Elitenetzwerk Bayern

UNIVERSITÄT BAYREUTH

Elite Study Program in Macromolecular Science

Start Module M041

Modern Research Topics in Macromolecular Science

Faculty of the Elite Study Program

Winter term 2015/16

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, technical terminology and methodologies in the individual subfields of Macromolecular Science in addition to their main focus. The offered topics cover the fields macromolecular chemistry, colloidal chemistry, biopolymers, biochemistry, polymer physics, biophysics, polymer technology, polymer engineering, and theory and simulation of macromolecules.
In the module 15 topics will be offered, compiled in three blocks A, B and C. They students have to select 8 topics. To meet the interdisciplinary intention of a module at least 2 of each block have to be selected. Each topic has a length of about 8 to 10 hours and includes lectures, seminars and laboratory tours. In addition the students will have a tour and brief introduction of the research facilities.

Block A:

A1: Design of supramolecular architectures for functional materials
Hans-Werner Schmidt, Macromolecular Chemistry I

A major challenge in polymer science, 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. Our 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, we explored in the past years the design and structure-property relations of molecules capable to self-assemble into supramolecular nano-fibers and nano-objects. The molecules were for example tailored to function as nucleating/clarifying agents for semi-crystalline polymers, as charge storage additives in electret materials, as nano-fibers for filtration applications and as efficient organo- and hydrogelators.

Date: will be arranged after consulting with the participants (one day)

A2: Inorganic Nanofillers
Josef Breu, Andreas Edenharter, Patrick Feicht, Inorganic Chemistry I

Compounding nanofillers generates huge specific interface areas that significantly alter the properties of commodity polymers. In particular low dimensional fillers with large aspect ratios allow for mechanical reinforcement, improvements in flame retardancy and in permeability. Several aspects of nanocomposites will be covered from a critical review of the literature, the choice of appropriate fillers, interface management, a comparison of compounding methods all the way to thorough characterization. The laboratory tour includes permeability measurement, cone calorimetry and LOI.

Date: will be arranged after consulting with the participants (one day)

A3: Multifunctional Colloids - From Simple Building Blocks to Modern Devices
Prof. Dr. Matthias Karg, Prof. Dr. 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.

Proposed dates: 1 full day, 23. March or 29. March (incl. experimental demonstrations)

A4: 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.

Proposed dates: 17. March or 23. March (one full day)

A5: Solar Energy Conversion and Energy Storage
Sven Hüttner (Juniorprof. Solar Energy), Keylab "Device Engineering"

The development of alternative ways for energy conversion and energy storage belongs to one of the great challenges we have to face in the 21st century. Solar energy conversion will make a significant contribution within the future mix of energy sources.
In this module we will give detailed presentation of the state of the art and developing solar cell technologies. The presentation is beyond a simple listening of technologies, and fundamental questions in chemistry, physics and material science

will be highlighted. This includes general concept of light harvesting – mimicking nature, materials for solar cells (inorganic, organic and hybrid semiconductors), enhancement of light absorption and charge generation, limitations in solar cells as well as fabrication and characterization techniques. A closely related field is energy storage. The future mobile devices, electro mobility and electric cars as well as the stabilization of our more and more complex growing energy supply grid will require new and sophisticated batteries. Out of the many promising concepts we will give an introduction to Li-Ion batteries and the ongoing research objectives.
This course will provide a substantial overview of current research in solar cells and Li-Ion batteries and demonstrate the ongoing research in the Keylab "Device Engineering" of the University Bayreuth. In a lab course (approx. 3h) we will explain the facilities within the Keylab and demonstrate the processing and characterization of a novel hybrid solar cell.

Date: will be arranged after consulting with the participants (one day)

Block B:

B1: Advanced Laser Techniques: Confocal Raman and Fluorescence Lifetime Imaging (FLIM) Microscopy and Holographic Methods
Lothar Kador, BIMF

Confocal microscopy is a powerful technique for imaging samples in all three dimensions of space. It can easily be 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.
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. In this context, we will address the formation of volume phase gratings and surface relief gratings and discuss the different properties of thin and thick holographic gratings.
The project part will be devoted to practical demonstrations of one of these techniques.

Date: will be arranged after consulting with the participants (one day) (except March 07 – 11)

B2: More than just scratching on the surface: Measuring interactions and mechanics in polymer systems by scanning probe microscopy
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 different experimental approaches based on the AFM, including practical demonstrations. The basic principles governing the stretching response of linear polymers, starting from the Gaussian chain model, will be covered as well as the desorption processes of adsorbed polymers from a solid substrate, which allows to probe the interactions on the monomer level. Moreover, we will explain how to measure locally mechanical properties of thin films or fibers.

Proposed dates: 3. March or 17. March (one full day)

B3: Diffusion in Polymers
Werner Köhler, Experimental Physics IV, 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. 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 diffusion and thermal diffusion. As experimental techniques, light scattering and transient holography will be covered.

Proposed dates: 31.March or 7.April (one full day)

B4: Kernmagnetische Resonanzspektroskopie und Polymerdynamik
Ernst Rößler, Experimentalphysik II

Seit einigen Jahren existiert ein kommerzielles Field-Cycling (FC) NMR-Spektrometer, das es erlaubt, die Frequenzabhängigkeit der Spin-Gitter-Relaxation (insbesondere ^{1}H) zu messen. Diese „NMR-Relaxometrie“ unterscheidet sich wesentlich von der konventionellen NMR. Im Gegensatz zu letzteren wird im Fall der FC-NMR das äußere Magnetfeld zwischen einem Polarisations-, Relaxations- und Detektionsfeld schnell (ms) geschaltet („Cycling“). Damit lassen sich u.a. Theorien der Polymerdynamik, wie z.B. das Doi-Edward´sche Tube-Repation-Modell, erstmals über einen großen mikroskopischen Zeitbereich überprüfen. In Analogie zu rheologischen Messungen werden aus den Relaxationszeiten $T_1(\omega)$ Masterkurven konstruiert, die nach Fourier-Transformation es erlauben, die segmentale

Korrelationsfunktionen über mehr als acht Dekaden in der Zeit zu verfolgen. Die Korrelationsfunktion weist unterschiedliche Potenzgesetzregime auf, die verschiedenen Arten der Polymerdynamik, wie Glas-, Rouse- und Entanglement-Dynamik, zugeordnet werden. Man kann hier von molekularer Rheologie sprechen. – Im experimentellen Teil werden Sie Messungen an einem solchen FC-NMR-Spektrometer durchführen, wobei die Kettenlänge (Molekulargewicht) des Polymers (Polybutadien) vom Grenzfall monomere Flüssigkeit bis hin zum Hochpolymeren variiert wird. Auf diese Weise wird der Übergang von einfacher Flüssigkeitsdynamik zur Polymerdynamik erkennbar und die besagten Relaxationsregime identifizierbar.

Date: will be arranged after consulting with the participants (2 half days including experiments)

B5: Single Molecule Spectroscopy and Superresolution Microscopy
Jürgen Köhler, Experimental Physics IV

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.

Proposed dates: 25. February and 26. February (two times half a day: 9:00 – 12:00)

Block C:

C1: Structure and Dynamics of Bio-Macromolecules
Claus Kuhn, Paul Rösch, Stephan Schwarzinger, Kristian Schweimer, Birgitta Wöhrl, Biopolymere

Biological macromolecules are essential for life. They are responsible for formation of soft and rigid structures, synthesis and degradation of molecules, and tight control of these events though signaling cascades. To understand their mode of action it is pivotal to obtain detailed insights into the 3D-structure of such bio-macromolecules. Moreover, many of the above-mentioned events require structural changes and conformational flexibility. Therefore, it is equally important to study the dynamic behavior of these molecules.
We present an overview of state-of-the-art methods for the production of bio-macromolecules for structural studies and give an introduction into nuclear magnetic resonance (NMR) spectroscopy and X-ray crystallography of proteins, nucleic acids, and carbohydrates. Introductory presentations will be complemented by experimental sessions and a lab tour through our facilities. Finally, emerging trends as well as remaining questions will be addressed in an open discussion.

Date: will be arranged after consulting with the participants (one day)

C2: Biopolymer-based biofabrication for regenerative tissue engineering
Thomas Scheibel, Kiran Pawar, Biomaterials

Modern regenerative medicine aims at the functional regeneration of tissue 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. Suitable biopolymers such as silk proteins can be processed using different technologies, involving various spinning and coating methods as well as hydrogel formation. The resulting material morphologies have to be both mechanically and physically tested as well as analyzed concerning their cell compatibility and ability to promote suitable 2- and 3-D scaffolds for tissue engineering. In this module, theoretical introductions into and demonstration of several processing methods of the model biopolymer spider silk protein including electro-spinning, dip-coating etc., biofabrication techniques, and biomedical characterization are given.

Proposed dates: 29. February and 01. March or 16. and 17. March (8:30 - 12:30)

C3: 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.

Proposed dates: 1. March or 2. March or 3. March (one full day)

C4: 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.

Proposed dates: 29. February - 4. March (two times half a day) or 4. April - 8. April (two times half a day)

C5: Principles of Selforganization

Walter Zimmermann, Theoretical Physics I

Patterns are ubiquitous in nature. Stripe patterns, for instance, are found in biology (skin pattern …), chemistry (Turing), Physics (convection, Taylor-vortices, wrinkles …) and geoscience (atmosphere, continental drift …). The driving mechanism of stripes in various systems is very different, but they follow common principles which are qualitatively explained as well as the driving mechanisms for selected examples. Besides stripes also hexagonal patterns (e. g. clouds, perma frost, vegetation patterns) squares, travelling or standing waves, oscillatory patterns, spirals (heart, chemical reactions etc.) or synchronization are explained. Most of the patterns are driven by dissipative (competing) processes and others by competing length scales. The formation of patterns is essentially a bifurcation. The generic types of bifurcation scenarios are discussed and analyzed by elementary textbook methods. What is a stability band of spatial patterns? What is the number $\sqrt{3}$ in this context, for instance for Turing patterns? Is the Eckhaus-stability ratio $\sqrt{3}$ also relevant for an understanding of the dynamics of the skin-pattern of the “zebra”-fish as it is for instance in fluids? Is biological pattern formation purely driven by genes?
Optional: Using Matlab software for simulation and visualization of the dynamics of a few patterns.

Date: will be arranged after consulting with the participants (one day)