# COURSE DATA

| Data Subject | |
|---|---|
| **Code** | 43996 |
| **Name** | Advanced computational techniques |
| **Cycle** | Master's degree |
| **ECTS Credits** | 6.0 |
| **Academic year** | 2022 - 2023 |

**Study (s)**

| Degree | Center | Acad. year | Period |
|---|---|---|---|
| 2184 - Master's Degree in Theoretical Chemistry and Computational Modelling | Faculty of Chemistry | 2 | Annual |

**Subject-matter**

| Degree | Subject-matter | Character |
|---|---|---|
| 2184 - Master's Degree in Theoretical Chemistry and Computational Modelling | 3 - Advanced aspects | Obligatory |

**Coordination**

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

# SUMMARY

The 13th edition of the Intensive Course of the Master in Theoretical Chemistry and Computational Modelling will be organized at the University of Perugia from 3rd to 28th September 2018.

# PREVIOUS KNOWLEDGE

**Relationship to other subjects of the same degree**

There are no specified enrollment restrictions with other subjects of the curriculum.

### Other requirements

There are no prerequisites

## COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

### 2184 - Master's Degree in Theoretical Chemistry and Computational Modelling

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- 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.
- El estudiante es capaz de adaptarse a diferentes entornos culturales.
- El estudiante debe ser capaz de mantener una conversación en una lengua extranjera, normalmente inglés, y se expresa correctamente tanto en forma oral como escrita.
- 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 - Master's Degree Erasmus Mundus in Theoretical Chemistry and Computational M

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.

- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- 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.
- 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.
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## LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

-Either set up or recognize the Schodinger equatio for model systems in the presence of external condiitions so that their resolution can be planned using computational media.

-To know how to use network-based High Performance Computation (HPC) facilities such as Grid or similar techniques.

-To know about some library of parallel computing routines and how to apply them to some kind of particular problems (e.g., magnetic systems)

## DESCRIPTION OF CONTENTS

### 1. 1.

-- To learn about the multi-configurational time-dependent Hartree (MCTDH) method for resolving time-dependent quantum dynamics problems
--- To focus on the transitions between different electronic states that occur without absorption or emission of photons (radiationless transitions)
-- To learn to process of realization of Digital Learning Objects

## WORKLOAD

| ACTIVITY | Hours | % To be attended |
|---|---|---|
| Theory classes | 32,00 | 100 |
| Tutorials | 10,00 | 100 |
| Development of individual work | 35,00 | 0 |
| Study and independent work | 50,00 | 0 |
| Preparation of practical classes and problem | 23,00 | 0 |
| **TOTAL** | **150,00** | |

## TEACHING METHODOLOGY

**Classes in computer classroom:** Teaching is conducted in a computer room. Classes in sessions of two hours, include a brief theoretical introduction in which the teacher sets out the basic concepts and practical applications, and a practical part, in which the student will learn through solving practical cases.

**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

- W. Schattke and R. Diez, Quantum Monte Carlo Programming, Wiley 2013.
- J. Singh, Electronic and optoelectronic properties of semiconductor structures, Cambridge University Press 2003.
- A. Costantini, S. Tasso, O. Gervasi (2009). Visualization and Web Services for Studying Molecular Properties. in O. GERVASI, D. TANIAR, Y. MUN, A. IGLESIAS, M.L. GAVRILOVA: Selected Papers of the 2009 Internationa Conference on Computational Science and Applications IEEE Computer Society Los Alamitos, CA 222-228
- A. Lagana'; Manuali C; N. Faginas Lago; O. Gervasi; S. Crocchianti; (2009). From Computer Assisted to Grid Empowered Teaching and Learning Activities in Higher Chemistry Education, Innovative Methods of Teaching and Learning Chemistry in Higher Education, 153-190
- Appropriate bibliographycal support material for all the subjects will be included in advance on the website of the Intensive Course .