UNIVERSIDAD AUTÓNOMA DE MADRID

32529 - DEEPENING THE THEORETICAL CHEMISTRY METHODS

Syllabus Information

Code - Course title: 32529 - DEEPENING THE THEORETICAL CHEMISTRY METHODS

Degree: 616 - Máster en Química Teórica y Modelización Computacional (2013)
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional

Faculty: 104 - Facultad de Ciencias

Academic year: 2019/20

1.Course details

1.1.Content area

Deepening in Methods of Theoretical Chemistry

1.2.Course nature

Optional

1.3.Course level

Máster (MECES 3)

1.4.Year of study

616 - Máster en Química Teórica y Modelización Computacional (2013): 1
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional: 1

1.5.Semester

Annual

1.6.ECTS Credit allotment

5.0

1.7.Language of instruction

English

1.8.Prerequisites

There are no previous prerequisites

1.9.Recommendations

There are no recommendations.

1.10.Minimum attendance requirement

Attendance is mandatory

1.11.Faculty data

a. Course coordinator

-Name and Surname: Marcos Mandado (Coordinator)

-Email: mandado@uvigo.es

-Institution: University of Vigo

b.- Lecturer

-Name and Surname: Paula Mori

-Email: paula.mori@uam.es

-Institution: Autonomous University of Madrid

c.- Lecturer

-Name and Surname: Ramón López Rodríguez

-Email: rlopez@uniovi.es

-Institution: University of Oviedo

d. Master's Coordinator

Sergio Díaz-Tendero: sergio.diaztendero@uam.es

Manuel Alcamí: manuel.alcami@uam.es

NOTE: The complete updated teaching team is published on the center's website.

1.12.Competences and learning outcomes

1.12.1.Competences

These learning objectives contribute to provide the following skills for the students:

BASIC AND GENERAL SKILLS

CB6 – To possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a research context.

CB7 – That students know how to apply the acquired knowledge and their ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their area of study.

CB8 – That students are able to integrate knowledge and face the complexity of making judgments from information that, incomplete or limited, includes reflections on the social and ethical responsibilities linked to the application of their knowledge and judgments.

CB9 – That students know how to communicate their conclusions and the knowledge and ultimate reasons that sustain them to specialized and non-specialized audiences in a clear and unambiguous way.

CB10 – That students have the learning skills that allow them to continue studying in a way that will be largely self-directed or autonomous.

CG01 – That students are able to promote, in academic and professional contexts, technological and scientific advancement 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 people with disabilities, and c) the values of a culture of peace and democratic values.

CG02 – That students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.

TRANVERSAL SKILLS

CT02 – That students are organized at work demonstrating that they know how to manage the time and resources available.

SPECIFIC SKILLS

CE01- Students demonstrate their knowledge and understanding of the facts by applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.

CE04 - To understand the theoretical and practical foundations of Computational techniques with which they can analyze the electronic, morphological and structural structure of a compound and properly interpret the results.

CE15 – To understand the basic principles of "ab initio" methodologies and Density Functional Theory.

CE16 - Students are able to discern between the different existing methods and know how to select the most appropriate method for each problem.

1.12.2.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.

1.13.Course contents

- 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 and fractional spins: delocalization error and static correlation error
-Time dependent DFT: linear response and explicit time propagation
-Challenges for currently used approximations in DFT: strong correlation
-The exact energy functional of DFT

1.14.Course bibliography

-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 manybody problem, Springer-Verlag (1990).
-Axel Becke, Perspective: Fifty years of density-functional theory in chemical physics J. Chem. Phys. 140, 18A301 (2014).

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

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Contact hours (minimum 33%)	35
Independent study time	90

2.2.List of training activities

Activity	# hours
Lectures	20
Seminars	15
Practical sessions	
Clinical sessions	
Computer lab	
Laboratory	
Work placement	
Supervised study	
Tutorials	
Assessment activities	
Other	

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.

3.Evaluation procedures and weight of components in the final grade

3.1.Regular assessment

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.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

3.2.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.

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

4.Proposed workplan

Please check the official schedule published on the Master's website.