



Universidad de Jaén

FACULTY OF EXPERIMENTAL SCIENCES

Applied physical chemistry

2024-2025
Grado en Química



GRATIS



Acceso Mayores 40

Guías docentes UJA

Horarios de tutorías

Llamamientos PEvAU

Movilidad (Coordinador)

P.O.D.

Solicitud bilingüismo

Syllabus 2024-25 - 10313004 - Applied Physical Chemistry (Química física aplicada a sistemas biológicos)

Caption

- Level 1: Tutorial support sessions, materials and exams in this language
- Level 2: Tutorial support sessions, materials, exams and seminars in this language
- Level 3: Tutorial support sessions, materials, exams, seminars and regular lectures in this language

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Full version (Spanish)

English

DEGREE:

Grado en Químicas

FACULTY:

FACULTY OF EXPERIMENTAL SCIENCES

ACADEMIC YEAR:

2024-25

COURSE:

Applied Physical Chemistry

SYLLABUS

1. COURSE BASIC INFORMATION

NAME: Applied Physical Chemistry

CODE: 10313004

ACADEMIC YEAR: 2024-25

LANGUAGE: English

LEVEL: 2

ECTS CREDITS: 6.0

YEAR: 4

SEMESTER: PC

2. LECTURER BASIC INFORMATION

NAME: PARTAL UREÑA, FRANCISCO

DEPARTMENT: U127 - QUÍMICA FÍSICA Y ANALÍTICA

FIELD OF STUDY: 755 - QUÍMICA FÍSICA

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E-MAIL: fpartal@ujaen.es

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WEBSITE: <http://www4.ujaen.es/~fpartal/>ORCID: <https://orcid.org/0000-0002-5554-1205>

LANGUAGE: English

LEVEL: 2

NAME: GRANADINO ROLDÁN, JOSÉ MANUEL

DEPARTMENT: U127 - QUÍMICA FÍSICA Y ANALÍTICA

FIELD OF STUDY: 755 - QUÍMICA FÍSICA

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E-MAIL: jmroldan@ujaen.es

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WEBSITE: -

ORCID: <https://orcid.org/0000-0002-9527-1158>

LANGUAGE: English

LEVEL: 2

3. CONTENT DESCRIPTION

THEORY:

CHAPTER 1: MOLECULAR INTERACTIONS

Electric properties of molecules. Magnetic properties of molecules. Inter- and intra-molecular interactions.

CHAPTER 2: PHOTOCHEMISTRY

Excited States. Photophysics: fluorescence, fosforescence, intra- and inter-molecular energy transfer, chemiluminescence. Excimer and exciplex. Photochemistry in Nature: vision, photosynthesis, DNA damage by UV radiation.

CHAPTER 3: MACROMOLECULES (I): MAIN PRINCIPLES

Introduction: synthetic and biological polymers. Macromolecular structure: structure levels, random coils. Properties of macromolecules: mechanical properties, thermal properties, electrical properties. Determination of shape and size: mean molar masses, experimental techniques for the determination of molar masses and molar mass distribution.

CHAPTER 4: MACROMOLECULES (II): BIOLOGICAL MACROMOLECULES

Structure of proteins. Structure of nucleic acids. Structure of polysaccharides. Structure of micelles and biological membranes. Computer-aided simulations: Molecular Mechanics calculations, Molecular Dynamics simulations, Monte Carlo simulations, Quantitative structure-activity relationship (QSAR).

CHAPTER 5: MOLECULAR RECOGNITION

Introduction. Theoretical models of binding: single-site, single-affinity binding; independent multiple-site, equal affinity binding; independent multiple-site, variable affinity binding; cooperative binding. Experimental analytical techniques.

ORIENTED ACTIVITIES:

Molecular properties from Computer-Assisted Molecular Modelling

LABORATORY EXPERIMENTS:

- 1) Applications of Magnetic Susceptibility measurement.
- 2) In silico prediction of the binding site of a drug to its target.
- 3) Dipolar moments in solution
- 4) Polymer characterisation from viscosity measurements

4. COURSE DESCRIPTION AND TEACHING METHODOLOGY

- 1) Lessons in the classroom. Theory contents and exercises related with them.
- 2) Seminars and tutorial where supporting activities will be developed.
- 3) Experimental sessions in the laboratory.

Students with special educational needs should contact the Student Attention Service (Servicio de Atención y Ayudas al Estudiante) in order to receive the appropriate academic support

5. ASSESSMENT METHODOLOGY

- 1) The theoretical concepts of the subject will be assessed through a written exam, which will be 50% of the final grade. With this instrument the B10 and C14 skills are assessed.
- 2) Targeted activities will be assessed through work and exercises. They account for 20% of the final grade. With this instrument the B8, B10 and Q5 skills are evaluated.
- 3) The laboratory sessions will be compulsory to pass the subject. Its weight in the final grade is 30% and will be evaluated continuously by the teacher. With this instrument the P5 skill is assessed.

6. BOOKLIST [\(Access the bibliography in the Library catalog\)](#)

MAIN BOOKLIST:

- Essentials of chemical biology: structure and dynamics of biological macromolecules . Edition: -. Author: Miller, Andrew, 1963-. Publisher: Chichester, England ; Hoboken, NJ : John Wiley & Sons, c2008 [\(Library\)](#)
- Photochemistry. Edition: 1st published, repr. (with corr.). Author: Wayne, Carol E.. Publisher: Oxford [etc.]: Oxford University Pres, 1999 [\(Library\)](#)
- Physical chemistry of macromolecules: basic principles and issues. Edition: -. Author: Sun, S.F.. Publisher: New York [etc.]: John Wiley & Sons, cop. 1994 [\(Library\)](#)
- Physical chemistry for the life sciences. Edition: 2nd ed. Author: Atkins, Peter William. Publisher: Oxford : Oxford University Press, 2011 [\(Library\)](#)
- Atkins' Physical Chemistry. Edition: 10th. Author: P. Atkins, J. de Paula. Publisher: Oxford University Press [\(Library\)](#)
- Computational Chemistry and Molecular Modeling [electronic resource] : Principles and Applications by K. I. Ramachandran, Gopakumar Deepa, Krishnan Namboori.. Edition: 1st ed. 2008.. Author: Ramachandran, K. I. author.. Publisher: Springer Berlin Heidelberg [\(Library\)](#)
- Computational Chemistry [electronic resource] : Introduction to the Theory and Applications of Molecular and Quantum Mechanics by Errol G. Lewars.. Edition: 2nd ed.. Author: Lewars, Errol G. author.. Publisher: Springer Netherlands [\(Library\)](#)

ADDITIONAL BOOKLIST:

- Experimental physical chemistry. Edition: Oxford: Clarendon Press, 1985. Author: Matthews, G. Peter. Publisher: - [\(Library\)](#)
- Experiments in physical chemistry. Edition: 8th ed.. Author: Garland, Carl W.. Publisher: Boston : McGraw-Hill Higher Education, c2009 [\(Library\)](#)

7. SUSTAINABLE DEVELOPMENT GOALS

Salud y bienestar

Industria, innovación e infraestructura

DETAILED INFORMATION

The contents of this subject connect with SDG-3.b (Support research and development of vaccines and medicines for communicable and non-communicable diseases that primarily affect developing countries and facilitate access to affordable essential medicines and vaccines in accordance with the Doha Declaration on the TRIPS Agreement and Public Health, which affirms the right of developing countries to make maximum use of the provisions of the Agreement on Trade-Related Aspects of Intellectual

Trade-Related Aspects of Intellectual Property Rights regarding flexibilities to protect public health and, in particular, provide access to medicines for all) and SDG-9.b (Support development of domestic technologies, research and innovation in developing countries, including by ensuring an enabling policy environment for industrial diversification and value addition to commodities, among other things).

8. VIRTUAL / CLASSROOM TEACHING SCENARIO

TEACHING METHODOLOGY AND TRAINING ACTIVITIES

Training Activities	Format (classroom / online)	Teaching methodology Description
32 Theory sessions on the contents of the program	On-site when it was possible	32 sessions of participatory master classes, one hour each.
5 sessions of Academically Directed Activities	On-site when it was possible	5 sessions of two hours each.
4 laboratory sessions	On-site when it was possible	Sessions of 4 hours each.
Tutoring	On-site when it was possible+ online	Some tutoring sessions will be conducted in person and others online (synchronous and asynchronous)

EVALUATION SYSTEM

Ordinary call

Assessment test	Format (face-to-face / online synchronous or asynchronous)	Description	Percentage
Final exam	On-site when it was possible	Written exam on theoretical content and problem solving	50%
Oriented Activities Exam	On-site when it was possible	Several tests during the semester	20%
Laboratory Exam	On-site when it was possible	Delivery of laboratory notebook and attendance	30%

Extraordinary call

Assessment test	Format (face-to-face / online synchronous or asynchronous)	Description	Percentage

Final exam	On-site when it was possible	Written exam on theoretical content and problem solving	50%
The qualifications obtained in the ordinary call for the laboratory practices and oriented activities will be maintained.			

MEANS

The resources to be used for non-contact activities will be those offered by the University of Jaén, such as the Learning Management System and the Google Suite applications.

Electronic bibliographic resources available to the University of Jaén Library have been included in the recommended bibliography.

9. VIRTUAL TEACHING SCENARIO

TEACHING METHODOLOGY AND TRAINING ACTIVITIES

Training Activities	Format (classroom / online)	Teaching methodology Description
32 Theory sessions on the contents of the program	Online	38 sessions of participatory master classes, one hour each, conducted by videoconference
5 sessions of Academically Directed Activities	Online	5 sessions of two hours each, conducted by videoconference
4 laboratory sessions	Online	Replacement of the 4 practical sessions (lasting 4 hours each session) with online training activities that will simulate the completion of laboratory practices (videos, tutorials, etc.). They will be held at the same time scheduled for the face-to-face sessions.
Tutoring	Online	Tutoring sessions will be conducted by videoconference (synchronous and asynchronous)

EVALUATION SYSTEM

Ordinary call

Assessment test	Format (face-to-face / online synchronous or asynchronous)	Description	Percentage
Final exam	Online synchronous	Written exam on theoretical content and problem solving	50%

Laboratory Exam	Asynchronous Online	Delivery of laboratory notebook and attendance	30%
Oriented Activities Exam	Asynchronous Online	Several tests during the semester	20%

Extraordinary call

Assessment test	Format (face-to-face / online synchronous or asynchronous)	Description	Percentage
Final exam	Online synchronous	Written exam on theoretical content and problem solving	50%
The qualifications obtained in the ordinary call for the laboratory practices, and oriented activities will be maintained.			

MEANS

The resources to be used will be those offered by the University of Jaén, such as the Learning Management System and the Google Suite applications.

Electronic bibliographic resources available to the University of Jaén Library have been included in the recommended bibliography.

DATA PROTECTION CLAUSE (on line exams)

Institution in charge of data processing: Universidad de Jaén, Campus Las Lagunillas, s/n, 23071 Jaén

Data Protection Delegate: dpo@ujaen.es

Purpose: In accordance with the Universities Law and other national and regional regulations in force, carrying out exams and assessment tests corresponding to the courses students are registered in. In order to avoid frauds while sitting the exam, the exam will be answered using a videoconference system, being able the academic staff of the University of Jaén to compare and contrast the image of the person who is answering the exam with the student's photographic files. Likewise, in order to provide the exam with evidential content for revisions or claims, in accordance with current regulation frameworks, the exam will be recorded and stored.

Legitimacy: compliance with legal obligations (Universities Law) and other national and regional regulations currently in force.

Addressees: service providers who are the owners of the platforms where the exams are carried out and with whom the University of Jaén has signed the corresponding data access contracts.

Storage periods: those established in current in force regulations. In the specific case of exam videoconference recordings, not before the examination records and transcripts are closed or the exam can still be reviewed or challenged.

Rights: you can exercise your right of access, amendment, cancellation, opposition, suppression, limitation and portability by sending a letter to the postal or electronic address indicated above. In the event that you consider that your rights have been violated, you may submit a complaint to the Andalusian Council for Transparency and Data Protection www.ctpdandalucia.es

CLASS RECORDING CLAUSE PERSONAL DATA PROTECTION

Person in charge: Universidad de Jaén, Paraje Las Lagunillas, s/n; Tel.953 212121; www.ujaen.es

Data protection delegate (DPO): TELEFÓNICA, S.A.U. ; Email: dpo@ujaen.es

Procedure aim: To manage proper recordings of teaching sessions with the aim of facilitating learning process under a multimodal and/or online teaching

Period for record storage: Images will be kept during legal term according to regulations in force

Legitimacy: Data will be managed according to legal regulations (Organic Law 6/2001, December 21, on Universities) and given consent provided by selecting corresponding box in legal admission documents

Data recipients (transfers or assignments): Any person allowed to get access to every teaching modality

Rights: You may exercise your rights of access, rectification, cancellation, portability, limitation of processing, deletion or, where appropriate, opposition. To exercise these rights, you must submit a written request to the Information, Registration and Electronic Administration Service of the University of Jaen at the address above, or by e-mail to the address above. You must specify which of these rights you are requesting to be satisfied and, at the same time, you must attach a photocopy of your ID card or equivalent identification document. In case you act through a representative, legal or voluntary, you must also provide a document that proves this representation and identification. Likewise, if you consider that your right to personal data protection has been violated, you may file a complaint with the Andalusian Data Protection and Transparency Council www.ctpdandalucia.es

Campus Las Lagunillas s/n | 23071 - Jaén

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