Master in Chemical Science and Technology
Faculty of Chemical Sciences
Universidad Complutense de Madrid

Syllabus:
Situation 1, 2 and 3
Advanced Experimentation and Modeling in Chemistry. Advanced Techniques in Physical Chemistry: Fundaments and Applications.

Code: 605197

FACULTY OF CHEMICAL SCIENCES
UNIVERSIDAD COMPLUTENSE DE MADRID
Term 2020-2021

Situation 1. In-person

Course name

Advanced experimentation and modeling in Chemistry. Advanced Techniques in Physical Chemistry: Fundaments and Applications.

Duration

First semester

ECTS credits/Character

6 credits/Compulsory

Course content

Applied spectroscopy. Techniques for the characterization of complex materials: colloids, plastics, paints, coatings, etc. Supercritical fluid techniques. Simulation methods for chemical systems and biomolecules.

Lecturers

The course lecturers belong to research groups within the department where the equipment and techniques mentioned in the program of the course are available.

Course coordinator	Andrés Guerrero
Group/Office	Química Supramolecular y Simulación/QA249
Lab/Office	QA-247-C
Email address	aguerrero@quim.ucm.es

Lecturer	Albertina Cabañas Poveda
Group/Office	QA-276
Lab/Office	Equilibrio de Fases y Fluidos Supercríticos/QB203-QB204
Email address	a.cabanas@quim.ucm.es

Lecturer	Elena Junquera
Group/Office	Química Coloidal y Supramolecular/QB250
Lab/Office	QB206-QB207
Email address	junquera@ucm.es

Lecturer	Francisco Ortega
Group/Office	Sistemas Complejos: Coloides, Polímeros e Interfases/QB212
Email address	fortega@ucm.es

Lecturer	Antonio Rey
Lab/Office	Simulación de Sistemas Poliméricos Complejos y Proteínas/QB251
Email address	areygayo@ucm.es

Lecturer	Eduardo Sanz García
Lab/Office	Termodinámica Estadística y Simulación/QB256
Email address	esa01@quim.ucm.es

Lecturer	Ana Rubio
Lab/Office	Simulación de Sistemas Poliméricos Complejos y Proteínas/QB252
Email address	amrubioc@ucm.es

Lecturer	Mercedes Taravillo
Group/Office	Altas Presiones: Determinación de Parámetros Termodinámicos y Espectroscópicos/QA258
Lab/Office	QB-218
Email address	mtaravil@ucm.es

Lecturer	Álvaro Lobato Fernández
Group/Office	Altas Presiones: Determinación de Parámetros Termodinámicos y Espectroscópicos/QA254
Lab/Office	QB-218
Email address	a.lobato@ucm.es

Lecturer	Eduardo Guzmán Solís
Group/Office	Sistemas Complejos: Coloides, Polímeros e Interfases/QB212
Email address	eguzmans@ucm.es

Aims and skills

Aims

In addition to the general aims of the Master (Aims 1–6), the following specific aims will be considered:

1. To provide a solid foundation of chemical-physical instrumentation not necessarily acquired during the Degree in Chemistry.
2. The development of experimental skills in multidisciplinary environments.
3. To become familiar with advanced characterization techniques for molecules, materials, and diverse chemical-physical processes.
4. An introduction to advanced molecular simulation techniques for the study of condensed matter, polymers, and biomolecules.

General Competences

The general competences of the Master GC1–GC10 apply:

GC1: To integrate scientific concepts and deal with the complexity of chemical problems.
GC2: To develop theoretical-practical skills to solve problems of scientific and social interest in the context of chemistry.
GC3: To interpret and analyse complex data in the environment of chemistry and chemical technology.
GC4: To recognize and evaluate the quality of theoretical and practical results using the appropriate tools.
GC5: To employ and recognize the technology of materials to solve problems in this field.
GC6: To know and understand the scientific fundaments of materials and the interrelation between their structure, properties, processing, and applications.
GC7: To correlate the composition with the structure and properties of substances.
GC8: To apply the appropriate characterization techniques to systems under study.
GC9: To recognize the importance and usefulness of chemical compounds in various fields.
GC10: To describe the processes underlying the diverse applications of chemical compounds.

Specific competences

The specific competences of the Master SC1–SC12 apply:

SC1: To develop theoretical-practical skills in instrumental techniques.
SC2: To plan experiments according to established theoretical or experimental models.
SC3: To use computer programs that allow to describe and solve chemical problems.
SC4: To develop theoretical-practical skills for the characterization and analysis of different chemical substances and materials.
SC5: To develop theoretical-practical skills to relate the structure and properties of substances of different complexity.
SC6: To apply both theoretical and practical knowledge to solve chemical problems in unfamiliar environments.

SC7: To formulate conclusions based on chemical information in progress, including reflections on social responsibilities.
SC8: To select and use different procedures to obtain materials and nanomaterials.
SC9: To discuss and investigate the influence of the microstructure on the properties of materials and correlate them to appropriate physical laws.
SC10: To use techniques for the design and self-organization of nanomaterials to prepare nanostructures with properties of technological interest.
SC11: To identify different processing technologies and discern the most appropriate in each case.
SC12: To know the fundaments behind the selection of materials and how to apply them in the design of components.

Transversal Competences

The transversal competences of the Master TC1–TC8 apply:

TC1: To prepare, write, and defend scientific and technical reports.
TC2: To work in a team.
TC3: To value the importance of sustainability and respect for the environment.
TC4: To demonstrate self-learning capacity.
TC5: To demonstrate ethical commitment.
TC6: To communicate results both orally and in writing.
TC7: To work safely in research laboratories.
TC8: To demonstrate motivation for scientific research.

Contextualization within the Master

The proposed contents complement those included in other courses of the modules of the Master: Nanoscience and Nanomaterials (Nanomaterials and Nanochemistry Courses), Instrumentation and Analysis (Sensors and Biosensors), and Fundamental Chemistry (Lasers and Nanochemistry).

This course aims to integrate both chemical and physical knowledge and apply it to advanced techniques for the characterization of molecules and materials. The student will advance in their learning in direct contact with active research groups, using a wide range of experimental and simulation techniques applied to very diverse topics. This scenario will help the student interpret the complexity of chemical phenomena from a multidisciplinary perspective.

Course program

Block 1. Spectroscopy techniques

1.1 Fluorescence and/or UV-VIS spectroscopy. Application of spectroscopy techniques to the characterization of self-assembled systems.

1.2 Raman spectroscopy applied to materials science. Fundaments and applications in materials science, gemology, and heritage conservation.

1.3 NMR spectroscopy applied to the study of diffusion processes: DOSY.

Block 2. Characterization techniques of complex materials and supercritical fluid techniques

2.1 Static and dynamic scattering of light. Application to colloidal and macromolecular systems.

2.2 Working with supercritical fluids. Variable volume observation cell, micronization device by antisolvent agent, high-pressure reactors, and isothermal flow calorimeter.

2.3 Assembly of supramolecular systems supported on solid substrates. Manufacture of monolayers and multilayers using the Langmuir–Blodgett (LB) technique. Characterization of LB films.

Block 3. Simulation techniques of chemical and biomolecular systems

3.1 Molecular visualization Representations and their information. Free access programs. Drawing of molecules (Avogadro). Complex structure representations and simulation results (VMD).

3.2 Molecular dynamics. Algorithms. Periodic boundary conditions. Thermostats. Analysis of trajectories.

3.3 Monte Carlo simulation method. Applications. Practice: Modeling diluted solutions of flexible polymers. Characterization of the dimensions of a polymer. Effects of molecular weight. Effects of solvent quality. Universal behavior.

Teaching methodology and program

The teaching activities related to this course consist of theoretical classes and seminars with equivalent weight. Next, the students will undertake the study and use of the techniques described in the syllabus according to a basic temporal division: one theoretical class or seminar (1 hour) (competences GC1, GC2, GC3, GC4, GC8, SC1, SC2, SC4, SC5, SC6, SC7, TC3, TC7, TC8), and two experimental sessions (2 hours) (competences GC2, GC4, GC8, SC1, SC2, SC3, SC4, SC5, SC6, SC7, TC1, TC2, TC3, TC7, TC8). The faculty responsible for presenting these techniques will explain the theoretical basis, main applications, and provide a basic bibliography. After this introduction, the students will carry out the corresponding laboratory work, which in most cases will include the following activities: a) presentation of the work plan to be followed, b) performing the experiments, and c) presenting the results. To carry out these activities, the students will have an experiment script prepared by each laboratory.

At the end of the course, each student will perform a final experiment previously discussed with their tutor. This professor will supervise the work in the laboratory that has proposed said experiment. These final experiments will be assigned by a draw.

Hours of work/credits of the main activities

Activity	In-person (h)	Individual work (h)	ECTS credits
Theory classes	10	15	1
Seminars	5	7,5	0,5
Tutorials	2	3	0,2
Lab	55	41	3,84
Realization and presentation of individual final experiment; exam	3	8,5	0,46
Total	**75**	**75**	**6**

Characterization techniques and methods (70 hours)

Block 1. Spectroscopic techniques (26 hours = 6 hours t/s + 20 hours l)
Block 2. Characterization techniques of complex materials and supercritical fluid techniques (27 hours = 7 hours t/s + 20 hours l)
Block 3. Simulation techniques of chemical and biomolecular systems (17 hours = 5 hours t / s + 12 hours l)

Tutorials (2 hours)

The student will share with their tutor all matters related to the development of the course, in order to ensure the completion of the final experiment.

Design, implementation and presentation of the final experiment (3 hours)

In the last two weeks of the course, the student must plan and perform an experiment that requires some of the techniques used in the course. The results will be presented in public.

Learning outcome

1. To solve problems in the different fields of application of the studied techniques.
2. To plan experiments that require the use of the studied techniques.
3. To use computer programs that simulate physical chemical systems.
4. To communicate the contents included in the course.
5. To value the contents of scientific reports on topics described in the course.

Learning assessment

For evaluation, the student must have participated in at least 70% of the in-person activities, and must have finished and presented the individual experiment. Students who do not pass in the ordinary call will be informed of those sections that will be evaluated again in the extraordinary call.

The evaluation will be made according to the following concepts and weighting coefficients:

Participation in tutorials and seminars:
1/10

The participation of the student in tutorials and seminars will be evaluated.

Practical test:
2/10

The theoretical-experimental skills acquired by the student will be evaluated through the design and execution of an experiment. This test will be carried out under the supervision of one of the course lecturers. Contents that will be considered are the understanding of the phenomena associated with the experiment, the ability to elaborate an experimental protocol, and the experiment execution, as well as the analysis and discussion of the results.

Public presentation of the final experiment:
2/10

The quality of the presentation will be evaluated (content, organization and clarity). The grade will be determined by the average of the grades awarded by the lecturers attending the presentation.

Personal work:
5/10

The work carried out by the student throughout the course will be taken into account, where both the quality of the results and the answers to the questions for each experiment will be considered. Each teacher will provide a score for their experiment and the average value will define the overall score of this section.

Teaching language(s)

English/Spanish. The English language will be used preferentially.

Bibliography and complementary resources

Basic:

- Atkins, P., de Paula, J.: “Atkins’s Physical Chemistry”, 8th ed., Oxford University Press, Oxford, 2006. Versión española: “Química Física”, Editorial Médica Panamericana, Buenos Aires, 2008.

- Bertrán Rusca, J.; Núñez Delgado, J. (coord.): "Química Física", Volumen I y II, Ariel Ciencia, 2002.
- Skoog D.A., Holler F.J. and Nieman T.A., "Principios de análisis instrumental", McGrawHill (1992).

Complementary:

- Lakowicz J.R., "Principles of fluorescence spectroscopy", Kluwer (1999).
- Perkampus H.H., "UV-Visible spectroscopy", Springer (1992).
- Sanders J.K.M. and Hunter B.K., "Modern NMR spectroscopy", Oxford (1993).
- Berger, S., Braun, S., "200 and More NMR Experiments", Wiley (2004).
- Smith E. and Dent G., "Modern Raman spectroscopy", Wiley (2005).
- Ferraro, J.R., Nakamoto, K., Brown C.W., "Introductory Raman spectroscopy", Academic Press (2003).
- Nakamoto K., "Infrared and Raman spectra of inorganic and coordination compounds", Part A and B, Wiley (2009).
- McCash E. M., "Surface chemistry", Oxford (2001).
- Øgendal, L. "Light Scattering Demystified, Theory and Practice", 2013 (disponible gratuitamente en internet).
- Berne B.J. and Pecora R., "Dynamic Light Scattering: With Applications to Chemistry, Biology, and Physics", Dover Books on Physics (2000).
- Prausnitz J.M., Lichtenthaler R.N., Gomes de Azevedo E., "Molecular thermodynamics of fluid phase equilibria", Edición 3ª, Prentice-Hall, New Jersey (2001).
- Haile J.M.,"Molecular dynamics simulation", Wiley (1992).
- Leach, A.R., "Molecular Modeling", 2ª Ed., Longman (2001).
- Petty, M.C., "Langmuir-Blodgett Films: An Introduction", Cambridge University Press (1996).
- Roberts, B., "Langmuir-Blodgett Films", Springer (1990).

Situation 2. Mixed in-person/online

Teaching methodology and program

The teaching activities related to the course do not undergo significant modifications in the case of a mixed in-person/online situation. The difference respect to the in-person situation is that, in the case of techniques explained at research labs with reduced dimensions, the students will be split in several groups that will work simultaneously. Then, the number of students per technique will be considerably reduced without any effect on the number of hours of work of the main activities of the students. Eventually, some of these techniques will be introduced through online sessions with the aim of guarantee a low number of students at the research labs.

Learning assessment

The learning assessment of the students, regarding the concepts and weighting coefficients, does not undergo significant changes respect to the in-person situation.

In the case of the public presentation, online sessions could be used for the learning assessment of the students.

Situation 3. Online

Teaching methodology and program

The teaching activities related to the course will undergo modifications in the case of a full online situation. All the teaching will be synchronously imparted through online tools such as Google Meet/Collaborate. The sessions will take place during the schedules already stablished at the in-person situation. With this purpose, the used material/activity will be: experimental tutorials; software program tutorials of the different techniques; data files with the results of experimental measurements; synchronous sessions through Google Meet/Collaborate; recording of the synchronous sessions; relevant papers of the technique; online videos of the techniques. All this material will be available for the students through the Virtual Campus.

At the end of the curse, the students will develop a specific experimental exercise, keeping online synchronous sessions with the corresponding advisor. In this exercise, the student will deeply study the experimental concepts of the technique. Such exercise will be presented in public in the presence of all the lectures of the course.

Learning assessment

The learning assessment of the students, regarding the concepts and and weighting coefficients, do not undergoes significant changes respect to the in-person situation.

In the case of the practical exam and the public presentation, online sessions will be used for the learning assessment.