Chemistry for Physicists

Code: 100147
ECTS Credits: 6

2024/2025

Degree	Type	Year
2500097 Physics	FB	1

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Teachers

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Teaching groups languages

You can view this information at the end of this document.

Prerequisites

There are no official prerequisites, however, it is highly advisable that the student has taken chemistry during high school.

Objectives and Contextualisation

The general goal of the subject is to awaken in the student interest in the phenomena of nature within the field of chemistry, that is: the study of matter from the atomistic point of view, and the awareness that this study is based on the general laws of the physical world.

At the same time, it is also intended that the knowledge acquired allows to expand the field of vision, and therefore, the job possibilities.

Partial objectives of the subject are:

1) Understand the "anomalous" behavior of electrons that leads to the concepts of quantized energy and atomic orbitals.

2) Understand chemical bonding and how molecular structure allows us to rationalize intermolecular interactions that lead to the existence of the different states of matter.

Competences

- Communicate complex information in an effective, clear and concise manner, either orally, in writing or through ICTs, and before both specialist and general publics
- Develop strategies for analysis, synthesis and communication that allow the concepts of physics to be transmitted in educational and dissemination-based contexts
- Develop the capacity for analysis and synthesis that allows the acquisition of knowledge and skills in different fields of physics, and apply to these fields the skills inherent within the degree of physics, contributing innovative and competitive proposals.
- Use critical reasoning, show analytical skills, correctly use technical language and develop logical arguments
- Work independently, have personal initiative and self-organisational skills in achieving results, in planning and in executing a project

Learning Outcomes

1. Apply knowledge of the structure of matter to explain the properties and reactivity of simple and complex substances.
2. Apply the principles of thermodynamics and kinetics in chemical processes.
3. Communicate complex information in an effective, clear and concise manner, either orally, in writing or through ICTs, in front of both specialist and general publics.
4. Identify different types of chemical reactions and determine the concentrations of the substances involved in the equilibrium.
5. Identify the factors determining the speed of chemical reactions.
6. Manage the information, planning and organization of individual and cooperative work in solving chemical problems.
7. Present and discuss with colleagues the same ideas on the nature of chemical processes studied.
8. Use critical reasoning, show analytical skills, correctly use technical language and develop logical arguments
9. Work independently, take initiative itself, be able to organize to achieve results and to plan and execute a project.

Content

Lesson 1 Background of quantum mechanics.

Waves and particles. Electromagnetic radiation. Blackbody radiation. Photoelectric effect. Wave-particle duality. Electron diffraction. Uncertainty principle. Schrödinger equation. Probabilistic interpretation of the wave function. Energy states.

Lesson 2. Atomic structure.

Resolution of the Schrödinger equation for the particle in a box model system. Solution of the Schródinger equation for the hydrogen atom. Quantum numbers and atomic orbitals. Physical meaning of orbitals. Mathematical analysis. Stern-Gerlach experiment: electronic spin. Polyelectronic atoms. Antisymmetry principle. Calculation of atomic orbitals of polyelectronic atoms. Screening. Electronic configurations. Periodic table. Periodic properties: atomic radii, ionization energy and electron affinity. Concept of electronegativity.

Lesson 3. Molecular structure I.

Molecular orbitals. LCAO method. Qualitative study of diatomic molecules. Extension to polyatomic systems. Walsh diagrams. The metallic bond. Band theory. Quantitative methods to obtain molecular orbitals. Computational chemistry.

Lesson 4. Molecular structure II.

Covalent bonding: Lewis theory. Bond forces. Bond polarity and electronegativity. Lewis acids and bases. Molecular geometry (VSEPR). Dipole moment.

Lesson 5. Intermolecular forces.

Interactions between charged molecules (ions). Ionic bonding. Interactions between polar molecules. Interactions between polar and nonpolar molecules: induced dipole moment. Interactions between nonpolar molecules. London dispersion forces. A phenomenon not entirely explained: hydrogen bonding.

Lesson 6. Structure of solids.

Aggregation states and intermolecular forces. Types of solids: covalent solids, ionic solids, metallic solids and molecular solids. Compact and non-compact crystal structures. Unit cell. Physical properties of solids. Ionic solids: Lattice energy and Born-Haber cycle.

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Problems classes	15	0.6	1, 2, 5, 8
Theory classes	30	1.2	4, 5, 8
Type: Supervised			
Preparation of theory contents	6	0.24	6, 7
Type: Autonomous			
Problem solving	39.5	1.58	1, 2, 4, 5, 6, 8
Study of theory fundamentals	50.5	2.02	6

The center of the learning process is the student's work. The student learns by working, and the mission of the teaching staff is to help him/her in this task (1) by providing information or showing him/her the sources where they can be obtained and (2) by accompanying his/her steps so that the learning process can be carried out effectively. In line with these ideas, and in accordance with the objectives of the subject, the development of the course is based on the following activities:

Theoretical classes:

The student acquires the scientific-technical knowledge of the subject by attending classes and participating in the construction of their own knowledge. In these, the explanations on the part of the teacher will alternate with posing questions and fostering discussion between the students. In order to complement them, it is necessary to study the topics of the subject. In the final classes 15 minute will be reserved so as the students may answer the survey about the course.

Classes of problems and exercises:

These sessions have a double mission, on the one hand, the scientific-technical concepts previously worked on in the theoretical classes are complemented by means of the resolution of problems. On the other hand, from the critical discussion of the exercises carried out, these classes are the natural forum in which to discuss the development of the work carried out by the student contributing the necessary knowledge to carry it out, or indicating where and how they can be acquired. The mission of the problem class is to act as a bridge between

theoretical classes and autonomous work, promoting the capacity for analysis, critical reasoning, and problem-solving.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Evidences	10%	0	0	3, 6, 7, 8, 9
Final exam	90%	3	0.12	1, 2, 8
Partial exams	90%	6	0.24	1, 2, 4, 5

In this subject, there will be a continuous evaluation. The final grade will be distributed among the following concepts:

- Evidences 10% (not recoverable)

- Partial Exams 90% (2 in total)

In order to pass the subject, the weighted mean of the two partial exams and the delivered evidences must be at least equal to 5.0. In addition, a minimum of 4 to each of the two partial exams is needed have presented all the works.

- Final examination of recovery 80%. Optional. It includes the whole subject matter, with the aim of recovering the subject or improving the final grade. The grade of the final exam will replace the grade obtained from the combination of the two partial exams. It should be noted that only 90% of the subject can be recovered, corresponding to the grade of partial examinations. The marks of the works to be delivered cannot be recovered. In order to take the final exam, the student must have taken at least 1 partial exam and all the works must have been handed in.

Non-evaluated result

A student will be considered to have obtained the non-evaluated qualification if he/she has not delivered the two partial exams nor the final exam.

SINGLE ASSESSMENT

Students who have opted for single assessment will have to take a final exam consisting of two parts: An exam where the theoretical knowledge acquired by the student will be assessed and exercises similar to those proposed as evidences to continuous assessment students where the ability to connect theory knowledge with its application to specific cases will be assessed. This final test will be carried out on the same day, time and place as the tests of the second partial of the continuous assessment modality. The student´s grade will be the one obtained from this final test.

If the grade is lower than 5 out of 10, the student has another opportunity to pass the subject through the recovery exam that will be held on the datesetby the degree coordination.

Bibliography

Most pertinent references

I.N. LEVINE, *Physical Chemistry* 6th Edition, McGraw Hill, 2009. ISBN: 978-0072538625

P. W. ATKINS *Physical Chemistry,* 8th Edition, Oxford University Press (2006) ISBN: 0-19-879285-9

J. CASABÓ, Estructura atómica y enlace químico, *Ed. Reverté*. 1997. ISBN: 84-291-7189-4

F. CENTELLES, E. BRILLAS, X. DOMÈNECH, R. M. BASTIDA, Fonaments d'estructura atòmica i de l'enllaç químic. Publicacions de la Universitat de Barcelona-Barcanova. 2002. ISBN: 9788475338064

J. M. COSTA, J. M. LLUCH, J. J. PÉREZ, Química. Estructura de la matèria. Enciclopèdia Catalana. Biblioteca Universitària. 1994. ISBN: 13: 9788477395164.

P. A. COX,Introduction to quantum theory and atomic structure, Oxford chemistry primers. 1998. ISBN: 0-19-855916-X

H. B.GRAY, Chemical bonds: an introduction to atomic and molecular structure, University Science Books. 1994. ISBN: 0-935702-35-0

Globally, any general physical chemistry book can be readily used as a reference for this general course.

Software

There is no specific software to be used in this course

Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	1	Catalan	first semester	morning-mixed
(PAUL) Classroom practices	2	Catalan	first semester	morning-mixed
(TE) Theory	1	Catalan	first semester	morning-mixed
(TE) Theory	2	Catalan	first semester	morning-mixed