Course Package

Molecular and Materials Science- Q1 + Q2

Name module	Molecular and Materials Science - Q1 + Q2
Educational programme	MSc Chemical Science & Engineering
Period	First semester (quartile Q1 + Q2)
Study load	30 EC
Coordinator	C. C. Diepenmaat

Molecular Science and Material Science			
Quartile 1	**Quartile 2**	**Quartile 3**	**Quartile 4**
Supramolecular Chemistry **202400372** (5 EC)	**Organic Materials & Polymer Science** **193700030** (5 EC)		
Characterization **193700010** (5 EC)	**Advanced Molecular Separations** **201300049** (5 EC)		
Advanced Colloids and Interfaces **201800083** (5 EC)	***Electives: choose 5 EC*** **Electrochemistry: Fundamentals & Techniques – 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 Kinetics; Basics of Physical Chemistry; Organic and Inorganic Chemistry; Molecular Biology; Basic knowledge of Thermodynamics; Materials Science; Polymer Science; Material Science; Advanced knowledge of Characterization Method; Chemistry & Technology of Organic Materials; basic knowledge of Chemical Engineering or Advanced Technology.

Quartile 1

202400372 - Supramolecular Chemistry

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

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

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.)

Quartile 2

193700030 - Organic Materials & Polymer 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 human-made polymers, nanoparticles, degradable polymers, polymer coatings and novel processing methods, e.g. 3D printing. We will also discuss the end-of-life of polymers and plastics and potentially sustainable alternatives.

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, assemblies, 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 that knowledge will be required. The course focuses on materials and materials properties, basic knowledge on polymer chemistry is expected but we also suggest the Polymer Synthesis and the Sustainable Organic Chemistry classes as a follow-up to this course with a focus on syntheses methods.

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: choose 5 EC

201800014 - Electrochemistry: Fundamentals & Techniques

Electrochemistry deals with chemical changes caused by electricity (as in electrolyzers), and with the generation of electricity through chemical reactions (as in galvanic cells, i.e., batteries under discharge). 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, aiming to phase out fossil-based fuels towards net zero carbon emission by 2050, the 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 needed.

The course consists of following activities:

- Lectures and tutorials deal with the fundamental principles of electrochemistry, including thermodynamics, double layer structure, electrode reactions, and mass transfer in electrochemical systems. The main experimental techniques to study electrode reactions are also discussed
- The students carry out group practical projects and prepare a report discussing and interpreting the obtained results. The report is structured in the form of a research article. This allows students to familiarize with learned fundamentals and apply theoretical concepts to laboratory experiments and case studies in electrochemistry.

193737010 - Advanced Ceramics

The structure of the course follows the different steps of the ceramic fabrication process starting first with a general introduction and then lectures related to the preparation of powder (Lectures 2 to 5), compact formation (Lecture 6), and sintering (Lecture 7). Basic phenomena such as particle size, interaction between particles, nucleation/crystallization, solid-state reactions, and transport phenomena in solid-state systems are also discussed in the course. In addition to lecture 1 to 7 which focuses on the theory, two additional guest lectures are also given. The first guest lecture is a presentation of a scientific article on ceramic nano-powder composites and is used to link theory and experimental results. The second guest lecture is about materials synthesis and production techniques

for functional ceramics at the Forschungszentrum Jülich in Germany. If possible, an excursion is organized at the Forschungszentrum Jülich following the lecture. Lecture notes are also made available.
Individual writing and reading home assignments are provided for the students to practice but are not mandatory.

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

In Statistical Thermodynamics, we describe the microscopic behavior of atoms and molecules, and we use this description to understand the macroscopic properties of materials and fluids. In the core of Statistical Thermodynamics, there is Statistical Mechanics - which is a mathematical structure with applications in various fields, in particular, classical and quantum physics, but not limited to those.

Via many applied examples and exercises from organic and inorganic materials science and daily life, you will get an accurate understanding of entropy, you will learn how to work within different statistical ensembles and make use of partition functions, and consider out-of-equilibrium thermodynamic processes.