UCLouvain

# lbrna2201

*2023*

# Principles in heterogeneous catalysis

| 5.00 credits | 52.5 h | Q1 |
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| Teacher(s) | Gaigneaux Eric ; |
| Language : | French<br>> English-friendly |
| Place of the course | Louvain-la-Neuve |
| Prerequisites | No prerequisite. The courses LBRNA2103 ' Chimie des solides and LBRNA2102 ' Caractérisation de la surface des matériaux, or equivalent courses, are however helpful. |
| Main themes | The course gives a complete overview of catalysis, in particular heterogeneous catalysis. The different categories of catalysts and catalytic processes are surveyed and situated in the context of industrial processes related to petrochemistry, fine chemistry, environmental protection (air and water depollution) and biomass conversion. Then, are addressed the principles dictating the efficiency of catalysts; are described, first the elementary steps of the catalytic cycle, then the kinetic laws related to the different main catalytic mechanisms. At the end, the main methods for the preparation of heterogeneous catalysts are addressed, distinguishing between bulk catalysts and supported ones, and mentioning the problematic of their scaling-up. |
| Learning outcomes | **At the end of this learning unit, the student is able to :**<br>a. Contribution de l'activité au référentiel AA (AA du programme)<br>1.2, 1.4<br>2.2, 2.3, 2.4<br>3.5, 3.6, 3.7<br>4.1, 4.2, 4.3, 4.4, 4.5<br>b. Formulation spécifique pour cette activité des AA du programme (**maximum 10**)<br>At the end of this activity, the student is able to :<br>- Explain the impact of a catalyst on the different indicators (enthalpy, free energy, equilibrium constant, reaction path, etc) of a chemical reaction<br>- Describe the working of a catalyst in a given chemical reaction among the major catalytic mechanisms and their elementary steps.<br>From there, the student is also able to:<br>1 - Deduce the role of the different co-reagents (and eventually the products) in a catalytic mechanism,<br>- Predict the impact of variations of operating conditions (temperature, pressure, concentrations, etc) on the performances (conversion, selectivity, specificity, lifespan, resistance to deactivation, etc) of a catalytic process,<br>- Propose the co-reagents and conditions allowing to optimize the latters;<br>- Deduce the roles of the different elements (atoms, clusters, crystalline phases, etc) constituting the formulation of an active catalyst in a given chemical reaction, and propose guidelines of improvements.<br>Moreover, the student is able to :<br>- Discriminate between specificity and selectivity (in particular their 'shape' variants) of a catalytic system, and propose different catalysts preparation strategies allowing to improve these performance indicators;<br>- Propose a method, and the conditions and reagents to utilize, allowing to prepare a catalyst meeting given specifications (bulk and surface compositions, texture, structure, oxidation stages of elements, performances, etc). |
| Evaluation methods | Written "open book" examination surveying systematically all the mentioned LO. |
| Teaching methods | Lecture supported by a powerpoint slideshow available on Moodle at the beginning of the course. A constant interaction via questions-answers is established with the students, leading them to debates, and allowing them to integrate the content during the lessons. Case studies of general interest (automotive catalysis) or more specific (examples of current researches) are also undertaken.. |
| Content | PART 1 ' Introduction, History and GEneralities<br>INTRODUCTION : Objectives of the course / Connection with chemistry of solids / Definition of heterogeneous catalysis / Catalysts application domains<br>HISTORy : The beginning of heterogeneous catalysis / Les 1st ideas / The 1st applications / The start of modern catalysis / Sabatier's works / Sabatier's descendants / Modern applications / The current situation |

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| | GENERALITIES : What is a catalyst ? / Major catalysts categories (homogeneous catalysis ' biocatalysis ' heterogeneous catalysis) / Comparaison and complementarity homo vs heterogeneous / Importance of catalysis (atom efficiency, E factor, EQ factor)<br>PART 2 ' Basic Principles<br>CATEGORIES OF HETEROGENEOUS CATALYSTS : Bulk catalysts / Supported catalysts / Malaxed-agglomerated catalysts<br>MORPHOLOGY OF HETEROGENEOUS CATALYSTS : Grain-micrograin-particule / Structuration / Concept of dispersion<br>PRINCIPLES FOR THE PREPARATION OF HETEROGENEOUS CATALYSTS: major operations for the preparation of bulk catalysts / major operations for the preparation of supported catalysts<br>STEPS OF THE HETEROGENOUS CATALYTIC REACTION : Reminder ' Steps ' Dependance to the temperature / Diffusion (importance of the diffusion ' external vs internal diffusion - consequences of diffusional limitations - preventing diffusional limitations) / Adsorption (importance of the adsorption - importance of the chimisorption) / Reaction mechanisms (Langmuir's monomolecular model ' Langmuir-Hinshelwood's, Eley 'Ridea's and Mars-van Krevelen's bimolecular models) / Connection with chemistry of solids / Connection with chemical engineering<br>PART 3 ' Environmental catalysis, the case of automotive catalysis<br>SOCIETAL NEEDS : Polluters & polluants / Challenges of environmental catalysis / Application domains<br>CONTEXT AUTOMOTIVE CATALYSIS : A few figures / Composition exhaust gases (gazoline vs diesel) / Standards<br>REACTIONS TO ACHIEVE : the 3 ways / effect of air/fuel ratio / concepts of richness : « Lambda » based and Schlater's / Effect of Lambda / Lambda probe<br>THE CATALYST : Typical composition / Variants / Causes of deactivation<br>OXIDATION OF CO : NO = poison, CO also / Langmuir Hinshelwood's mechanism / Effect of ceria<br>OXIDATION OF HC AND ALCOHOLs : Light-off and T50 / Adding ceria / Mechanis / Complications (1. dynamic effect - 2. reactions with water vapor and related reactions : reforming, water gas shift, PROX process, hydrocarbon steam reforming)<br>REDUCTION OF NOx : CO+NO / NO+H2 / Novel tendencies (1. novel engines ' 2. Towards the diesel engine) / NOx-trap (1. Toyota process ' 2. Particules and soots)<br>PART 4 ' Synthesis of heterogeneous catalysts<br>GENERALITIES & REMINDERS ' SUPPORTED CATALYSTS<br>IMPREGNATIONS WITHOUT INTERACTION PRECURSOR-SUPPORT : Capillary impregnation (principle - characteristics et problems ' industrial applications) / Diffusional impregnation (principle - duration)<br>IMPREGNATIONS WITH INTERACTION PRECURSOR-SUPPORT : Ion echange (principle - types of ion exchangers ' isoelectric point ' support dissolution ' simple ion exchange, with trapping, with acid-base reaction, multiple or competitive ' limitations) / Grafting (principle - grafting sur oxide support - conditions ' grafting on metals) / Deposition-precipitation (principle)<br>PART 5 ' Biomimetic catalysts<br>STARTING POINT : Reactions with O2 in nature / Enzymes and respiration / Heme center et oxidation enzymes / Specificity and selectivity<br>Towards biomimetic catalysts : mimicking the heme center : examples / deactivation / $1^{st}$ and $2^{nd}$ problems<br>SOLUTIONS : $1^{st}$ solution (picket fence) / $2^{nd}$ solution (encapsulation : principle - zeolites - examples ship in the bottle and performances)<br>CONCLUSIONS<br>Depending on the time available and the students interest, additional parts (of about 2 hours each) will address more punctual topics of research ; possible topics might be : the dynamic behavious of heterogeneous catalysts, optimization of catalytic formulations : the base of Bi-V-Sb-O, abatement of sulfur containing volatile organic compounds on MnO2, the reactivity of Sb-Re-O in selective oxidation, abatement of chloro-aromatic air polluants. |
| Inline resources | Moodle |
| Bibliography | Comme support de cours facultatif : Fundamentals of industrial catalytic processes (2nd edition) de C.H. Bartholomew and R.J. Farrauto (Wiley-Interscience, 2006), ISBN : 0-471-45713-2 |
| Other infos | This course can be given in English. |
| Faculty or entity in charge | AGRO |

| Programmes containing this learning unit (UE) | | | | |
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| Program title | Acronym | Credits | Prerequisite | Learning outcomes |
| Master [120] in Chemistry and Bioindustries | BIRC2M | 5 | | 🔍 |
| Advanced Master in Nanotechnologies | NANO2MC | 5 | | 🔍 |