COURSE DATA

Data Subject	
Code	44976
Name	Deepening of methods of theoretical chemistry
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

The goal is to provide a deeper knowledge of wave function and density functional methods to descriobe electronic structure

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

OUTCOMES

2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus

- 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 understand the basic principles of "ab initio" methodologies and Density Functional Theory
- 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 understand the theoretical and practical bases of computational techniques with which they can analyze the electronic, morphological and structural structure of a compound and interpret the results adequately.
- Students are able to discern between the different existing methods and know how to select the most appropriate method for each problem.

LEARNING OUTCOMES

The purpose of this course is to provide students a deeper insight into the methods used in theoretical chemistry, with particular emphasis on students to deepen in the following aspects:

- Knowledge of the specific problems of quantum mechanical methods applied to large systems.
- Understanding and ability to discriminate between different analytical methods useful for solving one-

electron and two-electron molecular integrals depending on the nature of these integrals.
- Understanding of the essential features of the numerical methods used to solve molecular integrals. As a result, ability to change parameters for each method in order to solve practical problems and to choose the most appropriate method for a
specific problem.
- Detailed knowledge of some methods that accelerate the process of solving selfconsistent equations.
- Knowledge of the fundamentals of local methods to evaluate the correlation energy.
- Detailed knowledge of the methodological grounds of most common methods
- Ability to estimate computational cost and scaling
- Estimation of the magnitude of the errors associated
- Ability to determine their applicability to a specific problem.
-Density functional theory: advanced math, functionals and recent concepts.
-Challenges for density functional theory.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	20,00	100
Seminars	15,00	100
TOTAL	**35,00**	

TEACHING METHODOLOGY

Lecture: The Professor will deliver face-to-face, or, online video 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 (https://posgrado.uam.es) 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

El aprendizaje y la formación adquirida por el estudiante serán evaluados a lo largo de todo el curso, intentando que el estudiante avance de forma regular y constante en la asimilación de los contenidos de la asignatura.
La nota final de la asignatura se basará en los ejercicios, trabajos y discusión de los mismos que se irá realizando durante el curso. Dichos trabajos se puntuarán en base a los siguientes porcentajes:

-90 % la memoria presentada por el estudiante.
-10 % la discusión que sobre la misma se realice con el profesor en tutorías y seminarios.

Resit

Contents that were failed in the ordinary assessment will be re-assessed through written reports focused on those contents. They will be done personally by the student in a fixed time period.

REFERENCES

Basic

- F. Jensen, Introduction to Computational Chemistry, John Wiley & Sons, Chichester, 1999

D. B. Cook, Handbook of Computational Quantum Chemistry, Oxford University Press, Oxford, 1998

A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover publications Mineola, 1996

T. Helgaker and P. R. Taylor, Gaussian basis sets and molecular integrals, World Sientific, Singapore, 1995

D. R. Yarkony (Ed.) Direct Methods in Electronic Structure Theory, Vol. part I, World Scientific, Sinapore, 1995

Helgaker, T., Jørgensen, P., Olsen, J.; Molecular Electronic-Structure Theory. John Wiley & Sons Ltd, 2000.

Roos, B. Editor; Lecture notes in quantum chemistry: European summer school in quantum chemistry. Springer-Verlag 1994. Chapters on CC, CI, MCSCF, calibration.

Robert G. Parr and Weitao Yang: Density Functional Theory for Atoms and Molecules. Oxford University Press, 1994.

A. J. Cohen, P. Mori-Sánchez and W. Yang, Challenges for Density Functional Theory, Chemical

Reviews, 112, 208 (2012).

Dreizler and Gross, Density Functional Theory: An approach to the quantum many-body problem, Springer-Verlag (1990)

Axel Becke, Perspective: Fifty years of density-functional theory in chemical physics J. Chem. Phys. 140, 18A301 (2014)