COURSE DATA

Data Subject	
Code	43998
Name	Applications
Cycle	Master's degree
ECTS Credits	6.0
Academic year	2021 - 2022

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 3th to the 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.
- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- 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.
- El estudiante tiene capacidad de generar nuevas ideas.
- 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 introduce some basic concepts related to the quantum-mechanical modelling of solids within so-called periodic-boundary conditions

-- To provide a broad overview of the main properties of materials that can be effectively computed with state-of-the-art algorithms within the density functional theory (DFT)

--- To know some basic concepts of crystallography will be recalled to introduce direct and reciprocal lattices. The need for periodic-boundary conditions to simplify the problem and the Bloch theorem

--To calculate the photoabsorption spectrum of a series of molecules and metal clusters.

-- To analyze different methods (based on the analysis of the electron density), carried out on the electron density distribution function closely related to the square of the wavefunction, to get information about the properties of the system, through the analysis of the wavefunction

- Recognize and practice how research funding and a job.

--To overview the interdisciplinary chemistry “outside the earth” (interstellar medium)

DESCRIPTION OF CONTENTS

1. 1.-

-- Modern Trends and Challenges in High-perfomance/hight-troughput Computing.
-- Quantum Mechanical approach to Materials Science. The CRYSTAL code at work.
-- Density Functional Theory Formalism and Applications.
-- Wavefunctions and binding analysis.
-- Surface Modelling, Adsorption and Reactivity.
-- COMMUNICATION SKILLS - Looking ahead: research funding, jobs and entrepreneurship
-- NEW TRENDS IN SCIENCE - The challenging rich chemistry in the interstellar medium

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	32,00	100
Seminars	10,00	100
Development of individual work	40,00	0
Study and independent work	44,00	0
Preparation of practical classes and problem	24,00	0
TOTAL	**150,00**	

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

- 1. R. F. W. Bader, Atoms in Molecules. A Quantum Theory, Clarendon Press, Oxford, 1990.
- 2. A. D. Becke and K. E. Edgecombe, J. Chem. Phys., 1990, 92, 5397-5403.
- 3. A. Savin, R. Nesper, S. Wengert and T. F. Fäsler, Angew. Chem. Int. Ed. Engl., 1997, 36, 1808-1832.
- 4. B. Silvi and A. Savin, Nature, 1994, 371, 683-686.
- 5. A. E. Reed, L. A. Curtiss and F. Weinhold, Chem. Rev., 1988, 88, 899-926.
- 6. M. Alcamí, O. Mó and M. Yáñez, in Molecular Electrostatic Potentials: Concepts and Applications, ed. J. S. Murray and K. Sen, Elsevier, Amsterdam, 1996, vol. 3, pp. 407-456.
- 7. M. D. Sicilia, O. Mo, M. Yanez, J. C. Guillemin, J. F. Gal and P. C. Maria, Eur. J. Mass Spectrom., 2003, 9, 245-255.
- 8. E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen, W. Yang, J. Am. Chem. Soc. 2010, 132(18), 6498-6506.

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