COURSE DESCRIPTION

Methods for the structural characterization of materials

Academic year 2026-2027

1. Programme-related data

1.1. Higher Education Institution	Universitatea Babeş-Bolyai din Cluj Napoca
1.2. Faculty	Chemistry and Chemical Engineering
1.3. Department	Chemical Engineering
1.4. Field	Chemical Engineering
1.5. Level of study	Master
1.6. Degree programme / Qualification	Advanced Process Chemical Engineering/ Master's Degree
1.7. Form of education	Full-time education

2. Course-related data

2.1. Course title	**Methods for the structural characterization of materials**			Course code	**CME7143**
2.2. Course coordinator	Prof. dr. Ion Grosu Conf. dr. Radu Silaghi-Dumitrescu Conf. dr. Gabriela Nemeş Conf. dr. Richard A. Varga Lecturer Dr. Cosmin Coteţ Conf. dr. Adrian Nicoara				
2.3. Seminar coordinator	Prof. dr. Ion Grosu Conf. dr. Radu Silaghi-Dumitrescu Conf. dr. Gabriela Nemeş Conf. dr. Richard A. Varga Lecturer Dr. Cosmin Coteţ Conf. dr. Adrian Nicoara				
2.4. Year of study	I	2.5. Semester	2	2.6. Type of assessment	Exam
2.7. Course status	Optional			2.8. Course type	Specialisation subject

3. Total estimated time (hours per semester of teaching activities)

3.1. Number of hours per week	**4**	of which: 3.2. course	**2**	3.3. seminar/ laboratory/ project	**2**
3.4. Total of hours in the curriculum	56	of which: 3.5. course	28	3.6. seminar/ laboratory	**28**
Time allocation for individual study (IS) and self-taught activities (ST)					**hours**
Learning from textbooks, course materials, bibliography, and notes (IS)					20
Additional research in the library, on subject-specific electronic platforms, and on-site					18
Preparing seminars/ laboratories/ projects, assignments, reports, portfolios, and essays					22
Tutoring (professional guidance)					6
Examinations					3
Other activities					
3.7. Total hours of individual study (IS) and self-taught activities (ST)				**69**	
3.8. Total hours per semester				**125**	
3.9. Number of credits				**5**	

4. Prerequisites (where applicable)

4.1. curriculum-related	Not the case
4.2 skills-related	Not the case

5. Specific conditions (where applicable)

5.1. course-related	
5.2. seminar/laboratory-related	

6.1. Competencies resulting from the completion of the degree programme *(as referred to in the curriculum)*[1]

Professional competencies	
Competency code	**Competency**
PC1	Descrierea, analiza şi utilizarea conceptelor şi teoriilor avansate din domeniul chimiei şi ingineriei chimice de proces. *Description, analysis and use of elaborate theories and concepts in the fields of chemistry and process advanced chemical engineering*
PC4	...
PC5	...
Transversal competencies	
Competency code	**Competency**
TC1	Executarea cu independenţă a sarcinilor profesionale complexe şi desfăşurarea autonomă de activităţi de cercetare-proiectare, utilizând tehnici asistate de calculator şi respectând normele de etică profesională şi de conduită morală. *Independent execution of complex professional assignments and autonomous development of project-research activities by using computer-assisted techniques and by observing the norms of professional ethics and moral conduct.*
TC3	...

6.2. Learning outcomes relevant to the degree programme (as referred to in the curriculum)[2]

Learning outcomes targeted by the subject		
Competency code	**Knowledge and comprehension**	**Specific academic skills**
CP1 **CP4** **CT1**	1. Formularea soluţiilor de rezolvare a problemelor complexe ale ingineriei chimice de proces pe baza cunoaşterii, identificării şi aplicării conceptelor, metodelor şi teoriilor avansate din domeniul ingineriei chimice şi chimiei *1. Formulation of solutions to solve complex chemical engineering problems based on knowledge, identification and application of advanced concepts, methods and theories in the field of chemical engineering and chemistry*	1. Analiza critică şi utilizarea principiilor, metodelor şi tehnicilor avansate pentru evaluarea, proiectarea şi dezvoltarea a noi produse/tehnologii1. *1. Critical analysis and application of advanced principles, methods, and techniques for the evaluation, design, and development of new products and technologies.*
PC4	2.	2.
PC5	3.	3.
TC2	...	...
TC3	...	...

[1] The professional and/or transversal skills targeted by the subject for which the course description is prepared will be copied from the curriculum of the degree programme. For each competency, the complete entry, including the competency code, will be copied with the exact wording that appears in the curriculum, without any changes. If no competency is copied from either of the two categories, the row corresponding to that category is deleted from the table.

[2] The learning outcomes relevant for the degree programme and targeted by the subject for which the course description is prepared will be listed. The entries, copied without any changes from the Curriculum by subject type (Core Subject/Specialisation Subject/Complementary Subject), are listed under the corresponding competency.

7. Subject-specific learning outcomes

Knowledge and comprehension
1. Realizarea unei analize critice bazată pe instrumente CAD, pentru identificarea de posibile rezolvări a problemelor complexe de proiectare a aparatelor şi utilajelor dintr-un proces chimic 1.*Performing a critical analysis based on CAD tools, to identify possible solutions to complex problems of designing equipment and plants in a chemical process*
2. ...
3. ...
4. ...
Specific academic skills
1. Elaborarea proiectelor integrate, bazate pe instrumente CAD, pentru dezvoltarea creativă a proiectării aparatelor, utilajelor şi instalaţiilor din industriile de proces chimic *1.Development of integrated projects, based on CAD tools, for the creative development of the design of devices, equipment and plants in the chemical process industries*
2. ...
3. ...

8. Contents

8.1. Course	**Teaching and learning methods**	**Remarks[3]**
MODULE 1 Spectroscopic methodes for structural characterization of organic and organometallic compounds		
8.1.1. Structural Characterization by NMR methods: NMR– principles. Solid State NMR. Interpretation of data and applications (2 hours)	Presentation; Explanation, Conversation; Description; Debate	4 hours
8.1.2. Structural Characterization by MS methods: Soft ionization techniques and investigation of multiple charged ions. (2 hours)	Presentation; Explanation, Conversation; Description; Debate	
8.1.3. Structural Characterization by EPR/ESR. Applicability and techniques. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	4 hours
8.1.4. Structural Characterization by ESR: experiments for materials characterization and biochemical applications (2 hours)	Presentation; Explanation, Conversation; Description; Debate	
8.1.5. Structural Characterization by UV-Vis spectroscopy. Applicability and techniques. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	4 hours
8.1.6. Structural Characterization by CD and vCD methods. Applicability and techniques. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
MODULE 2 Structural Characterization by DRX		
8.1.7. Single crystal and powder X ray diffractometry. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	4 hours
8.1.8. Interpretation of primary data. Atomic parameters, crystallographic	Presentation; Explanation, Conversation; Description; Debate	

[3] For example, organisational aspects, recommendations for students, specific aspects relating to the course/seminar, such as inviting experts in the field, etc.

tables intra and intermolecular connection (2 hours).		
MODULE 3. Structural Characterization by electrochimical methods.		
8.1.9. The principles of electrochemical investigations: classification of the methods using the nature and shape of perturbation and of the response. Electrochemical cell and specific equipments. Elementary stages and electrode processes. Thermodynamic and kinetic parameters which can be determined by electrochemical investigations. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	6 hours
8.1.10. Chronoamperommetic methods: principles and equipments. Hydrodynamic voltametry: principles and equipments. Levich and Koutecky-Levich relations and their applications. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
8.1.11. Cyclic voltammetry and impedance spectroscopy. Reversibility chriteria, experimental parameters and methods for the determination of characteristic phtsico-chemical properties. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
MODULE 4 – Characterization of materials and precursors using specific areas, pores distribution and the structure of the surface evaluated by microscopic methods (SEM, TEM). Termogravimetric methods and Differential Scanning Calorimetry		
8.1.12. Adsorption. Porous structure of solids. Determination of specific area and of the didtribution of the pores. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	6 hours
8.1.13. Structural characterization of solids by optic and electronic microscopies (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
8.1.14. Thermogravimetric analysis and differential thermogravimetric analysis. Differential Scanning Calorimetry. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	

Bibliography
Courses support

MODULE 1
1. N. E. Jacobsen, NMR Spectroscopy Explained, Ed Wiley-Interscience, 2007.
2. H Friebolin, Basic One- and Two-dimensional NMR Spectroscopy, Wiley-VCH, 2004.
3. S. Mager, Analiza Structurala Organică, Ed. Ştiinţifica si Enciclopedica, Bucureşti 1979.
4. David L., Crăciun C., Cozar O., Chiş V., Rezonanţă Electronică de Spin. Principii, metode, aplicaţii, Presa Univ. Clujeană, Cluj-Napoca, 2001.
5. H.H. Perkampus, UV-VIS spectroscopy and its applications, Springer-Verlag, 1992.
MODULE 2
1. W. Massa, Crystal Structure Determination, Editura Springer, Berlin, 2000. (accessible at the module holder)
MODULE 3
1. Oniciu L., Mureşan L., Electrochimie aplicată, Presa Universitară Clujeana, 1998.
2. A. J. Bard şi L. R. Faulkner, Electrochemical Methods. Fundamentals and Applications, John Wiley and Sons, New-York, 1980.
MODULE 4

1. E. Rouquerol, J. Rouquerol, K. Sing, Adsorption by Powders and Porous Solids. Principles, Methodology and Applications, Academic Press, San Diego, 1999.
2. J. M. Thomas, W. J. Thomas, Principles and Practice of Heterogeneous Catalysis, VCH, Weinheim, 1997.
3. J.W. Niemantsverdriet, Spectroscopy in Catalysis. An introduction, VCH, Weinheim, 1993.

8.2. Seminar/ laboratory	**Teaching and learning methods**	**Remarks**
Module 1		
8.2.1. – Interpretation of ^{1}H-RMN, ^{13}C-RMN, COSY, HMQC, HMBC, DNMR spectra and of the NMR spectra with other elements and those of heteronuclear correlations. - Interpretation of EI, CI, ESI, APCI, MALDI MS spectra	Conversation, Learning by discovery, Problem solving.	12 hours
8.2.2. - RES spectra, obtaining of samples, recording of spectra and their interpretation.	Conversation, Learning by discovery, Problem solving	
8.2.3. – Interpretation of UV-VIS, CD and vCD spectra for different materials.	Conversation, Learning by discovery, Problem solving	
Module 2		
8.2.4 Applications of specific programs and preparation of data for publication.	Conversation, Learning by discovery, Problem solving	4 hours
Module 3		
8.2.5 Investigation of redox systems by cyclic voltametry	Conversation, Learning by discovery, Problem solving	6 hours
8.2.6 Investigation of redox systems by chronoamperometry.	Conversation, Learning by discovery, Problem solving	
8.2.7 Spectroscopy of electrochemical impedance	Conversation, Learning by discovery, Problem solving	
Module 4		
8.2.8. Specific surface area determination for some carbon and zeolitic materials. OM/SEM/TEM/AFM images, obtaining and interpretation for some materials	Conversation, Learning by discovery, Problem solving	6 hours
8,2.9 Thermogravimetric analysis of some materials and the determination of the energy of secondary bonds by DSC.	Conversation, Learning by discovery, Problem solving	

Bibliography

MODULE 1
1. David L., Crăciun C., Cozar O., Chiş V., Rezonanţă Electronică de Spin. Principii, metode, aplicaţii, Presa Univ. Clujeană, Cluj-Napoca, 2001
2. R. M. Silverstein, F. X. Webster, D. J. Kiemle Spectrometric Identification of Organic Compounds, Wiley, New-York, 2005.
3. N. E. Jacobsen, NMR Spectroscopy Explained, Wiley-Interscience, 2007.
4. H.H. Perkampus, UV-VIS spectroscopy and its applications, Springer-Verlag, 1992.
5. Referate laborator şi fişe de lucru.
MODULE 2
1. W. Massa, Crystal Structure Determination, Editura Springer, Berlin, 2000. (accessible at the module holder)
MODULE 3
1. I.C. Popescu, G. Turdean, A. Nicoara, P. Ilea şi L. Muresan, Lucrări practice pentru Ciclul de Studii Aprofundate în Electrochimie, Lito. UBB, Cluj-Napoca, 1998.
MODULE 4
1. E. Rouquerol, J. Rouquerol, K. Sing, Adsorption by Powders and Porous Solids. Principles, Methodology and Applications, Academic Press, San Diego, 1999.
2. J. M. Thomas, W. J. Thomas, Principles and Practice of Heterogeneous Catalysis, VCH, Weinheim, 1997.
3. J.W. Niemantsverdriet, Spectroscopy in Catalysis. An introduction, VCH, Weinheim, 1993.

9. Evaluation

Type of activity	9.1 Evaluation criteria[4]	9.2 Evaluation methods[5]	9.3 Percentage in the final grade
9.4. Course	Correctness of answers –proper understanding and learning of notions and concepts discussed during lectures; Correct use of learned concept within new contexts. Correct solving of the problems as part of the examination subjects	Written examination. Proven or intended fraud is punished according to the ECST rules of UBB.	60%
9.5. Seminar/ laboratory	Correctness of answers –proper understanding and learning of notions and concepts discussed during lectures; Correct use of learned concept within new contexts.	Continuous assessment (session 6 and 7). Evaluated by means of problems to be solved	40%
9.6 Minimum standard for passing			
Grade 5 (five) at the written exam for each module. Adequate knowledge of at least one technique for each module.			

10. SDG labels (Sustainable Development Goals)[6]

	○	Sustainable Development Generic Label

								
			○					
								No label applies

[4] The evaluation criteria must directly reflect the learning outcomes targeted at the level of the degree programme respectively at the level of the subject. More specifically, the learning outcomes set out in the expected learning outcomes are assessed.

[5] Both final evaluation methods and ongoing evaluation strategies should be established.

[6] Select a single label which, according to the *Implementation of SDG labels in the academic process*, best matches the subject. If the subject addresses sustainable development in a generic manner (i.e. by presenting/introducing the general framework of sustainable development, etc.), then the Sustainable Development generic label may be applied. If none of the labels describe the **subject**, select the last option: *"No label applies."*

Date of entry:
17.04.2026

Signature of course coordinator

Prof. dr. Ion Grosu

Conf. dr. Radu Silaghi-Dumitrescu

Conf. dr. Gabriela Nemeş

Conf. Dr. Richard A. Varga.

Dr. Cosmin Coteţ

Conf. dr. Adrian Nicoara

Signature of seminar coordinator

Prof. dr. Ion Grosu

Conf. dr. Radu Silaghi-Dumitrescu

Conf. dr. Gabriela Nemeş

Conf. Dr. Richard A. Varga.

Dr. Cosmin Coteţ

Conf. dr. Adrian Nicoara

Date of approval in the department:
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Signature of the head of department

Prof. dr. ing. Graziella Liana Turdean

Prof. Dr. Monica Tosa

24.04.2026