

## SUBJECT TEACHING GUIDE

G56 - Quantum Physics and the Structure of Matter II: Atoms, Molecules and Solids  
Double Degree in Physics and Mathematics  
Degree in Physics

Academic year 2021-2022

| 1. IDENTIFYING DATA              |                                                                                   |                  |                    |                  |                                          |
|----------------------------------|-----------------------------------------------------------------------------------|------------------|--------------------|------------------|------------------------------------------|
| Degree                           | Double Degree in Physics and Mathematics<br>Degree in Physics                     |                  |                    | Type and Year    | Compulsory. Year 3<br>Compulsory. Year 3 |
| Faculty                          | Faculty of Sciences                                                               |                  |                    |                  |                                          |
| Discipline                       | Subject Area: Quantum Physics and the Structure of Matter<br>Central Module       |                  |                    |                  |                                          |
| Course unit title and code       | G56 - Quantum Physics and the Structure of Matter II: Atoms, Molecules and Solids |                  |                    |                  |                                          |
| Number of ECTS credits allocated | 6                                                                                 | Term             | Semester based (1) |                  |                                          |
| Web                              |                                                                                   |                  |                    |                  |                                          |
| 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                                        |  |  |  |  |
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| Office           | Facultad de Ciencias. Planta: + 3. DESPACHO PROFESORES (3008) |  |  |  |  |
| Other lecturers  | JOSE IGNACIO GONZALEZ SERRANO                                 |  |  |  |  |

### 3.1 LEARNING OUTCOMES

- Know the quantum description of hydrogen and helium atoms and learn how to generalize it to other atoms.
- Understand the main atomic periodic properties and apply it to know the different the bonds of molecular and solid compounds.
- Know the fundamentals of the photon absorption and emission by atoms.
- Know how to find the symmetry operations and the symmetry group of a molecule or a solid.
- Relate the symmetry of an atom, a molecule or a solid with its properties.
- Understand the concept of irreducible representation and know how to use the Character Tables of molecular point groups .
- To know the fundamental approximations for the resolution of the Schrödinger equation in simple molecules .
- To understand the fundamentals and limitations of the adiabatic approach and its implications in the separation of electronic , vibrational and rotational states.
- Know how to construct the molecular orbitals diagram of simple diatomic and polyatomic molecules, using symmetry. Learn to deduce basic properties of the link.
- Understand the microscopic differences between solid , liquid and gaseous states, state changes and phase transitions.
- To know the concepts of Bravais network, motif, primitive cell, conventional cell, Wigner-Seitz cell and first Brillouin zone.
- Know how to draw them in the case of simple structures.
- To know how to analyze a Debye-Scherrer diagram of X-ray diffraction of a simple structure , studying the rules of selection and analyzing simply the intensity.
- Know and apply the Born model for the ionic bond. Know how to apply the Born-Haber method.
- Distinguish a solid insulator, semiconductor and metallic, relating the electrical conductivity to the location of the electrons and the scheme of electronic bands.
- To know the basics of basic experimental techniques for the characterization of materials (solids, liquids and gases) and for the study of their electronic and vibrational structures: mass spectrometry, atomic absorption, infrared absorption, photoelectron spectroscopy, ...

### 4. OBJECTIVES

- Obtain an overview of the microscopic constitution of matter, starting from the electronic structure of atoms, to understand why they interact to form molecules and solids.
- Learn the quantum description of multielectronic atoms: The Helium atom
- Understanding the independent particle model in multielectronic atoms and the need for antisymmetrization of the wave function, the Hartree-Fock equations and the exchange energy concept.
- Describe the states of a multielectronic atom when including spin-orbit and hyperfine interactions.
- Understand the atom-radiation interaction.
- Know how to calculate transition probabilities in electric dipolar approximation.
- To understand from the first principles the microscopic origin of the molecular bond and the intermolecular forces , understanding the similarities and differences between the ionic and covalent bonds , as well as the intermolecular interactions of van der Waals and the hydrogen bonds.
- Be able to analyze and understand the microscopic origin of many relevant macroscopic properties (molecular reactivity, electrical conductivity, thermal expansion, piezoelectricity, hardness, ...).
- Acquire and understand the basic knowledge of the structure of crystalline solids, their symmetries and their structures of electronic bands.
- Understand the concepts and foundations of theories and models of the structure of matter, their approximations and limits, as well as the orders of magnitude of the properties analyzed.
- Acquire the fundamentals of relevant materials characterization techniques (solids, liquids and gases), paying special attention to X-ray diffraction in crystalline solids.

## 6. COURSE ORGANIZATION

| CONTENTS |                                              |
|----------|----------------------------------------------|
| 1        | One electron atoms                           |
| 2        | Interactions with fields                     |
| 3        | 2-electron atoms                             |
| 4        | Multielectronic atoms                        |
| 5        | Periodic Properties                          |
| 6        | Diatomic molecules and bonding               |
| 7        | Polyatomic molecules                         |
| 8        | Rotational and vibrational molecular spectra |
| 9        | Intermolecular forces                        |
| 10       | Crystalline structure of solids              |
| 11       | Reciprocal lattice and X-ray diffraction     |
| 12       | Basic approximations in the study of solids  |
| 13       | Vibrations in solids. Dispersion curves      |

## 7. ASSESSMENT METHODS AND CRITERIA

| Description                                                                                                                                                                                                                                                                                                                                                                                                                | Type         | Final Eval. | Reassessn | %             |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------|-------------|-----------|---------------|
| Topics 1-5: Theoretical questions and practical problems                                                                                                                                                                                                                                                                                                                                                                   | Written exam | No          | Yes       | 40,00         |
| Ordinary exam: Theoretical questions and practical problems                                                                                                                                                                                                                                                                                                                                                                | Written exam | Yes         | Yes       | 9,00          |
| Extraordinary exam: Theoretical questions and practical problems                                                                                                                                                                                                                                                                                                                                                           | Written exam | Yes         | No        | 0,00          |
| Partial exam. Lessons 6-11                                                                                                                                                                                                                                                                                                                                                                                                 | Written exam | No          | Yes       | 31,00         |
| Evaluation of proposed exercises                                                                                                                                                                                                                                                                                                                                                                                           | Others       | No          | Yes       | 20,00         |
| <b>TOTAL</b>                                                                                                                                                                                                                                                                                                                                                                                                               |              |             |           | <b>100,00</b> |
| <b>Observations</b>                                                                                                                                                                                                                                                                                                                                                                                                        |              |             |           |               |
| <p>The score of partial exams (with sufficient marks) along the evaluation of selected exercises will be kept up to the ordinary exam. It is possible to take the final exam to increase the score. It will be possible to choose whether the score in the exam is also used to re-evaluate the proposed hand-outs.</p> <p>If the extraordinary exam is taken its score will be 100% of the final marks in the course.</p> |              |             |           |               |
| <b>Observations for part-time students</b>                                                                                                                                                                                                                                                                                                                                                                                 |              |             |           |               |
| The professors will take care of special cases of students at partial time dedication (Working or high level sportives, etc)                                                                                                                                                                                                                                                                                               |              |             |           |               |

## 8. BIBLIOGRAPHY AND TEACHING MATERIALS

### BASIC

- R. Eisberg y R. Resnick, Física Cuántica. Átomos, Moléculas, Sólidos, Núcleos y Partículas, (Limusa, Noriega Editores, México, 2000).
- [R. Eisberg and R. Resnick. Quantum physics of atoms, molecules, solids, nuclei, and particles, 2nd Edition (Wiley-VCH, 1985)]
- C. Kittel. Introducción a la Física del Estado Sólido (Reverté, 1993)
- [C. Kittel, Introduction to solid state physics. 8th Ed.. (Wiley, 1976)]