SUBJECT TEACHING GUIDE

M1561 - Symmetry in Atoms, Molecules and Solids

Master's Degree in Theoretical Chemistry and Computional Modelling

Academic year 2017-2018

1. IDENTIFYING DATA					
Degree	Master's Degree in Theoretical Chemistry and Computional Modelling			Type and Year	Compulsory. Year 1
Faculty	Faculty of Sciences				
Discipline					
Course unit title and code	M1561 - Symmetry in Atoms, Molecules and Solids				
Number of ECTS credits allocated	5	Term		Annual based	
Web	https://moodle.uam.es/course/view.php?id=29724				
Language of instruction	Spanish	English Friendly	No	Mode of delivery	Face-to-face

Department	DPTO. CIENCIAS DE LA TIERRA Y FISICA DE LA MATERIA CONDENSADA
Name of lecturer	PABLO GARCIA FERNANDEZ
E-mail	pablo.garciafernandez@unican.es
Office	Facultad de Ciencias. Planta: + 3. DESPACHO PROFESORES (3008)
Other lecturers	PERE ALEMANY I CAHNER

3.1 LEARNING OUTCOMES

- - Adquire the general and specific skills of the course's subject and the theoretical/practical knowledge described in the contents section.
  Develop the ethical, personal and interpersonal skills associated to the job.

4. OBJECTIVES

Provide the student with the mathetical base to correctly treat symmetry in atoms, molecules and solids with great emphasis on possible applications.
1. Group theory and symmetry
- Symmetry in science
- Isommetry in Euclid space
- Introduction to abstract group theory
- Introduction to representation theory
- Matrix representation of symmetry groups.
- Irreducible representations.
2. Symmetry in molecules
- Groups and representations in quantum mechanics
- Applications of group theory in quantum chemistry
3. Symmetry in solids
- Spatial groups
- Isotropic and anisotropic structures
- The reciprocal lattice of a Bravais lattice
- Application on electronic wavefunctions

6. COURSE ORGANIZATION

CONTENTS	
1	Point groups - Symmetry in molecules (Barcelona University) - Group algebra - Symmetry operations - Molecule classification - Matrix representation - Characters and classes - Irreducible representations - Rotation group
2	Spatial groups- Symmetry in solids (University of Cantabria) - Spatial gruops - Isotropic and anisotropic structures - Applications on electronic wavefunctions

7. ASSESSMENT METHODS AND CRITERIA

Description	Type	Final Eval.	Reassessn	%
Solve proposed problems (crystal symmetry)	Work	No	Yes	30,00
Solve computational problems (crystal symmetry)	Work	No	Yes	20,00
Build molecular symmetry program.	Work	No	No	30,00
Report on the code development.	Work	No	No	20,00
TOTAL				100,00

Observations

The final exam in September will contain both practical and theoretical sections and will deal with the full content of the course. The practical part will consist in the use of the various programs employed during the whole course. The score in this exam will be 70% for the theoretical part and 30% for the practical part.

Observations for part-time students

8. BIBLIOGRAPHY AND TEACHING MATERIALS

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