UNIVERSITÄT BAYREUTH

Elitenetzwerk Bayern

Elite Study Program *Macromolecular Science*

Start Module M054

Modern Research Topics in Macromolecular Science

Faculty members of Elite Study Program
Macromolecular Science

Winter term 2019/20

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 14 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 at least one topic 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: Design of supramolecular architectures for functional materials
Hans-Werner Schmidt, Macromolecular Chemistry

A major challenge in polymer science and supramolecular chemistry, with respect to novel functional and even multifunctional materials, is the understanding and control of hierarchical structured supramolecular polymers and nano-objects created by (macro)molecular self-assembly. Such complex self-assembled structures will provide constant progress in materials science and play a key role for innovative solutions. A goal is to fine-tune specific and complex functionality across all length scales (nano to macro) through molecular design and novel hierarchically structured systems.
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 experiment part with respect to filtration based on supramolecular nanofiber networks and the nucleation of isotactic polypropylene as well as a laboratory tour.

A2: Polymer foams
Volker Altstädt, 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, a practical introduction into foam injection-molding and foam extrusion is given using commercial machines. Finally, new trends and promising approaches as well as remaining questions will be discussed with the "foaming experts" of Polymer Engineering group.

A3: Multifunctional Colloids - From Simple Building Blocks to Modern Devices
Anna Schenk, Markus Retsch, Physical Chemistry Department

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.

A4: Shape-changing polymers: molecular design & applications
Leonid Ionov, Biofabrication

Polymers are materials with broad range of applications ranging from medicine to airspace 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.

B1: Color Formation in Organic Light Emitting Devices (OLEDs) - A Combined Chemistry and Physics Approach

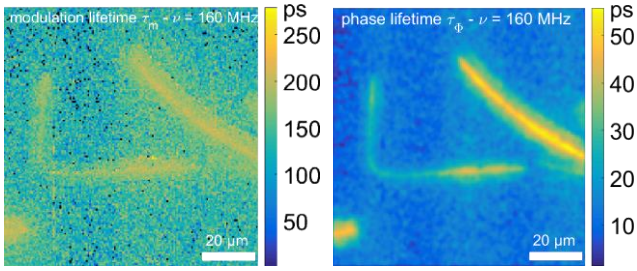
Peter Strohriegl, Macromolecular Chemistry I
Anna Köhler, Experimental Physics II

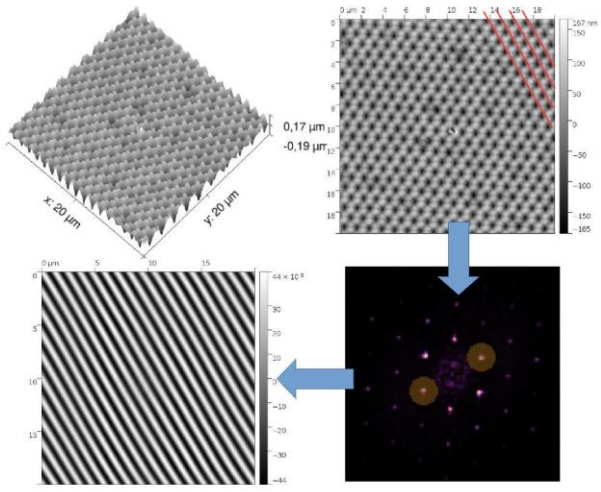
Colors have attracted people for thousands of years. In the first part of the interdisciplinary course, a short introduction in the basics of color formation and color mixing will be given. Afterwards, the principles of Organic-Light Emitting Devices (OLEDs) will be introduced with special emphasis on the different materials used.
The second part of the course gives an introduction to the photophysics of OLEDs. In such devices the physical principles of energy transfer from a host material to a guest molecule are used to generate different colors in an energy efficient way. The detailed understanding of the photophysics of organic semiconductors has paved the way to the commercialization of full color OLED-displays.

B2: Advanced Laser Techniques: Confocal Raman and Fluorescence Lifetime Imaging (FLIM) Microscopy and Holographic Methods

Lothar Kador, Bayreuth Institute of Macromolecular Research (BIMF)

Confocal microscopy is a powerful technique for imaging samples in all three dimensions of space. It can be easily combined with the analysis of secondary radiation such as, e.g., Raman scattering or fluorescence light. We will especially discuss the methods of confocal Raman microscopy and confocal fluorescence lifetime imaging (FLIM) microscopy. Whereas the former technique yields spatially resolved information about the chemical composition of the sample, the FLIM method maps the excited-state lifetime of fluorophores. Special emphasis will be laid on FLIM experiments in the frequency domain which use a cw laser amplitude-modulated in the radio-frequency (rf) regime rather than a pulsed laser. In this context, some fundamentals of rf experiments will be touched as well.





In the second part of the lecture, an introduction to holography and some of its possible applications will be given. As an important model system, we will consider the azobenzene molecule and its photophysics. We will address the formation of volume phase gratings and surface relief gratings and discuss the different properties of thin and thick holograms. The project part will be devoted to practical demonstrations of one of these techniques.

B3: Single Molecule Spectroscopy and Superresolution Microscopy
Jürgen Köhler, Spectroscopy of soft Matter (SsM)

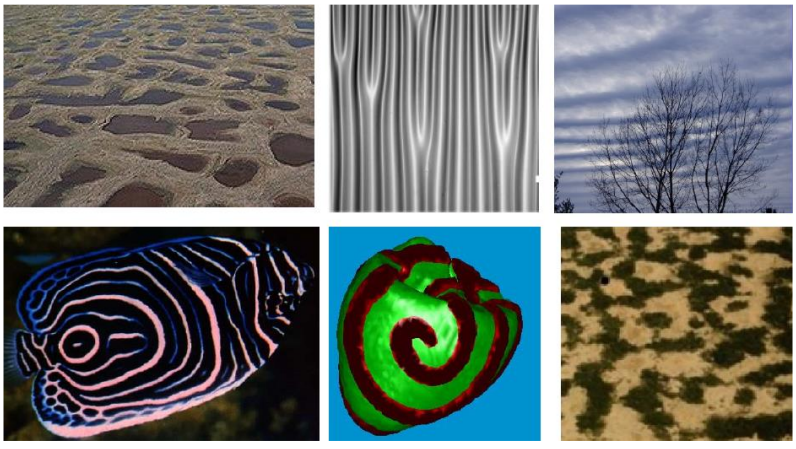
The Nobel Prize in Chemistry 2014 has been awarded to E. Betzig, W.E. Moerner, and S. Hell for the development of optical microscopy beyond the Abbe diffraction limit. The underlying techniques are based on fluorescence and exploit either single-molecule techniques or the delibarate depletion of electronically 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 a single-particle tracking experiment will be performed as a practical exercise.

C1: The fascination of pattern formation and self-organization: Basic principles, applications, possible directions
Walter Zimmermann, Theoretical Physics I

Pattern formation and self-organization are fundamental strategies in nature, which fascinate both the layman and researchers from many disciplines. In addition to their aesthetic appeal, the function of the patterns in nature are of central interest.

In this course I will give an introduction to the field and explain some main concepts in the context of experiments. Using several examples from physics, biology, chemistry or material science, I will illustrate that the mechanism driving a spatially extended pattern, like a stripe or traveling wave pattern, are vastly different in diverse systems. Stripe patterns, for instance, are found in biology (skin pattern, segmentation …), chemistry (Turing, microphases in Blockcopolymers…), Physics (convection, Taylor-vortices…), material science (wrinkles …) and geoscience (atmosphere, continental drift …). Traveling waves are found in fluids or they occur during cell division of E.coli. Further examples are explained, such as hexagonal patterns (e. g. cloud, perma frost or vegetation patterns), spirals or synchronization phenomena.

I will explain - qualitatively and in terms of basic models – that each nonlinear pattern has a number of robust and system-independent properties and that the concepts of pattern formation provide a framework for their system-independent, generic properties. Why are patterns of different wavenumbers stable in inhomogeneous systems (variability)? By which generic principles can a pattern be selected or controlled? How do patterns interact with their environment such as boundaries or inhomogeneities?
Which functions do patterns in nature fulfill? Besides addressing these elementary questions, I will highlight some recent developments and applications as well as possible future direction of pattern formation.



C2: Physical Properties of Liquid Crystals: From Low Molecular Weight Materials to Elastomers

Helmut R. Brand, Theoretical Physics III

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.

C3: 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 diffusion coefficients are discussed in the second part, and state of the art experiments can be seen in the laboratory.
The lectures will cover phenomenology of diffusion, including polymer models, linear laws, self diffusion, collective and thermal diffusion, and the Rouse and reptation model. As experimental techniques, light scattering and transient holography will be covered.

D1: Protein and DNA self-assembled functional nanostructures

Thomas Scheibel, Martin Humenik, Melanie Scheibel, Biomaterials

Novel assembly strategies and types of nanomaterials are required to solve nowadays-technological challenges. Self-assembly processes, which are independent of external energy sources and unlimited in dimensional scaling, became a very promising approach. Self-assembled biopolymers offer several advantages, since evolutionary gained monomer units possess well-tuned functions allowing self-assembled biopolymers with properties featured by chemical and physical addressability, specific recognition, functionality and higher order complexity, all of then defined in distinct monomers sequences.
In this module, we introduce recent developments in self-assembled DNA and protein polymers as well as hybrid entities thereof for constructing of complex hierarchical materials in “bottom up” approaches with nanoscale architecture and programmable functions.
In the practical part of the course, we will demonstrate possible analyses of a working DNAzyme nanomotor and self-assembly of spider silk protein into nanofibrils.

D2: Biopolymer-based biofabrication for regenerative tissue engineering
Thomas Scheibel, Sahar Salehi, Hendrik Bargel, 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, 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 various spinning and coating methods as well as hydrogel formation. The physical and mechanical properties of the materials as well as their morphologies and the cell compatibility can be analyzed to evaluate the suitability for development of 2- and 3-D scaffolds.
The overview of this module is 1) introduction and demonstration of several processing methods of the model biopolymer spider silk protein including electro-spinning, 3D printing etc., and 2) introduction to tissue engineering and specifically skeletal muscle tissue regeneration, as well as demonstration of different types of scaffolds cultured with muscle cells.

D3: From molecular detail to genome-wide view
Claus D. Kuhn, ENB Junior Research Group "Gene regulation by non-coding RNA"

Understanding biological processes in molecular detail is a pre-requisite for the development of modern treatments for disease. Since structural biology possesses the tools to reveal biological snapshots at atomic resolution, it is the method of choice to unravel molecular details. However, understanding the molecular details of a single molecular interaction does not allow for conclusions concerning an entire organism. This is why modern drug development has to bridge between understanding the molecular details of a given interaction and its organism-wide implications.

Therefore, the ENB beginner module will cover both aspects, modern techniques to unravel atomic details of biomolecules and their genome-wide impact. Specifically, the module will cover the interaction between nucleic acids and proteins with an emphasis on the interaction between non-coding RNAs and proteins.

In two half-day sessions the ENB students will gain insights into the theoretical and practical aspects of studying protein-RNA interactions in molecular detail and in a genome-wide context. In more detail, the module will cover biochemical aspects ranging from the recombinant production of protein complexes to their study using mass spectrometry, X-ray crystallography and cryo-electron microscopy. In addition, the students will be given an introduction to bioinformatics tools with which it is possible to study the impact of non-coding RNA molecules genome-wide.

D4: 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 producers 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 motived adulteration and NMR has become a main tool to battle EMA. 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. 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.