Elitenetzwerk Bayern

UNIVERSITÄT BAYREUTH

Elite Study Program in Macromolecular Science

Advanced Course

Modern Research Topics in Macromolecular Science

Faculty of the Elite Study Program

Winter term 2008/09

The scope of the advanced course on 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 underling concepts, technical terminology and methodologies in the individual subfields of Macromolecular Science beside their main focus. The offered topics cover the fields macromolecular chemistry, colloidal chemistry, biopolymers, biochemistry, microbiology, polymer physics, biophysics, polymer technology, polymer engineering, theory and simulation of macromolecules. The students will select 8 topics from 16 offered topics. Each individual topic has a length of 10 hours and includes lectures, seminars and laboratory illustrations. In addition the students will have a tour and brief introduction of the research facilities.

The following topics will be offered in the winter term 2008/09:

Polymer foams
Volker Altstädt, Polymer Engineering

Due to the unique properties of polymer foams, a large number of innovative applications can be realised. 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 dampening.
The first part of the module (5 hours) focuses on the fundamental physics of polymer foams, including a detailed discussion of the foaming processes currently utilised 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-moulded 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. Finally, the students will learn how to obtain tailored foam morphologies – and properties. Some special experimental techniques for a better understanding of the foaming processes are also highlighted.
This oral part is followed by an experimental session (5 hours) taking place in our laboratories. More precisely, a practical introduction into foam injection-moulding 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.

Structure and Dynamics in Polymer Colloids
Matthias Ballauff, Physical Chemistry I, Colloid chemistry

In our part we shall focus on research done recently in our group on polymer colloids. These systems consist of well-defined polymer particles of approximately 100nm in diameter that are dispersed in water. In our recent work we have synthesized these particles and characterized by various methods including electron microscopy and scattering methods. The present module will introduce into current work done on these particles. This will include: 1. a short lab course on the synthesis and the characterization of colloidal particles, 2. experimental work on the dynamics (dynamic light scattering and rheology) and a final seminar

Liquid Crystals: From Low Molecular Weight Materials to Elastomers
Helmut 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.

Forces on the nano-scale: From sensing to control
Andreas Fery, Physical Chemistry / Polymer Physics

Interfacial forces determine many properties like friction, adhesion, wetting or interaction with biological matter. In recent years, especially the Atomic force microscope (AFM) has developed into a versatile tool for measuring forces with nanometer resolution, like it is necessary for investigating interfaces. Above this, force measurements allow to explore mechanical properties of nano- and colloidal objects.
This module provides an overview of the most important concepts for measuring forces with a focus on AFM. It shows examples how the results can be used to gain control over interfacial interactions or to produce colloidal objects with tailored deformability and links the results to applications.

Stimuli-responsive materials for the life sciences
Ruth Freitag, Bioprozesstechnik

Stimuli-responsive materials show pronounced property changes in response to a small change in an environmental parameter such as the pH, the ionic strength, or the temperature. Lately molecules have been designed that correspond to light as stimulus. Such materials have various applications in the life sciences, e.g. in the area of bioprocessing, product isolation, drug delivery, tissue engineering, and medical technology. After a brief introduction into the synthesis of stimuli-responsive polymers we will prepare and characterize some linear and three-dimensional structures (hydrogels). Afterwards the most suitable structures will be used in the isolation of a recombinant protein from a cell culture supernatant and for storage and controlled release of insulin.

Confocal Raman and Fluorescence Lifetime Imaging (FLIM) Microscopy and Holographic Data Storage
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, which yields information on the chemical composition of the sample, and confocal fluorescence lifetime imaging (FLIM) microscopy, which maps the excited-state lifetime of fluorophores. In the latter case, emphasis will be laid on experiments in the frequency domain which use a cw laser amplitude-modulated in the radio-frequency (rf) regime. In this context, some fundamentals of rf experiments will be touched. In the second part of the lecture, an introduction to holography and its application to high-density data storage in polymers will be given. The project part will be devoted to practical demonstrations of one of these techniques.

Catalysts for Olefin Oligomerization and Polymerization
Rhett Kempe, Helmut Alt, Anorganische Chemie II

The topic covers general aspects of the importance and scope of catalyst research for olefin oligomerization and polymerization.
We give an introduction on synthesis and properties of potential catalysts and give an overview of the structure-property relationships in polymerization catalysis (empirical and theoretical approaches). Methods and tools to optimize catalysts and methods to heterogenize homogeneous catalysts will be explained. Latest developments in catalyst design and synthesis of new materials via chain transfer processes is discussed.

Organic Semiconductors
Anna Köhler, Experimental Physics II

Organic semiconductors such as soluble molecules and polymers combine the mechanical advantages of plastics (like flexibility or being robust) with electrical conductivity and the ability to emit light. Thus, they allow for the use of plastic technologies such as printing or reel-to-reel coating for the fabrication of semiconductor devices like solar cells, light-emitting diodes (LEDs) and field-effect transistors (FETs), and this makes them very attractive for the production of TVs and lighting applications. In the module, a lecture will give an overview on the photophysics of this new class of semiconductors with a view to the salient differences between organic and inorganic semiconductors. In a seminar, we will discuss recent developments in the field on the basis of current research papers. The practical exercise will be concerned with the study of energy transfer in phosphorescent host-guest systems.

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 because mass diffusion. Relevant experimental techniques for the measurement of diffusion coefficients are discussed in the second part. The last part takes place in the laboratory, where some experiments are performed together in the group, utilizing state-of-the-art equipment.
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.

Principles of ab initio electronic structure theory
Stephan Kümmel, Theoretical Physics

Understanding molecular processes often requires insight on the microscopic scale, i.e., on the atomic level. On the theoretical side, "ab initio" methods, i.e., theoretical approaches that employ only the fundamental laws of physics and work without empirical and adjustable parameters, are a valuable tool. This topic will give an elementary overview over such methods. After a recapitulation of the basic concepts of quantum mechanics, the challenges posed by realistic molecular problems will be discussed. The concepts of different ab initio approaches will be laid out and their successes and failures will be discussed using examples from physics and chemistry. Some insight into how electronic structure calculations are done in practice will be given. Depending on the students' interest and available technical facilities, an introduction into a frequently used electronic structure code will be given, offering the possibility for the students to run a few molecular calculations themselves.

Synthesis and Properties of Hybrid Nanostructures
Axel Müller, Macromolecular Chemistry II

We will demonstrate the synthesis and some important properties of well-defined polymer and hybrid structures. Here, we define hybrid structures as combinations of synthetic polymers with inorganic or biological moieties. After a short tutorial on the basics of controlled polymer synthesis (for those who had no contact with this topic so far) we will first focus on how to make some selected polymer structures (in particular branched polyelectrolytes and amphiphilic block and graft copolymers) and some special properties of these structures in bulk and solution. Then we will discus some amphiphilic colloid structures (e.g., Janus particles, cylindrical brushes), some organic-inorganic hybrids (e.g. polymers with silica, magnetic, or semiconducting nanoparticles, e.g., hybrid nanowires and nanotubes) and organic-protein hybrid structures (“chimeras”, e.g., polymer-protein conjugates and glycopolymers).

Structure and Dynamics of Bio-Macromolecules
Paul Rösch, Biopolymers

Proteins and nucleic acids are the polymeric building blocks of life. Their three-dimensional structures are investigated in the field of structural biology. In our department we focus on heteronuclear, multi-dimensional nuclear magnetic resonance (NMR) spectroscopy as main tool to elucidate structural and dynamic properties of bio-macromolecules. This technique is supplemented by optical spectroscopy (circular dichroism and fluorescence spectroscopy). The teaching module consists of a lecture series introducing biopolymer structure and concepts underlying the biophysical techniques used for structure determination. The lecture series will cover the following methodologies:

Birgitta Wöhrl: From gene to protein
Stephan Schwarzinger: Optical spectroscopy (from methods to results)
Kristian Schweimer: NMR spectroscopy (methodology)

The lectures will be completed by a lab tour dealing with the technical aspects of the techniques presented.

Challenges in Bioinorganic Chemistry
Holger Dobbek, Berta M. Martins, Lab. for Bioinorganic Chemistry

Life depends on the function of redox active bioinorganic cofactors like haem and Fe/S centres. These cofactors are integral components of so called metalloenzymes that work as catalysts in vital biological processes like fermentation, respiration and other redox processes.
We are interested in understanding how these bio-catalysts work. For that we use different approaches from structural biology and enzymology to determine the thermodynamic and kinetic parameters of their interaction with ligands, substrate and other proteins able to regulate their function.
The course will start with a tutorial on enzymatic catalysis where we will discuss metalloproteins, electron transport and radical chemistry. We will then have a lab practical on the last steps of structural enzymology: protein crystallization, structure determination, protein model refinement with 3-D visualization and graphical representation of the refined model.

Polymer dynamics studied by NMR field-cycling
E. Rößler, Experimentalphysik II

In a nuclear magnetic resonance (NMR) experiment, the spin-lattice relaxation time T1 describes the build-up of the nuclear magnetization in time, and T1 depends on the Larmor frequency being fixed by the external magnetic field B usually provided by a cryomagnetic. Only since recently, a commercial spectrometer, a so-called field-cycling spectrometer, is available which allows switching the B field of an electromagnet on the time scale of ms. This enables us to measure the dispersion of T1 = T1(ω) which is highly sensitive to slow dynamics in the liquid state. Thus, the method allows studying the collective dynamics in a polymer melt. The T1 dispersion shows certain relaxation regimes which are attributed to Rouse and reptation dynamics and which provide access to quantities like the smallest Rouse unit and the entanglement molecular weight. Experiments will be performed showing the crossover from a simple liquid to polymer, and they will be interpreted in terms of polymer physics.

Supramolecular Macromolecules
Hans-Werner Schmidt, Macromolecular Chemistry I

We will present in a series of introductory lectures the concepts and underling principles of supramolecular macromolecules and self-assembling of molecules. Special emphasis will be given on hydrogen bonded supramolecular polymers and assemblies. Low molecular weight organogelators and nucleating agents for semi-crystalline polymers will be reviewed as two special selected topics. The project afternoon includes experiments on polymer nucleation and gelation of organic solvents and a discussion on selected literature articles.

Color - Modern Aspects in Display Technology
Peter Strohriegl, Macromolecular Chemistry I

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 color formation in modern displays, both Liquid Crystal Displays (LCDs) - and Organic-Light Emitting Devices (OLEDs) will be discussed. In such devices the photophysical principles of energy transfer from a host material to a fluorescent or phosphorescent guest molecule are used in a clever way to manufacture full color displays.
The course ends with an experiment demonstrating the energy transfer from an organic host to a fluorescent dopant molecule. This experiment will be planned and accomplished by the students.

Zsigmondy Kolloquium

Andreas Fery, Thomas Hellweg, Alexander Wittemann

The „Zsigmondy Kolloquium“ in the field of Polymer and Colloid chemistry focuses on younger scientists as graduate students or post doctorate students working on this current research area. The two-day workshop is to bring together young scientists from different scientific backgrounds and offers them the opportunity to an exchange of experience and information on the research area of Polymer and Colloid Chemistry. In lectures and poster sessions the students have the possibility to present and to discuss their own research results along with academic and industrial researchers. Specialists from industry and university are invited to use this opportunity, in order to keep an eye on new results and young scientists.