# COURSE DATA

| Data Subject | |
|---|---|
| **Code** | 44002 |
| **Name** | Solids |
| **Cycle** | Master's degree |
| **ECTS Credits** | 5.0 |
| **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 | 1 | First term |

**Subject-matter**

| Degree | Subject-matter | Character |
|---|---|---|
| 2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1 | 5 - Optional subject area | Optional |

**Coordination**

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

# SUMMARY

**English version is not available**

# PREVIOUS KNOWLEDGE

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

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

**Other requirements**

## 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 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.
- 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.
- Skills in analysis and synthesis.
- 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.
- Comprender los fundamentos teóricos y prácticos de técnicas con las que puede analizar la estructura electrónica, morfológica y estructural de un compuesto.

## LEARNING OUTCOMES

To provide to the students the basic methodology to treat pure and defective periodic systems of condensed matter dealing with the following topics: Crystallography; Electronic structure; Thermodynamics; Phase transitions; Surfaces; Heterogeneous catalysis; Structural, optical and magnetical properties of defects; Magnetism. In the course the students will receive an intensive introduction to the modelization and treatment of all these issues in solids.

# DESCRIPTION OF CONTENTS

## 1. Topics and sub-topics

1. CRYSTALLOGRAPHY
1.1 Symmetry in crystals
1.2 Crystallography computing

2. ELECTRONIC STRUCTURE
2.1 Cluster and periodic models
2.2 Computational methodologies

3. THERMODYNAMICS
3.1 Static approximation and thermal models
3.2 Phase transitions

4. CHEMICAL BONDING
4.1 Scalar field induced topologies in crystals
4.2 Microscopic decomposition of observable properties

5. AB INITIO ELECTRONIC STRUCTURE CALCULATIONS IN SOLIDS
5.1 Comparison of wave function and density functional methods
5.2 From crystallographic data basis to electronic structure calculations

6. THERMODYNAMIC PROPERTIES OF CRYSTALLINE SOLIDS
6.1 E(V) curves and the static model
6.2 Phonons in crystals

7. AB INITIO SIMULATIONS OF STRUCTURAL, THERMODYNAMIC PROPERTIES AND REACTIVITY IN SURFACES
7.1 Cluster and periodic models
7.2 Adsorption and reactivity in surfaces

8. OPTICAL PROPERTIES
8.1 Quantum chemistry and the macroscopic Maxwell equations
8.2 Applications

9. ELEMENTS OF MOLECULAR AND CRYSTALLINE MAGNETISM
9.1 Model and effective hamiltonians
9.2 Applications

## WORKLOAD

| ACTIVITY | Hours | % To be attended |
|---|---|---|
| Theory classes | 50,00 | 100 |
| Development of individual work | 30,00 | 0 |
| Study and independent work | 45,00 | 0 |
| **TOTAL** | **125,00** | |

## TEACHING METHODOLOGY

**Lecture:** The Professor will deliver 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.

**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.).

**Solving practical exercises:** Numerical problems, multiple choice questions, interpretation and information processing, evaluation of scientific publications, etc..

**Written reports:** Orientation and supervision in the preparation of written reports.

## EVALUATION

**Ordinary 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 exercises that must be done during the course. The next criteria will be followed for assessment of student exercises:

- 60% from a practical exam on the course contents and practical session,
- 20% from discussions between the student and professor in tutoring sessions and seminars.
- 20 % from writing an essay based on a scientific paper

**Extraordinary assessment**

The student will have to face a final exam, including both theory and practical exercises. The student mark will be obtained from:

- 70% from the final exam,
- 30% from the individual work.
- 30% from the individual work.

## REFERENCES

### Basic

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- [21] P. Huang, and E. A. Carter, "Advances in Correlated Electronic Structure Methods for Solids, Surfaces and Nanostructures", Ann. Rev. Phys. Chem. 59 (2008) 261.
[22] G. Pacchioni, A. M. Ferrari, A. M. Márquez, and F. Illas, "Importance of Madelung Potential in Quantum Chemical Modeling of Ionic Surfaces", J. Comput. Chem. 18 (1997) 617.
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