COURSE DATA

Data Subject	
Code	43992
Name	Methods of theoretical chemistry 1
Cycle	Master's degree
ECTS Credits	5.0
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	1	Annual
3156 - Theoretical Chemistry and Computational Modelling	Doctoral School	0	First term

Subject-matter

Degree	Subject-matter	Character
2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1	2 - Methods	Obligatory
3156 - Theoretical Chemistry and Computational Modelling	1 - Complementos de Formación	Optional

Coordination

Name	Department
SANCHEZ MARIN, JOSE	315 - Physical Chemistry

SUMMARY

English version is not available

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 hay requisitos previos.

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.
- El estudiante es capaz de resolver problemas y tomar decisiones.
- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- Comprender los fundamentos teóricos y prácticos de técnicas con las que puede analizar la estructura electrónica, morfológica y estructural de un compuesto.
- Students understand the basic principles of "ab initio" methodologies and Density Functional Theory
- El estudiante es capaz de discernir entre los diferentes métodos existentes y cómo seleccionar el más adecuado para cada problema.

LEARNING OUTCOMES

As a result of participating in this course, students will be able to:

- Understand the theoretical and practical bases of computational techniques used in the electronic, structural and morphological analysis of a compound and interpret the results adequately.

- Understand the basic principles of "ab initio" methods, and Density Functional Theory.

- Shed light on what method is the most appropriate for each problem, considering the differences between them.

- Demonstrate knowledge and comprehension of the facts, applying concepts, principles and theories associated with Theorical Chemistry and Computational Modelling.

DESCRIPTION OF CONTENTS

1. Ab initio Methods

- Hartree-Fock methods: RHF y UHF
- Basis functions, pseudopotentials and effective potential.
- Variational savefunction-based Electron Correlation Methods: Configuration Interaction and multiconfigurationals methods
- Moller-Plesset Perturbation Theory
- Introduction to Coupled Cluster methods.

In the part of Quantum Chemical Methods we will formulate the main theorems in which the different methodologies are based and the most important "ab initio" methods will be studied.

2. Density Functional Theory

- Preliminary concepts. Hohenberg-Kohn Theorems.
- Kohn-Sham Method.
- Density Functional Approximations (DFAs; approximations to exchange-correlation functionals)

In the Functional Density Theory section the students should understand the basis ideas in which the theory is based. The student should understand how the different correlation-exchange functionals are developed and their main features. The student should know how to select the most adequate method for a fixed problem.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	20,00	100
Seminars	15,00	100
Development of individual work	30,00	0
Study and independent work	40,00	0
Preparation of practical classes and problem	20,00	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.

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.

Online Seminars: After the lecturing period, online seminars between the Professor and the students will be arranged at the *virtual classroom* in order to 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.

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 exercises that must be done during the course. The next criteria will be followed for assessment of student exercises:

- 70% from the student report,
- 30% from discussions between the student and professor in tutoring sessions and seminars.

Extraordinary assessment

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

- 70% from the final exam,
- 30% from the individual work.

REFERENCES

Basic

- - Helgaker, T., Jørgensen, P., Olsen, J.; Molecular Electronic-Structure Theory. John Wiley & Sons Ltd, 2000.
- Szabo, A., Ostlund, N. S.; Modern Quantum Chemistry. Introduction to Advanced Electronic Structure Theory. McGraw-Hill, 1989
- Roos, B. Editor; Lecture notes in quantum chemistry: European summer school in quantum chemistry. Springer-Verlag 1994. Chapters on CC, CI, MCSCF, calibration.
- Linear-Scaling Techniques in Computational Chemistry and Physics. Zaleny, R.; Papadopoulos, M.G.; Mezey, P.G.; Leszczynski, J. (Eds.). Springer (Berlin) 2011.
- A Chemist's Guide to Density Functional Theory. W. Koch and M.C. Holthausen, Wiley-VCH, 2001
- Density-Functional Theory of Atoms and Molecules. R.G. Parr and W. Yang, Oxford University Press, New York, 1989
- Electronic Structure. R.M. Martin, Cambridge University Press, Cambridge, 2004

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