

ȘCOALA DOCTORALĂ ÎN CHIMIE

**PhD Course Syllabus**

**1. Data about the program**

1.1 Higher Education Institution	UNIVERSITY OF BUCHAREST
1.2 Faculty	FACULTY OF CHEMISTRY
1.3 Department	DOCTORAL SCHOOL ON CHEMISTRY
1.4 Field of study	CHEMISTRY
1.5 Study cycle	DOCTORAT
1.6 Study program	CHEMISTRY

**2. Data about the discipline**

2.1 Discipline name	Sustainable development in chemistry: methods and strategies				
2.2 Holder of lecture activities	Prof. dr. Simona Margareta COMAN				
2.3 Holder of laboratory/seminar activities	-				
2.4 Year of study	I	2.5 Semester	I	2.6 Type of evaluation	V
				2.7 Discipline regime	C

**3. Total estimated time**

3.1 Number of hours per week	4	3.2 of which lectures	4	3.3 laboratory/seminar	-
3.4 Total curriculum hours	16	3.5 of which lectures	16	3.6 laboratory/seminar	-
Time distribution					hours
Study the textbook, course materials, bibliography, and notes.					50
Additional documentation in the library, on specialized electronic platforms, and work in the field					10
Seminar/lab preparation, homework, assignments, reports, portfolios, and essays					9
Tutoring					5
Other activities: Examinations					10
3.7 Total hours of individual study					84
3.8 Total hours per semester (3.4. + 3.7)					100
3.9. Number of credits					4

**4. Prerequisites (where applicable)**

4.1 of the curriculum	-General knowledge of General Chemistry, Inorganic Chemistry, Organic Chemistry, Physical Chemistry, Catalysis, and Materials Science
4.2 of skills	-Communication and understanding of specialized chemistry terms in English

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### 5. Conditions (where applicable)

<b>5.1 Course Conditions</b>	<ul style="list-style-type: none"> <li>-Classroom with blackboard, screen, computer, and projector or smartboard.</li> <li>-Attendance at all lectures is recommended.</li> <li>-Delay is accepted, within reasonable limits, avoiding the disruption of the educational process.</li> </ul>
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### 6. Learning outcomes

<b>6.1 Knowledge</b>	<p>Students will:</p> <ul style="list-style-type: none"> <li>✓ Recognize, understand, and reproduce concepts in the field of green chemistry and sustainability.</li> <li>✓ Identifies and develops methods to synthesize chemicals with improved, benign properties for specific applications.</li> <li>✓ Formulate solutions for complex problems in modern chemical research, including compliance with environmental standards.</li> <li>✓ Formulates scientific opinions on scientific research strategies in the area of green chemistry.</li> <li>✓ Describes and integrates specific and interdisciplinary knowledge into professional activity.</li> </ul>
<b>6.2 Skills</b>	<p>Students will be able to:</p> <ul style="list-style-type: none"> <li>✓ Accurately analyzes and applies major concepts in green chemistry and sustainability.</li> <li>✓ Understands chemical synthesis processes, controls structural, chemical, and physical characteristics, and develops creative solutions for emerging applications.</li> <li>✓ Uses logical, intuitive, and creative thinking to solve complex chemistry problems using methods specific to green chemistry and sustainability.</li> <li>✓ Applies scientific principles and research results to develop the specific, innovative skills required for new occupations emerging in sustainable chemistry.</li> <li>✓ Applies appropriate interdisciplinary methods to solve complex theoretical and practical chemical problems.</li> </ul>
<b>6.3 Responsibility and autonomy</b>	<p>Students will:</p> <ul style="list-style-type: none"> <li>✓ Works independently to study and apply scientific theories, taking initiative in applying fundamental principles to novel problems.</li> <li>✓ Makes informed decisions about chemical choices in the context of sustainable development.</li> <li>✓ Takes responsibility for implementing proposed solutions and justifies the approaches used by assessing operational risk and safety factors in the development of new benign chemicals.</li> <li>✓ Autonomously and responsibly applies the knowledge and skills acquired in chemistry while adhering to green chemistry principles.</li> <li>✓ Autonomously and responsibly applies knowledge and skills related to leading a work/research team, including the allocation of tasks and resources and the monitoring of project objective achievement.</li> </ul>

### 7. Contents

7.1 Course	Teaching methods	Comments
<b>Introductory notions. The need for sustainable development in chemistry:</b> Introduction to current global issues related to pollution, climate change, energy demand, waste and limited natural resources; Adverse effects of solvents (destruction of the stratospheric	Lecture Explanation Conversation	4 h

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ozone layer, global warming, formation of photochemical smog, formation of ozone in the troposphere); Use of hazardous chemicals. Case study: the Bhopal disaster; Concepts of process development and manufacture of chemicals with low impact on the environment: green chemistry, green engineering, sustainable development	Description	
<b>Notions of green chemistry:</b> Introduction to green chemistry; Concepts and terms; The principles of green chemistry; Evaluation of the green degree of chemical reactions: Mass parameters: efficiency, atom economy, factor E, reaction mass efficiency, atom efficiency, carbon efficiency, effective mass efficiency, mass intensity. Advantages and disadvantages of applying mass parameters in evaluating the degree of green; Energy parameters: energy intensity of the process, energy consumption in waste treatment, energy consumption in solvent recovery/recycling	Lecture Explanation Conversation Description	4 h
<b>Analysis of the green degree of chemical processes:</b> Radial Pentagon. Design, analysis and interpretation; EcoScale analysis for laboratory processes. Basic principles, calculation, analysis and interpretation; Green solvents: solvent-free chemical processes, water as reaction solvent, supercritical fluids, ionic liquids, fluorinated biphasic systems	Lecture Explanation Conversation Description	4 h
<b>Petrochemistry versus biorefinery / Notions of green engineering:</b> Biomass composition: chemistry, introduction to carbohydrate chemistry; The concept of biorefinery; Environmental issues related to wood ethanol production; Cellulose and lignin chemicals; Design of solid catalysts for biomass conversion; Platform molecules and value-added products; Notions of green engineering, economic importance of recycling reusable materials (plastics, paper, metals, etc.) worldwide; recycling in chemical processes (unprocessed raw materials, intermediates and additives). Linear economy versus circular economy: elementary sustainability.	Lecture Explanation Conversation Description	4 h
<p><b>Bibliography:</b></p> <ol style="list-style-type: none"> <li>1. Green Chemistry: An introductory text, Mike Lancaster (Ed.), The Royal Society of Chemistry, 2002.</li> <li>2. Handbook of Green Chemistry &amp; Technology, J. Clark and D. Macquarrie (Eds.), Blackwell Publishing, 2002</li> <li>3. Chemistry In Alternative Reaction Media, DJ Adams, PJ Dyson, SJ Tavener (Eds), John Wiley &amp; Sons Ltd, 2004</li> <li>4. The Role of Catalysis for the Sustainable Production of Bio-Fuels and Bio-Chemicals, KS Triantafyllis, AA Lappas, M. Stoecker (Eds.), Elsevier BV (2013)</li> </ol>		

### 8. The correlation of the subject contents with the expectations of the representatives of the epistemic community, professional associations and representative employers in the field related to the program

The course provides a wide range of fundamental and practical knowledge on:

- assessing the impact of chemical processes on the ecosystem
- modern and sustainable methods for achieving green chemical syntheses as alternatives to polluting and waste-generating chemical syntheses
- chemical transformation of renewable resources into value-added products on the consumer market

By mastering the theoretical-methodological concepts and approaching the practical aspects of the discipline, Sustainable development in chemistry: methods and strategies, students acquire consistent knowledge in accordance with the partial competencies required for possible occupations outlined in Grid 1 - RNCIS.

The course is designed and structured to enable the student, through the knowledge gained, to conduct research at a high level in any field of chemistry, in accordance with the fundamental concept of the 21st century: sustainable development.

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**9. Evaluation**

Type of activity	9.1 Evaluation criteria	9.2 Evaluation methods	9.3 Share of final grade
<b>9.4 Course</b>	Accuracy and quality of treatment of subjects  The accuracy of the knowledge acquired during the course	Written exam.	100%
<b>Minimum performance standard</b>			
The results of the evaluation of the discipline are expressed by the following grades: Very good / Good / Satisfactory / Insufficient. The grades "Very good", "Good", and "Satisfactory" allow the doctoral student to obtain the credits.			

Date 29/09/2025

Course holder's signature

Director of the Doctoral School in  
Chemistry

Prof. dr. Simona Margareta COMAN

Prof. dr. Camelia BALA

Approval date

29/09/2025

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**PhD Course Syllabus**

**1. Data about the program**

1.1 Higher Education Institution	UNIVERSITY OF BUCHAREST
1.2 Faculty	FACULTY OF CHEMISTRY
1.3 Department	DOCTORAL SCHOOL ON CHEMISTRY
1.4 Field of study	CHEMISTRY
1.5 Study cycle	DOCTORAT
1.6 Study program	CHEMISTRY

**2. Data about the discipline**

2.1 Discipline name	Compounds functionalized with paramagnetic species: synthesis and applications				
2.2 Holder of lecture activities	Prof. dr. Petre Ioniță				
2.3 Year of study	I	2.5 Semester	I	2.6 Type of evaluation	V
				2.7 Discipline regime	SD

**3. Total estimated time**

3.1 Number of hours per week	4	3.2 of which lectures	4	3.3 laboratory/seminar	-
3.4 Total curriculum hours	16	3.5 of which lectures	16	3.6 laboratory/seminar	-
Time distribution					hours
Study the textbook, course materials, bibliography, and notes.					40
Additional documentation in the library, on specialized electronic platforms, and work in the field					10
Seminar/lab preparation, homework, assignments, reports, portfolios, and essays					20
Tutoring					10
Other activities: Examinations					4
3.7 Total hours of individual study					84
3.8 Total hours per semester (3.4. + 3.7)					100
3.9. Number of credits					4

**4. Prerequisites (where applicable)**

4.1 of the curricula	Students are expected to have completed a Master's degree in Chemistry or a closely related field and to possess fundamental knowledge in: Electronic structure of atoms and molecules; Reaction mechanisms and synthetic methodologies; Basic spectroscopy and analytical chemistry; Physical chemistry principles (thermodynamics and kinetics)
4.2 of skills	Students should be able to: Understand and interpret scientific literature in inorganic and materials chemistry; Apply basic laboratory techniques for synthesis and purification of compounds; Use standard characterization methods (UV-Vis, IR, NMR) and understand their limitations in paramagnetic systems; Perform basic data processing and graphical representation of results

**5. Conditions (where applicable)**

5.1 Course Conditions	Not the case
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## ȘCOALA DOCTORALĂ ÎN CHIMIE

### 6. Learning outcomes

<b>6.1 Knowledge</b>	Students will: <ul style="list-style-type: none"> <li>✓ Demonstrate advanced understanding of the chemistry of paramagnetic species (transition metal ions, lanthanides, radicals) and their electronic structure.</li> <li>✓ Explain magnetic interactions, spin states, relaxation mechanisms, and structure-magnetic property relationships.</li> <li>✓ Understand synthetic strategies for functionalizing molecules and materials with paramagnetic centers.</li> <li>✓ Describe characterization techniques specific to paramagnetic systems (EPR/ESR spectroscopy, magnetic susceptibility measurements, magnetometry, NMR of paramagnetic systems).</li> <li>✓ Recognize current applications in catalysis, molecular magnetism, imaging (MRI contrast agents), sensing, and molecular electronics.</li> </ul>
<b>6.2 Skills</b>	Students will be able to: <ul style="list-style-type: none"> <li>✓ Design synthetic pathways to integrate paramagnetic centers into molecular or material frameworks.</li> <li>✓ Choose and utilize suitable characterization techniques for paramagnetic compounds.</li> <li>✓ Analyze EPR spectra, magnetic measurements, and spectroscopic signatures of paramagnetic species.</li> <li>✓ Link molecular structure to magnetic properties and functional behavior.</li> <li>✓ Critically assess literature data and compare experimental findings with theoretical models.</li> </ul>
<b>6.3 Responsibility and autonomy</b>	Students will: <ul style="list-style-type: none"> <li>✓ Independently design and execute research on paramagnetic compounds as part of their doctoral project.</li> <li>✓ Ensure safe handling of metal complexes and reactive intermediates.</li> <li>✓ Apply critical judgment when choosing methodologies and analyzing complex magnetic data.</li> <li>✓ Generate reliable, reproducible results and report findings with scientific integrity.</li> <li>✓ Offer original insights into the use of paramagnetic systems in advanced materials, catalysis, or biomedical applications.</li> </ul>

### 7. Contents

7.1 Course	Teaching methods	Comments
Introduction. History. Magnetism types. Free electron. Paramagnetism. Radicals in organic chemistry.	Lecture Explanation Conversation Description	4 h
Free radical formation. Types of free radicals. Factors affecting stability. Paramagnetic compounds. Synthesis. Reactivity.	Lecture Explanation Conversation Description	4 h
Stable organic free radicals. Organic compounds and materials functionalized with paramagnetic moieties.	Lecture Explanation Conversation Description	4 h
Application of paramagnetic compounds and materials: Electron paramagnetic resonance (electron spin resonance). Spectra simulation	Lecture Explanation Conversation Description	4 h

#### Bibliography:

1. Weil, J.A.; Bolton, J.R. *Electron Paramagnetic Resonance Spectroscopy: Elementary Theory and Applications*. Wiley-Interscience: Hoboken, NJ, USA, 2007.
2. Brustolon, M.; Giamello, E. *Electron Paramagnetic Resonance: A Practitioner's Toolkit*. John Wiley & Sons: Hoboken, NJ, USA, 2009.

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3. Chechik, V.; Carter, E.; Murphy, D.M. Electron Paramagnetic Resonance. Oxford Chemistry Primers; Oxford University Press: Oxford, UK, 2016.  
 4. Forrester, A.R.; Hay, J.M.; Thomson, R.H. Organic Chemistry of Stable Free Radicals. Academic Press: London, UK, 1968.  
 5. Hicks, R.G. Stable Radicals: Fundamentals and Applied Aspects of Odd-Electron Compounds. John Wiley & Sons, Ltd.: Chichester, UK, 2010.

### 8. The correlation of the subject contents with the expectations of the representatives of the epistemic community, professional associations and representative employers in the field related to the program

The discipline provides a broad foundation of fundamental and practical knowledge of the chemistry of paramagnetic compounds and their applications.

By mastering the theoretical-methodological concepts and approaching the practical aspects included in the discipline 'Compounds functionalized with paramagnetic species: synthesis and applications', students acquire a consistent knowledge, in accordance with the partial competencies required for the possible occupations provided in Grid 1 - RNCIS.

The course is designed and structured to enable the student, through the knowledge gained, to conduct high-quality research in any field of chemistry.

### 9. Evaluation

Type of activity	9.1 Evaluation criteria	9.2 Evaluation methods	9.3 Share of final grade
9.4 Course	-Accuracy and quality of treatment of exam subjects  - Acquiring the knowledge acquired in the course	Verification	100

#### Minimum performance standard

The results of the evaluation of the discipline are expressed by the following grades: Very good / Good / Satisfactory / Insufficient. The grades "Very good", "Good", and "Satisfactory" allow the doctoral student to obtain the credits.

Date 29/09/2025

Course holder's signature

Director of the Doctoral School in  
Chemistry

Prof. dr. Petre IONIȚĂ

Prof. dr. Camelia BALA

Approval date  
29/09/2025

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**PhD Course Syllabus**

**1. Data about the program**

1.1 Higher Education Institution	UNIVERSITY OF BUCHAREST
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1.4 Field of study	CHEMISTRY
1.5 Study cycle	DOCTORAT
1.6 Study program	CHEMISTRY

**2. Data about the discipline**

2.1 Discipline name	Structural characterization of solid materials						
2.2 Holder of lecture activities	Prof. dr. Vasile Pârvulescu						
2.3 Year of study	I	2.5 Semester	I	2.6 Type of evaluation	V	2.7 Discipline regime	C

**3. Total estimated time**

3.1 Number of hours per week	<b>4</b>	3.2 of which lectures	<b>4</b>	3.3 laboratory/seminar	-
3.4 Total curriculum hours	<b>16</b>	3.5 of which lectures	<b>16</b>	3.6 laboratory/seminar	-
Time distribution					
Study the textbook, course materials, bibliography, and notes.					
Additional documentation in the library, on specialized electronic platforms, and work in the field					
Seminar/lab preparation, homework, assignments, reports, portfolios, and essays					
Tutoring					
Other activities: Examinations					
3.7 Total hours of individual study					
3.8 Total hours per semester (3.4. + 3.7)					
3.9. Number of credits					

**4. Prerequisites (where applicable)**

<b>4.1 of the curricula</b>	-Graduate-level coursework in:Physical Chemistry (thermodynamics, quantum chemistry fundamentals), Solid State Chemistry or Materials Chemistry, Analytical Chemistry -A foundational understanding of atomic structure, chemical bonding, phase equilibria, and structure–property relationships in materials is required.
<b>4.2 of skills</b>	-Familiarity with spectroscopic techniques (e.g., IR, Raman, NMR – conceptual level). -Understanding of structure determination principles and data interpretation. -Ability to interpret graphical and numerical experimental data.

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### 5. Conditions (where applicable)

<b>5.1 Course Conditions</b>	<p>-Classroom with blackboard, screen, computer, and projector or smartboard. Attendance at all lectures is recommended. -Delays are accepted within reasonable limits, provided they do not disrupt the educational process.</p>
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### 6. Learning outcomes

<b>6.1 Knowledge</b>	Students will: <ul style="list-style-type: none"> <li>✓ Demonstrate advanced knowledge of the theoretical principles underlying structural characterization techniques for solid materials.</li> <li>✓ Explain the working principles, capabilities, and limitations of advanced techniques</li> <li>✓ Critically evaluate structural models and interpret complex structural data sets in the context of current scientific literature.</li> </ul>
<b>6.2 Skills</b>	Students will be able to: <ul style="list-style-type: none"> <li>✓ Select and justify appropriate structural characterization techniques for specific research problems.</li> <li>✓ Analyze and interpret experimental data.</li> <li>✓ Use specialized software for structural refinement, data processing, and crystallographic visualization.</li> <li>✓ Correlate structural information with chemical composition, physical properties, and material performance.</li> <li>✓ Critically assess the reliability, accuracy, and limitations of experimental results.</li> </ul>
<b>6.3 Responsibility and autonomy</b>	Students will: <ul style="list-style-type: none"> <li>✓ Independently design and conduct structural investigations within their doctoral research.</li> <li>✓ Take responsibility for data integrity, reproducibility, and accurate reporting of structural results.</li> <li>✓ Demonstrate critical judgment in selecting methodologies under complex and unpredictable research conditions.</li> <li>✓ Contribute original structural insights to the advancement of knowledge in solid-state chemistry or materials science.</li> <li>✓ Operate with high standards of scientific integrity and professional responsibility in collaborative research environments.</li> </ul>

### 7. Contents

<b>7.1 Course</b>	<b>Teaching methods</b>	<b>Comments</b>
<b>1. Diffraction-Based Characterization of Solid Materials:</b> Principles and applications of X-ray, neutron, and electron diffraction techniques; Phase identification, crystallinity, and structural refinement; Correlation of diffraction data with physicochemical properties; Integration of diffraction methods into operando experimental setups combined with complementary analytical techniques	Lecture Explanation Conversation Description	4 h
<b>2. Spectroscopic Characterization of Solid Materials:</b> Fundamentals of vibrational and electronic spectroscopy; Structural and electronic information obtained from spectral data; Coupling spectroscopic techniques with analytical methods in operando investigations	Lecture Explanation Conversation Description	4 h
<b>3. Experimental Conditions and Instrumental Adaptation:</b> Design of experiments under controlled environments; Adaptation of measurements to temperature-controlled, high-pressure, vacuum, and reactive atmospheres; In-situ vs. operando characterization	Lecture Explanation Conversation	4 h

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approaches and reactor-cell configurations	Description	
<p><b>4. Case Studies and Applications:</b> Analysis of representative materials (catalysts, functional materials, biomaterials, energy materials, environmental materials); Interpretation of multi-technique datasets; Discussion of structure–property relationships and real-world applications</p> <p><b>Bibliography:</b></p> <ol style="list-style-type: none"> <li>1. MA Bañares, Operando methodology: combination of in situ spectroscopy and simultaneous activity measurements under catalytic reaction conditions, - Catalysis today, 2005 - Elsevier</li> <li>2. M. Che, JC Védrine, Characterization of Solid Materials and Heterogeneous Catalysts: From Structure to Surface Reactivity, Wiley, 2012.</li> <li>3. van der Hoeven, J. E., &amp; Seshadri, R. (2023). "Advances in Structural Characterization for Complex Functional Oxides" - Review of cutting-edge diffraction and spectroscopy methods applied to materials science, Advanced Materials, <a href="https://onlinelibrary.wiley.com/journal/15214095">https://onlinelibrary.wiley.com/journal/15214095</a></li> <li>4. Zhang, T., et al. (2023). "Machine Learning in X-ray Diffraction Data Analysis"- Highlights data-driven approaches improving phase identification and refinement accuracy, Computational Materials, <a href="https://www.nature.com/articles/s41524-023-01024-z">https://www.nature.com/articles/s41524-023-01024-z</a></li> <li>5. Li, X., &amp; Wang, Y. (2024). "Integration of Spectroscopy and Microscopy for Nano-Scale Characterization"- Discusses combined structural analysis techniques and multi-modal data fusion, Chemical Reviews, <a href="https://pubs.acs.org/doi/10.1021/acs.chemrev.3c01041">https://pubs.acs.org/doi/10.1021/acs.chemrev.3c01041</a></li> </ol>	Lecture Explanation Conversation Description	4 h

### 8. The correlation of the subject contents with the expectations of the representatives of the epistemic community, professional associations and representative employers in the field related to the program

The course Structural Characterization of Solid Materials aligns with the expectations of the international epistemic community in solid-state chemistry and materials science by providing advanced knowledge and methodological expertise in structural analysis techniques. It responds to professional association standards by emphasizing accuracy, reproducibility, methodological rigor, and ethical data reporting.

The course meets the needs of representative employers (universities, research institutes, high-technology and materials industries) by developing the capacity to independently select, apply, and interpret advanced structural characterization methods. Graduates acquire competencies required for innovation-driven research environments, including critical evaluation of complex data, responsible research conduct, and autonomous decision-making in advanced analytical contexts.

### 9. Evaluation

Type of activity	9.1 Evaluation criteria	9.2 Evaluation methods	9.3 Share of final grade
9.4 Course	<p><b>1. Interpretation of Structural Characterization Data (50%)</b> Assessment of the student's ability to analyze and interpret experimental results obtained from diffraction and spectroscopic techniques: Correct identification of structural features; Correlation between different characterization techniques; Critical interpretation of operando/in-situ measurements; Scientific reasoning and rigor in conclusions</p> <p><b>2. Design of a Characterization Strategy (50%)</b> Assessment of the student's capacity to propose an appropriate experimental approach for a given solid material: Selection and justification of suitable techniques; Adaptation of experimental conditions (temperature, pressure, atmosphere, vacuum); Integration of complementary methods into a coherent analytical workflow; Feasibility and scientific relevance of the proposed methodology</p>	Verification	100

**ȘCOALA DOCTORALĂ ÎN CHIMIE**

<b>Minimum performance standard</b>			
The results of the evaluation of the discipline are expressed by the following grades: Very good / Good / Satisfactory / Insufficient. The grades "Very good", "Good", and "Satisfactory" allow the doctoral student to obtain the credits.			

Date of completion

29/09/2025

Course holder's signature

Prof. dr. Vasile Pârvulescu

Director of the Doctoral School on  
Chemistry

Prof. dr. Camelia BALA

Approval date

29/09/2025

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**PhD Course Syllabus**

**1. Data about the program**

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1.3 Department	DOCTORAL SCHOOL ON CHEMISTRY
1.4 Field of study	CHEMISTRY
1.5 Study cycle	DOCTORAT
1.6 Study program	CHEMISTRY

**2. Data about the discipline**

2.1 Discipline name	Ethics and Academic Integrity		
2.2 Holder of lecture activities	Prof. dr. Paul Vasos and Prof. dr. Camelia Bala		
2.3 Year of study	I	2.5 Semester	I

**3. Total estimated time**

3.1 Number of hours per week	<b>2</b>	3.2 of which lectures	<b>2</b>	3.3 laboratory/seminar	<b>-</b>
3.4 Total curriculum hours	<b>14</b>	3.5 of which lectures	<b>14</b>	3.6 laboratory/seminar	<b>-</b>
Time distribution					
Study the textbook, course materials, bibliography, and notes.					
Additional documentation in the library, on specialized electronic platforms, and work in the field					
Seminar/lab preparation, homework, assignments, reports, portfolios, and essays					
Tutoring					
Other activities: Examinations					
3.7 Total hours of individual study					
3.8 Total hours per semester (3.4. + 3.7)					
3.9. Number of credits					

**4. Prerequisites (where applicable)**

<b>4.1 of the curricula</b>	- Enrollment in a PhD program in Chemistry or a related field - Previous research experience (Master's thesis or equivalent)
<b>4.2 of skills</b>	- Ability to read and analyze scientific literature - Basic scientific writing skills - Familiarity with laboratory work and data recording practices

**5. Conditions (where applicable)**

<b>5.1 Course Conditions</b>	-Classroom with blackboard, screen, computer, and projector or smartboard. -Attendance at all lectures is recommended. -Delays are accepted within reasonable limits, provided they do not disrupt the educational process.
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## ȘCOALA DOCTORALĂ ÎN CHIMIE

### 6. Learning outcomes

<b>6.1 Knowledge</b>	Students will: <ul style="list-style-type: none"> <li>✓ Understand principles of research integrity and responsible conduct of research.</li> <li>✓ Recognize research misconduct and questionable research practices.</li> <li>✓ Understand authorship rules, peer review ethics, and publication standards.</li> <li>✓ Explain data management, reproducibility, and transparency requirements.</li> <li>✓ Understand intellectual property, confidentiality, and collaboration ethics.</li> <li>✓ Recognize ethical responsibilities related to chemical safety and societal impact.</li> </ul>
<b>6.2 Skills</b>	Students will be able to: <ul style="list-style-type: none"> <li>✓ Identify ethical risks in research activities and propose corrective actions.</li> <li>✓ Apply good practices in data recording, storage, and reporting.</li> <li>✓ Make justified authorship and publication decisions.</li> <li>✓ Evaluate journals, peer review processes, and publication credibility.</li> <li>✓ Resolve ethical dilemmas using structured decision-making approaches.</li> <li>✓ Communicate research results responsibly and transparently.</li> </ul>
<b>6.3 Responsibility and autonomy</b>	Students will: <ul style="list-style-type: none"> <li>✓ Demonstrate integrity and accountability in all research activities.</li> <li>✓ Take responsibility for accuracy, reproducibility, and transparency of results.</li> <li>✓ Act autonomously in ethical decision-making in complex research situations.</li> <li>✓ Respect intellectual property and collaborative responsibilities.</li> <li>✓ Promote ethical conduct within research teams and professional environments.</li> <li>✓ Contribute to maintaining public trust in science and responsible innovation.</li> </ul>

### 7. Contents

7.1 Course	Teaching methods	Comments
1. Responsible Conduct of Research: Principles of scientific ethics; Scientific responsibility in chemistry and society; Researcher accountability and public trust in science	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	2 h
2. Research Misconduct: Fabrication, falsification, plagiarism; Questionable research practices; Case studies from chemical research	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	2 h
3. Data Management and Reproducibility: Data recording and traceability (laboratory notebooks, raw data); Reproducibility and replicability in experimental sciences; Image and spectral data manipulation; FAIR principles and data sharing	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	2 h
4. Authorship and Publication Ethics: Authorship criteria and responsibilities; Duplicate publication and salami slicing; Predatory journals and peer-review ethics; Conflict of interest and disclosure practices	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	2 h
5. Intellectual Property and Confidentiality: Patents vs publication; Confidential information and collaborations; Research contracts and ownership of results	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	2 h

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6. Ethics in Collaboration and Supervision: Mentor–student relationships; Collaborative research and responsibilities; Diversity, equity, and respect in research environments	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	2 h
7. Safety, Environmental and Societal Responsibility: Ethical responsibilities in chemical safety; Environmental impact of research; Dual-use research considerations	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	1h
8. Case Studies and Ethical Decision-Making Workshop: Discussion of real ethical dilemmas; Ethical decision-making frameworks	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	1 h

### Bibliography:

#### International Guidelines and Reports

1. European Commission. (2017). The European Code of Conduct for Research Integrity (Revised Edition). <https://allea.org/code-of-conduct/>
2. National Academies of Sciences, Engineering, and Medicine. (2009). On Being a Scientist: A Guide to Responsible Conduct in Research (3rd ed.). <https://nap.nationalacademies.org/catalog/12192>
3. OECD. (2007). Best Practices for Ensuring Scientific Integrity and Preventing Misconduct.

#### Books

1. Haiduc I. (1996). Bunele Maniere in Stiinta, Culegere de Reguli si Norme, Academica.
2. Socaciu E, Vică C, Mihailov E., Gibeau T., Mureşan V., Constantinescu M. (2022) Etică și integritate academică, Editura Universității din București
3. Shamoo, A. E., & Resnik, D. B. (2015). Responsible Conduct of Research (3rd ed.). Oxford University Press.
4. Steneck, N. H. (2007). ORI Introduction to the Responsible Conduct of Research. U.S. Office of Research Integrity.
5. Macrina, F. L. (2014). Scientific Integrity (4th ed.). ASM Press.
6. Babbage, D. R. (2018). Research Ethics and Integrity for Chemists. Royal Society of Chemistry.

#### Articles and Educational Resources

1. Fanelli, D. (2018). Opinion: Is science really facing a reproducibility crisis? PNAS, 115(11), 2628–2631.
2. Ioannidis, J. P. A. (2014). How to make more published research true. PLoS Medicine, 11(10), e1001747.
3. OPE – Committee on Publication Ethics: <https://publicationethics.org/>
4. Office of Research Integrity Case Studies: <https://ori.hhs.gov/>

## 8. The correlation of the subject contents with the expectations of the representatives of the epistemic community, professional associations and representative employers in the field related to the program

The course Ethics and Academic Integrity is aligned with the expectations of the international scientific community, professional organizations in chemistry and research governance bodies, as well as representative employers in academia, research institutes, and industry.

The epistemic community requires doctoral researchers to conduct original research responsibly, ensuring credibility, reproducibility, and transparency of scientific results. The course addresses these expectations by providing training in responsible conduct of research, data management, authorship practices, peer review ethics, and prevention of research misconduct, thereby supporting the production of trustworthy and internationally competitive research.

Professional associations and regulatory frameworks emphasize adherence to research integrity codes, good laboratory practice, conflict-of-interest disclosure, and ethical publication standards. The course integrates these principles by developing the capacity to identify ethical risks, apply international integrity guidelines, and manage intellectual property and collaborative responsibilities appropriately.

Employers in research, pharmaceutical, chemical, environmental, and technological sectors require professionals capable of making ethically sound decisions, managing confidential data, and maintaining compliance with quality assurance and regulatory

### ȘCOALA DOCTORALĂ ÎN CHIMIE

requirements. The course contributes to these expectations by fostering autonomy in ethical decision-making, accountability in data handling, and responsible communication of scientific findings.

Overall, the discipline ensures that doctoral graduates possess the ethical awareness, professional responsibility, and decision-making autonomy necessary for advanced research environments and for maintaining public trust in science.

#### 9. Evaluation

Type of activity	9.1 Evaluation criteria	9.2 Evaluation methods	9.3 Share of final grade
9.4 Course	Student assessment is based on the ability to understand and apply ethical principles in research practice. Evaluation considers the correct identification of research misconduct and ethical risks, the capacity to analyze real or hypothetical case studies, and the justification of decisions according to responsible conduct of research standards. Students must demonstrate the ability to apply good practices in data management, authorship decisions, publication ethics, and collaboration. Clarity of argumentation, critical reasoning, and autonomy in proposing ethically sound solutions are essential components of the final evaluation.	Verification	100
<b>Minimum performance standard</b>			
The results of the evaluation of the discipline are expressed by the following grades: Very good / Good / Satisfactory / Insufficient. The grades "Very good", "Good", and "Satisfactory" allow the doctoral student to obtain the credits.			

Date 29/09/2025

Course holder's signature

Director of the Doctoral School on  
Chemistry

Prof. dr. Camelia BALA

Prof. dr. Paul VASOS

Prof. dr. Camelia BALA

Approval date  
29/09/2025

ȘCOALA DOCTORALĂ ÎN CHIMIE

**PhD Course Syllabus**

**1. Data about the program**

1.1 Higher Education Institution	UNIVERSITY OF BUCHAREST
1.2 Faculty	FACULTY OF CHEMISTRY
1.3 Department	DOCTORAL SCHOOL ON CHEMISTRY
1.4 Field of study	CHEMISTRY
1.5 Study cycle	DOCTORAT
1.6 Study program	CHEMISTRY

**2. Data about the discipline**

2.1 Discipline name	Biosurface analysis techniques		
2.2 Holder of lecture activities	Prof. dr. Camelia BALA		
2.3 Year of study	I	2.5 Semester	II

2.6 Type of evaluation

V

2.7 Discipline regime

FD

**3. Total estimated time**

3.1 Number of hours per week	4	3.2 of the lectures	4	3.3 laboratory/seminar	-
3.4 Total curriculum hours	16	3.5 of the lectures	16	3.6 laboratory/seminar	-
Time distribution					hours
Study the textbook, course materials, bibliography, and notes.					50
Additional documentation in the library, on specialized electronic platforms, and work in the field					30
Seminar/lab preparation, homework, assignments, reports, portfolios, and essays					10
Tutoring					10
Other activities: Examinations					9
3.7 Total hours of individual study					109
3.8 Total hours per semester (3.4. + 3.7)					125
3.9. Number of credits					5

**4. Prerequisites (where applicable)**

4.1 of the curricula	-Physical Chemistry (thermodynamics, kinetics, intermolecular interactions) -Analytical Chemistry and instrumental analysis -Basic spectroscopy and microscopy principles -Introductory biochemistry or molecular biology (proteins, membranes, biomolecular interactions) -Surface or colloid chemistry (recommended)
4.2 of skills	-Basic understanding of spectroscopic and imaging techniques (optical microscopy, UV-Vis, fluorescence) -Familiarity with data interpretation from analytical instruments -Knowledge of concentration, diffusion, and binding equilibria concepts -Ability to read and critically analyze scientific literature -Scientific writing and reporting skills

## ȘCOALA DOCTORALĂ ÎN CHIMIE

### 5. Conditions (where applicable)

<b>5.1 Course Conditions</b>	<ul style="list-style-type: none"> <li>-Classroom with blackboard, screen, computer, and projector or smartboard.</li> <li>-Attendance at all lectures is recommended.</li> <li>-Delays are accepted within reasonable limits, provided they do not disrupt the educational process</li> </ul>
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### 6. Learning outcomes

<b>6.1 Knowledge</b>	<p>Students will:</p> <ul style="list-style-type: none"> <li>✓ Demonstrate advanced understanding of physicochemical principles governing interactions at biological interfaces and surfaces.</li> <li>✓ Explain the operating principles, capabilities, and limitations of Atomic Force Microscopy (AFM), Confocal Microscopy, Surface Plasmon Resonance (SPR), and Fluorescence Correlation Spectroscopy (FCS).</li> <li>✓ Understand mechanisms of biomolecular adsorption, binding kinetics, diffusion, and surface organization at nano- and micro-scale levels.</li> <li>✓ Recognize the complementarity of imaging and spectroscopic techniques in characterizing biomolecular interactions and surface functionalization.</li> <li>✓ Evaluate the applicability of each technique for studying proteins, membranes, biofilms, and functionalized materials.</li> </ul>
<b>6.2 Skills</b>	<p>Students will be able to:</p> <ul style="list-style-type: none"> <li>✓ Select appropriate biosurface characterization techniques based on the research question and sample properties.</li> <li>✓ Interpret AFM topography and force spectroscopy data for biomolecular systems.</li> <li>✓ Analyze confocal microscopy images and spatial distributions of labeled biomolecules.</li> <li>✓ Extract kinetic and affinity parameters from SPR measurements.</li> <li>✓ Process correlation curves and diffusion data obtained by FCS.</li> <li>✓ Integrate information from multiple techniques to construct structure–function relationships at biological interfaces.</li> </ul>
<b>6.3 Responsibility and autonomy</b>	<p>Students will:</p> <ul style="list-style-type: none"> <li>✓ Independently design experimental strategies to investigate biomolecular interactions at surfaces within their doctoral research.</li> <li>✓ Critically assess measurement limitations, artifacts, and reproducibility of nanoscale characterization data.</li> <li>✓ Take responsibility for the correct interpretation and reporting of quantitative interaction parameters.</li> <li>✓ Apply good scientific practice in handling biological samples and sensitive instrumentation.</li> <li>✓ Contribute original insights to interdisciplinary research areas such as biomaterials, nanomedicine, sensors, or biointerfaces.</li> </ul>

### 7. Contents

<b>7.1 Course</b>	<b>Teaching methods</b>	<b>Comments</b>
<b>1. Atomic Force Microscopy (AFM) in the Investigation of Biomolecules</b> - Fundamentals of scanning probe microscopy and AFM instrumentation; Imaging modes: contact, tapping, non-contact, force spectroscopy; Sample preparation for biological materials (proteins, DNA, membranes, cells); AFM in liquid environments and dynamic biological processes; Applications: biomolecular recognition, protein aggregation, biofilm formation	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	4 h
<b>2. Confocal Microscopy – Principles and Applications</b> -Optical principles and instrumentation of laser scanning confocal microscopy; Fluorescence	Interactive Lectures Problem-Based Learning	4 h

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labeling strategies and probes for biomolecules; Optical sectioning and 3D reconstruction of biological samples; Applications: membrane organization, intracellular transport, biomaterial–cell interactions	Practical Workshops Reflective and Collaborative Learning	
<b>3. Surface Plasmon Resonance (SPR) - principle and applications</b> - Physical principles of plasmon resonance and surface-sensitive detection; Instrumental configuration and sensor chip functionalization; Kinetic analysis of biomolecular interactions (association/dissociation constants); Immobilization strategies and experimental design; Label-free detection and real-time monitoring; Applications: ligand–receptor binding, drug screening, biosensors, biomaterials	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	4 h
<b>4. Fluorescence Correlation Spectroscopy - principle and applications</b> - Theory of fluorescence fluctuations and autocorrelation analysis; Instrumentation and experimental setup; Detection of molecular interactions and aggregation processes; Combination with confocal microscopy and live-cell measurements; Applications: protein mobility, membrane dynamics, nanomedicine delivery systems	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	4 h
<b>Bibliography:</b> Books provide <b>methodological foundations</b> :		
<ol style="list-style-type: none"> <li>1. Dufrêne, Y. F. (Ed.). (2011). <i>Atomic force microscopy in molecular and cell biology</i>. Springer.</li> <li>2. Homola, J. (Ed.). (2006). <i>Surface plasmon resonance based sensors</i>. Springer.</li> <li>3. Lakowicz, J. R. (2006). <i>Principles of fluorescence spectroscopy</i> (3rd ed.). Springer.</li> <li>4. Pawley, J. B. (Ed.). (2006). <i>Handbook of biological confocal microscopy</i> (3rd ed.). Springer.</li> <li>5. Schasfoort, R. B. M. (Ed.). (2017). <i>Handbook of surface plasmon resonance</i> (2nd ed.). Royal Society of Chemistry.</li> </ol>		
<b>Selected Recent Articles &amp; Reviews:</b>		
<ol style="list-style-type: none"> <li>1. Dilsiz, N., et al. (2024). Analytical techniques for characterization of biological vesicles and interfaces. <i>TrAC Trends in Analytical Chemistry</i>, 170, 117430.</li> <li>2. Machán, R., &amp; Hof, M. (2010). Recent developments in fluorescence correlation spectroscopy for diffusion measurements in membranes. <i>International Journal of Molecular Sciences</i>, 11, 427–457.</li> <li>3. Parkkila, P. (2024). Confocal fluorescence microscopy and time-correlated single photon counting for intracellular analysis. <i>arXiv preprint</i>.</li> <li>4. Xia, F., et al. (2022). Advanced atomic force microscopy modes for biological applications. <i>Micromachines</i>, 13, 2035.</li> </ol>		

### 8. The correlation of the subject contents with the expectations of the representatives of the epistemic community, professional associations and representative employers in the field related to the program

The course **Biosurface Analysis Techniques** is aligned with the expectations of the international epistemic community in physical chemistry, biochemistry, nanoscience, and biomaterials research, as well as with professional associations and employers operating in research laboratories and high-technology industries.

Within the scientific community, advanced investigation of biomolecular interactions at interfaces is essential for modern research in nanomedicine, sensors, drug delivery, and functional materials. By covering Atomic Force Microscopy, Confocal Microscopy, Surface Plasmon Resonance, and Fluorescence Correlation Spectroscopy, the course develops the capacity to obtain quantitative structural and kinetic information at biointerfaces and to critically interpret complex experimental data.

Professional organizations emphasize methodological rigor, measurement reliability, and correct interpretation of nanoscale interaction parameters. The course integrates these principles through the evaluation of artifacts, reproducibility, quantitative kinetic analysis, and responsible reporting of results.

Representative employers in biotechnology, pharmaceutical, medical diagnostics, biomaterials, and analytical instrumentation sectors require specialists capable of independently selecting characterization techniques and integrating complementary analytical methods. The course supports these expectations by developing autonomy in experimental design, data interpretation, and interdisciplinary problem-solving.

Overall, the discipline ensures that doctoral graduates acquire competencies required for high-level research, innovation, and expert analytical roles at the interface of chemistry, biology, and materials science.

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**9. Evaluation**

Type of activity	9.1 Evaluation criteria	9.2 Evaluation methods	9.3 Share of final grade
9.4 Course	<p><b>1. Scientific Understanding and Data Interpretation (50%)</b> Assessment of the student's ability to correctly understand and interpret biosurface characterization methods:</p> <ul style="list-style-type: none"> <li>Correct explanation of the principles of AFM, Confocal Microscopy, SPR, and FCS</li> <li>Proper interpretation of experimental outputs (topography maps, fluorescence images, correlation curves, binding kinetics)</li> <li>Identification of limitations, artifacts, and measurement uncertainties</li> <li>Ability to correlate results with biomolecular interactions at interfaces</li> </ul> <p><b>2. Application to Research Problem and Critical Analysis (50%)</b> Assessment of the capacity to apply knowledge autonomously in a research context:</p> <ul style="list-style-type: none"> <li>Selection and justification of appropriate technique(s) for a given scientific problem</li> <li>Design of a coherent experimental strategy</li> <li>Critical comparison of complementary methods</li> <li>Scientific argumentation, clarity of presentation, and rigor of conclusions</li> </ul>	Verification	100
<b>Minimum performance standard</b>			
The results of the evaluation of the discipline are expressed by the following grades: Very good / Good / Satisfactory / Insufficient. The grades "Very good", "Good", and "Satisfactory" allow the doctoral student to obtain the credits.			

Date 29/09/2025

Course holder's signature

Director of the Doctoral School in Chemistry

Prof. dr. Camelia BALA

Prof. dr. Camelia BALA

Approval date

29/09/2025

ȘCOALA DOCTORALĂ ÎN CHIMIE

## PhD Course Syllabus

### 1. Data about the program

1.1 Higher Education Institution	UNIVERSITY OF BUCHAREST
1.2 Faculty	FACULTY OF CHEMISTRY
1.3 Department	DOCTORAL SCHOOL ON CHEMISTRY
1.4 Field of study	CHEMISTRY
1.5 Study cycle	DOCTORAT
1.6 Study program	CHEMISTRY

### 2. Data about the discipline

2.1 Discipline name	Mass spectrometry						
2.2 Holder of lecture activities	Prof. Dr. Andrei Medvedovici						
2.3 Year of study	I	2.5 Semester	II	2.6 Type of evaluation	V	2.7 Discipline regime	C

### 3. Total estimated time

3.1 Number of hours per week	4	3.2 of which lectures	4	3.3 laboratory/seminar	-
3.4 Total curriculum hours	16	3.5 of which lectures	16	3.6 laboratory/seminar	-
Time distribution					hours
Study the textbook, course materials, bibliography, and notes.					67
Additional documentation in the library, on specialized electronic platforms, and work in the field					40
Seminar/lab preparation, homework, assignments, reports, portfolios, and essays					0
Tutoring					0
Other activities: Examinations					2
3.7 Total hours of individual study					109
3.8 Total hours per semester (3.4. + 3.7)					125
3.9. Number of credits					5

### 4. Prerequisites (where applicable)

4.1 of the curricula	<ul style="list-style-type: none"> <li>Fundamentals in chromatography;</li> <li>Fundamentals in analytical instrumental analysis (more precisely, spectrometric techniques)</li> </ul>
4.2 of skills	<ul style="list-style-type: none"> <li>Operating abilities for PC and Word, Excel, and Origin applications.</li> <li>Ability for understanding a graphic functional representation and data processing modes.</li> <li>Communication abilities</li> </ul>

### 5. Conditions (where applicable)

5.1 Course Conditions	During the course, students will have their mobile phones switched off. Attendance of a minimum of 3 courses is considered mandatory. Course room with blackboard and video projector.
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## ȘCOALA DOCTORALĂ ÎN CHIMIE

### 6. Learning outcomes

<b>6.1 Knowledge</b>	Students will: <ul style="list-style-type: none"> <li>✓ Demonstrate advanced understanding of the physical principles of mass spectrometry, including ion formation, ion motion, ion detection, and mass-to-charge determination.</li> <li>✓ Explain gas-phase ionization methods and atmospheric/condensed phase ionization techniques.</li> <li>✓ Understand the operating principles, advantages, and limitations of mass analyzers and the distinction between low- and high-resolution systems.</li> <li>✓ Describe tandem MS and MS<sup>n</sup> experiments, fragmentation mechanisms, scan modes, and Fourier transform mass spectrometry.</li> <li>✓ Understand ion mobility MS, SIFT-MS principles, matrix effects, operational qualification, and the integration of MS with chromatographic techniques for structural confirmation.</li> </ul>
<b>6.2 Skills</b>	Students will be able to: <ul style="list-style-type: none"> <li>✓ Select appropriate ionization sources and analyzers according to analyte properties and research objectives.</li> <li>✓ Interpret mass spectra, isotopic patterns, and fragmentation pathways for structural elucidation.</li> <li>✓ Design and optimize MS and MS/MS experiments.</li> <li>✓ Evaluate matrix effects and analytical limitations and apply strategies to improve accuracy and sensitivity.</li> <li>✓ Integrate chromatographic separation with MS detection and critically assess data quality and reliability.</li> </ul>
<b>6.3 Responsibility and autonomy</b>	Students will: <ul style="list-style-type: none"> <li>✓ Independently design analytical strategies using mass spectrometry within their doctoral research.</li> <li>✓ Take responsibility for method validation, calibration, and reliable interpretation of analytical data.</li> <li>✓ Exercise critical judgment in selecting instrumentation and acquisition modes in complex analytical contexts.</li> <li>✓ Ensure reproducibility, traceability, and integrity of analytical results.</li> <li>✓ Contribute original analytical solutions to complex chemical, environmental, biological, or materials-related problems.</li> </ul>

### 7. Contents

7.1 Course	Teaching methods	Comments
Mass spectrometry: fundamental aspects. Use of mass spectrometry as a structural confirmation detector in chromatographic techniques; Gas phase ionization (electronic impact ionization - EI; chemical ionization - CI); Condensed phase ionization (atmospheric pressure ionization sources: ESI, APCI, MPI for liquid phase and MALDI and SIMS for solid phase). Direct ionization sources for real-time analysis (DART and DESI).	Lecture Explanation Conversation Description	4 h
Mass analyzers, basic operating principles: dual focusing (electrical and magnetic sectors), time of flight mass analyzer (ToF), distance of flight mass analyzer (DoF), linear quadrupole (Q), classic ion trap - quistor; linear ion trap (LIT); orbital ion trap (OIT); ion cyclotron resonance trap (ICR). Low-resolution mass analyzers versus high-resolution mass analyzers.	Lecture Explanation Conversation Description	4 h
Distinctive exploiting modes of a mass analyzer (full scan, single ion monitoring, multiple ion monitoring). Sequential scanning versus Fourier Transform MS. Tandem MS and MS <sup>n</sup> designs, space or time delayed. Collision cells. Distinctive exploiting modes of tandem mass systems (Product Ion Scan, Precursor Ion Scan; Neutral Scan Loss, Single Reaction Monitoring, Multiple Reaction Monitoring). Detection in mass spectrometry: ion current	Lecture Explanation Conversation Description	4 h

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detection versus image current monitoring.			
Operational qualification of a mass spectrometer. Matrix effects in atmospheric pressure ion sources. Ion Mobility Mass spectrometry. Fundamentals and instrumentation. SIFT-MS - Selected Ion Flow Tube Mass Spectrometry. Fundamentals and applications.	Lecture Explanation Conversation Description	4 h	

**Bibliography:**

1. A. Medvedovici, Fundamentals in mass spectrometry - course notes, personal web page. <https://unibuc.ro/user/Andrei.Medvedovici/?profiletab=documents>, 200 pgs. (2025).
2. WMA Niessen, Liquid chromatography - Mass Spectrometry, CRC Press, Taylor and Francis Group, Boca Raton (2006).
3. KL Busch, A glossary for Mass Spectrometry, Mass Spectrometry, 17 (6S), S26-S34 (2002).
4. JR Chapman (Ed.) - Mass Spectrometry of Protein and Peptides, vol.146 in Methods in molecular Biology, Humana Press Inc. (2000).
5. FW McLafferty, F. Turecek, Interpretation of Mass Spectra, 4th Edition, University Science Books (1993)

### 8. The correlation of the subject contents with the expectations of the representatives of the epistemic community, professional associations and representative employers in the field related to the program

The course Mass Spectrometry aligns with the expectations of the international analytical chemistry community by providing advanced knowledge and methodological competence in modern molecular characterization techniques. It reflects professional association standards by emphasizing instrument validation, measurement reliability, uncertainty evaluation, and responsible data interpretation.

The course meets the needs of representative employers (pharmaceutical, environmental, chemical, forensic, and biotechnology sectors) by developing the ability to independently select ionization techniques, design MS/MS experiments, and interpret complex analytical data. Graduates acquire competencies required for innovation-driven research environments, including autonomous decision-making, advanced analytical reasoning, and adherence to quality assurance practices.

### 9. Evaluation

Type of activity	9.1 Evaluation criteria	9.2 Evaluation methods	9.3 Share of final grade
9.4 Course	-Accuracy and quality of treatment of exam subjects  -Awareness of the knowledge acquired in the course	Verification	100

#### Minimum performance standard

The results of the evaluation of the discipline are expressed by the following grades: Very good / Good / Satisfactory / Insufficient. The grades "Very good", "Good", and "Satisfactory" allow the doctoral student to obtain the credits.

Date 29/09/2025

Course holder's signature

Director of the Doctoral School in  
Chemistry

Prof. dr. Andrei MEDVEDOVICI

Prof. dr. Camelia BALA

Approval date  
29/09/2025

ȘCOALA DOCTORALĂ ÎN CHIMIE

**PhD Course Syllabus**

**1. Data about the program**

1.1 Higher Education Institution	UNIVERSITY OF BUCHAREST
1.2 Faculty	FACULTY OF CHEMISTRY
1.3 Department	DOCTORAL SCHOOL ON CHEMISTRY
1.4 Field of study	CHEMISTRY
1.5 Study cycle	DOCTORAT
1.6 Study program	CHEMISTRY

**2. Data about the discipline**

2.1 Discipline name	Management of Scientific Research in Chemistry						
2.2 Holder of lecture activities	Prof. dr. Camelia BALA						
2.3 Year of study	I	2.5 Semester	II	2.6 Type of evaluation	V	2.7 Discipline regime	S

**3. Total estimated time**

3.1 Number of hours per week	4	3.2 of which lectures	4	3.3 laboratory/seminar	-
3.4 Total curriculum hours	16	3.5 of which lectures	16	3.6 laboratory/seminar	-
Time distribution					
Study the textbook, course materials, bibliography, and notes.					
Additional documentation in the library, on specialized electronic platforms, and work in the field					
Seminar/lab preparation, homework, assignments, reports, portfolios, and essays					
Tutoring					
Other activities: Examinations					
3.7 Total hours of individual study					
3.8 Total hours per semester (3.4. + 3.7)					
3.9. Number of credits					

**4. Prerequisites (where applicable)**

4.1 of the curricula	-Fundamental knowledge of experimental design and analytical techniques in chemistry. -Basic understanding of scientific methodology and statistical data interpretation. -Prior experience in conducting laboratory research and writing scientific reports or a Master's thesis.
4.2 of skills	-Basic scientific writing skills (literature review, citation, manuscript structure). -Familiarity with bibliographic databases (e.g., Web of Science, Scopus, SciFinder). -Introductory knowledge of laboratory safety procedures. -Basic digital competencies (data handling, use of reference management software, spreadsheet tools).

**5. Conditions (where applicable)**

5.1 Course Conditions	-Classroom with blackboard, screen, computer, and projector or smartboard. -Attendance at all lectures is recommended. -Delays are accepted within reasonable limits, provided they do not disrupt the educational process.
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## ȘCOALA DOCTORALĂ ÎN CHIMIE

### 6. Learning outcomes

<b>6.1 Knowledge</b>	Students will: <ul style="list-style-type: none"> <li>✓ Explain the principles of research planning and project design in chemical sciences.</li> <li>✓ Describe funding mechanisms, grant writing structures, and research ethics in chemistry.</li> <li>✓ Understand laboratory management, safety regulations, data management, and intellectual property concepts.</li> <li>✓ Recognize quality assurance, reproducibility standards, and publication strategies in chemical research.</li> </ul>
<b>6.2 Skills</b>	Students will be able to: <ul style="list-style-type: none"> <li>✓ Develop a structured research proposal with clear objectives, methodology, timeline, and budget.</li> <li>✓ Apply project management tools (e.g., Gantt charts, risk assessment, milestone tracking) to chemical research projects.</li> <li>✓ Manage research data according to FAIR principles and good scientific practice.</li> <li>✓ Prepare manuscripts, respond to peer review, and communicate research effectively to scientific and non-scientific audiences.</li> </ul>
<b>6.3 Responsibility and autonomy</b>	Students will: <ul style="list-style-type: none"> <li>✓ Conduct and manage research activities independently while adhering to ethical and safety standards.</li> <li>✓ Take responsibility for data integrity, reproducibility, and responsible conduct of research.</li> <li>✓ Lead small research tasks or laboratory teams effectively.</li> <li>✓ Make informed decisions regarding resource allocation, collaboration, and dissemination of research outcomes.</li> </ul>

### 7. Contents

<b>7.1 Course</b>	<b>Teaching methods</b>	<b>Comments</b>
Research Strategy in Chemical Sciences; Research Proposal Development; Project Planning Tools; Risk assessment in chemical research	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	4 h
Laboratory Organization & Resource Management; Chemical Safety & Regulatory Framework; Responsible Conduct of Research (RCR)§ Case Studies & Discussion	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	4 h
Data Management, Quality & Reproducibility; FAIR principles; Quality Assurance & Reproducibility; Intellectual Property & Technology Transfer; Practical Component - Drafting a data management plan (DMP)	Interactive Lectures Problem-Based Learning Practical Workshops Reflective and Collaborative Learning	4 h
Funding, Scientific Communication & Leadership; Research Funding & Grant Writing; Scientific Publishing Strategy; Scientific Communication; Leadership, Collaboration & Career Management - Team management in research groups,	Interactive Lectures Problem-Based Learning Practical Workshops	4 h

## ȘCOALA DOCTORALĂ ÎN CHIMIE

Supervising students, International collaboration, Building scientific reputation (ORCID, research profiles), Time management for PhD researchers	Reflective and Collaborative Learning	
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### Bibliography:

1. **The Emerald Handbook of Research Management and Administration Around the World (2023)** — comprehensive coverage of research management as a profession and global research administration practice. Open-access version available as PDF. *Link: <https://library.oapen.org/handle/20.500.12657/86164>*
2. **Project Management for Scholarly Researchers: Systems, Innovation, and Technologies (2023)** — a practical guide on project and research management, including planning, risk analysis, and administration in academic research, Adedeji B. Badiru, CRC Press (Taylor & Francis)
4. **Research Policy (Journal)** — monthly peer-reviewed journal focused on science, technology and innovation management — essential source for up-to-date articles on research systems and policy. *Link: <https://www.sciencedirect.com/journal/research-policy>*
3. **“Research information in the light of artificial intelligence: quality and data ecologies” (2024)** — discusses AI tools for managing research information systems, data quality and university research support structures. Otmane Azeroual, Tibor Koltay, *https://arxiv.org/abs/2405.12997* (open access)

## 8. The correlation of the subject contents with the expectations of the representatives of the epistemic community, professional associations and representative employers in the field related to the program

The course **Management of Scientific Research in Chemistry** aligns with the expectations of the epistemic community (academic researchers and research institutions), professional associations in chemistry and research administration, and representative employers (universities, research institutes, and industry R&D departments).

The course content addresses key competencies required at the doctoral level, including research planning, grant writing, laboratory management, research ethics, data management, intellectual property, and scientific communication. These areas reflect international standards for responsible conduct of research, quality assurance, reproducibility, and innovation management.

Academic institutions expect PhD graduates to independently design and manage research projects, secure funding, publish in peer-reviewed journals, and collaborate internationally. Professional associations emphasize ethical conduct, compliance with safety standards, and adherence to good laboratory and data management practices. Employers in industry and research organizations require project management skills, risk assessment capability, regulatory awareness, teamwork, and efficient resource allocation.

By integrating project management tools, ethical frameworks, data governance principles, and leadership training, the course ensures that graduates acquire competencies that meet labor market demands while supporting excellence in scientific research and innovation.

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**9. Evaluation**

Type of activity	9.1 Evaluation criteria	9.2 Evaluation methods	9.3 Share of final grade
9.4 Course	<p><b>1. Quality and Feasibility of the Research Management Project (50%).</b> Assessment of the student's ability to design a structured research management plan related to their PhD topic, including: Clarity and coherence of objectives, Logical alignment between objectives, methodology, timeline, and resources; Appropriate risk assessment and mitigation strategy; Realistic budgeting and planning; Integration of ethical, safety, and data management principles.</p> <p><b>2. Critical Analysis and Application of Research Management Principles (50%).</b> Assessment of the student's capacity to: Apply project management tools appropriately (e.g., Gantt chart, DMP, risk matrix); Demonstrate understanding of research ethics, reproducibility, and intellectual property; Critically evaluate funding strategies and publication plans; Present and justify decisions with scientific rigor and autonomy.</p>	Verification	100
<b>Minimum performance standard</b>			
The results of the evaluation of the discipline are expressed by the following grades: Very good / Good / Satisfactory / Insufficient. The grades "Very good", "Good", and "Satisfactory" allow the doctoral student to obtain the credits.			

Date 29/09/2025

Course holder's signature

Director of the Doctoral School in  
Chemistry

Prof. dr. Camelia BALA

Prof. dr. Camelia BALA

Approval date

29/09/2025