1.2.Course nature

Compulsory

1.3.Course level

Máster (MECES 3)

1.4.Year of study

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

1.5.Semester

Annual

1.6.ECTS Credit allotment

6.0

1.7.Language of instruction

English

1.8.Prerequisites

There are no previous prerequisites.

1.9.Recommendations

There are no recommendations.

1.10.Minimum attendance requirement

Attendance is mandatory.

1.11.Faculty data

a. Lecturer:
- Name and surname: Giovanni Granucci
- Institution: University of Pisa

b. Lecturer:
- Name and surname: Filippo De Angelis
- Institution: Institute of Molecular Science and Technologies (ISTM-CNR)

c. Lecturer:
- Name and surname: Edoardo Mosconi
- Institution: Institute of Molecular Science and Technologies (ISTM-CNR)

d. Lecturer:
- Name and surname: Stefano Evangelisti
- Institution: University Toulouse III Paul Sabatier

e. Lecturer:
- Name and surname: Dimitrios Skouteris
- Institution: Scuola Normale Superiore

f. Lecturer:
- Name and surname: Stefano Pasqua
- Institution: University of Perugia

g. Lecturer:
- Name and surname: Alessandro Moriconi
- Institution: University of Perugia

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

1.12.Competences and learning outcomes

1.12.1.Competences

BASIC AND GENERAL COMPETENCES

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.

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 COMPETENCES

CT01 - Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.

SPECIFIC COMPETENCES

CE22 – Students know the existence of advanced computational techniques such as instruction and data channeling, superscalar and multiscalar processors, chain operations, parallel platforms, etc.

1.12.2.Learning outcomes

- Either set up or recognize the Schrödinger equation for model systems in the presence of external conditions so that their resolution can be planned using computational media.
- To know how to use network-based High Performance Computation (HPC) facilities such as Grid or similar techniques.
- To know about some library of parallel computing routines and how to apply them to some kind of particular problems (e.g., magnetic systems).

1.13.Course contents

- To learn about the multi-configurational time-dependent Hartree (MCTDH) method for resolving time-dependent quantum dynamics problems.
- To focus on the transitions between different electronic states that occur without absorption or emission of photons (“radiationless transitions”).
- To learn to process of realization of Digital Learning Objects.

1.14.Course bibliography

The consultation material for all the subjects will be informed in advance on the website of the Intensive Course.

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	42
Independent study time	108

2.2.List of training activities

Activity	# hours
Lectures	32
Seminars	
Practical sessions	
Clinical sessions	
Computer lab	
Laboratory	
Work placement	
Supervised study	
Tutorials	10
Assessment activities	
Other	

Classes in computer science classroom: Teaching will be taught in a computer classroom. The classes, in two-hour sessions, will include a brief theoretical introduction, in which the teacher will explain the basic concepts and practical applications, and a practical part, in which the student will learn through the resolution of practical case.

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.

Tutoring sessions: The professor can organize either individual or group tutoring sessions about particular topics and questions raised by students.

Network teaching: All the tools available at the Moodle website (https://posgrado.uam.es) will be used (uploading of teaching materials, utilization of work team strategies, wiki, blogs, e-mail, etc.).

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

3.1.Regular assessment

The next criteria will be followed for assessment of student exercises:

- 60% Elaboration of a memory based on the exercises proposed in class.

- 40% Discussions between the student and professor in tutoring sessions and seminars about the exercises proposed in class.

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

The 13th edition of the Intensive Course of the Master in Theoretical Chemistry and Computational Modelling will be organized at the Università degli Studi di Perugia (Italy) from 3rd to 28th September 2018.

Further information of the Intensive Course, lectures, schedule on: http://www.chm.unipg.it/chimgen/mb/theo2//TCCM2018/EM-TCCM2018/EM-TCCM/Welcome.html