

# KOLOKVIUM 2022

**Ústav makromolekulární  
chemie AV ČR, v. v. i.**

Heyrovského náměstí 2  
162 06 Praha 6

**21. – 24. 2. 2022**

# 30. KOLOKVIUM



# K O L O K V I U M

Kolokvia jsou od roku 1992 výroční interní konferencí Ústavu makromolekulární chemie AV ČR, v. v. i.

Reflektují celosvětové trendy základního a aplikovaného výzkumu v oboru makromolekulární chemie a hlavní směry výzkumu ÚMCH AV ČR.

Nabízejí zaměstnancům ústavu a dalším hostům prostor pro odbornou diskuzi nad aktuálními výsledky řešených výzkumných projektů s možností rozvíjet vzájemnou spolupráci.

Součástí 30. Kolokvia jsou také přednášky pracovníků ústavu oceněných v minulém roce – Jiřího Bruse a Rafała Łukasze Konefała.

Těšíme se na Vás na našem 30. Kolokviu

# P R O G R A M

## Pondělí 21. 2.

9:00 **Jiří Kotek, Petr Šálek**  
Zahájení

9:10

9:10 **L1 Anna Golunova**

Development of advanced bioinks for 4D bioprinting

9:35 **L2 Petr Šálek**

Dispersion polymerization in Cellosolve/water medium:  
Universal method for various hydrophilic nanogels

10:00 **L3 Richard Laga**

Polymer-colloidal systems as MRI-detectable  
nanocarriers for antigen vaccine delivery

10:25 **L4 Michal Babič**

Polymer particles as contrast agents for photoacoustic  
tomography

CENTRUM Biomakromolekulární a  
bioanalogické systémy

10:50 **PŘESTÁVKA** Káva a diskuze u posterů

11:15 **L5 Ognen Pop-Georgievski**

Biofunctional polymer brush coatings at the nanoscale

11:40 **L6 Jan Svoboda**

Preparation and characterization of surface adherent  
polydopamine films on various substrates

12:05 **L7 Radoslava Sivkova**

Surface-grafted polymer brushes as platform  
for post-polymerization modification reactions

CENTRUM  
Biomakromolekulární a  
bioanalogické systémy

12:30 **PŘESTÁVKA** Oběd

13:30

13:30 **L8 Dana Kubies**

Polyelectrolyte assemblies for delivery of bioactive  
proteins supporting cell responses

13:55 **L9 Tomáš Riedel**

Complement activation dramatically accelerates blood  
plasma fouling on antifouling polymer brush surfaces

14:20 **L10 Miroslava Dušková Smrčková**

Synthesis of sec.-amine binders for high-performance  
and environmentally sustainable polyurea coatings and  
their curing with polyisocyanates

CENTRUM Biomakromolekulární  
a bioanalogické systémy

14:45 **L11 Miroslav Vetrík**

Fluorinated diselenide nanoparticles for the therapy  
of cancer



# P R O G R A M

## Úterý 22. 2.

9:00

- 9:00 **L12 Marina Rodrigues Tavares** (studentská prezentace)  
Glycopolymers as efficient inhibitors of galectin-induced tumor progression
- 9:25 **L13 Eliška Grosmanová** (studentská prezentace)  
Fluorescently labeled HPMA-based conjugates for enhanced tumor localization and penetration
- 9:50 **L14 Mykhailo Nahorniak** (studentská prezentace)  
Rose Bengal-modified light-upconverting nanoparticles for biomedical applications

CENTRUM  
Biomakromolekulární a  
bioanalógické systémy

10:15 **PŘESTÁVKA** Káva a diskuze u posterů

- 10:45 **L15 Zdeněk Starý**  
Nové polymerní materiály pro teleskopické kryty obráběcích strojů
- 11:10 **L16 Ehsan Naderi Kalali**  
Advanced multifunctional flame retardants
- 11:35 **L17 Hynek Beneš**  
Bio-based and bio-degradable polyurethane foams for environmental applications

CENTRUM Polymerní  
materiály a technologie

12:00 **PŘESTÁVKA** Oběd

13:30

- 13:30 **L18 Josef Jůza**  
Effect of a block copolymer on the interfacial tension in polymer blends
- 13:55 **L19 Abdelmohsen Abdellatif**  
Collagen/chitosan-glucon hollow fiber wound dressing: Preparation, characterization and medical applications
- 14:20 **L20 Miroslav Šlouf**  
New microscopic method developed at IMC: Powder electron diffraction in SEM

CENTRUM Polymerní  
materiály a technologie

- 14:50 **L21 Zulfiya Černochová**  
Tunned melittin encapsulation and release by complex formation with supramolecular polymer carriers

# P R O G R A M

## Středa 23. 2.

9:00

9:00 **L22 Johanna Elter**

Keeping everything in place - strategies for particle stabilization in nanomedicine

9:25 **L23 Volodymyr Lobaz**

Improving receptor targeting by anchoring to cell membranes

9:50 **L24 Svetlana Lukáš Petrova**

RAFT polymerization of N-(2-hydroxypropyl) methacrylamide as a macroCTA via microwave-assisted irradiation and their pH-responsive diblock copolymers respectively nano-objects

10:15 **L25 Sachin Gupta** (studentská prezentace)

Trichloroacetyl isocyanate adducts as a new class of initiators for copper-mediated RDRP

CENTRUM Nadmolekulární struktury a samoasociační procesy

10:40 **PŘESTÁVKA** Káva a diskuze u posterů

11:10 **Přednášky oceněných pracovníků**

11:10 **L26 Jiří Brus**

From solid-state NMR spectroscopy of organic solids to energy-related materials

11:35 **L27 Rafał Lukasz Konefal**

High-resolution NMR spectroscopy of polymers

12:00 **PŘESTÁVKA** Oběd

13:30

13:30 **L28 Islam Minisy** (studentská prezentace)

Polypyrrole: A fascinating example of conducting polymers

13:55 **L29 Iryna Ivanko** (studentská prezentace)

Conjugated redox polymer with poly(3,4-ethylenedioxythiophene) backbone and hydroquinone pendant groups as the solid contact in potassium-selective electrodes

14:20 **L30 Lukáš Pavlovec** (studentská prezentace)

Nové polymerní materiály pro separační membrány

CENTRUM Polymery pro optoelektronické a energetické aplikace



# P R O G R A M

## Čtvrtek 24. 2.

9:00		CENTRUM Polymery pro optoelektronické a energetické aplikace
9:00	<b>L31 Jiří Pflieger</b> Polymer memristors for neurosynaptic elements	
9:25	<b>L32 Adriana Šturcová</b> Dissolution of cellulose, a semi-crystalline polymer	
9:50	<b>L33 Miroslav Menšík</b> Vibrational beatings during singlet fission in butyl-substituted bis(thienyl)-diketopyrrolopyrrole derivatives	
10:15 <b>PŘESTÁVKA</b> Káva a diskuze u posterů		
10:45 <b>L34 Jiří Czernek</b> On the structure of $\alpha$ and $\beta$ forms of poly(3-hydroxybutyrate)		CENTRUM Struktura a dynamika makromolekul / Laboratoř analytické chemie
11:10	<b>L35 Olga Trhlíková</b> ICP-MS and cryogenic mill – improvement in polymer analysis	
11:35	<b>L36 Miloš Netopilík</b> Fast and efficient single step liquid chromatography separation of parent homopolymers from block copolymers	
12:00	<b>Vyhlášení ceny za nejlepší studentskou prezentaci a zakončení Kolokvia</b>	

# Seznam posterových prezentací

**P1 Abdelmohsen Abdellatif**

Collagen dressing reinforced by chitosan-glucan hollow fibers with high-performance properties for tissue engineering applications

**P2 Veronika Gajdošová**

Morphology and micromechanical properties of polyolefins

**P3 Sonal Gupta**

Tuning the conductivity, morphology, and capacitance with enhanced antibacterial properties of polypyrrole by acriflavine hydrochloride

**P4 Yadu Ram Panthi**

Resistive memory effect in methacrylate polymer derivatized with alkylated carbazole

**P5 Rasha Radwan**

Hyaluronan biofilms reinforced with partially deacetylated chitin nanowhiskers

**P6 Iryna Romanenko**

Conformational behavior of ethylene glycol based polymer brushes when exposed to anions of the Hofmeister series

**P7 Doebner von Tumacder**

Acid blue dyes in the electropolymerization of polypyrrole films

**P8 Yu-Min Wang**

Grafting-to vs. grafting-from: Grafting density and fouling resistance of poly(HPMA) brushes

**30. Kolokvium se uskuteční v přednáškovém sále A,  
s možností sledovat přenos v klubu B.**

**Posterová sekce bude instalována v galerii Makráč (chodba  
před kluby B a C).**

**Prosíme, dodržujte platná epidemiologická opatření.**

Informace o konání Kolokvia 2022, epidemiologických opatřeních a případné změny  
v programu lze nalézt na: <https://www.imc.cas.cz/events/22kolok/>

**KOLOKVIUM  
2022**



# Abstrakty přednášek

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## L1 Anna Golunova

### Development of advanced bioinks for 4D bioprinting

The proper selection of the bioink is crucial to the main parameters and is of the main challenges in the fast-growing field of 4D printing.

The most common commercial bioink is methacrylated gelatin crosslinked under UV light. The main flaws of this method are: 1) batch-to-batch incoherence in the structure of gelatin, 2) low tunability of the system, and 3) potential phototoxicity of the UV light.

To overcome mentioned flaws in this work we focused on the development of the synthetic and biodegradable bioink based on polyaminoacids able to crosslink under the visible light. We synthesized and characterized the poly[N5-(2-hydroxyethyl)-L-glutamine] based polymer precursor and gels made of it.

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## L2 Petr Šálek

### Dispersion polymerization in Cellosolve/water medium: Universal method for various hydrophilic nanogels

Dispersion polymerization is conventionally used for producing various micron-sized polymeric particles. Moreover, a tuning of polymerization parameters leads to sub-micron polymeric particles and even particles with diameter below 100 nm. This presentation will focus on the dispersion polymerization of 2-(dimethylamino)ethyl methacrylate, N-(2-hydroxypropyl) methacrylamide, and 2-hydroxyethyl methacrylate for the preparation of hydrophilic nanogels and their basic biological applications.

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## L3 Richard Laga

### Polymer-colloidal systems as MRI-detectable nanocarriers for antigen vaccine delivery

In this work, novel biocompatible polymer-colloidal carriers based on maghemite ( $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>) nanoparticles coated with poly[N-(2-hydroxypropyl)methacrylamide] (PHPMA) polymers for antigen vaccine delivery have been developed. The resulting materials were stable, well-defined, bio-responsive nanoparticles characterized by negligible toxicity and suitable hydrodynamic size and shape for efficient uptake by immune cells. A minimal peptide antigen derived from the HIV-1 binding site (V3) was successfully conjugated to the exemplary carrier to demonstrate its suitability for vaccine delivery. In addition, the superparamagnetic properties of the carrier enabled the detection of the vaccine by MRI.

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## L4 Michal Babič

### Polymer particles as contrast agents for photoacoustic tomography

Photoacoustic tomography is valuable technique for imaging of blood vessels, injuries, perfusion, oxygen saturation quantification, and lipid detection in vessels. Application of exogenous contrast agents can greatly improve the imaging effectivity and opens thus an opportunity to obtain diagnostic images originating on cellular and molecular level. To maximize the contrast effect of the exogenous agents, it is necessary to suppress the tissue contribution to the PA signal. The optical absorption of endogenous soft structures shows the minimum in the near-infrared (NIR) region from ~700 to 1100 nm. Therefore, a selection of suitable contrast agents is crucial.

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## L5 Ognen Pop-Georgievski

### Biofunctional polymer brush coatings at the nanoscale

Antifouling polymer layers containing extracellular matrix-derived peptide motifs offer promising new options for biomimetic surface engineering. In this contribution, we report the design of antifouling polymer brushes bearing biofunctional peptide motifs for tissue regeneration applications. We utilize grafting-to and grafting-from synthesis methods for attaining the polymer brush conformation, and further functionalize the brushes with various biomimetic peptide sequences, such as RGD and TYRAY. The characterization of obtained systems goes beyond the state-of-the-art findings based on far-field analytical techniques for proving the brush character of the synthesized polymer structures, their antifouling character and the biofunctionality induced by the presence of various peptide motifs. By utilizing mid-infrared nanoscopy methods of scattering-type scanning near-field optical microscopy (s-SNOM) and near-field infrared spectroscopy (nano-FTIR) we unravel the conformation and orientation of the individual polymer chains constituting the polymer brush films and directly determine the distribution of bifunctional peptides with a nanoscale resolution. We foresee that measurements under controlled temperature, humidity, or in liquids will give further physicochemical insights into bioactivity of these polymer brushes architectures.

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## L6 Jan Svoboda

### Preparation and characterization of surface adherent polydopamine films on various substrates

Polydopamine (PDA), is widely used as a biomimetic anchoring layer for the modification of various solid substrates. The growth of PDA layer was studied using surface sensitive techniques such as spectroscopic ellipsometry, AFM, XPS, grazing angle attenuated total reflection FTIR spectroscopy, scattering-type scanning near field optical microscopy and Fourier-transform infrared nanospectroscopy. We have particularly focused on the effects of polymerization time and substrate on the PDA structure. We found notable differences in the chemical composition of PDA formed on gold and on surfaces terminated with oxides/reactive hydroxides in the early stages of the layer formation.

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## L7 Radoslava Sivkova

### Surface-grafted polymer brushes as platform for post-polymerization modification reactions

In this contribution we present a method for the SI-ATRP polymerization of active esters based on N-methacryloxysuccinimide in mild conditions. The obtained active ester brushes show quantitative conversion under amidation conditions with various primary amines, including fluoroamines and amine-containing fluorophores. The effectiveness of the amidation reaction was studied in details utilizing spectroscopic ellipsometry (SE), infrared reflection-absorption (IRRAS) and X-ray photoelectron (XPS) spectroscopies.

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## L8 Dana Kubies

### Polyelectrolyte assemblies for delivery of bioactive proteins supporting cell responses

Complementary support of vascularization of implants and tissue-engineering (TE) constructs as well as modulation of the recipient's immune response are considered to be the key issues for the successful implementation of the TE concept. These processes can be supported by a local delivery of growth factors or chemokines that are incorporated into specific coatings or particles. The lecture will give a brief overview of the preparation and physico-chemical characterization of several types of polyelectrolyte assemblies in the form of layered-by-layered (LbL) films and nanoparticles, which we have recently designed as platforms for delivery of heparin-binding growth factors and chemokines.

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## L9 Tomáš Riedel

### Complement activation dramatically accelerates blood plasma fouling on antifouling polymer brush surfaces

Non-specific protein adsorption triggers a number of deleterious events in the application of biomaterials. Antifouling polymer brushes successfully suppress fouling, however for some coatings an extremely high variability of fouling for different donors remains unexplained. We report that this variability is due to the complement system activation that causes massive acceleration in the fouling kinetics of blood plasma. The results indicate that the alternative complement pathway plays a significant role in the fouling on poly(HEMA) through the “tick-over” mechanism of spontaneous C3 activation. The generated C3b binds to the polymer surface and amplifies complement activation locally.

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## L10 Miroslava Dušková Smrčková

### Synthesis of sec.-amine binders for high-performance and environmentally sustainable polyurea coatings and their curing with polyisocyanates

Polyurea-based materials serve as advanced materials suitable for various demanding applications: e.g., coatings of industrial equipment in exterior, architectural coatings, coatings for traffic means, etc. The properties of PU layers and ease of their application overbeat some coating systems based on epoxy chemistry or polyurethanes. The film-forming properties and the long-term performance much depend on the structure of the macromolecular network. We have varied chemistry of the aspartate resin to establish the relations between formation–structure–properties of final networks. Thus we will present our intermediate results on resins for films prepared by the aza-Michael addition, curing of these resins, role of side reactions during curing, and some crucial properties of final films.

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## L11 Miroslav Vetrík

### Fluorinated diselenide nanoparticles for the therapy of cancer

Radiation resistance of cancer cells represents one of the major challenges in cancer treatment. The novel fluoralkylated diselenide molecules based on seleno-L-cystine underwent self-assembled process. The redox-active diselenide molecules autocatalytically decompose hydrogen peroxide ( $H_2O_2$ ) and oxidize the intracellular glutathione (GSH) that results in the regulation of cellular oxidative stress. Alkylfluorinated diselenide nanoparticles showed a significant cytotoxic and radiosensitizing effect on cancer cells. C56BL/6 mice treated with fluoralkylated diselenides followed by fractionated radiation treatment (4x 2Gy) completely suppressed tumor growth. Our results suggest that described diselenide system behaves as a potent radiosensitizing agent targeting tumor growth and preventing tumor recurrence.

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## L12 Marina Rodrigues Tavares

### Glycopolymers as efficient inhibitors of galectin-induced tumor progression

Galectins are prospective targets for therapeutical applications due to their role in tumor progression. In this study, we describe the synthesis, physico-chemical characterization, and structure-activity relationship of various HPMA copolymers decorated with different carbohydrates derived from N-acetylated lactosamine. Their binding affinity to Gal-1 and Gal-3, as well as their inhibitory efficacy on selected galectin-positive or negative cancer cell lines were proved.

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### **L13 Eliška Grosmanová**

#### **Fluorescently labeled HPMA-based conjugates for enhanced tumor localization and penetration**

The present study brings fluorescently labeled high-molecular weight conjugates with RGD-based tumor homing specificity. The HPMA-based copolymers were decorated with wide range of RGD-based structures (linear, cyclic, branched). Their integrin-targeting potential was evaluated in vitro. The second aim was also to study, if the selectivity of cell-penetrating peptide bearing polymer carrier could be increased using RGD-based targeting strategy, so that could be used as a triple synergistic system combining passive accumulation, active targeting and increased penetration. The best fluorescently labeled system was also tested in vivo in tumor-bearing mice intended for accurate tumor boundaries visualization.

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### **L14 Mykhailo Nahorniak**

#### **Rose Bengal-modified light-upconverting nanoparticles for biomedical applications**

Upconverting nanoparticles (UCNPs) with unique ability to convert infrared light into visible one offer new possibilities in biomedical imaging or light-activated drug release and therapy.

Here, the NaYF<sub>4</sub>: Yb,Er UCNPs were synthesized and surface-modified with Rose Bengal, serving as a photosensitizer of xanthan type. The irradiation of particles with near-infrared light at 980 nm produced reactive oxygen species (ROS), which can kill cancer cells. Nevertheless, many challenges remain to be solved, including particle size regulation, reduced toxicity, good colloidal stability in aqueous media, improved quantum yield, and effective ROS generation.

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### **L15 Zdeněk Starý**

#### **Nové polymerní materiály pro teleskopické kryty obráběcích strojů**

Příspěvek shrnuje výsledky získané při řešení projektu aplikovaného výzkumu podpořeného MPO. Představen bude výzkum v oblasti modifikace termoplastických polyurethanů za účelem snížení tření během provozu teleskopických krytů obráběcích strojů a v oblasti povrchové úpravy pěnových tlumicích elementů.

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### **L16 Ehsan Naderi Kalali**

#### **Advanced multifunctional flame retardants**

Polymers are widely used in different advanced applications such as electronic, constructions, aeronautics, etc. due to their outstanding performance in mechanical behavior, electrical insulating, strong possibility of tailoring structure with desired functionalities. However, the flammability of most of polymers exists as a major drawback which has restricted their applications. Synthesis of new novel flame retardants based on the combination of bio-based or Eco-friendly nano-materials and organic/inorganic compounds with multi-functional task feature considered and high-performance polymer composites will be designed and developed. This presentation will explain and share the new ideas.

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## L17 Hynek Beněš

### **Bio-based and bio-degradable polyurethane foams for environmental applications**

Open-pore materials are highly desirable in many biotechnological and environmentally-oriented processes as substrates and carriers of microbial biomass. Herein, flexible fully-aliphatic polyurethane foam having porous structure with high open cell content was designed, prepared, characterized and tested as (bio)degradable cellular carrier of microorganisms (fungus *Fusarium solani* and bacterium *Pseudomonas* sp.) for biofiltration and wastewater biological treatment.

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## L18 Josef Jůza

### **Effect of a block copolymer on the interfacial tension in polymer blends**

Block and graft copolymers with blocks that are identical, miscible with or adhere to related components of a polymer blend can serve as compatibilizers. In the previously used models established by Leibler and Noolandi, simple solutions were published for special cases called dry brush and wet brush regime. We have tried to find a more general solution which is still relatively uncomplicated. The solution found is consistent with the dry brush regime for higher copolymer concentrations at the interface and shorter copolymer, and with the wet brush regime for lower copolymer concentrations and longer copolymer.

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## L19 Abdelmohsen Abdellatif

### **Collagen/chitosan-glucan hollow fiber wound dressing: Preparation, characterization and medical applications**

A multifunctional wound dressing based on complex chitosan-glucan (CSGC) hollow fiber/collagen (CO) in the presence of aloe vera (AV). CSGC hollow fiber exhibited inner diameter of  $(600 \pm 250 \text{ nm})$  and outer fiber diameter of  $(2.5 \mu\text{m})$ . The morphology and swelling ability of the wound dressing was investigated. The obtained composite dressing exhibited high hydrolytic stability sufficient mechanical properties compared to the native collagen. The hemostatic property of wound dressing was significantly enhanced compared to native CO with excellent biocompatibility. In-vivo assays showed that the novel dressing promoted wound healing compared with native CO.

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## L20 Miroslav Šlouf

### **New microscopic method developed at IMC: Powder electron diffraction in SEM**

Electron diffraction is performed in transmission electron microscopes (TEM), while in scanning electron microscopes (SEM) it has not been available until recently. We introduced a novel method that yields powder electron diffractograms in modern SEM microscopes as well. The method was developed in collaboration with Institute of Scientific Instruments and called 4D-STEM/PNBD, as it converts large 4D-STEM datasets (2D-arrays of 2D-nanobeam diffraction patterns) to a single PNBD pattern (powder nanobeam diffraction pattern, analogous to powder diffractograms from TEM). Unlike the complex 4D-STEM datasets, the PNBD patterns are easy to process even without deep crystallographic knowledge.

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## L21 **Zulfiya Černochová**

### **Tunned melittin encapsulation and release by complex formation with supramolecular polymer carriers**

In order to produce a biodegradable biocompatible well-defined nanoencapsulator of polycationic cargos, a series of modified anionic glycogens were synthesized by acylation of oyster glycogen with selected dicarboxylic acid anhydrides, possessing different hydrophobicity (bicyclo[2,2,2]-2,3:5,6-dibenzo-2,5-octadiene-7,8-dicarboxylic, 1,2-cyclohexanedicarboxylic, phthalic and succinic anhydrides). TEM imaging demonstrated that modification of glycogen took place in whole volume of the particles. Selfassembly behavior was studied with DLS as a function of solution temperature and pH. DLS autotitration with model cationic amphiphile cargo – honeybee poison peptide melittin in buffered solution revealed that melittin-modified glycogen polyplex formation occurs in the solution in the ratio 1/3, and survives further increasing of melittin concentration up to 1/9.8 weight ratio. In vitro experiments on erythrocytes clearly showed that modified glycogens efficiently suppress hemolytic activity of melittin serving as melittin antidotes or may, in opposite use, serve as controlled release carriers.

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## L22 **Johanna Elter**

### **Keeping everything in place - strategies for particle stabilization in nanomedicine**

Numerous variables need to be adjusted to create suitable particles for drug delivery applications. They have to be biocompatible and stable, but still able to release the encapsulated drug under certain conditions. The stability of the particles can be increased by crosslinking. It is possible to either apply click reactions (Diels-Alder reaction), and release drug molecules by other mechanisms in the particle (swelling), or to introduce groups for reversible, covalent crosslinking (disulfides). On the other hand, particle stabilization can also be achieved using non-covalent methods instead. The talk covers the mentioned strategies for particle stabilization, focusing on covalent methods.

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## L23 **Volodymyr Lobaz**

### **Improving receptor targeting by anchoring to cell membranes**

Block copolymers, from alkyl oxazolines, where the hydrophobic block is for embedding into phospholipid membrane and hydrophilic block carries the glutamate carboxypeptidase II inhibitor as an end group.

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## L24 **Svetlana Lukáš Petrova**

### **RAFT polymerization of N-(2-hydroxypropyl) methacrylamide as a macroCTA via microwave-assisted irradiation and their pH-responsive diblock copolymers respectively nano-objects**

A rapid and eco-friendly reversible addition-fragmentation chain transfer (RAFT) polymerization reaction of the N-(2-hydroxypropyl) methacrylamide (HPMA) monomer under microwave irradiation (MWI) is demonstrated. The polymerization kinetics were obtained using two different chain transfer agents (CTAs), namely, commercial 4-cyano-4-(phenylcarbonothioylthio)pentanoic acid and synthesized 4-cyano-4-(((ethylthio)-carbonothioyl)thio)pentanoic acid, in the presence of 4,4'-azobis(4-cyanovaleric acid) as the initiator in various solvents. In addition, the ability of MWI to facilitate copolymer formation was demonstrated by the preparation of relevant copolymers, such as poly(HPMA-b-bocAPMA), poly(HPMA-b-MABH) and poly(HPMA-b-PDPA). Furthermore, PHPMA-mCTA was used in a versatile platform for the synthesis of pH-responsive PHPMA-b-PDPA nano-objects obtained via MWI-RAFT polymerization-induced self-assembly (microwave-PISA).

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## L25 Sachin Gupta

### Trichloroacetyl isocyanate adducts as a new class of initiators for copper-mediated RDRP

The application of copper-mediated reversible-deactivation radical polymerization (Cu-RDRP) in the synthesis of complex polymeric architectures is often complicated by the inefficient attachment of initiating groups to the desired substrate. In this work, we introduce a novel class of Cu-RDRP initiators derived from trichloroacetyl isocyanate (TAI) that enable rapid, clean, and controllable functionalization of various substrates. We report on the optimization of Cu-RDRP conditions for model monomers, reveal the functionality of the initiators, and assess the hydrolytic stability of TAI adducts. The application of TAI in the modification of complex substrates will be also exemplified.

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## L26 Jiří Brus (oceněný pracovník)

### From solid-state NMR spectroscopy of organic solids to energy-related materials

Metal-organic frameworks (MOFs), owing to their unique architecture, attract consistent attention in the design of high-performance Li-battery materials. Here, we report a new category of crystalline materials based on the MIL53(Al) framework featuring metallocarborane (Li+CoD-) salt and present quantitative data on Li+ ion sites, local dynamics, chemical exchange, and charge-transfer pathways. We used multinuclear ss-NMR spectroscopy to examine the mechanism of ionic conductivity at atomic resolution and to elucidate order-disorder processes, framework-ion interactions and framework breathing during the loading of Li+CoD- species and transfer of Li+ ions.

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## L27 Rafał Łukasz Konefał (oceněný pracovník)

### High-resolution NMR spectroscopy of polymers

## L28 Islam Minisy

### Polypyrrole: A fascinating example of conducting polymers

Since conducting polymers were appreciated by the Nobel prize in chemistry in 2000, tremendous efforts were made for developing new types with highly improved properties. Conducting polymers show very attractive physicochemical properties. Alongside their high conductivity, they are chemically and environmentally stable, easily prepared with low-cost. CPs have been used in myriad of applications in various fields e.g., energy storage, conversion and harvesting, sensors, catalysis, wastewater treatment, etc. Polypyrrole (PPy) showed the highest conductivity among the conducting polymers with facile preparation procedure. However, its infusibility and insolubility highly limited its processability, and hence restricted its practical applications. Various approaches were used to overcome PPy drawbacks such as preparation of PPy nanostructures and/or composites. Herein, PPy was prepared in the presence of various organic dyes, as morphology-guiding agents, to form various nanostructures. The presence of organic dyes showed positive impact on PPy conductivity as well. The polymerization conditions, such as oxidant to monomer mole ratio, type of the organic dye and polymerization temperature have significantly influenced the physicochemical properties of the prepared PPy. The highest conductivity was achieved by frozen-polymerization technique, where the low temperature affects the rate of crosslinking, molecular weight and the ordering of PPy chains.

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## L29 Iryna Ivanko

### Conjugated redox polymer with poly(3,4-ethylenedioxythiophene) backbone and hydroquinone pendant groups as the solid contact in potassium-selective electrodes

The wide demand for semiconducting polymers, as ion-to-electron transducers, for analytes detection requires materials with reasonable properties. For that purpose, a conjugated polymer poly(3,4-ethylenedioxythiophene) with a covalently bonded hydroquinone group was used. Redox couples are one of the ways to adjust the  $E^\circ$  of solid contact ion-selective electrodes. Typically, the initially high  $E^\circ$  reproducibility is lost due to leaching out of non-covalently bounded redox molecules from SCISE. The introduction of covalently attached HQ groups in PEDOT-HQ prevents the leaching and simultaneously allows additional charge storage in PEDOT-HQ that is 25 times higher than for unsubstituted PEDOT.

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## L30 Lukáš Pavlovec

### Nové polymerní materiály pro separační membrány

První část práce se zabývá syntézou komonomeru bis(4 aminobenzyl)-hexabenzylbambus[4]juriu a následnou přípravou polyimidových membrán, vhodných k separaci plynů. Zakomponování tohoto komonomeru bylo potvrzeno NMR technikou. Polyimidové membrány byly charakterizovány metodami FTIR, DMTA, DSC a TGA, taktéž byly změřeny permeační vlastnosti v závislosti na obsahu zmíněného komonomeru. Druhá část práce se zabývá polymer-analogickými reakcemi na poly(epichlorhydrinu). Zesítním sekundárními aminy a následnými reakcemi s 1,4 diazabicyclo[2.2.2]oktanem a methyljodidem vznikly iontovýměnné membrány, u kterých byla změřena vodivost Cl<sup>-</sup> a OH<sup>-</sup> aniontu impedanční spektroskopii. Vodivost Li<sup>+</sup> byla prokázána difúzní NMR sondou.

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## L31 Jiří Pflieger

### Polymer memristors for neurosynaptic elements

Contrary to classical binary electronic devices memristors with neurosynaptic functionality take a continuity of resistance values with synaptic weights modulated by the number and frequency of homogeneous spikes. In order to mimic neural synapse memristors must exhibit reliable analog properties including non-abrupt switching transitions, continuously variable resistance states, and predictable response. We will show that PMMA derivatives with charge transporting group separated from the polymer backbone by an alkyl chain change their electrical characteristics from a bistable to analog behavior, depending on the length and flexibility of the side chain.

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## L32 Adriana Šturcová

### Dissolution of cellulose, a semi-crystalline polymer

Cellulose in cell walls forms microfibrils – they consist of amorphous domains and of highly ordered crystalline domains, which do not favour solubility. Treatments involving harsh conditions are necessary to dissolve this polymer. Driving forces and mechanisms of cellulose dissolution are not yet fully understood.

We compare behaviour of cellulose in either of two cellulose solvent systems: an organic solvent N,N-dimethylacetamide with addition of lithium chloride salt and an ionic liquid 1-butyl-3-methylimidazolium chloride. By the means of vibrational spectroscopy and X-ray diffraction, the structural differences in cellulose chains solubilised by these two solvent systems are explained.

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### L33 Miroslav Menšík

#### Vibrational beatings during singlet fission in butyl-substituted bis(thienyl)-diketopyrrolopyrrole derivatives

The transient optical absorption in 2,5-bis(butyl)3,6-bis(thiophen-2-yl)diketopyrrolopyrrole crystalline thin solid films at short delay time after photoexcitation was found to be modulated with the period of 1.6 ps. This behavior was explained in frame of the singlet fission process as a strong coupling between a particular intermolecular vibrational mode and electronic states of singlet and triplet pair excitons. For different wavelengths of the probe pulse a notable antiphase shift was explained by vibrationally controlled population exchange between singlet and triplet pair excitations.

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### L34 Jiří Czernek

#### On the structure of $\alpha$ and $\beta$ forms of poly(3-hydroxybutyrate)

In this work, the recently solved (10.1021/acs.macromol.9b00225) crystal structure of the  $\alpha$  form of poly(3-hydroxybutyrate) and the previously known  $\beta$  form (10.1021/acs.macromol.5b02310) were investigated by means of high-level quantum chemical calculations, which were performed for dimeric models comprising 58 atoms. In particular, the breakdown into electrostatic, induction, and dispersion contributions to a total stabilization of these two crystalline forms was reliably described. This will be discussed in the context of interchain interactions in crystals of polyesters with a general aim of understanding the structure – mechanical properties relationship.

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### L35 Olga Trhlíková

#### ICP-MS and cryogenic mill – improvement in polymer analysis

The Laboratory of Analytical Chemistry has procured two important instruments for improving polymer analysis. (i) The ICP-MS technique allows for the quantitative analysis of a wide range of elements (Li-U) at very low concentrations (at the ppb and ppt levels) and with the simultaneous determination of several elements. (ii) With the cryogenic mill, material soft at ambient temperatures can be finely ground to powders in liquid nitrogen, i.e. under the glass transition temperature. Better sample homogeneity is achieved resulting in higher precision and reliability of analysis (e.g., elemental).

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### L36 Miloš Netopilík

#### Fast and efficient single step liquid chromatography separation of parent homopolymers from block copolymers

The modified layout of the barrier method called liquid chromatography under limiting conditions of enthalpic interactions is presented. It enables automated quantitative separation of blends of synthetic polymers, for example, the single-step discrimination of both parent homopolymers from the block copolymers. Moreover, this method enables the estimation of molar mass and molar mass distribution of the block copolymer precursor. Adjacent large sequences of mobile phase of different compositions are applied as barriers. They are created by a computer-controlled pair of pumping systems in the form of longitudinal profiles along the column. The home synthesized block copolymers polystyrene-block-poly(2-vinylpyridine) served as model examples of the method application.

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