Course Package

Materials Science

Name module	Materials Science – 2A
Educational programme	MSc Chemical Engineering
Period	First block of first semester (block 2A)
Study load	15 ECTS
Coordinator	C. C. Diepenmaat

Materials Science			
block 1A	**block 1B**	**block 2A**	**block 2B**
		Polymer Physics **193730060** (5 EC)	
		Advanced Organic Chemistry **201900123** (5 EC)	
		Electives: choose 5 EC **Chemical Process Analysis** **201800328** (2,5 EC) **Physical Organic Chemistry** **201800448** (2,5 EC) **Electrochemical Engineering** **201800326** (2,5 EC) **Advanced Reaction Kinetics -** **202300234** (2,5 EC)	

Required preliminary knowledge: Organic Chemistry; Mathematics (among others Statistics for Chem. Process Analysis); Molecular & Biomolecular Chemistry and Technology; Thermodynamics; and Chemical Reaction Engineering; Langmuir-Hinshelwood kinetics.

193730060 - Polymer Physics

A coherent introduction at the graduate student level is offered into the properties and behavior of soft matter with a specific focus on the modelling polymer(-dynamics). The treatment follows the book of H. Gedde and / or M. Rubinstein, but is mainly based on the lecture slides, which will be provided during the course. Polymers are an essential component in many industrial applications, but also in biological systems. In this course, you will learn the fundamentals of polymer physics, which are required to predict the static and dynamic properties of such polymeric structures. We will use many examples to illustrate the relevance of these fundamental concepts. Moreover, you will learn how to test and visualize the discussed theories using molecular dynamics (MD) simulations. In the second half of the course, we will explore how we can employ the acquired fundamental knowledge to aid the design of potential applications and help in the investigation of unexplored scientific research areas.

201900123 - Advanced Organic Chemistry

- Give insight in reaction mechanisms;
- Reacive groups, competing mechanisms;
- Structures of amino acids and proteins;

- Peptides and their chemical synthesis;
- Orthogonal chemistry;
- Protein modification;
- Chemistry on surfaces;
- Cell surface engineering;
- Protein arrays, protein sensors
- Antifouling and bio-activation of biomaterials.

Electives: choose 5 EC

201800328 - Chemical Process Analysis

This course intends to provide an understanding of how experiments on a chemical process should be designed, so that data collection will lead to statistically meaningfull conclusions in an efficient and effective way. A methodology for the optimization of the parameters in a chemical process or of a chemical product will be developed, and analytical strategies for continuous monitoring of the status of a chemical process, product or instrument will be elaborated. Chemometric data analysis concepts including pattern recognition and multivariate analysis will be discussed in the context of chemical process or product performance characterization and process model selection, verification and validation. The concept of statistical process control will be explained.

The obtained knowledge and skills will be practiced by applying them to real (industrial) cases.

201800448 - Physical Organic Chemistry

At the end of the module, you will be able to:

- Understand basic concepts in Physical Organic Chemistry (e.g., mass-action kinetics, acid-base equilibria, enzymatic conversions, photochemical processes), and
- Formulate, as well as solve, equations governing these basic concepts.
- Understand how to analyze the influence of changes to molecular structures in Linear Free Energy Relationships (such as Hammett Plots, Grunwald- Winstein Plots, or Swain-Scott Parameters).
- Apply key concepts in Physical Organic Chemistry in real-world problems. That is, translate complex problems into verifiable hypotheses that can be tested: i) within the organic framework (i.e., by designing a set molecular structures and experimental methods), and ii) within the physical framework (i.e., by determining the set of differential equations that govern the dynamics).

201800326 - Electrochemical Engineering

The student should be able to understand and make suggestions to improve electrochemical processes (e.g. low and high temperature fuel cells and electrolysers) on the basis of thermodynamics, kinetics and physical transport phenomena.

202300234 - Advanced Reaction Kinetics

Catalytic reactors are essential for the circular economy and the energy transition. We need to develop better catalysts that can convert plastic waste to added value chemicals, electrify highly endothermic processes, and create new processes that can convert electricity into chemical energy vectors (e.g. methane, methanol and ammonia). In this course, we will learn how to test catalysts in a systematic manner allowing us to properly select the best materials for the conversion of interest.

We will first review basic concepts of Langmuir-Hinshelwood (LH) reaction mechanisms on heterogeneous catalysis. Then, we will discuss the complexities associated to the measurement of reaction kinetics in the absence of mass and heat transfer limitations together with the experimental and theoretical tests that can be done to prove that the system operates in the kinetic regime. We will learn how we should design experiments to get data that can help us to discriminate between different reaction mechanisms using kinetic modelling.

This knowledge on LH mechanisms will be then applied to a real experimental system. You will acquire lab data in a flow reactor coupled to an on-line GC-FID system. For this reason, you will have to design the experimental matrix with the aim of determining the main kinetics of the process (Ea and reaction orders). This information will be used to discriminate between different reaction mechanisms. The results from the experimental section and the kinetic modelling will be compiled in a written report that together with an oral exam will compute for the final grade of the course.

The attendance to the lab is mandatory in this course as you will be paired in groups of two people to conduct the experiments in the flow reactor. Safety training will be conducted before the starting of the course to ensure that all the experiments are conducted in a safe manner.

The modules are tentative and subject to change. Please check [the website] *regularly.*