



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

**Syllabus:**

*Advanced Experimentation and  
Modeling in Chemistry. Advanced  
Techniques in Physical Chemistry:  
Fundamentals and Applications.*

**Code: 605197**

**FACULTY OF CHEMICAL SCIENCES  
UNIVERSIDAD COMPLUTENSE DE  
MADRID  
Term 2019-2020**

### Course name

*Advanced experimentation and modeling in Chemistry. Advanced Techniques in Physical Chemistry: Fundamentals 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.*

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*Master in Chemical Science and Technology*

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## 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 fundamentals 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 fundamentals 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. Fundamentals 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 Characterization of materials by DSC. Study of phase transitions (poly and mesomorphism), glass transitions, and crystallization by means of DSC and polarized light microscopy.
- 2.3 Working with supercritical fluids. Variable volume observation cell, micronization device by antisolvent agent, high-pressure reactors, and isothermal flow calorimeter.
- 2.4 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**

<b>Activity</b>	<b>Presential (h)</b>	<b>Individual work (h)</b>	<b>ECTS credits</b>
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
<b>Total</b>	<b>75</b>	<b>75</b>	<b>6</b>

### **Characterization techniques and methods (70 hours)**

Block 1. Spectroscopic techniques (23.5 hours = 4.5 hours t/s + 19 hours l)

Block 2. Characterization techniques of complex materials and supercritical fluid techniques (29.5 hours = 5.5 hours t/s + 24 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 presential activities. 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).

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).

Berger, S., Braun, S., "200 and More NMR Experiments", Wiley (2004).

McCash E. M., "Surface chemistry", Oxford (2001).

Øgandal, 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).