UNIVERSIDAD AUTÓNOMA DE MADRID

31238 - APPLICATIONS

Syllabus Information

Code - Course title: 31238 - APPLICATIONS

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

Applications

1.2.Course nature

Compulsory

1.3.Course level

Máster (MECES 3)

1.4.Year of study

616 - Máster en Química Teórica y Modelización Computacional (2013): 2
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional: 2

1.5.Semester

Annual

1.6.ECTS Credit allotment

6.0

1.7.Language of instruction

English

1.8.Prerequisites

There are no prerequisites.

1.9.Recommendations

There are no recommendations.

1.10.Minimum attendance requirement

Attendace is mandatory.

1.11.Faculty data

a. Professor:
- Name and Surname: Osvaldo Gervasi.
- Institution: University of Perugia.

b. Professor:
- Name and Surname: Jefferson Maul.
- Institution: University of Turín.

c. Professor:
- Name and Surname: Alessandro Erba.
- Institution: University of Turín.

d. Professor:
- Name and Surname: Mauro Stener.
- Institution: University of Triste.

e. Professor:
- Name and Surname: Manuel Yáñez.
- Institution: Autonomous University of Madrid.

f. Professor:
- Name and Surname: Albert Rimola.
- Institution: Autonomous University of Barcelona.

g. Professor:
- Name and Surname: Antonio Laganà.
- Institution: Master-UP.

h. Professor:
- Name and Surname: Cecilia Ceccarelli.
- Institution: Institute of Planetology and Astrophysics of Grenoble

i. Master's Coordinators:

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

Manuel Alcamí: manuel.alcami@uam.es

NOTE: The complete updated teaching team is published on the school'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 – 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 a 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.
CG04 - Students develop a critical thinking and reasoning and know how to communicate them in an egalitarian and non-sexist way both in oral and written form, in their own language and in a foreign language.

CROSS-COMPREHENSIVE SKILLS
CT01 - Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
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.
CT04 - Students are able to generate new ideas based on their own decisions.

SPECIFIC SKILLS
CE01- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
CE03 – Students acquire an overview of the different applications of the Theoretical Chemistry and modeling in the fields of Chemistry, Biochemistry, Materials Sciences, Astrophysics and Catalysis.

1.12.3.Course objectives

-To introduce some basic concepts related to the quantum-mechanical modelling of solids within so-called periodic-boundary conditions.
-To provide a broad overview of the main properties of materials that can be effectively computed with state-of-the-art algorithms within the density functional theory (DFT).
-To know some basic concepts of crystallography will be recalled to introduce direct and reciprocal lattices. The need for periodic-boundary conditions to simplify the problem and the Bloch theorem.
-To calculate the photoabsorption spectrum of a series of molecules and metal clusters.
-To analyze different methods (based on the analysis of the electron density), carried out on the electron density distribution function closely related to the square of the wavefunction, to get information about the properties of the system, through the analysis of the wavefunction.
-Recognize and practice how research funding and a job.
-To overview the interdisciplinary chemistry “outside the earth” (interstellar medium).

1.13.Course contents

-Modern Trends and Challenges in High-perfomance/hight-troughput Computing.
-Quantum Mechanical approach to Materials Science. The CRYSTAL code at work.
-Density Functional Theory Formalism and Applications.
-Wavefunctions and binding analysis.
-Surface Modelling, Adsorption and Reactivity.
-Communications Skills - Looking ahead: research funding, jobs and entrepreneurship.
-New Trends in Science - The challenging rich chemistry in the interstellar médium.

1.14.Course bibliography

1. R. F. W. Bader, Atoms in Molecules. A Quantum Theory, Clarendon Press, Oxford, 1990.
2. A. D. Becke and K. E. Edgecombe, J. Chem. Phys., 1990, 92, 5397-5403.
3. A. Savin, R. Nesper, S. Wengert and T. F. Fässler, Angew. Chem. Int. Ed. Engl., 1997, 36, 1808-1832.
4. B. Silvi and A. Savin, Nature, 1994, 371, 683-686.
5. A. E. Reed, L. A. Curtiss and F. Weinhold, Chem. Rev., 1988, 88, 899-926.
6. M. Alcamí, O. Mó and M. Yáñez, in Molecular Electrostatic Potentials: Concepts and Applications, ed. J. S. Murray and K. Sen, Elsevier, Amsterdam, 1996, vol. 3, pp. 407-456.
7. M. D. Sicilia, O. Mo, M. Yanez, J. C. Guillemin, J. F. Gal and P. C. Maria, Eur. J. Mass Spectrom., 2003, 9, 245-255.
8. E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen, W. Yang, J. Am. Chem. Soc. 2010, 132(18), 6498-6506.

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

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Contact hours (minimum 33%)	42
Independent study time	108

2.2.List of training activities

Activity	# hours
Lectures	32
Seminars	10
Practical sessions	
Clinical sessions	
Computer lab	
Laboratory	

Work placement	
Supervised study	
Tutorials	
Assessment activities	
Other	

Lecture: The Professor will deliver lectures about the theoretical contents of the course.

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.).

Seminars: The Professor and the students will 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.

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 next criteria will be followed for assessment of student exercises:
- 60% Elaboration of a memory based on the exercises proposed in class.
- 40% Discussions between the student and professor in tutoring sessions and seminars about the exercises proposed in class.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

4.Proposed workplan

The 13th edition of the Intensive Course of the Master in Theoretical Chemistry and Computational Modelling will be organized at the Università degli Studi di Perugia (Italy) from 3rd to 28th September 2018.

Further information of the Intensive Course, lectures, schedule on:
http://www.chm.unipg.it/chimgen/mb/theo2//TCCM2018/EM-TCCM2018/EM-TCCM/Welcome.html