

## SUBJECT TEACHING GUIDE

M1561 - Symmetry in Atoms, Molecules and Solids

Master's Degree in Theoretical Chemistry and Computational Modelling

Academic year 2021-2022

| 1. IDENTIFYING DATA              |   |                  |              |                  |                    |
|----------------------------------|---|------------------|--------------|------------------|--------------------|
| Degree                           | Master's Degree in Theoretical Chemistry and Computational 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                              | <a href="https://moodle.uam.es/course/view.php?id=29724">https://moodle.uam.es/course/view.php?id=29724</a> |                  |              |                  |                    |
| Language of instruction          | Spanish   | English Friendly | Yes          | 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  | IGNACIO SOLÁ REIJA  |  |  |  |  |

### 3.1 LEARNING OUTCOMES

- Acquire 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 mathematical base to correctly treat symmetry in atoms, molecules and solids with great emphasis on possible applications.

1. Group theory and symmetry
  - Symmetry in science
  - Isometry 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) <ul style="list-style-type: none"> <li>- Group algebra</li> <li>- Symmetry operations</li> <li>- Molecule classification</li> <li>- Matrix representation</li> <li>- Characters and classes</li> <li>- Irreducible representations</li> <li>- Rotation group</li> </ul> |
| 2 | Spatial groups- Symmetry in solids (University of Cantabria) <ul style="list-style-type: none"> <li>- Spatial groups</li> <li>- Isotropic and anisotropic structures</li> <li>- Applications on electronic wavefunctions</li> </ul>   |

#### 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 |
| Solve point symmetry problems                   | Work | No          | No        | 50,00 |

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

For part-time students, deadlines will be flexible to adapt to their schedules.

## 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)