



UNIVERSITÄT
BAYREUTH



Elite Network
of Bavaria

Elite Study Program *Macromolecular Science*

Start Module M063

**Modern Research Topics in
Macromolecular Science**

Faculty members of Elite Study Program
Macromolecular Science

Winter term 2022/23

The scope of the Start Module “*Modern Research Topics in Macromolecular Science*” is to introduce the students, coming from different backgrounds, to various facets of the broad and interdisciplinary field of Macromolecular Science. It is intended that the students will get a basic understanding of underlying concepts, terminology and methodologies in the individual subfields of Macromolecular Science. The offered topics cover the fields macromolecular chemistry, colloidal chemistry, biopolymers, biochemistry, polymer physics, biophysics, polymer technology, polymer engineering, electronic and optical devices, advanced characterization methods, and theory and simulation of macromolecules.

In the start module 17 topics are offered, compiled in four blocks A, B, C and D. Each student has to select 8 topics. To meet the interdisciplinary intention of the module two topics of each block has to be selected. Each topic has a length of about 8 to 10 hours and includes lectures, seminars and laboratory tours.

A1: Multifunctional Colloids - From Simple Building Blocks to Modern Devices

Anna Schenk, Markus Retsch, *Physical Chemistry*

Colloidal particles represent a materials class with a vast range of composition, size, and shape. The unique properties of colloids can mainly be related to their enormous surface to volume ratio and differ significantly from their respective bulk materials. The functionality of such particles can be further enhanced by self-assembly of such building blocks into regular films or arrays, which for instance are known as colloidal crystals.

In this module, we give a detailed introduction into the synthesis, characterization and application of colloidal particles. We will focus on a range of materials such as polymers, metals, and metal oxides, which can also be combined to yield composite materials. Important concepts in colloidal science, in particular the stability of colloidal dispersions and forces influencing colloidal stability, will be introduced. The relevance of these concepts will be discussed in the light of self-assembled materials consisting of colloidal building blocks. Such materials are promising platforms for modern sensors and photovoltaic devices.

A2: Polymer foams

Holger Ruckdäschel, *Polymer Engineering*

Due to the unique properties of polymer foams, a large number of innovative applications can be realized. These include packaging with reduced material costs, aerospace and automotive parts with good property-to-weight ratios, decreased thermal conductivity, and enhanced acoustic and mechanical damping.

The first part of the module focuses on the fundamental physics of polymer foams, including a detailed discussion of the foaming processes currently utilized both in academia and in industry as well as the resulting structure-property-relationships.

Thereby, different types of polymer foams (particle foams, reactive polyurethane foams (PUR), extruded and injection-molded foams) and their typical properties and applications are introduced. In addition, current scientific approaches towards the control of cell nucleation, cell growth and volume expansion will be presented. Innovations (micro- to nano-cellular) and the hierarchical structuring of polymeric foams are also highlighted. Finally, the students will learn how to obtain tailored foam morphologies – and properties.

This oral part is followed by an experimental session taking place in our laboratories and pilot plant stations. More precisely, an introduction into foam injection-molding and foam extrusion is given. Finally, new trends and promising approaches as well as remaining questions will be discussed with the working group “Polymer Foams” of Polymer Engineering group.

A3: Design of supramolecular architectures for functional materials

Hans-Werner Schmidt, *Macromolecular Chemistry*

Nature uses precisely arranged complex macromolecular structures, often representing superstructures, to accomplish a specific functionality. In this context, supramolecular chemistry allows to achieve defined supramolecular nanostructures with tailored functionalities via controlled self-assembly of (macro)molecular building blocks. The realization of (multi)functional hierarchical structures across all length scales with increasing complexity is a major perspective in materials science and play a key role for innovative solutions.

In this context, the module will provide an introduction to supramolecular chemistry and an overview on the design of supramolecular architectures for functional materials. This includes, in particular, the design and structure property relations of supramolecular nanofibers for filtration applications, single supramolecular nanofibers for long-range transport of excitonic energy and hierarchically structured supramolecular nanofibers as functional polymer additives. The module will also comprise an experimental part with respect to filtration based on supramolecular nanofiber networks and the nucleation of isotactic polypropylene as well as a laboratory tour.

B1: From Interaction Forces to Nanorobotics

Georg Papastavrou, *Physical Chemistry II*

Interfacial forces determine many properties like friction, adhesion, or wetting. In recent years, the atomic force microscope (AFM) has developed into a versatile tool for measuring such forces at the nanometer scale with force resolutions in the order of few tenths of a pico-Newton. Such force measurements allow not only to determine the interaction on the level of single polymer chains but as well to explore mechanical properties of nano- and colloidal objects not accessible by other techniques.

In this module, we will demonstrate how the increasing miniaturization of devices becomes on one hand limited by the aforementioned surface forces but on the other hand these allow for radically new types of technology, which until some years ago would be attributed to science fiction. Such fields included micro- and nanorobotics, self-propelling colloids or new types of analytical devices that can flow in blood vessels. The participants will have the possibility to measure and “feel” surface forces, such as the extension of a single polymer chain, aspirate colloidal particles by nanofluidics and to manipulate colloidal objects.

B2: Solid-state NMR spectroscopy for probing structural functional materials for a sustainable energy economy

Jürgen Senker, Helen Grüninger, *Inorganic Chemistry III*

The turnover to a sustainable energy economy, that is based on renewable sources, is one of the main challenges our society needs to solve in the near future. This includes better solutions for energy conversion and energy storage. For efficient devices, such as batteries, solar cells or fuel cells, novel multifunctional materials need to be developed and understood to meet the challenging criteria with respect to ionic and electronic conductivities and simultaneous high material stabilities. Solid-state NMR spectroscopy can probe local structural features, which are often disordered, and the local dynamics and long-range diffusion in solids without changing the sample environment. In combination these aspects aid to understand the materials and derive structure-property relations, which are the key for the design of sustainable and efficient next-generation devices.

In this context, the module will introduce you to how to probe structural and dynamical properties of functional material by solid-state NMR spectroscopy. The focus will be set on a variety of solid-state NMR experiments to probe i) local structural information, such as distances between functional groups or their orientation, and ii) ion dynamics and transport in materials for *proton-conducting membranes* for fuel cell applications and *hybrid perovskites* for future solar cell designs. The module will also provide a laboratory tour around the solid-state NMR spectroscopic laboratories at the UBT including the high-field 1 GHz magnet and a hyperpolarization machine.

B3: Morphology control and characterisation of nanostructured functional organic thin films – how to make plastic solar cells work

Eva M. Herzig, *Dynamics and Structure Formation, Experimental Physics*

The nanostructure and morphology of organic molecules strongly influences the function of organic solar cells. Charge transport in these materials depends on the relative position of organic semiconducting molecules with respect to each other, as do various loss mechanisms. We will look into the processing of thin films and examine which aspects of the nanomorphology we can address via processing by getting to know current literature examples.

In the second part of the one-day course we are looking into how to characterize the nanostructure using x-rays. We will look into some standard methods also applied to other material systems with the goal of equipping the students with the basic concepts of scattering which will aid to plan future experiments in research and industrial contexts.

A lab tour and information on how to apply for measurement times at large scale experimental facilities conclude the day.

C1: Physical Properties of Liquid Crystals: From Low Molecular Weight Materials to Elastomers

Helmut R. Brand, *Theoretical Physics*

The field of liquid crystals will be introduced. In one special topic we cover selected LC phases. The second special topic deals with physical properties and methods. In the project afternoon we will discuss selected literature and in particular the derivation of the Frank elastic energy for a nematic liquid crystal.

C2: Diffusion and Dynamics in Polymers

Werner Köhler, *Experimental Physics, Polymer Physics*

Diffusion, the uncorrelated motion of molecules, plays a key role in understanding dynamic processes in macromolecular systems. In the first part of this topic basic concepts of how polymers diffuse in the bulk and in solution are introduced. The difference between self and collective diffusion is discussed and it is shown that a temperature gradient can also induce mass diffusion. Basic models for the description of polymer dynamics are introduced. Relevant experimental techniques for the measurement of various diffusion coefficients are briefly discussed. The lectures covers phenomenology of diffusion, including polymer models, linear laws, self diffusion, collective and thermal diffusion, and the Rouse and reptation model.

C3: Single Molecule Spectroscopy and Superresolution Microscopy

Jürgen Köhler, *Spectroscopy of soft Matter (SsM)*

The Nobel Prize in Chemistry 2014 has been awarded to E. Betzig, W.E. Moerner, and S. Hell for the development of optical microscopy beyond the Abbe diffraction limit. The underlying techniques are based on fluorescence and exploit either single-molecule techniques or the deliberate depletion of electronically excited states.

The topic provides a general background about fluorescence and its application for superresolution microscopy, in particular single-molecule spectroscopy, and stimulated emission depletion. On the second day some experiments will be performed as a practical exercise.

D1: Biopolymer-based biofabrication for regenerative tissue engineering

Thomas Scheibel, Sahar Salehi-Müller, Hendrik Bargel, *Chair Biomaterials*

Modern regenerative medicine aims at the functional regeneration of tissues through stimulation and support of the endogenous regeneration potential of the human body. This approach longs for novel materials for bone, muscle, ligament, and skin substitutes or nerve regeneration characterized by their defined three-dimensional structure, a tissue-related hierarchical morphology, and an adjusted biochemical composition. In order to gain such biomaterials, multidisciplinary approaches combining materials science and processing technologies, natural sciences, and medicine are necessary. Biofabrication is an emerging field in the area of biomaterials, aiming at the generation of three-dimensional structures from materials that may contain vital cells and that allow the generation of scaffolds with high survival rates of the embedded cells. Different biopolymers such as gelatin, collagen, silk, or alginate are extensively used for biofabricating and they can be processed using different technologies, involving 3D-printing, various spinning and coating methods, as well as hydrogel formation. The physical and mechanical properties of the materials as well as their morphologies and cell compatibility are then analyzed to evaluate the suitability for the development of 2- and 3-D scaffolds.

The overview of this module is 1) an introduction and demonstration of several processing methods of the model biopolymer spider silk protein including 3D printing, electro-spinning, etc., and 2) an introduction to tissue engineering, specifically skeletal muscle tissue regeneration, as well as demonstration of different types of scaffolds cultured with muscle cells and their analysis.

D2: Shape-changing polymers: molecular design & applications

Leonid Ionov, *Biofabrication*

Polymers are materials with broad range of applications ranging from medicine to aerospace industry. Polymers are able to offer a number of vivid advantages, such as improved flexibility, adaptability and reconfigurability, which is intrinsic to living systems. An additional degree of freedom for design of materials can be provided by use of intelligent polymers, which are able to change their structure, macroscopic properties and shape in response to change of condition or under influence of external signal. Shape-changing materials are of potential application for surgery, soft robotics, drug delivery, tissue engineering and many other fields.

In this module, molecular principles of design of shape-changing polymer, correlation between their molecular structure and their physico-chemical properties as well as application for a variety of fields will be discussed. The module will cover the most important classes of shape-changing polymers such as hydrogels, shape-memory polymers, liquid crystalline elastomers, electroactive polymers, elastomers and others. We will also discuss ways to combine shape transformation with additive manufacturing (3D printing) that opens new horizons for engineering.

D3: NMR in Food Science – From General Quality Control to Food-Polymer Analysis

Stephan Schwarzinger, *Nordbayerisches NMR Zentrum (NBNC)*

Food is essential for us. In Germany, we enjoy easy access to safe food of high quality, which very often also comes with a low price. It is actually the producer's responsibility to ensure safety and quality of the food put to the market. Because of the price pressure in the market analysis also should be cost-efficient. It may thus be surprising that a technology such as NMR has recently found entry into routine-analysis of food. But NMR has a significant advantage in analyzing difficult to handle samples, which include complex mixtures such as food. Hence, NMR is highly efficient in establishing quantitative ingredient profiles and for assessing the quality of raw components. Ingredient profiles in combination with advanced chemometric methods (including application of AI and machine learning) have become a standard to test for adulteration of food. In recent times this has become an important issue as the promises made on labels of food often do not match the content of the package. Deliberate mis-labeling in order to increase profit is known economically motivated adulteration and NMR has become a main tool to battle EMA (Economically Motivated Adulteration, which is a criminal statement of facts according to European law). An important part here is testing of raw materials for quality, i.e., whether or not specifications have been met. Carbohydrate based polymers play an important role in food industry as gels and thickeners – but are extremely difficult to analyze. NMR can provide insights into purity and composition of such materials.

We present an introduction into food fraud and how chemometrics (with focus on NMR and IR) can be used to detect numerous quality parameters within a single measurement and at the same time test for authenticity. Insight is provided how machine learning and AI (neural networks) as well as combination of methods (e.g. NMR+IR) help improving quality of chemical analysis (chemometrics). We will put a particular emphasis on prerequisites for such an approach and when it is not indicated/ possible. Finally, we give a brief introduction into the field of carbohydrate-based gels and thickeners used in food industry and show examples of NMR-analysis of these compounds. A lab-tour highlighting the needs for developing novel analytical applications for food – including quality management – closes the module.