

## FISA DISCIPLINEI

### 1. Information regarding the program

1.1 Higher education institution	Babeş-Bolyai University, Cluj-Napoca
1.2 Faculty	Chemistry and Chemical Engineering
1.3 Department	Chemistry
1.4 Field of study	Chemical Engineering
1.5 Study cycle	Master
1.6 Study programme / Qualification	Advanced Process Chemical Engineering/ Master's Degree

### 2. Information regarding the discipline

2.1 Name of the discipline	Methods for the structural characterization of materials – CME 7143						
2.2 Course coordinator	Prof. dr. Ion Grosu Prof. dr. Radu Silaghi-Dumitrescu Conf. dr. Gabriela Nemeş Conf. dr. Richard A. Varga Lect. dr. Cosmin Coteţ Conf. dr. Adrian Nicoara						
2.3 Seminar coordinator	Prof. dr. Ion Grosu Prof. dr. Radu Silaghi-Dumitrescu Conf. dr. Gabriela Nemeş Conf. dr. Richard A. Varga Lect. dr. Cosmin Coteţ Conf. dr. Adrian Nicoara						
2.4 Year of study	I	2.5 Semester	2	2.6. Type of evaluation	C	2.7 Type of discipline	DS/Opt.

### 3. Total estimated time (hours/semester of didactic activities)

3.1 Hours per week	4	Of which: 3.2 course	2	3.3 seminar/laboratory	2
3.4 Total hours in the curriculum	56	Of which: 3.5 course	28	3.6 seminar/laboratory	28
Time allotment:					ore
Learning using manual, course support, bibliography, course notes					20
Additional documentation (in libraries, on electronic platforms, field documentation)					20
Preparation for seminars/labs, homework, papers, portfolios and essays					20
Tutorship					6
Evaluations					3
Other activities: not the case					-
3.7 Total individual study hours	69				
3.8 Total hours per semester	125				
3.9 Number of ECTS credits	5				

### 4. Prerequisites (if necessary)

4.1 curriculum	<ul style="list-style-type: none"> <li>• Not the case</li> </ul>
4.2 competencies	<ul style="list-style-type: none"> <li>• Not the case</li> </ul>

## 5. Conditions (if necessary)

5.1 for the course	<ul style="list-style-type: none"> <li>• Students will attend the courses having the materials made available prior to each course</li> <li>• Students will turn off their mobile phones</li> </ul>
5.2 for the seminar /lab activities	<ul style="list-style-type: none"> <li>• Students will attend the seminar with the course notes referring to the seminar topic</li> <li>• Students will turn off their mobile phones</li> </ul>

## 6. Specific competencies acquired

Professional competencies	<ul style="list-style-type: none"> <li>• Definition of notions, concepts, theories and advanced models in the field of Methods for the structural characterization of materials as well as their proper use within the professional community.</li> <li>• Application and interpretation of the structural properties of materials as well as concepts, approaches and phenomena.</li> <li>• Identification and proper usage of concepts, method and theories for solving new complex problems of materials and environmental sciences.</li> <li>• Use of advanced knowledge in the field of chemistry and structural analysis to determine, explain and interpret the applications in the fields of materials and environmental sciences</li> <li>• Critical analysis and usage of principles, methods and advanced work techniques to solve specific problems of materials and environmental sciences.</li> <li>• Ability of understanding the techniques and for the interpretation of data obtained with spectroscopic methods for the structural characterization of materials using NMR and MS.</li> <li>• Ability of understanding the techniques and for the interpretation of data obtained with spectroscopic methods for the structural characterization of materials using RES and CD.</li> <li>• Ability of understanding the techniques and for the interpretation of data obtained with spectroscopic methods for the structural characterization of materials using X-ray and UV-vis methods</li> <li>• Ability of understanding the techniques and for the interpretation of data obtained with spectroscopic methods for the structural characterization of materials using electrochemical methods.</li> <li>• Ability of understanding the techniques and for the interpretation of data obtained with spectroscopic methods for the structural characterization of materials using thermal analysis data.</li> <li>• Familiarization with BET method and similar techniques, determination of specific areas, pores size and distribution, correlations BET-SEM.</li> </ul>
Transversal competencies	<ul style="list-style-type: none"> <li>• Analysis , interpretation and communication of scientific information and comply with professional ethics and moral</li> <li>• Planning, monitoring and assuming professional duties of underline group. Proving the coordination capabilities, analytical thinking, adaptability and flexibility, team work abilities.</li> <li>• Self-evaluation of professional performances and establish the needs of continuous learning, documentation in the work fields in correlation to the labour market</li> <li>• Responsible activities for solving the tasks and adaptation for group activities</li> <li>• The ability to write and defend reports.</li> </ul>

## 7. Objectives of the discipline (outcome of the acquired competencies)

7. General objective of the discipline	<ul style="list-style-type: none"> <li>Familiarize students with the basics notions, concepts and techniques used in the identification, structural characterization and reactivity of materials by spectroscopic methods</li> </ul>
7.2 Specific objective of the discipline	<ul style="list-style-type: none"> <li>Assimilation of the requested knowledge to be able to use NMR and MS techniques for the characterization of materials.</li> <li>Assimilation of the requested knowledge to be able to use RES and CV techniques for the characterization of materials .</li> <li>Assimilation of the requested knowledge to be able to use UV Vis and X-ray techniques for the characterization of materials .</li> <li>Assimilation of the requested knowledge to be able to use electrochemical techniques for the characterization of materials</li> <li>Assimilation of the requested knowledge to be able to use nitrogen adsorption-desorption, thermogravimetric, OM, TEM, SEM and AFM techniques for the characterization of materials</li> </ul>

## 8. Content

8.1. Course	Teaching methods	Remarks
<b>MODULE 1 Spectroscopic methodes for structural characterization of organic and organometallic compounds</b>		12 hours
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	
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 RES. Applicability and techniques. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
8.1.4. Structural Characterization by RES: experiments for materials characterization and biochemical applications (2 hours)		
8.1.5. Structural Characterization by UV-Vis spectroscopy.. Applicability and techniques. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
8.1.6. Structural Characterization by CD and vCD methods. Applicability and techniques. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
<b>MODULE 2 Structural Characterization by DRX</b>		4 hours
8.1.7. Single crystal and powder X ray diffractometry. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
8.1.8. Interpretation of primary data. Atomic parameters, crystallographic tables intra and intermolecular connection (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
<b>MODULE 3. Structural Characterization by electrochimical methods.</b>		6 hours
8.1.9. The principles of electrochemical investigations:	Presentation; Explanation,	

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).	Conversation; Description; Debate	
8.1.10. Classic and non-conventional polarography: 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, chronoamperometry and impedance spectroscopy. Reversibility criteria, experimental parameters and methods for the determination of characteristic physico-chemical properties. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
<b>MODULE 4 – Characterization of materials and precursors using specific areas, pores distribution and the structure of the surface evaluated by microscopic methods (SEM, TEM). Thermogravimetric methods and Differential Scanning Calorimetry</b>		6 hours
8.1.12. Adsorption. Porous structure of solids. Determination of specific area and of the distribution of the pores. (2 hours).	Presentation; Explanation, Conversation; Description; Debate	
8.1.13. Structural characterization of solids by electronic microscopy. (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	
<b>Bibliography</b> Bibliografie Courses support MODULE 1 1. N. E. Jacobsen, <i>NMR Spectroscopy Explained</i> , Ed Wiley-Interscience, 2007. 2. H Friebolin, <i>Basic One- and Two-dimensional NMR Spectroscopy</i> , Wiley-VCH, 2004. 3. S. Mager, <i>Analiza Structurala Organică</i> , Ed. Științifică și Enciclopedică, București 1979. 4. David L., Crăciun C., Cozar O., Chiș V., <i>Rezonanță Electronică de Spin. Principii, metode, aplicații</i> , Presa Univ. Clujeană, Cluj-Napoca, 2001. 5. H.H. Perkampus, <i>UV-VIS spectroscopy and its applications</i> , Springer-Verlag, 1992. Bibliography MODULE 2 1. W. Massa, <i>Crystal Structure Determination</i> , Editura Springer, Berlin, 2000. (accessible at the module holder) Bibliografie MODULE 3 1. Oniciu L., Mureșan L., <i>Electrochimie aplicată</i> , Presa Universitară Clujeană, 1998. 2. A. J. Bard și L. R. Faulkner, <i>Electrochemical Methods. Fundamentals and Applications</i> , John Wiley and Sons, New-York, 1980. Bibliografie MODULE 4 1. E. Rouquerol, J. Rouquerol, K. Sing, <i>Adsorption by Powders and Porous Solids. Principles, Methodology and Applications</i> , Academic Press, San Diego, 1999. 2. J. M. Thomas, W. J. Thomas, <i>Principles and Practice of Heterogeneous Catalysis</i> , VCH, Weinheim, 1997. 3. J.W. Niemantsverdriet, <i>Spectroscopy in Catalysis. An introduction</i> , VCH, Weinheim, 1993.		

8.2 Seminar / Laboratory	Teaching methods	Remarks
<b>Module 1</b>		12 hours
8.2.1. – Interpretation of $^1\text{H}$ -RMN, $^{13}\text{C}$ -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.	
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	
<b>Module 2</b>		
8.2.4 Applications of specific programs and preparation of data for publication.	Conversation, Learning by discovery, Problem solving	4 hours
<b>Module 3</b>		
8.2.5 Investigation of redox systems by cyclic voltametry	Conversation, Learning by discovery, Problem solving	6 hours
8.2.6 Spectroscopy of electrochemical impedance	Conversation, Learning by discovery, Problem solving	
<b>Module 4</b>		
8.2.7. Specific surface area determination for some carbon and zeolitic materials. SEM/TEM/OM images, obtaining and interpretation for some natural porous materials	Conversation, Learning by discovery, Problem solving	6 hours
8.2.8 Thermogravimetric analysis of some materials and the determination of the energy of secondary bonds by DSC.	Conversation, Learning by discovery, Problem solving	
<b>Bibliography</b> <b>MODULE 1</b> 1. David L., Crăciun C., Cozar O., Chiș V., <i>Rezonanță Electronică de Spin. Principii, metode, aplicații</i> , Presa Univ. Clujeană, Cluj-Napoca, 2001 2. R. M. Silverstein, F. X. Webster, D. J. Kiemle <i>Spectrometric Identification of Organic Compounds</i> , Wiley, New-York, 2005. 3. N. E. Jacobsen, <i>NMR Spectroscopy Explained</i> , Wiley-Interscience, 2007. 4. H.H. Perkampus, <i>UV-VIS spectroscopy and its applications</i> , Springer-Verlag, 1992. 5. Referate laborator și fișe de lucru. <b>Bibliography MODULE 2</b> 1. W. Massa, <i>Crystal Structure Determination</i> , Editura Springer, Berlin, 2000. (accessible at the module holder) <b>Bibliografie MODULE 3</b> 1. I.C. Popescu, G. Turdean, A. Nicoara, P. Ilea și L. Muresan, <i>Lucrări practice pentru Ciclul de Studii Aprofundate în Electrochimie</i> , Lito. UBB, Cluj-Napoca, 1998. <b>Bibliografie MODULE 4</b> 1. E. Rouquerol, J. Rouquerol, K. Sing, <i>Adsorption by Powders and Porous Solids. Principles, Methodology and Applications</i> , Academic Press, San Diego, 1999. 2. J. M. Thomas, W. J. Thomas, <i>Principles and Practice of Heterogeneous Catalysis</i> , VCH, Weinheim, 1997. 3. J.W. Niemantsverdriet, <i>Spectroscopy in Catalysis. An introduction</i> , VCH, Weinheim, 1993.		

**9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program**

- Acquirement of the theoretical and practical concepts of **Methods for the structural characterization of materials** course will provide the students with the competencies requested by ARN.

**10. Evaluation**


Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the final grade (%)
10.4 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%
10.5 Seminar/laboratory	Correctness of answers –proper understanding and learning of notions and concepts discussed during lectures; Correct use of learned concept within new contexts. Quality of reports	Continuous assessment (session 6 and 7). Evaluated by means of problems to be solved,	40%
10.6 Minimum performance standards			
<ul style="list-style-type: none"> <li>Grade 5 (five) at the written exam for each module.</li> <li>Adequate knowledge of at least one technique for each module.</li> </ul>			

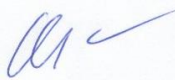
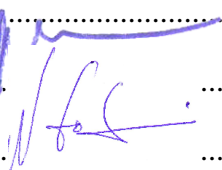


Date

Signature of course coordinators

Signature of seminar coordinators

06.04.2021


  
.....  
  
.....  
  
.....  
  
.....

  
.....  
  
.....  
  
.....  
  
.....

Date,

Approval in Department

May 07, 2021

.....  
  
.....

.....  
  
.....

Signature,  
Head of Chemistry Department

Acad. Cristian Silvestru



Date of approval

Signature of the head of department

April 25, 2021



Prof. dr. ing. Graziella Liana Turdean