



32531 - LABORATORY IN APPLIED THEORETICAL CHEMISTRY

Syllabus Information

Code - Course title: 32531 - LABORATORY IN APPLIED THEORETICAL CHEMISTRY

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

Applied Theoretical Chemistry Laboratory

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.

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1.10. Minimum attendance requirement

Attendance is mandatory.

1.11. Faculty data

a. Subject's coordinator:

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- Department: Chemistry
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b. Lecturer:

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- Institution: Universidad Autónoma de Madrid
- Department: Chemistry

c. Lecturer:

- Name and surname: Etienne Plesiat
- Email: etienne.plesiat@uam.es
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d. Lecturer:

- Name and surname: Michele Pisarra
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e. Lecturer:

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f. Master's coordinators:

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

1.12. Competences and learning outcomes

1.12.1. Competences

BASIC AND GENERAL COMPETENCES

CB6 – Students 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 - Students know how to apply the acquired knowledge and their problem solving capacity in new or little known environments within broader (or multidisciplinary) contexts related to their area of study.

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

CB9 - Students know how to communicate their conclusions and the knowledge and reasons that support them to specialized and non-specialized audiences in a clear and unambiguous way.

CB10 - Students possess the learning skills that allow them to continue studying in way that will be self-directed or autonomous.

CG01 - 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.

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

CROSS-COMPREHENSIVE COMPETENCES

CT02 - Students are organized at work demonstrating that they know how to manage their time and resources.

CT03 - 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.

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1.12.2.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. Analysis of the information relevant to the wavefunction and other properties from the output of these programs.
5. Reinforce the concepts of static and dynamic correlation.
6. Get familiar with molecular orbital visualization programs
7. Periodic systems: basic physical concepts
8. Get familiar with periodic boundary conditions codes.

1.13.Course contents

1. Basic tools for scientific work: : plotting tools (xmgrace), reference managers (Mendeley, BibTeX), document preparation with LaTeX (text, equations, figures, tables and bibliography) .
2. Brief introduction to Python programing.
3. Introduction to conventional quantum chemistry programs: Gaussian, Mopac and Molcas
4. Programs for dynamics simulations: Venus
5. Periodic boundary conditions codes: VASP
6. Programs for result visualization: Gview, Molden.

1.14.Course bibliography

1. Consulta de documentación actualizada en línea en lenguajes de programación y aplicaciones: Python: www.python.org
2. J. B. Foreman y E. Frisch, Exploring chemistry with Electronic Structure Methods. 2nd Edition. Gaussian, Inc. Pittsburgh, 1996.
3. MOLCAS v. 7.8 Users' manual, Lund University, 2012.
4. Mopac manual: <http://openmopac.net/manual/>
5. L. Sun and W. Hase, Born-Oppenheimer Direct Dynamics Classical Trajectory Simulations.
6. Charles Kittel Introduction to solid state physics.
7. Neil W. Ashcroft and N. David Mermin Solid state physics.
8. Gaussian manual www.gaussian.com

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	50
Independent study time	75

2.2.List of training activities

Activity	# hours
Lectures	
Seminars	
Practical sessions	40
Clinical sessions	
Computer lab	
Laboratory	
Work placement	
Supervised study	
Tutorials	10

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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.

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 (<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

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

3.1.Regular 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.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

3.2.Resit

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.

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

4.Proposed workplan

Learning topic	Lecturer
Introduction to scientific research	1
Computer tools	2 and 12
Quantum Chemistry Software: Gaussian, Mopac	3
Quantum Chemistry Software: Molcas	4, 5 and 6
Dynamics software: Venus	7 and 8

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Periodic systems software: VASP

9, 10 and 11

Please, check the official schedule posted on the master website.

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