31235 - ADVANCED THEORIES IN ELECTRONIC STRUCTURE AND CONDESED MATTER

Syllabus Information

Code - Course title: 31235 - ADVANCED THEORIES IN ELECTRONIC STRUCTURE AND CONDESED MATTER

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

Advanced Electronic Structure and Condensed Matter Theory

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

9.0

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. Lecturer:
- Name and surname: Marzio Rosi
- Institution: University of Perugia

b. Lecturer:
- Name and surname: Coen de Graaf
- Institution: University of Groningen

c. Lecturer:
- Name and surname: Remco Havenith
- Institution: University of Groningen

d. Lecturer:
- Name and surname: Jaime Suarez
- Institution: University of Milan

e. Lecturer:
- Name and surname: Alfredo Sánchez
- Institution: University of Valencia

f. Lecturer:
- Name and surname: Inmaculada Cuesta
- Institution: University of Valencia

g. Lecturer:
- Name and surname: Leonardo Belpassi
- Institution: Institute of Molecular Science and Technologies (ISTM-CNR)

h. Lecturer:
- Name and surname: Ivan Carnimeo
- Institution: International School for Advanced Studies

i. Master's coordinators:
- Manuel Alcamí. manuel.alcami@uam.es
- 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 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 COMPETENCES

CT01 - Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.

SPECIFIC COMPETENCES

CE20 - Students know and critically evaluate the applicability of advanced methods of quantum chemistry to quasi-generated systems, such as systems with transition metals or excited states (their spectroscopy and reactivity).

CE21 – Students know the theories and calculation methods for the study of solids and surfaces. Critical evaluation of its applicability to problems of catalysis, magnetism, conductivity, etc

1.12.2.Learning outcomes

- To familiarize the students with the possibilities that coupled cluster offers for the computation of a variety of molecular properties, which essentially represent the answer of the molecular system to an electromagnetic perturbation
- To learn the theoretical basis of the methods, providing insights about the plane wave-pseudo potential method and Fast Fourier Transform techniques.
- To calculate, using DFT methods, of molecular properties of large systems, both for molecules and materials
- To obtain a theoretical description of the electronic structure that can be used to interpret experimental data, predict interesting phenomena and/or develop new theoretical concepts
- To introduce to Valence Bond (VB) theory
- To learn how to interpret the results of different Valence Bond calculations using different orbital models
- To learn theoretical and computational tools for solving the Quantum Molecular Dynamics in Nuclear Vibrational Spectroscopy

1.13.Course contents

- Introduction to computational chemistry: density functional theory for geometry optimizations and coupled cluster approach for energies.
- Advanced electron structure theory related with the post Hartree-Fock methods. Electronic Excited States.
- Introduction to Valence Bond Theory.
- Quantum dynamics for Nuclear Vibrational Spectroscopy.
- Determination of molecular properties in the coupled cluster approach.
- Relativistic quantum chemistry.
- Modelling large molecular systems with plane waves basis sets.

1.14.Course bibliography

[1] Introduction to quantum mechanics, David J. Tannor, University Science Books (2007).

[2] A method for solving the molecular Schrödinger equation in Cartesian coordinates via angular momentum projection operators. J. Suarez, S. Stamatiadis, L. Lathouwers, S.C. Farantos, Comp. Phys. Comm. 180, p225 (2009).

[3] Quantum Molecular Dynamics on Grids, R. Kosloff, Dynamics of Molecules and Chemical Reactions (editors R. E. Wyatt and J. Z. H. Zhang), CRC Press (1996).

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	64
Independent study time	161

2.2.List of training activities

Activity	# hours
Lectures	56
Seminars	8
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