

CURRICULUM

Master: Chemistry of Advanced Materials

FACULTY OF CHEMISTRY

UNIVERSITY OF BUCHAREST

First year of study, semester I

	Course name	No. hours
1	Liquid crystals	56
2	Catalytic materials	56
3	Physical chemistry of the solid state	56
4	Ethics and academic integrity	14
5	Biobased and biodegradable materials	28

First year of study, semester II

	Course name	No. hours
1	Micro and nanostructured polymer-based materials. Thermal analysis	56
2	Polynuclear Complexes and Molecular Materials	56
3	Physical chemistry of mesogens	56
4	Chemocatalytic concepts for biomass valorization	28

Second year of study, semester I

	Course name	No. hours
1	Characterisation of materials	56
2	Chemical sensors and biosensors	56
3	Research activity	168

Second year of study, semester II

	Course name	No. hours
1	Nanomaterials	40
2	Clusters, polymers and inorganic rings chemistry	40
3	Research activity	180
4	Biomass valorization based on biocatalysis	20

UNIVERSITY OF BUCHAREST
FACULTY OF CHEMISTRY
Master: Chemistry of Advanced Materials

SYLLABUS

Dicipline: CATALYTIC MATERIALS

Lecturer: Prof. Dr. Habil. Ioan-Cezar MARCU

No. of lecture hours: 28

No. of hours for practical activities: 28

Nr. of credits: 5

Form of examination: Written examination

Lectures: 28 hours

No.	Lecture topic	No. of hours
1	Introduction. Placing catalytic materials in the group of functional materials. Definition of the concepts of material, functional material and catalytic material. Definition of the catalytic action. Fundamental properties of the solid catalysts: activity, selectivity and stability. Classification of solid catalysts.	1
2	Catalysts based on metals and metallic alloys. Preparation of metallic catalysts. Specific features regarding the structure and properties of metallic catalysts. The nature of the active sites. Structure sensitivity of catalytic reactions. Supported metal catalysts. Metal-support interaction. Reaction mechanisms in catalysis on metals. Fundamentals of kinetics of heterogeneous catalytic reactions. Case study: the ammonia synthesis catalyst and the reaction mechanism involved.	6
3	Oxide-based catalytic materials. Preparation techniques. Structure of oxide catalysts. Oxides with variable valence state. Oxide non-stoichiometry – structural defects. Semiconductor character. Consequences for heterogeneous catalysis. Catalytic oxidation. The Mars – van Krevelen reaction mechanism and the corresponding rate law.	6
4	Acidic oxides. Origin of acidity. Lewis and Brønsted acidity in oxides. Control of acidity. Reaction mechanisms of acid-catalyzed reactions. Examples of acid catalysts. Alumina – catalyst and support.	4
5	Base oxides. Layered double hydroxydes – precursors for base oxides. Synthesis. Structure. Memory effect. Origin of basicity. Other base oxides. Applications in catalysis.	2
6	Sulfide-based catalytic materials. Preparation. Structure. Nature of active sites. Applications in catalysis.	2
7	Porous materials for catalyst support. Ordered porous materials. Techniques of preparation. Techniques of deposition of active component.	3

8	Biocatalytic materials. Enzyme as biocatalyst. Enzyme immobilization techniques. Biocatalytic aspects of immobilized enzymes (applications of the immobilized enzymes). Biocatalysis supporting natural products chemistry.	4
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Practical activities: 28 hours

No.	Practical activity subject	No. of hours
1	Safety rules in the laboratory. Brief presentation of practical activities and experimental set-ups	2
2	Preparation of a mixed oxide catalyst by coprecipitation	6
3	Characterization of oxides with variable valence state by electrical conductivity measurements as a function of temperature and oxygen partial pressure. Determination of structural defects.	8
4	Study of the catalytic oxidation of light alkanes over oxide-based catalysts in a continuous-flow reactor.	6
5	Multifunctional catalytic materials. Applications in catalytic conversion of ethanol in a batch reactor.	4
6	Discussion of the practical work reports and experimental results. Conclusions.	2

Recommended bibliography*

FOR LECTURERS

1. G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp (Eds.), *Handbook of Heterogeneous Catalysis*, 2nd Edition, Wiley-VCH, Weinheim, 2008.
2. F. Schüth, K. S. W. Sing, J. Weitkamp, (Eds.), *Handbook of Porous Solids*, Wiley-VCH, Weinheim, 2002.
3. J.M. Thomas, W.J. Thomas, *Principles and Practice of Heterogeneous Catalysis*, Wiley, 1996.
4. J.A. Anderson, M. Fernandez Garcia (Eds.), *Supported Metals in Catalysis*, Imperial College Press, 2005.
5. M.A. Vannice, *Kinetics of Catalytic Reactions*, Springer, 2005.
6. G.C. Bond, *Metal-catalysed reactions of hydrocarbons*, Springer, 2005.
7. M. Misono (Ed.), Heterogeneous Catalysis of Mixed Oxides Perovskite and Heteropoly Catalysts, *Stud. Surf. Sci. Catal.* 176 (2013) 1-181.
8. J.L.G. Fierro (Ed.), *Metal Oxides - Chemistry and Applications*, CRC Press, 2006.
9. A. Trovarelli (Ed.), *Catalysis by Ceria and Related Materials*, Imperial College Press, 2002.
10. K. Kosuge, *Chemistry of non-stoichiometric compounds*, Oxford University Press, 2001.

11. J.M. Herrmann, *Les techniques physiques d'étude des catalyseurs* (Imelik, B., Védrine, J.C. – éditeurs), Ed. Technip, Paris, 1988, Ch. 22.
12. M.A. Vannice, An analysis of the Mars – van Krevelen rate expression, *Catalysis Today*, 123 (2007) 18-22.
13. S.M. Coman, V.I. Pârvulescu, *Cataliză Acido-Bazică*, Editura Academiei Române, București, 2010.
14. D.G. Evans, X. Duan (Eds.), *Layered Double Hydroxides*, Springer-Verlag Berlin, 2006.
15. F. Cavani, F. Trifiro, A. Vaccari, Hydrotalcite-type anionic clays: preparation, properties and applications, *Catalysis Today*, 11 (1991) 173-301.
16. K. Faber, *Biotransformations in Organic Chemistry*, Springer-Verlag Berlin 2001.
17. K. B. G. Torssell, *Natural Product Chemistry*, 2nd ed., Apotekersocieteten/Taylor & Francis, 1997.

FOR PRACTICAL ACTIVITIES

1. S. Tanasoi, G. Mitran, N. Tanchoux, T. Cacciaguerra, F. Fajula, I. Săndulescu, D. Tichit, I.-C. Marcu, „Transition metal-containing mixed oxides catalysts derived from LDH precursors for short-chain hydrocarbons oxidation”, *Appl. Catal. A* 395 (2011) 78-86 (DOI: 10.1016/j.apcata.2011.01.028).
2. I.-C. Marcu, N. Tanchoux, F. Fajula, D. Tichit, „Catalytic conversion of ethanol into butanol over M-Mg-Al mixed oxide catalysts (M = Pd, Ag, Mn, Fe, Cu, Sm, Yb) obtained from LDH precursors”, *Catal. Lett.* 143 (2013) 23-30 (DOI: 10.1007/s10562-012-0935-9).
3. I. Popescu, E. Heracleous, Z. Skoufa, A. Lemonidou, I.-C. Marcu, „Study by electrical conductivity measurements of semiconductive and redox properties of M-doped NiO (M = Li, Mg, Al, Ga, Ti, Nb) catalysts for the oxidative dehydrogenation of ethane”, *Phys. Chem. Chem. Phys.* 16 (2014) 4962-4970 (DOI: 10.1039/C3CP54817A).
4. M. Răciulete, G. Layrac, F. Papa, C. Negrilă, D. Tichit, I.-C. Marcu, „Influence of Mn content on the catalytic properties of Cu-(Mn)-Zn-Mg-Al mixed oxides derived from LDH precursors in the total oxidation of methane”, *Catal. Today* 306 (2018) 276-286 (DOI: 10.1016/j.cattod.2017.01.013).
5. I. Popescu, J.C. Martínez-Munuera, A. García-García, I.-C. Marcu, „Insights into the relationship between the catalytic oxidation performances of Ce-Pr mixed oxides and their semiconductive and redox properties” *Appl. Catal. A* 578 (2019) 30-39 (DOI: 10.1016/j.apcata.2019.03.021).

* Available at the library of the Laboratory of Chemical Technology & Catalysis.

UNIVERSITY OF BUCHAREST
 FACULTY OF CHEMISTRY
Master: Chemistry of Advanced Materials

SYLLABUS

Discipline: BIOBASED AND BIODEGRADABLE MATERIALS

Lecturer: Dr. Delia-Laura POPESCU

No. of lecture hours: 28

No. of hours for practical activities: -

Nr. of credits: 3 ECTS

Form of examination: Written examination

Lectures: 28 hours

No.	Lecture topic	No. of hours
1.	Introduction to the course. Biobased and biodegradable materials: general characteristics and classifications	2
2.	Biomass properties and limitations/challenges for producing biobased materials. Transition towards a biobased economy. From linear bioeconomy to circular bioeconomy. Policies in a biobased economy. Sustainable biomass use	4
3.	Mechanisms of biodegradation. Methods for evaluating the biodegradability, environmental fate and ecotoxicity assessment of biodegradable materials. International and national norms on biodegradability and certification procedures	6
4.	Types of biodegradable materials - synthesis, physical and chemical properties, applications, biodegradation	4
5.	Biobased and biodegradable materials with industrial applications	4
6.	Biobased and biodegradable materials with environmental applications	4
7.	Biobased and biodegradable materials with medical applications	4

Recommended bibliography

1. *Biomass in the Bioeconomy*, J.L. Wertz, P. Mengal, S. Perez, CRC Press, 2022
2. *Biomaterials Science: An Introduction to Materials in Medicine*, 2nd Edition, Editors: B.D. Ratner, A.S. Hoffman, F.J. Schoen, J.E. Lemons, Elsevier Academic Press, USA, 2004.
3. *Biodegradable Materials: Production, Properties, and Applications*, B.M. Johnson, Z.E. Berkel, Nova Science Publishers, USA, 2011.
4. *The Complete Book on Biodegradable Plastics and Polymers (Recent Developments, Properties, Analysis, Materials & Processes)*, NIIR Board, Asia Pacific Business Press Inc., 2006.
5. *Biodegradable and Bio-based Polymers for Environmental and Biomedical Applications*, Ed. S. Kalia and L. Averous, Scrivener Publishing, 2016.
6. Articole științifice publicate în jurnale ale editurilor Elsevier, Wiley, Springer etc.

UNIVERSITY OF BUCHAREST
 FACULTY OF CHEMISTRY
Master: Chemistry of Advanced Materials

SYLLABUS

Dicipline: BIOMASS VALORIZATION BASED ON BIOCATALYSIS

Lecturer: Assoc. prof. Madalina SANDULESCU-TUDORACHE

No. of lecture hours: 20

Form of examination: Written examination

Lectures: 20 hours

No.	Lecture topic	No. of hours
1	Introduction. Basic concepts related to recycle (bio)-economy	2
2	Biomass: definition, classification, examples; discussion on biomass cocept.	2
3	Biocatalysis: definition, classification; aspects specific for biotechnology; discussion on the enzyme biocatalysis.	4
4	Homogeneous biocatalysis. Applications of biomass valorization	4
5	Heterogeneous biocatalysis. Applications of biomass valorization	4
6	Tune biocatalysts for biomass conversion	2
7	Critically evauation of biobased conversion route vs. fossil-based conversion route.	2

Recommended bibliography

1. R. Sheldon and D. Brady, Green chemistry, biocatalysis and the chemical industry of the future, 2022, ed. Wiley, doi.org/10.1002/cssc.202102628.
2. A.S. Bommarius and B.R. Riebel, Biocatalysis, 2004, ed. Wiley-Blackwell, ISBN-13 : 978-3527303441.
3. D. Ravelli and C. Samori, Biomass valorization: Sustainable methods for the production of chemicals, 2021, Wiley-VCH, ISBN: 9783527347179.
4. C. Baskar, S. Ranjit, R.S. Dhillon, Biomass conversion. The interface of biotechnology, chemistry and materials science, 2014, Springer-Verlag Berlin and Heidelberg GmbH & Co. KG, ISBN: 3642444490.

UNIVERSITY OF BUCHAREST
 FACULTY OF CHEMISTRY
Master: Chemistry of Advanced Materials

SYLLABUS

Dicipline: Chemo-catalytic concepts for biomass valorization

Lecturer: Prof. Dr. Habil. Simona Margareta COMAN

No. of lecture hours: 28

No. of hours for practical activities: 28

Nr. of credits: 5

Form of examination: Written examination

Lectures: 28 hours

No.	Lecture topic	No. of hours
1	Introduction. Sustainability for the twenty-first century: challenges; dematerialization versus transmaterialisation; sustainability in chemistry	2
2	Introduction in green chemistry: principles, evaluating the greenness of a chemical reaction (metrics, radial pentagon).	4
3	Introduction in green solvents: water as reaction solvent, ionic liquids, supercritical fluids, fluoruous solvents.	4
4	Heterogeneous catalysis in the context of green chemistry and sustainability. Critical elements. Case studies: catalysis in fine chemicals (vitamin E and menthol) and pharmaceutical (ibuprofen) synthesis.	4
5	Renewable resources: from biomass to bio-chemicals (platform molecules) and bio-fuels. Bio-refinery concept	4
6	Strategies to approach the renewable chemical industry: product-targeted and platform-molecule approaches	4
7	Towards a greener industry: liquid-phase conversion of biomass	2
8	Catalysts design for biomass valorization: metal oxides, metal oxide-supported metals, carbon-supported metals, acid-functionalized mesoporous materials, ion-exchange resins, zeolites and zeolite-supported metals	4

Practical activities: 28 hours

No.	Practical activity subject	No. of hours
1	Safety rules in the laboratory. Brief presentation of practical activities and experimental set-ups. Seminar: green metrics calculation for different organic reaction types and their evaluation from green chemistry point of view.	4
2	Catalytic transfer hydrogenation of castor oil	4

3	Synthesis of imidazolium room-temperature ionic liquids	4
4	Valorization of coffee grounds for biodiesel production	8
5	The catalytic one-pot synthesis of menthol from citronellal. The Wender principle: "reaction step economy".	4
6	Discussion of the practical work reports and experimental results. Conclusions.	4

Recommended bibliography

1. J. Clark, D. Macquarrie, *Handbook of green chemistry and technology*, Blackwell Science Ltd Ed., 2002
2. J. Clark, F. Deswarte, *Introduction to chemicals from biomass*, 2015, John Wiley & Sons, Ltd ISBN: 978-1-118-71448-5
3. S.M. Coman, V.I. Pârvulescu, *Cataliză Acido-Bazică*, Editura Academiei Române, București, 2010
4. P. Sudarsanam, R. Zhong, S. Van den Bosch, S. M. Coman, V. I. Parvulescu, B. F. Sels, *Functionalized heterogeneous catalysts for sustainable biomass upgrading to high-value chemicals*, *Chem. Soc. Rev.*, 2018, 47, 8349-8402

UNIVERSITY OF BUCHAREST
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Master: Chemistry of Advanced Materials

SYLLABUS

Dicipline: NANOMATERIALS

Lecturer: Dr. Octavian Pavel DUMITRU

No. of lecture hours: 20

No. of hours for practical activities: 20

Nr. of credits: 5

Form of examination: Written examination

Lectures: 20 hours

No.	Lecture topic	No. of hours
1	States of the art: the concept of nanomaterials, nanoscale, nanopores and nanostructures.	1
2	Nanomaterials synthesis by chemical, physical and biomimetics way. Synthesis of metallic and polymeric nanomaterials. Correlation structure - properties.	4
3	Classification of nanomaterials. Present and future applications of nanomaterials	2
4	Carbon Nanotubes - description, properties and applications.	2
5	Nanoparticles / nanopowder - description, properties and applications.	2
6	Nanocomposites - description, properties and applications.	2
7	Nanocapsules - description, properties and applications	2
8	Nanodots - description, properties and applications	2
9	Characterization of nanomaterials (SEM and AFM techniques)	1
10	Nanomaterials application: bio-nanomaterials with catalytic properties	2

Practical activities: 20 hours

No.	Practical activity subject	No. of
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		hours
1	Presentation of the laboratory: practical concepts, equipment and facilities. Laboratory work safety rules and fire protection.	2
2	Preparation of Ni nanoparticles using microwaves.	4
3	Determining the network parameters of a nanocrystalline structure. Analysis of crystalline solids by X-ray diffraction method	4
4	Determination of nanoparticle size.	4
5	Nanomaterials with catalytic properties. Application: hydrogenation reaction in the presence of Ni nanoparticles	4
6	Laboratory knowledge evaluation	2

Recommended bibliography

<ol style="list-style-type: none"> 1. Nanomaterials – Mechanics and Mechanisms ; K.T. Ramesh ; DOI 10.1007/978-0-387-09783-1 ; Springer Dordrecht Heidelberg London New York 2. Nanomaterials Handbook ; Edited by Yury Gogotsi 2006 by Taylor & Francis Group, LLC 3. Nanomaterials and Nanochemistry ; C. Brechignac, P. Houdy, M. Lahmani (Eds.) ; ISBN 978-3-540-72992-1 Springer Berlin Heidelberg New York 4. Nanomaterials - Synthesis, Properties and Applications ; Edited by A. S. Edelstein and R. C. Cammarata; ISBN 0 7503 0358 1 5. Nanomaterial Characterization – An Introduction; Edited by Ratna Tantra ; Published by John Willey & Sons, Inc., Hoboken, New Jersey 6. Nanomaterials Chemistry - Recent Developments and New Directions ; Edited by C.N.R. Rao, A. Müller, and A.K. Cheetham ; ISBN 978-3-527-31664-9 7. Introduction to Carbon Science ; Editor Professor Harry Marsh ; ISBN 0-408-03837-3

UNIVERSITY OF BUCHAREST
FACULTY OF CHEMISTRY
Master: Chemistry of Advanced Materials

SYLLABUS

Dicipline: MICRO AND NANOSTRUCTURED POLYMER MATERIALS. THERMAL ANALYSIS

Lecturer: Assoc. prof. Bogdan JURCA and Assoc. prof. Marian MICUT

No. of lecture hours: 28

No. of hours for practical activities: 28

Nr. of credits: 5

Form of examination: Written examination

Lectures: 20 hours

No.	Lecture topic	No. of hours
1	Introductory notions. Defining macrometric and nanometric domains in obtaining structured materials. General features and peculiarities on descendant (top-down) and ascendant (bottom-up) technologies in micro and nanostructured materials fabricati	2
2	Thermodynamic stability of binary mixtures: regular solutions, polymer solutions, polymer blends	2
3	Phase separation – an optimal approach in obtaining micro and nanostructured polymer-based films	2
4	Binodals and spinodals. Micro and nanostructures resulted via spinodal decomposition	2
5	Block copolymer self-assembly and nanostructures formation	2
6	Miniemulsion polymerization and synthesis of polymer nanoparticles	2
7	Polymer-based biomaterials used in tissue engineering	2
8	General principles of thermal analysis. Presentation of commonly used methods (TG, DTA and DSC). Physico-chemical informations obtained from these methods (exampl	2
9	Heterogeneous reactions with participation of solid phases. Kinetic	2

	influence of nucleation and diffusion. Isothermal heterogeneous processes: derivation of kinetic equations, parallelism with the kinetic treatment of homogeneous systems, differential/integral forms of the conversion function.	
10	Nonisothermal heterogeneous processes: differential/integral forms of the kinetic equation, temperature integral evaluation problem.	2
11	Calculation of the conversion degree from experimental TG and DSC data; classification of methods to determine the nonisothermal kinetic parameters. Methods to determine the nonisothermal kinetic parameters from a single heating rate experiment: differential methods.	2
12	Methods to determine the nonisothermal kinetic parameters from a single heating rate experiment: integral methods. Drawbacks of the methods based on a single heating.	2
13	Isoconversional methods to determine the activation energy: Linear isoconversional (integral and differential) methods. Nonlinear isoconversional (integral and differential) methods.	2
14	Methods to discriminate the expression of the conversion function Compensation effect in nonisothermal kinetics. Invariant kinetic parameters method	2

Practical activities: 28 hours

No.	Practical activity subject	No. Of hours
1	General safety and security rules. Viscoelastic behavior of a polymeric hydrogel revealed by dynamic-oscillatory rheology.	2
2	Study of in vitro fibrillogenesis of type I collagen	4
3	Synthesis of polymer nanoparticles: miniemulsion polymerization of methyl methacrylate	4
4	Obtaining a colloidal crystal by quasistatic self-assembly, from aqueous suspension, of monodisperse PMMA spheres onto a borosilicate glass	4

	substrate. Visible light diffraction as a method of assessing freshly deposited colloidal crystal: transparency to visible light and particle size estimat.	
5	Presentation of the thermal analysis experimental setup. Experimental study of the decomposition of calcium oxalate. Interpretation of the experimental curves (attribution and validation of the thermal decomposition mechanism).	4
6	Kinetic interpretation of the data obtained at thermal decomposition of calcium oxalate: methods based on a single heating rate. Critical analysis of the obtained results.	4
7	Study of the thermal decomposition of polyvinyl chloride by TG, DTG and DTA. Calculation of the kinetic parameters by isoconversional methods from multiple heating rate experiments. Critical analysis of the obtained result.	4
8	Discrimination of the conversion function expression for thermal decomposition of polyvinyl chloride in nonisothermal condition.	2

Recommended bibliography

<p>1. Course notes 2. W.T.S. Huck (editor) – Nanoscale Assembly. Chemical Techniques, Springer Science+Business Media, Inc., New York, 2005 3. B. Bhushan (editor) – Springer Handbook of Nanotechnology, Springer Science+Business Media, Inc., Heidelberg, 2004 4. M. Di Ventra, S. Evoy, J.R. Heflin, Jr. (editori) – Introduction to Nanoscale Science and Technology, Springer Science+Business Media, Inc., Boston, 2004 5. I.G. Murgulescu, E. Segal - Introducere în Chimia Fizică, vol.II.1, Teoria Molecular-Cinetică a Materiei, Editura Academiei, București, 1979 6. I.G. Murgulescu, T. Oncescu, E. Segal - Introducere în Chimia Fizică, vol.II.2, Cinetică Chimică și Cataliză, Editura Academiei, București, 1981 7. E. Segal, D. Fătu - Introducere în Cinetica Neizotermă, Editura Academiei, București, 1983 8. W. M. Groenewoud – Characterisation of Polymers by Thermal Analysis, Elsevier, 2001 9. Michael E. Brown (editor) – Handbook of Thermal Analysis and Calorimetry – vol.1 – Principles and Practice, Elsevier 1998 10. Stephen Z. D. Cheng (editor) - Handbook of Thermal Analysis and Calorimetry – vol.3 – Applications to Polymers and Plastics, Elsevier 2002 11. Michael E. Brown, Patrick K. Gallagher (editors) - Handbook of Thermal Analysis and</p>

Calorimetry – vol.5 – Advances, Techniques
and Application, Elsevier 2008

12. Michael E. Brown (editor) – Hot Topics in Thermal Analysis and Calorimetry – vol.1 –
Introduction to Thermal Analysis –

Techniques and Applications, Kluwer Academic Publishers, 2001

13. Judit Simon (editor) – Hot Topics in Thermal Analysis and Calorimetry – vol.7 – Thermal
Decomposition of Solids and Melts,
Kluwer Academic Publishers, 2007

14. Paul Gabbott (editor) – Principles and Applications of Thermal Analysis, Blackwell
Publishing, 2008

15. T. Hatakeyama, F.X. Quinn - Thermal Analysis - Fundamentals and Applications to
Polymer Science, 2nd edition, John Wiley and
Sons, 1999

16. P. J. Haines (editor) - Principles of Thermal Analysis And Calorimetry, Royal Society of
Chemistry, 2002

17. Bernhard Wunderlich - Thermal Analysis of Polymeric Materials, Springer 2005

18. A. K. Galwey, M. E. Brown – Thermal Decomposition of Ionic Solids, Elsevier 199