VNIVERSITAT DE VALÈNCIA

Course Guide
43995 Advanced theory of electronic structure and condensed matter

COURSE DATA

Data Subject	
Code	43995
Name	Advanced theory of electronic structure and condensed matter
Cycle	Master's degree
ECTS Credits	9.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1	Faculty of Chemistry	2	Annual

Subject-matter

Degree	Subject-matter	Character
2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1	3 - Advanced aspects	Obligatory

Coordination

Name	Department
SANCHEZ MARIN, JOSE	315 - Physical Chemistry
TUÑON GARCIA DE VICUÑA, IGNACIO NILO	315 - Physical Chemistry

SUMMARY

The 12th edition of the Intensive Course of the Master in Theoretical Chemistry and Computational Modeling will take place at the University of Valencia from September 4 to September 30, 2017.

Web: http://www.icmol.es/EMTCCM2017/

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 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.
- Know a foreign language.
- 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.
- 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).
- 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.
- Students know the existence of advanced computational techniques such as instruction and data channeling, superscalar and multiscalar processors, chain operations, parallel platforms, etc.

2193 - M.ErasmMund en Química Teórica y Modelización Computacional

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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

DESCRIPTION OF CONTENTS

1. 1. Advanced Electronic Structure Theory

-- 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.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	56,00	100
Seminars	8,00	100
TOTAL	**64,00**	

TEACHING METHODOLOGY

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

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.).

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.

EVALUATION

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.

REFERENCES

Basic

- [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)