32525 - SYMMETRY IN ATOMS, MOLECULES AND SOLIDS

Syllabus Information

Code - Course title: 32525 - SYMMETRY IN ATOMS, MOLECULES AND SOLIDS

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

Symmetry in atoms, molecules and solids.

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): 1
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional: 1

1.5.Semester

Annual

1.6.ECTS Credit allotment

5.0

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. Subject's coordinator:
- Name and surname: Pablo García Fernández
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- Department: Earth Sciences and Solid State Physics
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b. Lecturer:
- Name and surname: Ignacio Solá Reija
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c. Master's coordinators:
- Mauel Alcamí. manuel.alcami@uam.es
- Sergio Díaz-Tendero. sergio.diaztendedor@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.

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

CE11 - Students possess the necessary mathematical basis for the correct treatment of the symmetry in atoms, molecules and solids, with emphasis in the possible applications.

CE17 - Students understand and manage the mathematical tools required for the development of theoretical chemistry both in fundamental aspects and applications

1.12.2.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.

1.13.Course 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

1.14.Course bibliography

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).

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	40
Independent study time	85

2.2.List of training activities

Activity	# hours
Lectures	20
Seminars	20
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 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 .

3.Evaluation procedures and weight of components in the final grade

3.1.Regular 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 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.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

3.2.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.

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	70
Continuous assessment	30

4.Proposed workplan

Please, check the official schedule posted on the master website.