Course Package

Materials Science – Q3

Name module	Materials Science – Q3
Educational programme	MSc Chemical Science & Engineering
Period	Third quartile of second semester – Q3
Study load	15 EC
Coordinator	C. C. Diepenmaat

Materials Science			
Quartile 1	**Quartile 2**	**Quartile 3**	**Quartile 4**
		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

Polymer materials have intriguing properties due to their peculiar chained structure and large molecular weight. In the first part of this course, we discuss the fundamental physics that describes and predicts static and dynamic properties of polymeric structures. This treatment follows the instruction in the book of M. Rubinstein and covers the physical behavior of single polymer chains; mixing of binary liquids, polymer solutions, and polymer blends; and the dynamics of polymer chains. In the second part of the course, you will apply the concepts in polymer physics by writing a research proposal with a group of fellow students. This proposal will propose research aimed to answer a previously unanswered problem in polymer physics.

201900123 - Advanced Organic Chemistry

- Reacive groups, competing mechanisms;
- Structures of amino acids and proteins;
- Peptides and their chemical synthesis;
- Orthogonal chemistry;
- Protein modification;

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

- 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 aims to equip students with the knowledge and skills to design experiments for chemical processes that prioritize sustainability. Emphasizing efficient and effective data collection, the course will guide participants in developing methodologies to optimize parameters in chemical processes and products while minimizing environmental impact.

Students will explore analytical strategies for continuously monitoring chemical processes, products, and instruments, ensuring that sustainability metrics are integrated into performance evaluations. The course will cover chemometric data analysis concepts, including pattern recognition and multivariate analysis, within the context of characterizing chemical process performance and selecting, verifying, and validating chemical models. Additionally, the principles of statistical process control will be discussed, highlighting their role in maintaining quality and efficiency in sustainable manufacturing practices. Students will be able to apply their acquired knowledge and skills to real-world industrial cases, focusing on innovative solutions that enhance sustainability in chemical engineering.

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 course will comprise of lectures and tutorials on the following topics:

- Thermodynamics of electrochemical devices (Gibbs free energy, electrical work, Nernst equation)
- Definition of real cell potential (thermodynamics vs kinetics), losses in electrochemical devices
- Novel applications of electrochemistry to replace traditional chemical processes
- Industrial electrolysis – chlor-alkali and chlorate processes: energy and cost considerations, cell configurations, operating conditions
- Hydrogen fuel cells and water/steam electrolysers – working principles of Alkaline, PEM and solid oxide cells, advantages and disadvantages of each technology
- Model-guided design of electrochemical cells using PEM/solid oxide cells as an example – relevant reaction kinetic and transport phenomena and theories used to study them, performance metrics
- Low temperature electrochemical CO2 reduction to valuable chemicals – technological advances, pH effects, operating modes and conditions, deactivation and its mediation.

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.