COURSE DATA

Data Subject	
Code	44981
Name	Applied Theoretical Chemistry Laboratory
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	3 - Optativas de primero	Optional

Coordination

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

SUMMARY

English version is not available

Lección Magistral: El profesor expondrá los contenidos del curso en sesiones presenciales de dos horas basándose en los materiales docentes publicados en la plataforma Moodle.

Clases en aula de informática. La docencia se impartirá en un aula de informática. Las clases, en sesiones de dos horas, incluirán una introducción teórica breve, en la que el profesor o profesora expondrá los conceptos básicos, y aplicaciones prácticas, y una parte práctica, en la que el estudiante aprenderá a través de la resolución de casos prácticos.

Docencia en red. Se utilizará las distintas herramientas que ofrece la plataforma moodle (http://www.uam.es/moodle). Publicación de contenidos de la asignatura, herramientas de trabajo en grupo: foros de discusión y wiki, correo electrónico

Tutorías. El profesor realizará tutorías individuales o con grupos reducidos sobre cuestiones puntuales que los estudiantes puedan plantear.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

No pre-requisites

OUTCOMES

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- Students can apply the knowledge acquired and their ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study.
- Students are able to integrate knowledge and handle the complexity of formulating judgments based on information that, while being incomplete or limited, includes reflection on social and ethical responsibilities linked to the application of their knowledge and judgments.
- Students can communicate their conclusions, and the knowledge and rationale underpinning these, to specialist and non-specialist audiences, clearly and unambiguously.
- Students have the learning skills that will allow them to continue studying in a way that will be largely self-directed or autonomous.
- Students have the knowledge and understanding that provide a basis or an opportunity for originality in developing and/or applying ideas, often within a research context.
- 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 are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.
- Students are organized at work demonstrating that they know how to manage their time and resources.
- 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.

LEARNING OUTCOMES

1. Introduction to scientific research: literature searches and presentation of scientific documents.

2. Basic informatic tools: visualization tools, graphing tools and math tools.

3. Introduction to quantum chemical packages aiming at the description of the ground and excited states.

4.-Reinforce the concepts of static and dynamic correlation.

5.-Introduction to Molecular Dynamics packages.

6.-Periodic systems: basic physical concepts

7.- Introduction to packages oriented to Periodic Systems.

8. Analysis of the information relevant to the wavefunction and other properties from the outputs of the different packages.

9. To get familiar with visualization programs for the results of the different packages

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Tutorials	10,00	100
Development of individual work	30,00	0
Study and independent work	45,00	0
TOTAL	**125,00**	

TEACHING METHODOLOGY

Lecture: The Professor will deliver lectures about the theoretical contents of the course during two-hour sessions. The presentations will be based on the different materials available at the Moodle platform.

Teaching in computer room. Teaching will be conducted in a computer room. The classes, in sessions from two to four hours, will include a brief theoretical introduction, in which the teacher will present the basic concepts, followed by practical applications, in which the student will learn through the resolution of practical examples.

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.).

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

EVALUATION

Ordinary assessment

The knowledge acquired by the student will be evaluated along the course. The educational model to follow will emphasize a continuous effort and advance in training and learning.

The final student mark will be based on evaluation of a research project (proposed and supervised during in-person lessons) covering the knowledge acquired throughout the course. Class participation will also be evaluated. The next criteria will be followed for evaluation:

- 60% A report of the practices or exercises related to the subject. Of this percentage, 40% corresponds to the completion of the report and 20% classroom activities.

- 40% Discussion about the exercises, works of practices carried out in the subject, which may be in the form of an oral presentation of the report made.

Extraordinary assessment

The student will have to face a final exam, including both theory and practical exercises. The student mark will be obtained from:

- 60% from the student report,

- 40% from classroom activities

REFERENCES

Basic

- . Consulta de documentación actualizada en línea en lenguajes de programación y aplicaciones: Python: www.python.org
- B. Foreman y E. Frisch, Exploring chemistry with Electronic Structure Methods. 2nd Edition. Gaussian, Inc. Pittsburgh, 1996.
- MOLCAS v. 7.8 Users manual, Lund University, 2012.
- Charles Kittel Introduction to solid state physics
- Neil W. Ashcroft and N. David Mermin Solid state physics

- 1. Mopac manual: http://openmopac.net/manual/
- L. Sun and W. Hase, Born-Oppenheimer Direct Dynamics Classical Trajectory Simulations.
- Neil W. Ashcroft and N. David Mermin Solid state physics
- Gaussian manual www.gaussian.com