VNIVERSITAT DE VALÈNCIA

Course Guide
43999 Further study of methods of theoretical chemistry

COURSE DATA

Data Subject	
Code	43999
Name	Further study of methods of theoretical chemistry
Cycle	Master's degree
ECTS Credits	5.0
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	1	Annual

Subject-matter

Degree	Subject-matter	Character
2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1	5 - Optional subject area	Optional

Coordination

Name	Department
SANCHEZ MARIN, JOSE	315 - Physical Chemistry
TUÑON GARCIA DE VICUÑA, IGNACIO NILO	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 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.
- El estudiante es capaz de resolver problemas y tomar decisiones.
- El estudiante es organizado en el trabajo y sabe gestionar el tiempo.
- 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

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 self-consistent 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.

DESCRIPTION OF CONTENTS

1. Topics

- One-electron molecular integrals. Properties and analytical and numerical techniques.
- Two-electron molecular integrals. Screening, direct methods, decomposition techniques. Pseudospectral methods. Use of multipolar expansion.
- SCF Equations. Convergence. Methods adapted to sparse matrices.
- Efficiency of the method and scaling. Computational Cost.

- Introduction to electron correlation.
- Wavefunction-based methods:
Configuration Interaction
Coupled Cluster
Perturbation theory. MPn methods
Multireference methods
- Basis sets for electron correlation
- Introduction to explicitly correlated methods.
- Local methods for electron correlation.
- Intermolecular systems. Interaction energy partitioning methods.

-Density Functional Theory (DFT)
- Exchange-correlation functional development: from LDA, GGA, hybrids to recent ideas
- Exact conditions, adiabatic connection and other approaches

-Kohn-Sham eigenvalues and the OEP method
-Extension of DFT to fractional particle numbers
-Time dependent DFT: linear response and explicit time propagation
-Challenges for currently used approximations in DFT: strong correlation
-The exact energy functional of DFT

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:

- 90% from the student report,
- 10% from discussions between the student and professor in tutoring sessions and seminars.

Extraordinary assessment

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)

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