COURSE DATA

Data Subject	
Code	44972
Name	Symmetry in atoms, molecules and solids
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	1 - Fundamentos	Obligatory

Coordination

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

SUMMARY

The goal of this subject is to provide the students with the mathematical background necessary to adequately treat the symmetry in atoms, molecules and solids with special emphasis in posible applications.

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

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- 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.
- Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
- Students possess the necessary mathematical basis for the correct treatment of the symmetry in atoms, molecules and solids, with emphasis in the possible applications.
- Students understand and manage the mathematical tools required for the development of theoretical chemistry both in fundamental aspects and applications.

LEARNING OUTCOMES

To provide the students with the mathematical background necessary to adequately treat the symmetry in atoms, molecules and solids with special emphasis in posible applications.

DESCRIPTION OF CONTENTS

1. Group theory and symmetry

Introduction to abstract group theory
Introduction to representation theory
Matrix representations of symmetry groups
Irreducible representations

2. Symmetry in molecules

Groups and representations in quantum mechanics
Application of group theory in quantum chemistry
Rotation group SO(3)

3. Symmetry in solids

Space-group symmetry
Isotropic and anisotropic structures
Reciprocal lattice of a Bravais lattice
Application to electronic wavefunctions

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	20,00	100
Seminars	20,00	100
TOTAL	**40,00**	

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 (https://posgrado.uam.es) will be used (uploading of teaching materials, utilization of work team strategies, wiki, blogs, e-mail, etc.).

Tutoring sessions: The professor can organize either individual or group tutoring sessions about particular topics and questions raised by students.

Online Seminars: After the lecturing period, online seminars between the Professor and the students will be arranged at the *virtual classroom* in order to 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 .

EVALUATION

he 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 and tests carried out mid-semester and at the end of the course. The next criteria will be followed for assessment of student exercises:

- 50 % Symmetry in atoms and molecules
  - Resolution of problems that will be specified throughout the course. The problems will be of mixed nature, involving both practical and theoretical aspects.
- 50 % Symmetry in solids
  - 30% solution of 2 standard problems associated to the theory provided before the intensive course and to be handed out during the intensive course.
  - 20% solution of an advanced exercise using computational resources, both a program to calculate band structures and the Bilbao crystallographic server.

Resit

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.

REFERENCES

Basic

- Charles C. Pinter A Book of Abstract Algebra, Dover, (New York) 2010

Roy Mc Weeny Symmetry. An Introduction to Group Theory and its Applications, Dover (New York) 2002

Philip R. Bunker Molecular Symmetry and Spectroscopy, Academic Press (London) 1979

D.M. Bishop, Group Theory and Chemistry. Clarendon Press (New York) 1973

D. Schonland, Molecular Symmetry. An introduction to Group Theory and it uses in Chemistry, Van Nostrand 1965

M. Tinkham. Group Theory and Quantum Mechanics. MacGraw Hill (New York) 1974 Dove, Structure and Dynamics. Oxford University Press (Oxford) 2003

C. Hammond. The Basics of Crystallography and Diffraction. Oxford University Press (Oxford) 2001

C. Kittel. Introduction to Solid State Physics. Wiley (New York) 2004

N.W. Ashcroft y N.D. Mermin. Solid State Physics. Saunders College () 1976

M.S. Dresselhaus, G. Dresselhaus y A. Jorio, Group Theory: Applications to the Physics of Condensed Matter, Springer (2008)