UNIVERSIDAD AUTÓNOMA DE MADRID

31237 - MOLECULAR DYNAMICS AND COMPUTER SIMULATION AND MODELIZATION

Syllabus Information

Code - Course title: 31237 - MOLECULAR DYNAMICS AND COMPUTER SIMULATION AND MODELIZATION

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

Chemistry and Molecular Dynamics – Simulation and Modelling

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

9.0

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: Cecilia Colleti
- Institution: University of Chieti

b. Lecturer:
- Name and surname: José M. Hermida
- Institution: University of Vigo

c. Lecturer:
- Name and surname: György Lendvay
- Institution: Hungarian Academic of Sciences

d. Lecturer:
- Name and surname: Pedro A. Enríquez
- Institution: University of La Rioja

e. Lecturer:
- Name and surname: Fermin Huarte
- Institution: University of Barcelona

f. Lecturer:
- Name and surname: Manuel Lara
- Institution: Autonomous University of Madrid

g. 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 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.

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.

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.

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.

1.12.2.Learning outcomes

- To outline the basics of the time-dependent wave-packet approach, that will be exemplified through the simulation of simple wave-packet propagations in one dimension.
- To know the fundamentals of classical Molecular Dynamics and the steps to prepare MD calculations.
- Time-dependent wavepacket approach: obtaining scattering information.
- To overview of the theories of reaction rates: The basic properties of elementary reactions as obtained from reaction kinetics experiments.
- The quasiclassical trajectory method(Principles and Applications).
- Theoretical description of collisional energy transfer.

1.13.Course contents

- Mixed quantum-classical methods in collisional dynamics.
- Intermolecular Forces, explicit solvent models and QM/MM statistical calculations.
- Reaction Rate Theory.
- The QCT method. From principles and to applications in Reaction Dynamics.
- Molecular Dynamics: Fundamentals and Gas Physisorption Simulations.
- Time-dependent wavepacket approach: obtaining scattering information.

1.14.Course bibliography

- “Introduction to quantum mechanics: a time-dependent perspective”, by David J. Tannor. 2007. University Science Books.
- "Elements of Molecular Dynamics”, by W. Smith 2014.

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	63
Independent study time	162

2.2.List of training activities

Activity	# hours
Lectures	56
Seminars	7
Practical sessions	
Clinical sessions	
Computer lab	
Laboratory	
Work placement	
Supervised study	
Tutorials	
Assessment activities	
Other	

Lecture: The Professor will deliver lectures about the theoretical contents of the course.

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.).

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.

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