

27213 - Physical Chemistry II

Syllabus Information

Academic year: 2023/24

Subject: 27213 - Physical Chemistry II

Faculty / School: 100 - Facultad de Ciencias

Degree: 452 - Degree in Chemistry

ECTS: 11.0

Year: 3

Semester: Annual

Subject type: Compulsory

Module:

1. General information

The subject deals with basic contents of Quantum Chemistry and Surface Phenomena, Heterogeneous Catalysis and Electron Kinetics

The objectives of the subject are:

1. To know the fundamentals of quantum mechanics and their application in systems of interest in chemistry, among others, molecular orbital theory
2. To know the fundamental concepts of the physical chemistry of surfaces and to apply them to the study of systems of interest and to the resolution of questions and problems.
3. Introduction to the use of computer programs for the study of the electronic structure of atoms and molecules
4. To apply different experimental techniques for the study of chemical-physical phenomena that take place at interfaces

These approaches are aligned with the following Sustainable Development Goals (SDGs):

- Goal 4: Quality education
- Goal 7: Affordable and non-polluting energy
- Goal 9: Industry, Innovation and Infrastructure
- Goal 12: Responsible Production and Consumption

In order to enrol in this subject, it is necessary to have taken Physical Chemistry I.

2. Learning results

The competencies and learning outcomes are described in the verification report (https://academico.unizar.es/sites/academico.unizar.es/files/archivos/ofiplan/memorias/grado/ciencias/mv_127.pdf), Once the student has passed the subject, they is expected to:

1. Understand and handle the basic terminology of Quantum Chemistry and Physical Chemistry of Surfaces.
2. Is able to solve simple problems using the quantum-mechanical method with application in Spectroscopy.
3. Explains the structure of matter at the atomic level and learns the quantum interpretation of chemical bonding using molecular orbital theory.
4. Manages computer calculation programs for the quantum chemical study of molecules.
5. Explains the thermodynamic and kinetic aspects of processes and reactions taking place at interfaces.
6. Is able to use chemical-physical techniques in studies related to the theoretical contents of Physical Chemistry of Surfaces.

3. Syllabus

The program of the subject is divided into four blocks:

QC1. Quantum Chemistry: Fundamentals and atoms

- Introduction to Quantum Mechanics
- Mathematical Foundations and Postulates
- Quantum-mechanical study of simple systems
- The hydrogen atom.
- Approximate methods. Polyelectrolyte atoms. Atomic Spectroscopy

QC2. Quantum Chemistry: Chemical Bonding

- Introduction to molecular structure through the theory of molecular orbitals: chemical bonding

QS1. Physical Chemistry of Surfaces: Theory and problems

- Physical Chemistry of Surfaces
- Surface phenomena
- Gas-solid adsorption and heterogeneous catalysis
- The electrified interface

QS2. Physical Chemistry of Surfaces Practices

4. Academic activities

The learning process will consist of the following training activities:

1. Acquisition of theoretical knowledge (6 ECTS) in large group participative lectures.
2. Problem solving classes and seminars (2 ECTS) in small groups.
3. Practical computer classes (2 ECTS), where students will work individually.
4. Practical laboratory classes (1 ECTS). The work will be organized, as a general rule, in groups of two students.

For each thematic block, the activities are:

- QC1: 35 hours of theoretical class, 14 hours of problems and 4 hours of computer practice.
- QC2: 8 hours of theoretical class and 16 hours of computer practice.
- QS1: 17 hours of lectures and 6 hours of problems.
- QS2: 10 hours of chemical laboratory practice.

5. Assessment system

Requirements to pass the subject

To pass the subject it is necessary to pass independently, with a minimum grade of 5 points (out of 10), each of the four blocks described above: QC1, QC2, QS1 and QS2. The compensation of a single block will be admitted, if it has a minimum grade of 4 points, provided that the final grade [equation (1)] is at least 5 points. The grades of the past or compensable blocks are saved until the Second call

Completion of the computer practices is required to pass or compensate QC1 and QC2. Otherwise, a practical computer test may be taken in the first and second calls.

Evaluation activities

1. **QC1** block exam. It will be held during the examination period at the end of the first semester.
2. **QC2** block exam. It will take place at the end of the computer practices and will consist of two parts: theory and practice. In order to pass or compensate this block it is necessary to obtain a minimum grade of 3.5 out of 10 in the theory questions.
3. Evaluation of the laboratory practices of the **QS2** block by means of reports/questionnaires. It is necessary to have completed the lab practices and submitted all required reports/questionnaires.
4. On the official date of the first call, the **QS1** block exam will be held, as well as the rest of the blocks of the subject (**QC1**, **QC2** and **QS2**) that have not been passed previously. The **QS2** block exam will consist of a practical test in the laboratory and processing of the results obtained. Students may sit for the exam of any of the blocks to improve their grade.
5. On the official date of the second call, the written exam of blocks **QC1**, **QC2** and **QS1** will be held, together with a practical exam of **QS2** block.

Final grade of the subject

The final grade for the subject will be calculated with the following formula:

Final grade = QC1*0.52 + QC2*0.18 + QS1*0.21 + QS2*0.09 (equation 1)

Students who did not take any of the blocks in the first or second call will be listed in the minutes as "*No Shown*"

When, having taken the 1st or 2nd call, the requirements to pass the subject are not met, because any of the block has not been passed or compensated, the grade will be *Failed*, even if the weighted average when applying equation 1 is equal to or higher than 5 points. In this case, a numerical grade of 4.5 points will appear in the records.