COURSE DESCRIPTION

COURSE DETAILS

Title (of the course): **FÍSICA ATÓMICA Y MOLECULAR**
Code: 100515
Degree/Master: **GRADO DE FÍSICA** Year: 4
Name of the module to which it belongs: MÓDULO ESPECÍFICO
Field: AMPLIACIÓN DE FÍSICA
Character: OBLIGATORIA Duration: FIRST TERM
ECTS Credits: 6.0 Classroom hours: 60
Face-to-face classroom percentage: 40.0% Study hours: 90
Online platform: http://moodle.uco.es/moodlemap/

LECTURER INFORMATION

Name: BERENGUER ANTEQUERA, JORGE (Coordinator)
Department: FÍSICA
Area: FÍSICA ATÓMICA, MOLECULAR Y NUCLEAR
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PREREQUISITES AND RECOMMENDATIONS

Prerequisites established in the study plan

To have, at least, B1 Level in English to take this course in the bilingual group.

Recommendations

- Math and numerical methods skills up to second course level.
- Quantum Physics knowledge.
- General and specific competences up to this level.

This is a subject of the last undergraduate course. It shares many of the competences with previous courses. This means that a certain level of math and physics knowledge and skill have been attained by the students. Our goal is to fix and improve this level.

It is highly recommended to have taken previously the course "Quantum Physics II". The tools covered in that course (perturbative method, variational method, Schrödinger equation in 3d, orbital and spin angular momenta, harmonic oscillator...) are applied here in this course. Besides, it is also recommended to take (or have taken) the course "Quantum Mechanics", since the coupling of angular momenta will be often used in this course.

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INTENDED LEARNING OUTCOMES

CB1	Capacity to analyse and synthesise.
CB2	Capacity to organise and plan.
CB3	Oral and/or written communication.
CB4	Capable of information management.
CB5	Resolution of problems.
CB6	Team work.
CB8	Independent learning.
CB9	Creativity.
CE1	Knowledge and comprehension of phenomena and the most important physical theories.
CE2	Capacity to estimate orders of magnitude to interpret different phenomena.
CE5	Capacity to model complex phenomena, translating a physical problem into mathematical lanaguage.
CE7	Capacity to transmit knowledge in a clear manner both in educational and in non-educational environments.
CE8	Capacity to use computing tools to resolve and model problems and to present the results.

OBJECTIVES

Study of the electronic structure of many-electron atoms (mean field model and variational approximation) and understanding of its role in the periodic properties of the elements. Multiplets. Selection rules and phenomenology of atomic spectra. Study the phenomenology of the molecular spectra and identification of excitation modes giving rise to the molecular band structure. Born-Oppenheimer approximation. Quantum foundations of chemical bonds.

CONTENT

1. Theory contents

1.- Two electron atoms
1.1.- Statement of the problem for two electron atoms.
1.2.- Solution for two electron atoms: independent particle model, perturbative and variational methods.
2.- Multielectronic atoms.
2.1.- Statement of the problem for multielectronic atoms.
2.2.- Solution for multielectronic atoms: Slater deteminants, mean field model and predictions.
2.3.- Hartree-Fock and the self-consistent method.
2.4.- Corrections to the mean field model: electrostatic multiplets, fine and hyperfine structure.

3.- Atoms in electromagnetic fields.
3.1.- Hydrogenic systems in electromagnetic fields.
3.2.- Transitions processes: absortion, stimulated emission and spotaneous emission.
3.3.- Dipole approximation.
3.4.- Rule selection for hydrogenic atoms.
3.5.- Rul selection for multielectronic atoms.

4.- Introduction to the molecular Physics.
4.1.- General description to the molecular structure.
4.2.- Born-Oppenheimer approximation for diatomic molecules.

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4.3.- electronic orbitals, rotovibrational levelsfor diatomic molecules: Harmonic Oscilator approximation, Morse potential and centrifugal distortion.
4.4.- Electronic sttructure for poliatomic molecules.

2. Practical contents

In each thematic block, some practical content will be worked on by solving problem relationships and exercises corresponding to the theoretical content. Solving more complex problems through the use of computer programs is also included.

SUSTAINABLE DEVELOPMENT GOALS RELATED TO THE CONTENT

Quality education
Gender equality
Reduced inequalities
Partnerships for the goals

METHODOLOGY

General clarifications on the methodology (optional)

In face-tp-face activities, master classes with theoretical contents will be presented, seeking and valuing the participation of the students through questions. In problem lectures (they are called Case Studies and should not be confused with the evaluation instrument with the same name), a set of problems, previously known by students, will be solved. About non-presetial hours, students will develop different activities such as: information search, bibliographical consulting, problem solving, personal study activities.

Methodological adaptations for part-time students and students with disabilities and special educational needs

The methodological adaptations for part-time students and students with disabilities will consist of:
1.- For part-time students: their assistance will be provided to the group that best suits their needs.
2.- For students with disabilities, the teaching staff will hold meetings with the affected party to establish the most appropriate adaptations for each case, following the indications of the report issued by the Inclusive Education Unit.

Face-to-face activities

Activity	Large group	Medium group	Total
Assessment activities	3	-	3
Lectures	33	-	33
Seminar	-	24	24
Total hours:	***36***	***24***	***60***

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Off-site activities

Activity	Total
Exercises	20
Group work	10
Information search	5
Reference search	5
Self-study	50
Total hours	***90***

WORK MATERIALS FOR STUDENTS

Case studies
Coursebook
Exercises and activities
Lessons summary
References

EVALUATION

Intended learning	Case study/clinical case discussion/scientific work discussion	Exams	Problem solving
CB1	X	X	X
CB2	X	X	X
CB3	X	X	X
CB4	X	X	X
CB5		X	X
CB6	X		
CB8	X		X
CB9	X	X	X
CE1		X	X
CE2	X		X
CE5		X	X
CE7	X	X	
CE8	X		X

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Intended learning	Case study/clinical case discussion/scientific work discussion	Exams	Problem solving
Total (100%)	*10%*	*80%*	*10%*
Minimum grade	*5*	*5*	*5*

(*)Minimum mark (out of 10) needed for the assessment tool to be weighted in the course final mark. In any case, final mark must be 5,0 or higher to pass the course.

Attendance will be assessed?:

No

General clarifications on instruments for evaluation:

The evaluation instrument "Exams" corresponds to 80% of the evaluation and is made up of three parts: a part of theoretical and/or application questions with multiple answers, another part of questions and short-answer exercises and a last part of questions and larger problems. The grade of the evaluation instrument "Exams" will be the arithmetic mean of the three parts described above if and only if in each of the three parts that make up the evaluation instrument "Exams", at least, the grade of 45% is reached. In the cases in which in one of the three parts (or in several of them) the corresponding quota of 45% is not achieved, the evaluation instrument "Exams" will not be taken into account in the final grade. In addition, and in any case, the minimum grade of the evaluation instrument "Exams" must be 5.0 to be considered for purposes of computing the final grade.
The other instruments are used for continuous assessment:

-- It is mandatory to turn in "Problem solving" tasks in order to pass this course. A well-argued and original solution is needed to get the maximum grade.

-- "Case study" consists of the application of computational techniques to advanced problems, using the knowledge and skills developed in this course. "Scientific work discussion" consists of the study and presentation by the students of a topic of practical interest. This will be assessed according to the level, contents and skills of the course. It is mandatory to turn in both tasks in order to pass this course. Both tasks have the same weight in this assessment instrument.

The grades obtained in the continuous evaluation will remain valid for all the ordinary calls of this academic year.

Clarifications on the methodology for part-time students and students with disabilities and special educational needs:

For part time students, special evaluation tools will be taylored according to the specific teaching methodology selected for them.

Clarifications on the evaluation of the extraordinary call and extra-ordinary call for completion studies:

The extraordinary call and the completion of studies call will be assessed using the same criteria as in the other calls of the year. The continuous evaluation grades for extraordinary calls will correspond to the current academic year.

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Qualifying criteria for obtaining honors:

An overall qualification of 9.0 is required (Artículo 80.3 del Reglamento de Régimen Académico de la Universidad de Córdoba).

BIBLIOGRAPHY

1. Basic Bibliography

Bransden, B. H., & Joachain, C. J. (2003). *Physics of atoms and molecules*. Pearson Education India.
Weissbluth, M. (2012). *Atoms and molecules*. Elsevier.
del Río, C. S. (1977). *Introducción a la teoría del átomo*. Alhambra.
Requena Rodríguez, A., & Zúñiga Román, J. (2020) *Espectroscopía*. García Maroto.
Pilar, F. L. (2001). *Elementary quantum chemistry*. Courier Corporation.
Bernath, P. F. (2020). *Spectra of atoms and molecules*. Oxford university press.

2. Further reading

Slater, J. C. (1960). Quantum theory of atomic structure, Vols. I and II. McGraw-Hill.
Slater, J. C. (1963). Quantum Theory of Molecules and Solids. Vol. 1: Electronic Structure of Molecules. McGraw-Hill.
Landau, L. D., & Lifshitz, E. M. (2013). Quantum mechanics: non-relativistic theory (Vol. 3). Elsevier.
Bethe, H. A., & Jackiw, R. (1997). Intermediate quantum mechanics. CRC Press.
Alonso, M. & Finn, E. J. (1971). Física Vol. III: Fundamentos cuánticos y estadísticos. Fondo educativo interamericano.

COORDINATION CRITERIA

Common evaluation criteria
Joint activities: lectures, seminars, visits ...
Tasks deadlines
Tasks performance

SCHEDULE

Period	Assessment activities	Lectures	Seminar
1# Fortnight	0,0	3,0	0,0
2# Fortnight	0,0	5,0	2,0
3# Fortnight	0,0	5,0	5,0
4# Fortnight	0,0	5,0	4,0
5# Fortnight	0,0	5,0	4,0
6# Fortnight	0,0	5,0	4,0
7# Fortnight	3,0	5,0	5,0

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Period	Assessment activities	Lectures	Seminar
Total hours:	***3,0***	***33,0***	***24,0***

The methodological strategies and the evaluation system contemplated in this Course Description will be adapted according to the needs presented by students with disabilities and special educational needs in the cases that are required.