Course Package

Molecular and Materials Science

Name module	Molecular and Materials Science - 1A + 1B
Educational programme	MSc Chemical Engineering
Period	First semester (block 1A + 1B)
Study load	30 ECTS
Coordinator	C. C. Diepenmaat

Molecular Science and Material Science			
block 1A	**block 1B**	**block 2A**	**block 2B**
AMM Molecular & Biomolecular CT **193700020** (5 EC)	**AMM Organic Materials Science** **193700030** (5 EC)		
AMM Characterization **193700010** (5 EC)	**Advanced Molecular Separations** **201300049** (5 EC)		
Advanced Colloids and Interfaces **201800083** (5 EC)	***Electives: (1 of the 5 EC or 2 of the 2,5 EC)***		
	Electrochemistry Fundamentals and Techn. - 201800014 (5 EC)		
	Advanced Ceramics - 193737010 (5 EC)		
	Ion Transport in Fluids - 201800327 (2,5 EC)		
	Statistical Thermo - 201800332 (2,5 EC)		

Required preliminary knowledge: To do this course package you need to have completed at least the first two years of your BSc. Basic knowledge of Catalysis and Kinetic, Basics of Physical Chemistry, Organic and Inorganic Chemistry, Molecular Biology, Basic knowledge of Thermodynamics, materials science and molecular biology. This is an advanced-level graduate course, thus basic knowledge of Organic Chemistry and Polymer Science taught in the bachelor curriculum is a prerequisite and will be assumed. Basic knowledge of Catalysis and Kinetic, Basics of Physical Chemistry, Organic and Inorganic Chemistry, Material Science and Molecular Biology, Basic knowledge of Thermodynamics, Advanced knowledge of Characterization Method, Chemistry & Technology of Organic Materials, basic knowledge of chemical engineering or advanced technology. If you choose to do Statistical Thermo and Molecular Modelling you need to have a knowledge of Statistics and Matlab.

Block 1A

193700020 - AMM - Molecular and Biomolecular Chem. and Techn.

1. Noncovalent interactions, development of supramolecular chemistry (incl. the Excel modeling of thermodynamec equilibria)

2. Synthetic host-guest chemistry I: cation-binding hosts
3. Synthetic host-guest chemistry II: binding of guests in solution
4. Molecular recognition in biological systems, enzyme catalysis
5. Sensor concepts and sensor devices
6. Cooperativity: molecular and biomolecular (e.g. hemoglobin) examples
7. Multivalency: effective molarity concept, cyclization, cell membrane recognition
8. Polyvalent systems I: macromolecular assembly + supramolecular polymers
9. Polyvalent systems II: coordination polymers, MOFs
10. Polyvalent systems III: proteins an protein folding
11. Polyvalent systems IV: virus assembly
12. Polyvalent systems V: DNA + artificial DNA constructs
13. Polyvalent systems VI: layer-by-layer assembly
14. Polyvalent systems VII: supramolecular materials

193700010 - AMM Characterization

In this module a palette of state-of-the-art characterization techniques to investigate structure and properties of nanostructures will be introduced and applied. The module consists of 3 courses: Surface characterization (35 %), X-ray diffraction (30 %) and Microscopy and Spectroscopy (35 %). Recent publications on metal halide perovskite photovoltaics will be used as case study to illustrate the potential and complementarity of all techniques discussed in this module.

201800083 - Advanced Colloids and Interfaces

Description of colloids, surfaces and interfaces. All kinds of interfaces between different phases are treated. Thermodynamic descriptions of these interfaces are deduced. Several techniques for characterizing interfaces are discussed. During contact hours, the contents of will be presented and discussed, and exercises will be made and discussed. For each topic, a case assignment will be offered. Topics include:

- Lifshitz-van der Waals Interactions
- Polar/Acid-Base Interactions
- Wetting and Contact Angles
- Electrostatics
- DLVO and XDLVO interaction
- Electrokinetic Phenomena
- Electrostatic and Polymeric Stabilization of Colloids
- Colloidal Phenomena (Marangoni-Effect, Ouzo effect, etc.)

Block 1B

193700030 - AMM Organic Materials Science

1920-2020 – a century of polymers and organic materials! Organic materials feature enormous variations in their physical properties as a result of the tremendous wealth of the different possible existing molecular structures of carbon based compounds. The consequence of this plethora of properties is that function and use of organic materials can be tailored by controlling molecular structure virtually at will by using modern synthetic approaches, allowing one to realize many advanced applications, which belonged to the realm of phantasy just a few decades ago. In this lecture course molecular structure-property relations will be discussed for the different types of (advanced) synthetic and natural (macromolecular) organic materials, including man-made polymers, nanoparticles, degradable polymers, polymer coatings and novel processing methods, e.g. 3D printing.

The course starts with a history of polymer science and the peculiar molar mass and molar mass distributions inherent to synthetic and also certain natural polymers. The determination of molar masses is a critical factor for all organic materials and will be covered to set a basis for the coming topics. Approaches will be treated which allow materials engineers to quantitatively estimate physical properties based on the molecular structure. Effects of processing on structure (texture) and hence on properties will be demonstrated (coatings, processing techniques but also by synthetic means). A description and comparison of the major classes of the most frequently used industrial polymers for different function will complement this course. In addition to single-component single-phase systems, polymer blends (mixtures), block copolymers and polymer composites will also be discussed. These materials allow one to combine the useful properties of individual constituents in one system and achieve targeted improved properties. The physical principles of multicomponent phase diagrams of polymers, and microphase separation in block copolymers will be treated. One particular advantage of polymers is related to their ease of processability. Processing introduces texture in the material, hence processing-structure (orientation) effects need attention. For demanding structural applications (sports, aerospace, etc...) the mechanical properties must be further enhanced. Polymer (nano)composites can combine the easy processing with superior mechanical (and other improved physical) performance. Hence a section on polymer (nano)composites will also be included in the course. Major classes of advanced soft matter, e.g. in electroactive and nanomaterial applications will be elucidated. The class will end with a student minisymposium on current interesting and relevant topics of modern soft matter and polymer science.

This is an advanced level graduate course, thus basic knowledge of organic chemistry, materials science and polymer science taught in the bachelor curriculum is a prerequisite and will be assumed.

201300049 - Advanced Molecular Separations

In Advanced Molecular Separations, separation technology is discussed starting from molecular properties up to full scale processes. The focus is on choosing a separation technology for given molecular properties, and the subsequent molecular design of more advanced separation technologies. For two separation technologies, fluid separations and membrane technology, the molecular design and separation process are treated in much greater detail, including a discussion on useful models to describe thermodynamics and mass transfer. The course will include two tests, one on fluid separations and one on barrier separations, but will also include two assignments on selecting the right separation technology for a given separation case.

Electives: (1 of the 5 EC or 2 of the 2,5 EC)

201800014 - Electrochemistry Fundamentals and Techn.

Electrochemistry deals with chemical changes caused by electrical energy. Electrochemical processes are highly used in various branches of the industry and have an ever-increasing impact in our everyday life. Think, for example, of consumer products like batteries (e.g., in notebooks, smart phones or cars), electrosynthesis (or electrochemical conversion), electroplating or production of hydrogen by electrolysis of water. With more electrical energy being produced from solar and wind energy, a sustainable electricity supply will rely on storage. Additionally, noting that fossil-based fuels will be phased out, production of chemicals and fuels by alternative means will be required. Here, electrochemistry offers sustainable solutions, but further improvement of current and emerging electrochemical conversion techniques is certainly needed.

The course consists of three parts:

- Lectures and tutorials deal with the fundamental principles of electrochemistry, including thermodynamics, double layer structure, electrode reactions, and mass transport in electrochemical systems. Main experimental techniques for the study of electrode reactions will also be discussed.
- The students (e.g. in groups of 4 students) will carry out two practical (experimental) projects and prepare reports discussing and interpreting the obtained results. The report will be structured in the

form of a research article. This allows students to familiarize with learned fundamentals and to apply theoretical concepts to laboratory experiments and case studies in electrochemistry.

- Topical lectures (1x or 2x, if time allows) will expose students to relevant electrochemical research activities carried out by researchers within our faculty/in the Netherlands.

193737010 - Advanced Ceramics

Several steps in the fabrication process of ceramic materials are discussed and the importance to understand the effects of processing variables on the evolution of microstructural parameters is emphasized. Basic processes are treated like powder preparation, powder treatments (milling and mixing), forming into a green shape and sintering. Basic phenomena are e.g.: particle size, interaction between particles, nucleation/crystallization, solid state reactions and transport phenomena in solid state systems.

The objective in materials process engineering is to find relations between (desired) materials properties and relevant microstructural parameters on one side and to understand which process parameter changes a certain microstructural parameter on the other hand.

The basic processes and phenomena, as indicated above, will be treated in lecture notes and tutorials. An important aspect of the course is the in-depth treatment by the student of a specific part of a ceramic fabrication process. This project will be presented by means of a literature and a presentation essay.

201800327 - Ion Transport in Fluids

Starting from the electrochemical potential, the Nernst-Planck equation will be derived and then used to understand the relative contribution of electromigration and diffusion. The validity of assuming electroneutrality in a fluid phase is discussed and investigated by introduction of the Poisson equation. In double layers and interfaces, the potential and ion distributions can be studied further. Next, the effect of fluid transport on ion transport and vice-versa will be introduced by combining the Poisson-Nernst-Planck equations with the Navier-Stokes equations. From this, electrokinetic mechanisms such as electro-osmosis can be derived. Finally, the use of these frameworks in relevant industrial procesess where ion transport plays a crucial role is explored.

201800332 - Statistical Thermo

Statistical thermodynamics provides the fundamental concepts that allow us to predict macroscopic thermodynamic variables and materials properties. Via many applied examples from organic and inorganic material science, you will get a microscopic understanding of entropy, you learn how to work within different ensembles, you will learn how to work with partition functions as well as out-of-equilibrium thermodynamics.