VNIVERSITAT DE VALÈNCIA

Course Guide
43997 Chemical and molecular dynamics and computer modelling

COURSE DATA

Data Subject	
Code	43997
Name	Chemical and molecular dynamics and computer modelling
Cycle	Master's degree
ECTS Credits	9.0
Academic year	2020 - 2021

Study (s)

Degree	Center	Acad. year	Period
2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1	Faculty of Chemistry	2	Annual

Subject-matter

Degree	Subject-matter	Character
2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1	4 - Advanced modelling and applications	Obligatory

Coordination

Name	Department
SANCHEZ MARIN, JOSE	315 - Physical Chemistry
TUÑON GARCIA DE VICUÑA, IGNACIO NILO	315 - Physical Chemistry

SUMMARY

The 13th edition of the Intensive Course of the Master in Theoretical Chemistry and Computational Modelling will be organized at the University of Perugia from the 3rd to 28th September 2018.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

There are no pre-requisites

OUTCOMES

2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1

- 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.
- El estudiante es capaz de adaptarse a diferentes entornos culturales.
- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- 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.

2193 - M.ErasmMund en Química Teórica y Modelización Computacional

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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

DESCRIPTION OF CONTENTS

1. 1.

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.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	56,00	100
Seminars	7,00	100
Development of individual work	60,00	0
Study and independent work	66,00	0
Preparation of practical classes and problem	36,00	0
TOTAL	**225,00**	

TEACHING METHODOLOGY

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

Network teaching: All the tools available at the Moodle website (http://www.uam.es/moodle) 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.

EVALUATION

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.

REFERENCES

Basic

- Juan Andrés, J, Bertran, Eds. (several authors) Theoretical and Computational Chemistry. Fundations, Methods and Techniques. Publicacions de la Universitat Jaume I. Castellon (Spain). 2007
- F. Jensen. Introduction to Computational Chemistry, 2nd Ed. .Wiley, 2007
- A. Szabo, N. Ostlund. Modern Quantum Chemistry. Macmillan. 1982
- G. C. Schatz and M. A. Ratner, editors. Quantum Mechanics in Chemistry . Dover, New York, USA, 2002
- H.-D. Meyer, F. Gatti, and G. A. Worth, editors. M C T D H: Basic Theory, Extensions, and Applications toMultidimensional Quantum Dynamics . VCH, Weinheim, Germany, 2009
- Introduction to quantum mechanics: a time-dependent perspective, by David J. Tannor. 2007. University Science Books.
- Elements of Molecular Dynamics, by W. Smith 2014

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

English version is not available