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.	2
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	2

	sites. Applications in catalysis.	
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).	3

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, Bucureşti, 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.

Disclaimer: This Summer School is realised with the EEA Financial Mechanism 2014-2021 financial support. Its content (text, photos, videos) does not reflect the official opinion of the Programme Operator, the National Contact Point and the Financial Mechanism Office. Responsibility for the information and views expressed therein lies entirely with the author(s)