



Book of Abstracts

CEITEC PhD Retreat

23-24 April 2015

Valtice, Czech Republic

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CEITEC



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Welcome address

Dear participants of the CEITEC PhD Retreat

We would like to welcome you to the first CEITEC PhD Retreat that follows the tradition of similar events taking place within many renowned research institutes around the world. This event is organized by PhD students under the patronage of the Central European Institute of Technology (CEITEC). The main objective of CEITEC is to create environment for high level scientific discovery and interdisciplinary cooperation. To accomplish these goals, we believe that motivating scientists at the very beginning of their career plays an absolutely crucial role. The CEITEC PhD Retreat is a conference for young scientists aiming to promote collaboration of PhD students from different scientific areas.

This retreat offers a unique opportunity for you to meet and get to know colleagues working in the fields of life and material sciences, to present and discuss your work. You will gather and share inspiring ideas, learn about the exciting science that other students are working on, draw inspiration from the invited speakers, and make new friends. CEITEC itself is a multidisciplinary scientific centre, covering a wide range of biological, material and technology research. Therefore, the programme also includes various topics, such as molecular medicine, physics and mathematics in medicine, novel materials, biosensing, plant biology as well as off-topic lectures covering the other aspects of the life of a PhD student.

We sincerely hope that the first CEITEC PhD Retreat will be a productive meeting full of excellent science and inspiring discussions and that you will enjoy your stay in the beautiful setting of Valtice Château.

The organizing committee

Michaela Fojtů
Kristýna Hudcová
Ondřej Chmela
Marian Márik
Adam Obrusník
Jelena Pejović
Monika Sieberová



Practical information

General information

» Internet connection

WiFi connection is available in both hotels where participants will be accommodated. Since Valtice Château is an old, historical building, the internet connection at the venue will unfortunately be limited.

» Emergency Phone Numbers

The emergency phone number is 112.

» Insurance

The organizers of the event do not accept liability for any injury, loss or damage, arising from accidents or other situations during the event. Participants are, therefore, advised to arrange accident and health insurance.

» Departure from Brno

Bus transfer to and from Valtice is provided by the organisers. Detailed information regarding the departures will be sent to the participants by e-mail one week before the conference.

Retreat information

» Registration

The registration desk is located on the third floor of Valtice Château. See the back cover of this book for the exact location. The registration takes place on **Thursday, 9am – 10am.**

» Badge

All participants will receive a name badge upon registration. Everyone is kindly requested to wear his name badge during the whole event. Only participants who are wearing their name badges will be admitted to the conference premises.

» Language

The official language of the CEITEC PhD Retreat is English.

» Programme changes

The organizers cannot assume liability for any changes in the programme due to external or unforeseen circumstances.

Poster session

The student poster session will take place on **Thursday, 23 April at 19.30**. The participants are strongly encouraged to hang their posters as early in the morning as possible (right after the registration or during one of the coffee breaks). The participants can find their poster stand number at the end of this book.

The posters will be peer-reviewed and the best-rated poster from each section will be awarded with a prize. In their conference package, each participant will find a voting ticket with a ticket ID which is assigned randomly (i.e. the peer-review is anonymous).

The participants are kindly asked to write down the numbers of **two posters** that they found most interesting and best presented onto the voting ticket. **One of these has to be from the Life sciences** section (poster numbers L01-L49) **and the other from the Material sciences and physics** section (poster numbers M01-M46). By the end of the poster session, the tickets have to be thrown into a ballot box located at the door to the poster room.




The results of the poster session will be announced just before the closing of the conference. In case of a draw, the better poster will be chosen by the speakers.





Programme

Thursday, 23 April 2015

- 9.00 – 10.00 Registration
- 10.00 – 10.15 Opening speech
- Plenary 1: Novel materials**
- 10.15 – 11.00 **Ronald Zirbs** (*BOKU Vienna, AT*) - Core-shell nanoparticles with ultra-high dispersant densities for advanced material sciences
- 11.00 – 11.45 **Martin Hanczyc** (*CIBIO Trento, IT*) - Materials inspired from biology: perspectives from artificial life
- 11.45 – 13.15  Lunch
- Plenary 2: Physics and mathematics in biomedicine**
- 13.15 - 14.00 **Deborah O'Connell** (*University of York, UK*) - Plasma medicine
- 14.00 - 14.45 **Irena Koutná** (*Masaryk University Brno, CZ*) - Derivation of human induced pluripotent stem cells and advanced methods of image processing
- 14.45 - 15.15  Coffee break
- Plenary 3: Molecular medicine**
- 15.15 - 16.00 **Anki Östlund Farrants** (*Stockholm University, SWE*) - The ups and downs with studying ribosomal genes
- 16.00 - 16.45 **Ladislav Vyklický** (*Czech Academy of Sciences Prague, CZ*) - Block of NMDA receptor channels by endogenous neurosteroids: implications for the agonist induced conformational states of the channel vestibule
- 16.45 - 17.15  Coffee break
- 17.15 - 18.30 **Student session** - short talks by students
- 19.30 - 23.00 **Poster session** - informal networking and music with buffet

Friday, 24 April 2015

9.00 - 9.30 Presentations of sponsors

Plenary 4: Off-topic

9.30 - 10.15 **Roman Badík** (*CEITEC Brno, CZ*) - Individual funding opportunities for PhD students and postdocs

10.15 - 11.00 **Markus Dettenhofer** (*CEITEC Brno, CZ*) - Opening doors to your career with a science PhD

11.00 - 12.30 🍴 Lunch

Plenary 5: Biosensing and bioelectronics

12.30 - 13.15 **Peter Ertl** (*AIT Vienna, AT*) - Advanced in vitro diagnostics to organ-on-a-chip technology

13.15 - 14.00 **Martin Weiter** (*Brno University of Technology, CZ*) - Organic semiconductors for bioelectronics: organic and printed electronics meets biology

14.00 - 14.30 ☕ Coffee break

Plenary 6: Plant biology

14.30 - 15.15 **Petr Babula** (*Masaryk University Brno, CZ*) - Biological activity of naphthoquinone and its derivatives as promising cytotoxic compounds promoting cell death

15.15 - 16.00 **Karel Říha** (*CEITEC Brno, CZ*) - Telomeres, DNA repair and genome stability: taking an engineer approach

16.00 - 16.30 **Student poster award**

16.30 Departure



Invited talks

Abstracts and speaker biographies



Panel: Novel materials

Core-Shell nanoparticles with Ultra-High Dispersant Densities for Advanced Material Sciences

Ronald Zirbs

University of Natural Resources and Life Sciences Vienna, Austria

Superparamagnetic Fe_3O_4 nanoparticles (NPs) are used in a rapidly expanding number of applications in e.g. the biomedical field, for which brushes of biocompatible polymers such as poly(ethylene glycol) (PEG) have to be densely grafted to the core. Grafting of such shells to monodisperse Fe_3O_4 NPs has remained a challenge mainly due to the conflicting requirements to replace the ligand shell of as-synthesized NPs with irreversibly bound PEG dispersants. We introduce a general two-step method to graft PEG and other dispersants from a melt to Fe_3O_4 NPs first functionalized with nitrodopamine (NDA). This method yields uniquely dense (3 chains/nm²) and stable spherical PEG-brushes compared to existing methods, and remarkably colloidally stable NPs.



Ronald Zirbs, Ph.D.

Senior Scientist

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Biography

Ronald Zirbs received his Ph.D. in Technical Chemistry at Vienna University of Technology in 2006. He is currently working on his habilitation on nanoparticle actuated membrane materials at the Institute for Biologically inspired materials of the University of Natural Resources and Life Sciences Vienna.



Panel: Novel materials

Materials inspired from biology: perspectives from artificial life

Martin Hanczyc

CIBIO, University of Trento, Italy

My work is focused on understanding the fundamental principles of living and evolving systems through experimental science. To this end, I build synthetic systems where dynamic life-like properties emerge when self-assembled systems are pushed away from equilibrium. I will present an experimental model of bottom-up synthetic biology: the dynamic oil droplet. This system is able to sense, metabolize and potentially evolve. I will present how sensory-motor coupling can produce chemotactic motile droplets and may form the basis for smart materials. The general principle of this work is to develop new, dynamic, far from equilibrium materials.



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Biography

Martin Hanczyc is a Principal Investigator at the University of Trento, Italy. He formally was an Honorary Senior Lecturer at the Bartlett School of Architecture, University College London, Chief Chemist at ProtoLife and Associate Professor at the University of Southern Denmark. He received a bachelor's degree in Biology from Pennsylvania State University, a doctorate in Genetics from Yale University and was a postdoctorate fellow under Jack Szostak at Harvard University. He has published in the area of protocells, complex systems, evolution and the origin of life in specialized journals including JACS and Langmuir as well as PNAS and Science. He was also a mentor for the first iGEM synthetic biology student team from Denmark. He is developing novel synthetic chemical systems based on the properties of living systems.

Martin actively develops outreach for his research by giving several public lectures and collaborating with architects and artists in several exhibitions world wide including the Architecture Biennale in Venice Italy in 2010 to bring experiments out of the lab and into the public space. His approach to science has been integrative, multidisciplinary and publicly visible with over 20 press items including Nature News, Scientific American, Discovery Channel, WIRED and BBC Radio. Martin gave an invited public lecture at TED in 2011, which now has over 600,000 views.



Panel: Physics and mathematics in biomedicine

Plasma medicine

Deborah O'Connell

Department of Physics, University of York, United Kingdom

In recent years, investigations into the application of atmospheric pressure low temperature plasmas (LTPs) for biomedical purposes have demonstrated great potential in areas such as surface sterilisation, wound healing, biofilm inactivation, and cancer therapy. Low temperature plasmas can be generated by applying a high electric field across a gas, which breaks down the gas to form a plasma. This creates a complex, unique reactive environment containing high concentrations of reactive oxygen and nitrogen species (RONS). Operated at atmospheric pressure and around room temperature, the delivery of RONS, to a target, is a key mediator of oxidative damage and cell death in biological systems. RONS are already known to play an important role in many existing therapeutics. Plasmas have the advantage they can simultaneously produce and deliver a range of these species, potentially accessing superior pathways and mechanisms. This presentation will provide an introduction and overview of the field of plasma medicine, including recent investigations of interactions with prostate cancer cells. Taking both healthy prostate cells and prostate cancer tissue cells from a single patient, this study allows for a direct comparison of the effectiveness of the treatment. Using clinically relevant, close-to-patient samples, we show evidence promoting the potential of LTP as a future focal cancer therapy treatment for patients with early stage prostate cancer.



Deborah O'Connell, Ph.D.

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Biography

Deborah O'Connell leads an inter-disciplinary research group on low-temperature plasmas for biomedical applications at the York Plasma Institute (YPI), Department of Physics, University of York, UK. She joined the YPI in 2011 with an EPSRC Career Acceleration Fellowship (CAF) and holds a permanent faculty position. Prior to this she was at Queen's University Belfast, where she brought a EU Marie Curie Intra-European fellowship award. She also held postdoc positions at the Ruhr University Bochum in Germany and received her Ph.D. from Dublin City University, Ireland in 2004.

Since joining York her research group has grown to currently 8 Ph.D. students and 3 postdocs (including many cross-departmental positions between Physics, Chemistry, Biology and the Hull York Medical School). Her scientific contributions to the research community have been recognized through the 'Noah Hershkowitz Early Career Award 2013'. She sits on many international committees (including EU COST Action Bioplasma steering committee, International Symposium of Plasma Chemistry (ISPC), AVS PST Division Executive committee) and has organised national and international conferences (e.g. co-Chair ICPIG). She is a member of the editorial board of *Plasma Sources Science and Technology (IoP Publishing)* and *Plasma Medicine (Begell House Publishing)* and is currently a guest editor for *Biointerfaces (AVS publications)*. She has published over 45 publications in peer-reviewed journals and is a regular invited speaker with over 35 invited talks at major international conferences, overseas national conferences and leading institutions in the field.

Panel: Physics and mathematics in biomedicine

Derivation of human induced pluripotent stem cells and advanced methods of image processing

I. Koutná, P. Šimara, P. Matula, L. Tesařová, B. Šalingová

CBIA - Centre for Biomedical Image Analysis, Faculty of Informatics, Masaryk University, Brno, Czech Republic

Human induced pluripotent stem cells (hiPSCs) possess a great potential for clinical application. Various reprogramming techniques were presented during 7 years of hiPSCs research. Genome non-integrating and completely xeno-free protocols from the first biopsy to stable hiPSCs clones are highly preferable in terms of future clinical application. In CBIA lab we successfully generated hiPSCs using STEMCCA lentivirus, Sendai virus or episomal vectors. Human fibroblasts and CD34+ blood progenitors were used as a source cells and were maintained either on mouse embryonic feeder cells or in feeder-free conditions. The reprogramming efficiency was comparable for all three methods and both cell types, while the best results were obtained in feeder-free conditions. The pluripotency of our hiPSCs was verified by differentiation into all three germ layers and by teratoma assay. In order to study genomic integrity, we monitored DNA damage response (DDR). Image analysis of immunohistochemical or ImunoFISH experiments is very important step of iPSCs evaluation in the context of their genome integrity and stability. In CBIA lab we develop unique software "Acquarium" for this advanced image analysis.

Acquarium is open source software (GPL) for carrying out the common pipeline of many spatial cell studies using fluorescence microscopy. It addresses image capture, raw image correction, image segmentation, quantification of segmented objects and their spatial arrangement, volume rendering, and statistical evaluation. It is focused on quantification of spatial properties of many objects and their mutual spatial relations in a collection of many 3D images. It can be used for analysis of a collection of 2D images or time lapse series of 2D or 3D images as well. It has a modular design and is extensible via plug-ins. It is a stand-alone, easy to install application written in C++ language. The GUI is written using cross-platform wxWidgets library.



Assoc. Prof. Irena Koutná, Ph.D.

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Biography

University studies and diplomas obtained

1997 (MSc.) Department of Biochemistry, Faculty of Sciences, Masaryk University
2001 (RNDr.) Department of Biology, Faculty of Biology, JČU České Budějovice
2001 (Ph.D.) Department of Molecular Biology and Genetics, Faculty of Sciences MU
2014 Associate Professor of Molecular Biology and Genetics, Faculty of Sciences MU

Employment

1995 - 1997 – Masaryk Memorial Cancer Institute, Brno
1997 - 1998 – Lachema, a.s., Brno,
1999 - now – Science-research, group leader, CBIA, Faculty of Informatics, Masaryk University Brno
2011 - now – Junior Researcher, FNUUSA – ICRC-ICCT

Research scope

Pluripotent stem cells, hematopoietic stem cell, embryonic stem cell, iPS, hematopoiesis, driven differentiation, molecular cytogenetics, genomics of population, topology of genes and chromosomes in human cell, epigenetics, microarrays technology, flow cytometry.

International cooperation

Laboratory of Dr. Kaufman, associate professor of medicine in the Division of Hematology, Oncology, and Transplantation and associate director of the Stem Cell Institute at the University of Minnesota. Laboratory of Professor Majlinda Lako at the Institute of Genetic Medicine Newcastle University.

Research projects and grants (running)

Responsible member of research team of grants: Ministry of Education of the Czech Republic grant CZ.1.07/2.3.00/30.0030 and Grant Agency of the Czech Republic 302/12/G157



Panel: Molecular medicine

The ups and downs with studying ribosomal genes

Ann-Kristin Östlund Farrants

Department of Molecular Biosciences, Stockholm University

Ribosomal genes are heavily transcribed, and 80% of the RNA in eukaryotic cells is ribosomal RNA. Ribosomal RNAs are major parts of ribosomes and therefore involved in protein synthesis, something all cells need. The number of ribosomes is supposed to be higher in dividing and growing cells, and lower in cells that are resting. Since there is so much of the gene product it is hard to study and have been neglected for long. These genes are difficult to study also in high through put methods, since they are repetitive in nature and not aligned in the genomes. In my second project, studying the human response to malaria antigens, we are studying protein coding genes but also genes such as ribosomal genes. The two projects face different problems which I will address.



Prof. Ann-Kristin Östlund Farrants, Ph.D.

Professor

Stockholm University

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Biography

- BSc, Stockholm University – 1979
- Exchange student, DAAD-fellow in Universität Konstanz, Germany, 1981-1983, working on the mitochondrial outer membrane. Master Sc – 1984
- Technician at University of Leeds, UK, 1985, working on lipoprotein lipase
- Exchange student at Middlesex hospital Medical School, UK, 1986, working on glutathione transferases
- Technician at University in Oslo, Norway, 1987, working on a twin study to elucidate genetical variations in heart attacks
- PhD awarded, University in Oslo, Norway – 1992, Peroxisomes and bile acid synthesis
- Post-doc at Karolinska Institutet, Sweden, 1993-1997, working on chromatin remodeling and transcription
- Junior Lecturer, 1997 – 2003, establishing my own group on chromatin remodelling complexes in transcription
- Lecturer, 2003 – 2010, working on chromatin remodelling in transcription and RNA processing
- Professor, 2011 – date, working on chromatin remodelling, ribosomal transcription and RNA processing/ Genetic and epigenetic factors in the response to malaria.

Panel: Molecular medicine

Block of NMDA receptor channels by endogenous neurosteroids: implications for the agonist induced conformational states of the channel vestibule

Ladislav Vyklický

Institute of Physiology, Academy of Science of the Czech Republic

N-methyl-D-aspartate receptors (NMDAR) are glutamate-gated ion channels involved in excitatory synaptic transmission, synaptic plasticity and excitotoxicity. Their activity can be influenced by several allosteric modulators, including neurosteroids, which inhibit responses of NMDAR in a use-dependent (requiring receptor activation) but voltage-independent manner. However, attempts to identify the site of action for steroids with the inhibitory effect on NMDA receptors have so far failed. Our aim was therefore to elucidate the molecular mechanism of steroid action at NMDA receptors using electrophysiological and molecular biological techniques in combination with molecular modeling.

The results of our experiments show that two mutations (GluN1(T648A) and GluN1(A649T)) within the highly conserved M₃ SYTANLAAF motif considerably reduce the inhibitory effect of negatively charged steroids at NMDA receptors. In contrast, inhibition of mutated NMDA receptors by positively charged steroids is voltage-dependent. Moreover, GluN1(T648A)/GluN2B and GluN1(A649T)/GluN2B receptors showed to be spontaneously active and were insensitive to other inhibitors, suggesting that these mutations have greatly altered the receptor channel function.

These results indicate that the extracellular mouth of the NMDAR channel is the site of action for steroids with the inhibitory effect and further have implications for the arrangement of the channel in the open configuration. We have used this to propose a model of the open state of the NMDA receptor channel. Detailed understanding of the mechanism of action of neurosteroids on NMDA receptors has therapeutic importance for the development of drugs with neuroprotective properties.



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Biography

Ladislav Vyklický Jr. studied Medicine at Charles University in Prague. He gained postdoctoral experience as a Fogarty Visiting Fellow and Fogarty Visiting Scientist at the Laboratory of Developmental Neurobiology, National Institutes of Health, Bethesda, Maryland, USA (Mark L. Mayer) and as a Visiting Scientist in Max-Planck Institute for Cellular Physiology, Heidelberg, Germany (Professor Bert Sakmann). In 1995 he received prestige International Research Scholar of the Howard Hughes Medical Institute. He is currently Head of Department of Cellular Neurophysiology (Institute of Physiology ASCR), Member of the Scientific Board of the Central European Institute of Technology Masaryk University CEITEC MU, and Member of the Board for Ph.D. studies in the field of Neuroscience. The major goal of his research group is to comprehend the relationship between structure and function of ion channels, including those activated during synaptic transmission, to characterize the actions of pharmacologically active substances and to explain the molecular mechanism by which they influence ligand-gated ion channels using quantitative analytical techniques.



Panel: Biosensing and bioelectronics

Advanced in vitro diagnostics to organ-on-a-chip technology

Peter Ertl

AIT Austrian Institute of Technology GmbH

Microchip technology is vital for cell analysis because it is the only technology capable of simulating the physiological environment of cells and cell assemblies to investigate cellular transport mechanisms and cell proliferation events in the presence of specific reagent concentrations, temperature or shear force conditions. In light of the benefits of biochip technology and its potential future applications, my research group at AIT is developing lab-on-a-chip systems for various biomedical applications. My research is focused on the heterogeneous integration of micro- and nanosensors, miniaturized fluid handling systems and electronic components to establish higher level system architecture needed for advanced micro-Total Analysis Systems (μ TAS), organ-on-a-chip technologies and smart implants. In course of the seminar various lab-on-a-chip components for cell analysis and cell chip applications including multilevel cell analysis, tumour invasion studies and nanomedicine will be presented.



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Biography

Initially, Peter Ertl studied Food Sciences and Biotechnology at the University of Natural Resources and Life Sciences Vienna, Austria. In 1997 Dr. Ertl entered a Ph.D. program in Chemistry at the University of Waterloo (Ontario, Canada) focusing on biosensor and bioassay development for the rapid identification of microorganisms. Following the completion of his Ph.D. in 2001, he worked as a postdoctoral fellow at the University of California at Berkeley (CA, US) developing capillary electrophoresis chips (CE) for DNA analysis and fragment sizing. In 2003, he co-founded *RapidLabs Inc.* (Kitchener Ontario, Canada) a medical diagnostic device company in the field of antibiotic susceptibility testing where he worked as Director of Product Development until 2005. He then joined the Austrian Institute of Technology, Vienna Austria where his research investigates the dynamic adaptive cellular responses to systemic stress factors as well as cell-to-matrix and cell-to-cell interactions that perpetuate tissue healing and dysfunctions. He lectures various courses at the Technical University Vienna, University of Life Sciences Vienna and University of Applied Sciences. In 2011 he was appointed Adj. Assoc. Prof. (habilitation) in the field of Nanobiotechnology at the University of Life Sciences Vienna. In 2012 Dr. Ertl was awarded Fulbright Visiting Scholar at the Department of Chemistry of the University of California at Berkeley and in 2013 he was invited Visiting Scientist at the Nanyang Technological University, Center of Biomimetic Sensor Science, Singapore. Dr. Ertl currently heads the Cell Chip research group at the Biosensor Technologies unit with the focus on developing advanced *in vitro* and *in vivo* diagnostic systems.

Panel: Biosensing and bioelectronics

Organic Semiconductors for Bioelectronics: Organic and Printed Electronics Meets Biology

Martin Weiter

Materials Research Centre, Brno University of Technology, Czech Republic

Organic electronics is a platform technology based on the combination of new materials and cost-effective, large area production processes that open up new fields of application. The remarkable progress in the field of organic and molecular electronics brings new insights and possibilities for detection of biological processes by electronic means which should lead to effective, more sensitive, cheap and thus more competitive devices and sensors. Organic semiconductors show a number of key enabling features, such as electronic and ionic transport, easy functionalization as well as biocompatibility, biodegradability and conformability. Based on these materials a novel bioelectronic devices should be proposed. The lecture will focus on several examples of applications of organic materials and devices in bioelectronics. The operation principle and materials requirements will be discussed.



Prof. Martin Weiter, Ph.D.

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Biography

Specialization: organic electronics and photonics, printed electronics, advanced materials and biomaterials

Position: Head of Research Group, Materials Research Centre, Brno University of Technology Dean of Faculty of Chemistry, Brno University of Technology

Scientific work: In his scientific work he focuses on the preparation and characterization of organic semiconductor materials with properties suitable for electronic and optoelectronic applications, electron phenomena in organic semiconductors, optical and electrical properties of organic semiconductors (in particular transport and photogeneration of charge carriers) and applications of advanced organic and biological materials in optical, electronic and sensor devices.

Education: He received his Diploma in 1994 from the Brno University of Technology (BUT), Faculty of Electrotechnics (CZ) and his Ph.D. degree in Material Engineering at the same university. From 1998 he works at the BUT, Faculty of Chemistry, Institute of Physical and Applied Chemistry. In 2002 one year stay as postdoc at Phillips University Marburg, Germany. Since 2006 he is the Vice Dean for External Relations, since 2010 Head of Research Group at established Materials Research Centre BUT. In 2003 he received the Rector's award for excellence in teaching and scientific work.

Publication Activity: He is author and co-author of more than 60 original scientific papers of which 44 papers in international impacted journals, 14 papers in peer-reviewed journals with total 282 citations of published articles.

Other results: Principal investigator of many national and international (FP7, ESF, GACR, TACR, ...) projects targeted to the basic and applied research in materials science and nanotechnology.

Panel: Plant biology

Biological activity of naphthoquinone and its derivatives as promising cytotoxic compounds promoting cell death

Petr Babula

Department of Physiology, Masaryk University, Brno, Czech Republic

Nature products represent an alternative source of biologically active compounds, especially in the sphere of cancer chemotherapy. These new compounds frequently seem to be more potent and less toxic. Interest in naphthoquinones, a group of plant and fungal secondary metabolites, increased in connection with lapachol and β -lapachone, two naphthoquinone derivatives with interesting biological properties. Compared to lapachol, β -lapachone demonstrates strong cytotoxicity that was shown not only on many tumour cell lines, but also on *in vivo* models. As ARQ 501, β -lapachone was or is studied in ten phase I-II studies. The studies performed also show that naphthoquinones are able to modify effect of commonly used antineoplastic agents, and, in addition, are able to induce different types of non-apoptotic cell deaths. The lecture will be aimed at new challenges and possibilities of plant secondary metabolites in anticancer therapy.



Assoc. Prof. Petr Babula, Ph.D.

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Biography

Petr Babula studied Pharmacy at Veterinary and Pharmaceutical University in Brno. He completed his PhD in Pharmacognosy and became there an Associate Professor. Then he held a group leader position in a Laboratory of Explants Cultures and in 2009 became a Head of Section of Botany. Since 2014 he is as Head of Department of Physiology at Masaryk University in Brno. His research is primarily focused on pharmacological studies investigating secondary metabolites and their biological activity (naphthoquinones in particular), cardioprotective properties of plant secondary metabolites, and plant and plant cell stress physiology. Besides that he addresses the mechanisms by which heavy metal ions affect living organisms and is also particularly interested in fluorescence and confocal microscopy techniques.

Panel: Plant biology

Telomeres, DNA repair and genome stability: taking an engineer approach

Karel Říha

Plant Molecular Biology at CEITEC, Masaryk University, Brno, Czech Republic

Telomeres form termini of chromosomes, which are linear DNA molecules that store our genetic information. Chromosomes can break, and such damage is very efficiently recognized and repaired. Formally, ends of linear chromosome may resemble broken DNA and the primary function of telomeres is to protect natural chromosome ends from being treated as DNA damage. If telomeres fail doing so, chromosome ends become unstable and trigger strong cellular responses that contribute to tumor formation or organismal aging. I will talk about molecules involved in chromosome end protection and put a particular emphasis on a dual role of DNA repair proteins in this process.



Karel Říha, Ph.D.

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Biography

I graduated here at Masaryk University in 1998 in genetics. Then I went for a postdoctoral stay at the Department of Biochemistry at Texas A&M University where I used plants to study telomere structure and function. In 2003 I decided to join a newly founded Gregor Mendel Institute in Vienna, Austria, where I became a Junior Group leader in 2005. My research interests were mainly focused on telomeres, DNA repair and meiosis. Since 2014 I am a group leader at CEITEC.

Panel: Off-topic

Opening Doors to your Career with a Science PhD

Markus Dettenhofer, Ph.D.

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Biography

Markus Dettenhofer, Ph.D. has been the Executive Director of the Central European Institute of Technology (CEITEC) since 2012. Prior to joining CEITEC, Markus was Project Leader for viral vaccine and antibody discovery at Crucell (Johnson & Johnson), where he led teams to discover antibodies and vaccines against respiratory syncytial virus, which causes serious diseases of the airways in small children. He has additionally held management roles with several small and mid-sized biotechnology companies. In 2009, as a Lecturer in Genetics with Harvard Medical School, he led a study analysing the conditions for the successful development of a sustainable innovative biomedical economy in Panama. Markus was a Howard Hughes Post-Doctoral Fellow at Harvard Medical School, carrying out genetic research involving cellular, molecular and tissue experiments, including research into the gene *Formin 1* and its significance for bone development, and the gene *Formin 2* in memory function. He was a visiting scholar at the Institut de Biologie Moléculaire et Cellulaire in Strasbourg, France in 2000–2001. He received a Ph.D. from Johns Hopkins University, and a B.S. from UC Berkeley. Additionally, his work has been published in a range of scientific journals such as *Science*, *the Journal of Biological Chemistry*, and *Human Molecular Genetics*.



Panel: Off-topic

Individual funding opportunities for PhD students and Postdocs

Roman Badík

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Biography

Roman Badík has been the Grants Manager of the Central European Institute of Technology since 2011. Prior to joining CEITEC, Roman worked as a Project Manager in a consulting company dealing with the whole process of receiving and managing grants from EU Structural Funds. Roman managed to coordinate the preparation of projects with a total budget of 60 million EUR to be requested for funding from the Operational Programme R&D for Innovation. After joining CEITEC, Roman became responsible for coordinating the grants services throughout all CEITEC partners. After coordinating the preparation of projects worth 7 mil. EUR from the EU Structural Funds (all of them approved for funding), he started to deal with international grants, mainly FP7/Horizon 2020. He was coordinating the preparation of the FP7 ERA Chair proposal which was approved as the only project in the Czech Republic. He is also responsible for the support of researchers applying for ERC Grants and therefore created the ERC Support Scheme inspired by the experience of top European research organizations. With the help of this support scheme, CEITEC at Masaryk University received two ERC grants which was for the first time in the history of the university.





Life sciences

Students' abstracts





L01: Diffusion kurtosis imaging detecting changes in white and gray matter induced by alpha-synuclein accumulation in TNWT-61 mouse model of Parkinson's disease

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Introduction: One of Parkinson's disease (PD) big concern is finding a biomarker to diagnose the early stage. Diffusion kurtosis imaging (DKI) by measuring non-Gaussian diffusion may better characterize the microstructural brain changes as compared to diffusion tensor imaging (DTI). The aim of this study was to evaluate the capability of DKI for detecting the microstructural changes induced by alpha-synuclein accumulation in both gray matter (GM) and white matter (WM) in TNWT-61 mice using the tract based spatial statistics (TBSS) and region of interest (ROI) analyses.

Results: The principle findings of this study were increase in mean kurtosis and decrease in mean diffusivity in thalamus, sensorimotor cortex, hippocampus, external capsule and basolateral amygdaloid nucleus in 14 month TNWT-61 mice as compared to WT littermates. We also found significant correlations between alpha-synuclein accumulation and increase in kurtosis and decrease in diffusivity in the thalamus.

Methods: Fourteen month old alpha-synuclein overexpressing transgenic (TNWT-61) mice and wild-type (WT) littermates underwent DKI scanning using 9.4 Tesla system in vivo. TBSS analysis was used to compare kurtosis, diffusivity and fractional anisotropy maps in both GM and WM of TNWT-61 mice as compared to WT mice. In addition, ROI analysis for alpha-synuclein was performed for substantia nigra, striatum, hippocampus, sensorimotor cortex, and thalamus.

Conclusion: Our finding suggest the DKI should be preferred over DTI in PD patients due to that DKI reveal to show more sensitivity than DTI in detecting microstructural changes due to alpha-synuclein accumulation in both GM and WM in PD animal model.



Lo2: Cell nuclei localization and 3D reconstruction of plant cell cultures from confocal images

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Counting of single plant cells is used as a method to evaluate cell concentration in a plant cell suspension. Our goal was to create a 3D reconstruction of plant cell cultures from confocal images and automatize process of determination of cell nuclei localization. In our experiments a plant suspension cultures of *Chenopodium rubrum* has been used. The cell nuclei were stained by SYBR[®] Green fluorescent DNA binding marker. Experiments were performed on the confocal microscope Leica TCS SP8 X. A hundred slices with spatial resolution of 1024×1024 pixels were selected. The projection image is acquired by the first step where the maximal intensities are situated on areas where nuclei are located. Proposed segmentation steps allow reduction of noise and artefacts. Z-axis position is obtained as a location of peak maxima from mean intensity profile. Finally model of scene can be created by emplacement of spheres with adequate diameter to found 3D coordinates. The results were verified by manual counting.

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Lo3: Analysis of immunoglobulin gene rearrangements at the single cell level – proof of chronic lymphocytic leukemia oligoclonality

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Immunoglobulin (IG) receptor is a distinctive feature of B-cells and is crucial for their survival. Due to the stochastic rearrangements of IG loci (IGH, IGK and IGL) and their hypermutations, each B-cell bears a unique IG receptor structure. In chronic lymphocytic leukemia (CLL), leukemic clone originates from a single mature B-cell and therefore can be characterized by a specific IG gene rearrangement, common for all leukemic cells.

CLL is usually a monoclonal disease, however, in 2-5% of CLL cases, multiple productive IGH rearrangements (MP-IGH) are present. In 35% of MP-IGH cases, coexistence of at least two leukemic clones was revealed by flow cytometry, based on clonal IGK/IGL restriction [1]. In the remaining 65% of cases, it is difficult to clarify underlying biological cause of MP-IGH. To further investigate causal mechanisms of MP-IGH, we developed a technique for IG analysis in single cells.

Using this technique, transcribed IGH, IGK and IGL gene rearrangements from single sorted B-cells are co-amplified in nested multiplex PCR and sequenced, with 90% success rate on average. In 2 biclonal CLL controls and also in 6/6 analyzed MP-IGH CLL cases, we detected at least two separated IGH/IGK/IGL combinations recurrently, suggesting expansion of multiple B-cell clones. We assume that oligoclonality is the major cause of MP-IGH detection in CLL.

Acknowledgement: Work is supported from MUNI/A/1180/2014, IGA MZCR NT13493-4/2012 and MŠMT VaVPI CZ.1.05/1.1.00/02.0068.

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Lo4: Glyco-biosensing by surface plasmon resonance: Focus on lectin-based immunosensor for prostate cancer

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Conventional assays for clinical diagnostic are mostly based on sandwich strategy involving a monoclonal or a polyclonal antibody. However, such approaches have several disadvantages including the sensitivity, the reproducibility and the necessity of labeling. Furthermore, the biospecific interaction could not be observed in the real-time. Clinical diagnostics can be effectively addressed using immunosensor-based approaches. Such biosensor technology enable fast and efficient determination of various cancer biomarkers. Nowadays, surface plasmon resonance (SPR) is one of the most effective optical label-free biosensing techniques for both quantitative and qualitative parameters of the biosensing event. One of the frontiers in cancer research aims at glycosylation. Since altered glycosylation is a common feature of tumorigenesis, the objective of this study was to develop sandwich-based assay for glycoprofiling of the prostate cancer biomarker, free prostate specific antigen (fPSA). Thus paving way for the personalized medicine. Experiments with capture antibody (anti-PSA) specific against fPSA followed by glycoprofiling using glycan-binding protein (lectin) were performed. Future perspectives include improving the sensitivity using lectin-gold nanoparticle conjugates.

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Lo5: Haemoparasites of chelonians

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Chelonians have higher expected biodiversity of haemoprotozoa due to the more restricted habitats and lower mobility [1]. Most commonly identified haematozoa of chelonians are apicomplexans of the genera *Haemogregarina*, *Haemoproteus* and *Hemolivia*, often characterized by high intensity of infection. Extraerythrocytic trypanosomes are also often observed, nevertheless, generally in low numbers [2]. The prevalence and the intensity of infection in affected individual reveal the status and possible influence of parasites in the host population in natural conditions [3]. Haemoprotozoa are transmitted by vectors or through intermediate hosts, for that may be the cause of their significant decline. Confirmed definitive hosts and vectors of haemoprotozoa are leeches, ticks, and dipterans. Chelonian haemoparasites are mostly not strictly host-specific, their occurrence is bound to the vector.

Haemogregarina parasites have been reported worldwide in all families of freshwater turtles and terrestrial tortoises [4]. The life cycle includes erythrocytic gamogony and sporogony taking place intracellularly in leeches and erythrocytic and extra-erythrocytic merogony in the vertebrate host. Until recently, evolutionary relationships among *Haemogregarina* species have been studied using molecular-genetic methods based on partial 18S rDNA sequences. Species of *Haemoproteus* are characterized by the ability to produce haemozoin in the form of pigment granules [5]. *Hemolivia mauritanica* is the only known haemogregarine infecting tortoises *T. graeca* and *T. marginata* in western Palaearctic region. Low parasitaemias of trypanosomes is typical for naturally infected chelonian hosts. Although wild tortoises and turtles are commonly infected with haemoprotozoa, the effect is very rarely reported and pathogenicity is still poorly known.

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Lo6: ROS-Auxin interplay in regulation of photosynthesis under stress

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Environmental cues represent the major hardships to crop productivity worldwide. Plant cells integrate photosynthetic, developmental and environmental stress signals through the modulation of reactive oxygen species (ROS) and hormone network signals. Particularly, ROS and auxin pathways are the main players that impact on plant stress adaptation responses [1]. Owing to the vital importance of photosynthetic processes for plant growth and survival, a complex signaling network operates to control photosynthesis in response to biotic and abiotic stress which directly affects ROS and auxin homeostasis. Notwithstanding the large number of evidence showing interplay between ROS and auxin on photosynthesis, molecular insight into the nature of ROS-auxin crosstalk remains scarce. Therefore future studies are necessary to shed light on crosstalk between chloroplast and auxin network. Previously, it was demonstrated that the expression of a cyanobacterial flavodoxin (Fld) in chloroplasts prevents ROS accumulation under a wide range of environmental challenges, protecting thus photosynthesis from photo-inhibition [2]. Therefore, Arabidopsis transgenic plants (*pfld*) can be used as an innovative tool to dissect the auxin-plastid ROS crosstalk regulatory network involved in photosynthesis regulation under stress by genetic screen.

As photosynthesis is one of the most relevant traits in plant breeding programs, the identification of genes involved in stress-induced photosynthesis regulation will bring novel approaches to optimize crop performance in changing environmental field conditions.

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Lo7: Elemental analysis, FTIR and ^{13}C NMR of humic substances isolated from forest soil

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The aim of this work was study chemical composition, chemical properties and humification degree of different soil humic substances (HS). The object of our study were three various samples of HS. HAs and FA were isolated from forest soil Humic Podzol (locality Krkonoše, Czech Republic). Isolation of soil HS was performed according to the procedure recommended by the International Humic Substances Society (IHSS). The humic and fulvic acids were characterized and compared using chemical methods and spectroscopic techniques, including Fourier transform infrared (FTIR) and liquid-state ^{13}C nuclear magnetic resonance (^{13}C NMR). Infrared spectroscopy is a useful technique in characterization of structure, functional groups and formation modes of HS. ^{13}C NMR spectra of soil HS were obtained with a Bruker Avance III NMR spectrometer at an observation frequency of 125.8 MHz for ^{13}C . The approximate number of scans was 25.000. For data analysis, the spectra were divided into chemical shift regions assigned to the following classes of chemical groups: alkyl C (0–45 ppm), O-alkyl C (45–106 ppm), aromatic C (106–165 ppm), and carbonyl and carboxyl C (165–220 ppm), respectively. Aromaticity (f_a), hydrophilicity and hydrophobicity ratio (Hfi/Hfo) and biological activity (BiA) of HS were calculated from the area of the NMR spectra.



Lo8: ATM mutations are stable during the course of chronic lymphocytic leukemia

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Mutations in *ATM* gene are associated with inferior prognosis in CLL patients. We noted very good response of *ATM* mutated CLL samples to anti-CD20 antibodies rituximab and ofatumumab in our recent study [1]. Therefore, we analyzed “*in vivo* destiny” of *ATM* mutations during the course of CLL. We selected 25 patients covering the whole spectrum of *ATM* defects involving mutations: missense and other types of mutations, with and without 11q-. In these patients, the presence of particular mutations was analyzed in subsequent time point during the disease course. Nineteen cases were monitored in a relapse (median follow-up 42 months; therapy involved anti-CD20 antibodies in 15 cases), while there was no therapeutic intervention in period between samplings in six patients (median follow-up 18 months). Among the new samples, we detected *ATM* mutations in 24/25 patients. In the remaining patient (treated with ofatumumab and chemotherapy) we observed loss of a partially selected (original proportion about 15%) missense mutation. In other two patients we noted disappearance of 1 out of 2 mutations, in one case after rituximab with chemotherapy and in one case spontaneously. We also confirmed the stability of *ATM* mutations in other two patients analyzed retrospectively at diagnosis (median between samplings 55 months); the same mutations were again present at both analyzed time points. Altogether, our results clearly document that *ATM* mutations are stable during the course of CLL. Their elimination by therapy is rare, despite using most potent regimens involving monoclonal antibodies.

Acknowledgement: Supported by MUNI/A/1180/2014.

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Log: Decreasing doxorubicin-induced oxidative stress using nanocarriers

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Doxorubicin is an anthracycline antibiotic that belongs to one of the most widely prescribed anticancer drugs [1]. However, its administration is accompanied by several serious side effects. The most crucial one is associated cardiotoxicity. The major hypothesis regarding the pathophysiology of doxorubicin-induced cardiac damage is related to mechanism of oxidative stress as the outcome of altered function of antioxidant system resulting in generation of reactive oxygen species [2, 3]. Liposomal and apoferritin nanocarriers investigated within this study hold a great potential to enhance specificity and bioavailability of treatment, and therefore to reduce side effects of therapy. This study revealed significant decrease in gene expression of *ALHD3A1* and *TXNRD2* in liver as a main detoxification organ, and influence on the expression of these enzymes in left heart ventricle as a potential target of toxicity.

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L10: Phospholipids from *Coxiella burnetii* analyzed by Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry

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Coxiella burnetii is ethiological agent of Q fever which is endemic throughout the world. Phospholipids from *C. burnetii* strain Nine Mile virulent phase I (NM I) and low-virulent phase II (NM II) cell were analyzed by Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry. FT-ICR mass spectrometry has provided very high mass accuracy that permits a detailed and comprehensive characterization of ions. Phospholipids from the phase I *C. burnetii* cells were much more complex than those from the phase II cells. Moreover, in the latter, the absence of phospholipids of the phosphatidylinositol class could be noticed. Phospholipids as glycerophosphoethanolamines, glycerophosphocholines and glycerophosphoglycerols are presented in both forms (NM I and NM II). The difference is in the presence of glycerophosphates and glycerophosphoserines. In NM I were detected glycerophosphates but not the glycerophosphoserines. However, NM II phospholipids contain glycerophosphoserines but not the glycerophosphates. This study showed that complex phospholipids mixtures extracted from *C. burnetii* cell extracts analyzed by FT-ICR mass spectrometry. These are important findings since it has been believed so far that a lipopolisaccharide is the only outer membrane component that undergoes modifications during the phase variation of the microorganism. Modifications of the outer membrane macromolecules enable the bacterium to be a more versatile, more heterogeneous microorganism that can cope better with a variety of different environments.

L11: Partial atomic charges for chemoinformatics applications

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Partial atomic charges describe a distribution of electron density in a molecule and therefore provide clues regarding the chemical behavior of molecules. In chemoinformatics, they started to be used recently [1] and especially their fast and accurate calculation via Electronegativity Equalization Method (EEM) [2,3] seems very promisingly. Unfortunately, this method can be currently used only for small fraction of drug-like molecules – main objects of chemoinformatics research.

In our work, we accepted this challenge and prepared EEM parameters, which cover most of the drug-like molecules and yield very accurate partial atomic charges. In parallel, these parameters are applicable for at least 95% of molecules in key drug databases (Drugbank, ChEMBL, Pubchem and ZINC). Additionally, we provide a software solution for easy computation of EEM charges, which allows a direct application of this method in chemoinformatics.

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L12: Telomere methylation analyses in *Nicotiana tabacum*

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Telomeres are nucleoprotein complex structures at the end of chromosomes and are composed of microsatellite DNA formed by short repeated unit varying in dependence of organism. Plants such as *Arabidopsis thaliana* or *Nicotiana tabacum* have telomeres formed by tandem repeats (TTTAGGG)_n. The presence of methylcytosines in telomeric DNA was first described in *Arabidopsis thaliana* by Cokus et al. (2008) [1]: There is a preference of methylation of the inner Cytosine (CCCMTAAA) with a frequency of about 10%. Methylation of tobacco telomeres was already observed by Majerova et al. (2011) [2]. The importance of these epigenetic marks remains poorly understood and *Nicotiana tabacum* is a very useful and common model for analysis of epigenetic properties of plant telomeric chromatin. Here, the presence of methylcytosines in bisulfite-treated isolated telomeric DNA from tobacco was detected with extension of a set of primers corresponding to repetitive methylation patterns. First results have shown that telomeric DNA of tobacco is mainly non-methylated, but the methylation occurs following repetitive patterns, with a clear preference for methylation of the inner cytosines (CCCMTAAA)_n. Currently, electrochemistry by square wave voltammetry with pyrolytic graphite electrode is performed to detect the A:G ratio in bisulfite-treated isolated telomeric DNA in order to quantify the methylcytosine level in tobacco and to contribute to the understanding of the role of these epigenetic marks in plant telomeres.

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L13: Optimization of asymmetric PCR-SSCP for single-copy nuclear markers in Brassicaceae species with different ploidy levels

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The potential of single-copy nuclear genes to uncover evolutionary relationships increases their application in phylogenetic studies. In comparison to ribosomal and chloroplast gene markers, single-copy gene markers are informative in tracking the relationships in plant lineages with a high incidence of hybridization and subsequent allopolyploidization. Here we present a unique approach to elucidate phylogenetic relationships and putative parental genomes in ancient allopolyploid lineages in the family Brassicaceae. We detected allelic variants of selected single-copy nuclear genes by asymmetric PCR-SSCP (Polymerase Chain Reaction Single-Strand Conformation Polymorphism) in Brassicaceae species with different ploidy levels. Described protocols are applicable in phylogenetic studies of allopolyploids and autopolyploids in the Brassicaceae as well as in other plant groups. Optimized conditions of asymmetric PCR-SSCP will potentially contribute to a broader application of the method on phylogenetic analyses based on single-copy gene markers.

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L14: What determines chromosome breakpoints in crucifer species?

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The ancestral genomes of crucifer species (Brassicaceae) have been altered by chromosome rearrangements, such as inversions, duplications/deletions, transpositions, chromosome fissions and “fusions”. The incidence of these rearrangements is associated with chromosome breakage and breakpoints. The extensive inter-species chromosome collinearity across the mustard family and a number of sequenced genomes allow us to compare underlying sequences at chromosome breakpoints. In this multi-species comparison, we compared the arrangement of genomic blocks and chromosome breakpoint sequences among the sequenced genomes of *Arabidopsis lyrata* (n = 8), *A. thaliana* (n = 5), *Brassica rapa* (n = 10), *Camelina sativa* (n = 20) and *Schrenkiella parvula* (n = 7). Using various bioinformatics approaches, we aimed to identify and characterize chromosome breakpoints, to compare the individual breakpoints with the rest of genome landscapes, and to analyze whether specific sequence motifs or features are associated with chromosome breakpoints.

Our analyses suggest that most of chromosome breakpoint regions in the analyzed Brassicaceae species exhibit a lower GC content (Mann-Whitney U test, $p < 0.05$) and an enrichment in tandem repeats and LINE elements (Mann-Whitney U test, $p < 0.05$), compared to genomic regions outside chromosome rearrangements. These results suggest that repeat-rich chromosome regions are potentially prone to become breakpoints of larger-scale rearrangements shuffling genomes of crucifer species.

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L15: NMR relaxation studies of receiver domain of cytokinin receptor CKI_{1RD} mutants from *Arabidopsis thaliana*

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In our project, we studied the signaling pathway, called multistep phosphorelay signaling system in the plant *Arabidopsis thaliana*. The multistep phosphorelay signaling pathway has a great influence on many aspects of growth and development of plants. This signaling system is based on phosphate transfer between the cytoplasmic membrane and nucleus. In the plant *Arabidopsis thaliana*, histidine kinase is phosphorylated upon signal recognition, and forwards the phosphate group through histidine phosphotransfer proteins to a response regulator protein located in nucleus, where the response take place. The input signal can be light, osmotic changes or hormones.

Aspartic acid 137 present in active centre of CKI_{1RD} plays an important role in the signaling pathway. This Asp 137 residue binds phosphate and transfers it to next protein involved in the signaling pathway. Two CKI_{1RD} proteins with mutations in their active sites (CKI_{1RD} -D137A and CKI_{1RD} - D137E) were studied by NMR relaxation experiments. The proteins were expressed in *E.coli* and labeled by stable isotope ¹⁵N.

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L16: Determination of the reference genes in *Streptococcus equi subsp. zooepidemicus* for real-time PCR

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Real-time polymerase chain reaction (qPCR) has become a powerful technique for gene expression monitoring. *Streptococcus equi subsp. zooepidemicus* (SEZ) is the pathogen most commonly isolated from horses. It is known as hyaluronic acid (HA) producer [1]. The whole genome expression analysis of *Streptococcus equi subsp. zooepidemicus* strain ATCC 35246 was performed using DNA microarrays. According to the stability of gene expression 10 genes including *gyrA* and *gyrB* were chosen as potential reference genes. Further analysis of expression stability of selected genes was done by real-time PCR [2]. C_t values from PCR analysis were processed in Microsoft Excel; our conclusions were additionally confirmed by GeNorm normalization [3]. Three biological replicates in two technical replicates were analyzed in total. Three reference genes were determined: SeseC_02327 (*mscS*, NCBI gene ID 14004807), SeseC_00767 (NCBI gene ID 14003568), SeseC_01348 (*gyrA*, NCBI gene ID 14004035). We have chosen *gyrA* gene as reference for our qPCR experiments with SEZ strain ATCC 35246.

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L17: Electrochemical detection of miR-34a-5p as a promising tool for HNC and PCa diagnosis

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MicroRNAs (miRNAs) are a class of non-coding RNAs that are intensively studied as biomarkers of various diseases. In this study, the attention was aimed at the research of miR-34a-5p related to head and neck cancer (HNC) and prostate cancer (PCa). MiR-34a-5p belongs to the miR-34 family and is directly linked to p53 and Wnt pathways. Beside the classical molecular biology techniques of miRNAs study (PCR, Northern Blotting, microarrays technologies), new biophysical approaches were applied. The results from the PCR analysis were complemented with UV absorption spectra, CD spectra and linear sweep voltammetry in connection with adsorptive transfer stripping (AdTS) technique indicating significant differences in miR-34a-5p expression status.

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L18: Production of bioethanol from waste bread

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Increasing prices of traditional raw material for ethanol production is reason to search new materials for ethanol production. Food waste seems to be one of the inexpensive suitable fermentation feed used in distilleries. Mainly bakery waste offers good composition for fermentation. It follows that waste bread is suitable for ethanol production. [1]

We used for the experiment waste bread from household. It was pretreated by grinding. 100 mL of 15% (w/v) bread and water suspension was prepared for experiment. pH of solution was adjusted to 5.5. Then α -amylase was added to bread suspension and flasks were placed into tempered shaker. After 2 hours of exposure α -amylase was added to the flask glucoamylase. After addition, the suspension was hydrolyzed for 1.5 hours. Hydrolysis took place under 65°C with shaking (130 min⁻¹).

Hydrolysates were inoculated with *Saccharomyces cerevisiae*. After inoculation, flasks were placed into a thermostat heated to 30°C. Fermentation took place for 66 hours. The experiment was taken at two different values of pH - with adjustment to 5.0 and without adjustment. Yields of glucose and ethanol were analysed by HPLC with RI detector.

Concentration of glucose before fermentation was 84.45 g·L⁻¹. We obtained 31.46 g·L⁻¹ of ethanol in hydrolysate without pH adjustment. In hydrolysate with adjusted pH we obtained 30.84 g·L⁻¹ of ethanol. It was found that highest yield of ethanol was obtain at hydrolysates without pH adjustment.

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L19: Study of glycan-protein interactions with glycan biosensors

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Glycans have important role in many of intra- and extracellular processes. Glycan biosensors can be used for the study of glycan-protein interactions. Gold is the most widespread surface for biosensor fabrication due to the ability for strong binding with thiols. Thiols are used for the formation of self-assembled monolayer (SAM), which is the most important step in biosensor preparation. With SAM immobilization of glycans can be controlled together with ligand density and surface inertness. Glycans are immobilized onto surface through functional groups such COOH, OH, azide etc.. Biosensors have beneficial properties such as their ability to study interactions with label-free detection methods in a sensitive way. Electrochemical impedance spectroscopy (EIS) is one of the most sensitive detection method measuring changes in surface resistance. Glycan with terminal sialic acid was immobilized onto gold surface which was previously modified with a mixture of 11-mercaptoundecanoic acid and 6-mercapto-1-hexanol. This glycan biosensor was used to detect lectins and viral hemagglutinins down to aM (10^{-18} M) level. EIS, atomic force microscopy (AFM) and surface plasmon resonance (SPR) were used to study interactions between the biosensor and two lectins and two hemagglutinins isolated from avian and human influenza viruses.

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L2o: chromDraw: an R package for visualization of linear and circular karyotypes

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Species-specific sets of chromosomes - karyotypes - are traditionally depicted as linear ideograms comprising individual chromosomes represented by vertical bars. However, linear visualization has its limitations when two or more karyotypes have to be shown and compared. In these instances, circular visualization might provide easier comprehension and interpretation of inter-species chromosome collinearity and homologous rearrangements, which are described by conserved genomic blocks. The package chromDraw is designed to visualize linear and circular karyotypes in the same graphic design without a need to use to different tools for each type of chromosome visualization.

The program is freely distributed under GNU General Public License (GPL) and can be installed from Bioconductor or the web page www.plantcytogenomics.org. The source code of the tool and its online version are available from the same web site.

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L21: Reaction mechanism of ppGalNAcT2: QM/MM Metadynamics and String Method

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Polypeptide UDP-GalNAc transferase (ppGalNAcT2) is a metal dependent retaining glycosyltransferase of GT-A fold that catalyzes the first step in mucin type O-glycosylation. It transfers GalNAc moiety from UDP-GalNAc to the hydroxyl group of either threonine or serine residue on the target protein. We use hybrid QM/MM Car-Parrinello molecular dynamics simulations in order to study the reaction mechanism. In this approach the key region where the enzymatic reaction is occurring is treated at a DFT level of theory, while the rest of the system is described by computationally less demanding force field. The free energy surface of the reaction is roughly explored by metadynamics methodology and the minimum free energy path between reactants and products is optimized using string method. Combining these two methods we obtain relatively rough overview of the free energy landscape and an accurate estimation of the free energy barrier for the glycosyltransferase reaction.



L22: Focal adhesion kinase regulation and expression in malignant B cells

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Microenvironmental interactions in lymph nodes and bone marrow are crucial for biology and aggressiveness of B-cell chronic lymphocytic leukaemia (CLL). In particular, the cell adhesion and integrin-associated kinase FAK could be potentially important for therapy resistance. We examined FAK expression in CLL B cells sorted according to the surface expression of CXCR4/CD5. The CXCR4^{dim}/CD5^{bright} cells have recently exited the lymph nodes to circulate in peripheral blood, and we observed that they have lower FAK levels than CXCR4^{bright}/CD5^{dim} cells that have been circulating in blood for a long time (fold change 1.5; P<0.05). This suggests that microenvironmental interactions down-modulate FAK. Notably, CLL patients at lower disease stage (RAI 0-II; n=34) had significantly higher FAK expression than patients at higher stage (RAI III-IV; n=27; P<0.05). The patients with relatively lower expression of FAK also tend to have shorter overall survival in comparison to cases with high-level FAK (n=63, median survival 9 vs. 14.5 years; P=0.09). Other clinical-biological characteristics (p53, IGHV, cytogenetics) did not significantly correlate with FAK expression. In conclusion, FAK levels are regulated by microenvironmental interactions thus affecting CLL prognosis. We are currently testing approaches that block such interactions with integrin signalling inhibitors to target this therapeutically.

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L23: Blood - cerebrospinal fluid barrier in rat after peripheral nerve injury

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The unilateral chronic constriction injury (CCI) used as a neuropathic pain model causes the elevation of proinflammatory cytokines levels not only in the dorsal root ganglia (DRG) related to damaged nerve, but also in remote DRG and central nervous system structures. We purpose that one of the possible pathways for spread of neuroinflammation could be over the blood-cerebrospinal fluid barrier present in choroid plexus (CP). We used the intravenous injection of fluorescent conjugated dextrane (FluoroEmerald - FE) to clarify our hypothesis.

Twelve Wistar male rats were divided to the 3 days (n=5) and 21 days (n=5) of CCI groups, two rats were naive. The FE was intravenously applied at time of CCI survival and rats were sacrificed after 18 hours of FE circulation, perfused transcardially by Zamboni's fixative. Distribution of FE and simultaneous immunohistochemical detection for resident (ED2) and activated (ED1) macrophages, antigen presenting cells (APC; MHC-II) and microglia (OX-42) was studied in CP using coronal cryostat sections through the brain.

FluoroEmerald particles were presented in cuboidal epithelial cells of CP. The activated macrophages, microglia and APC positive for FE were found in CP stroma. Epilexal Kolmer cells immunostained for ED2 and MHC-II were loaded by FE. In addition, FE particles were also found in ventricular ependymal cells (EC). Our results suggest that composite effect of CCI and FE causes immune reaction in CP followed by diffusion of FE particles into EC.

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L24: Self-assembly of amphiphilic peptides

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Proteins can self-assemble into a wide variety of quaternary structures, both compact and extended. Size and shape of these aggregates are determined by geometry of interacting proteins and by positions and type of their interaction sites. However, a priori prediction of the self-assembled structure of proteins remains challenging due to the complex nature of proteins. The complexity could be reduced by focus on specific class of proteins and their general features. We investigated aggregation of amphiphilic alpha-helical proteins at various conditions using recently developed coarse-grained model of amphiphilic rod-like particles [1] with one or two attractive (hydrophobic) stripes. We have observed formation of finite clusters of different sizes up to heptamers depending on the size of the hydrophobic stripe or the angle between stripes. Proteins with one hydrophobic stripe formed clusters with hydrophobic core reflecting generic coiled-coils [2], while proteins with two hydrophobic stripes formed clusters with hydrophilic tunnel. Highest yield conditions for different clusters can be calculated using our relative cluster populations. These results provide a generic insight into the relation between the features of amphiphilic alpha-helical proteins and morphology of their aggregates.

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L25: Gelatin templated gold nanostructured electrodes for sensitive glucose detection

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Due to the importance of glucose in physiological processes, sensitive, rapid and reliable methods for its detection are required. The biocatalytic sensors provide low limits of detection but the enzymatic layer is volatile. Sensors that are not based on enzymes are very stable in all conditions, however worse detection limits are typically obtained. One of the ways to achieve an improved sensitivity of the detection is by developing of a sensor with optimized surface morphology. In this work gelatin templated gold nanostructures were fabricated in order to improve the sensitivity of glucose detection. The 3D cavities were made by crosslinking of gelatine layer on the gold surface and nanostructured surface was formed in these cavities by electrodeposition of gold from the electroplating solution. Gel layers on the electrodes were cleaned by KOH and chromic acid. Scanning electron microscopy and atomic force microscopy were used for characterisation of the created surfaces. The glucose was detected by a direct electrochemical oxidation during cyclic voltammetry in alkaline solution. Limit of detection of 10 μM was achieved in water samples. For the detection of glucose in serum, the samples were first deproteinized in acetone, centrifugated and the pH was adjusted by KOH. The sensor was able to detect 1.3 mM glucose in diluted deproteinised human serum samples with negligible effect of interferents present in human blood serum. The results were verified using commercial glucometer ACCU-CHEK Active[®] and the standard kit for photometrical detection of glucose BioLaTest GLU L 500 S.



L26: The affectation of endothelial occludin expression by carotenoids per inflammation

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Tight junctions (TJs) regulate endothelial paracellular transport of substances from blood into subintimal space. Occludin, one of TJ proteins, regulate their function. Changes in its expression contributes to increased TJ permeability and endothelial barrier function. Bacterial inflammation is a risk factor for atherosclerosis. Carotenoids of yeast biomass are natural substances which can protect the endothelial function and to reduce of atherosclerosis. The aim of our pilot study was to investigate antioxidant effects of carotenoids on expression of occludin in endothelium of aorta of endotoxemic Wistar rats. The inflammation was induced by a single dose of bacterial lipopolysaccharide (LPS) (1 mg/kg i.p.). Subsequently, rats were fed with a yeast biomass containing carotenoids (10 mg/kg/day) for 10 days. LPS slightly decreased occludin expression and its location in endothelium comparing with the controls. It was associated with worse endothelium-dependent relaxation of the aorta, increased activity of NOS in aorta. LPS increased levels of TNF- α , MDA and NAGA activity in plasma. Carotenoids increased occludin expression in LPS rats, decreased levels of inflammatory markers and improved aortic relaxation. Our results suggest that short-term supplementation of natural carotenoids of yeast biomass had antioxidant and anti-inflammatory effects which may positively affect barrier function of vascular endothelium.

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L27: Deciphering splicing regulators in the *SERPING1* exon 3

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C1 inhibitor (C1INH) is a serpin-type protease inhibitor playing an important role in human plasma. Its major function is the inhibition of the complement system to prevent its spontaneous activation. Mutations in the gene encoding C1INH, *SERPING1*, can lead to hereditary angioedema (HAE) which is rare but potentially life-threatening disease.

As diagnostics is often based on the changes in amino acid sequence the importance of pre-mRNA splicing and its regulation was underestimated for a long time. However, there is an increasing evidence of connection between splicing aberration and human diseases. Cell-specific alternative splicing of exon 3 of the *SERPING1* gene showing interesting variations between different groups of HAE patients has been described (Cruz *et al.*, 2012). Our hypothesis is that exon 3 (as alternative exon and extraordinary long exon) might be regulated by higher number of regulatory elements that make it more prone to splicing aberrations caused by its mutations. In accordance with this hypothesis our results revealed altered splicing in two HAE patients with mutations in exon 3 of the *SERPING1* (outside the exon-intron boundaries). For the purpose of thorough analysis of splicing regulators, set of deleted minigenes composed of exon 3 *SERPING1*+pET01 vector was prepared. By means of these deletion experiments and further minigene analyses the most important splicing regulatory elements in exon 3 should be determined.

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L28: Prepare your dog – canine babesiosis at the door!

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Canine babesiosis has been considered as an emerging infectious disease in multiple European countries during last decades [1]. The most frequent causative agent in Central Europe is *B. canis* predominantly transmitted by *D. reticulatus* ticks. Clinical signs of the disease are connected with intravascular and extravascular haemolysis, developing within 10-21 days after a tick bite, and can range from a subclinical form to acute renal failure and death [2]. Autochthonous canine babesiosis has never been described in the Czech Republic compared to neighbouring Slovakia where clinical cases are frequently reported. This phenomenon poses opportunity for studying the environmental factors influencing further pathogen spreading. A wide-ranging task required a complex approach comprising the study of vector, pathogen and host. Between April 2009 and November 2011 we have collected 14 355 ticks at 270 localities situated in selected parts of Moravia and Slovakia and clinical samples from 235 dogs. A considerable number of samples and field data enabled us: (i) to characterize ecological niche, exact distribution limits and abundances of *D. reticulatus* in the studied area; (ii) to define the geographic distribution of natural foci of canine babesiosis and to assess the risk level of *B. canis* infection in different parts of studied regions; (iii) and to compare the reliability of different diagnostic approaches to canine babesiosis detection.

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L29: Characterization of plant cuticles for a study of foliar fertilizers

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Nowadays, foliar uptakes belong to the most widespread fertilizers application over the world. The surface of plant is formed by thin layers, which are called cuticles. This layer is limiting barrier for sprayed solution on the leaves surface. The characterization of plant cuticles is very important for understanding their function in case of penetration the substances into the structure of plant (the penetration of humic acids and the influence of modification in our research). First part of our research is focused on morphology of these barriers. We use fluorescence lifetime imaging microscopy (FLIM) and determination of fluorescence lifetime of groups. Further method, we use optical and fluorescence microscopy for study the change of structure and effect of applied substances. Other important parameter is thickness of layer, which is usually determined by profilometry measurements.

Next part of research is focused on simple diffusion techniques, which were enabled to simulate of foliar uptake in the nature. Moreover presented diffusion techniques can be used for the determination of fundamental diffusion parameters (e.g. effective diffusion coefficient) through thin plant cuticles.

Our work focused on the problem with nutrients overloading in soil and degradation not only soil, but ground water too.



L30: Chronobiology of acute cardiovascular events

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Incidence of acute cardiovascular diseases shows chronobiological variations, although little is known about its influence on further prognosis and mortality [1]. Circadian rhythms are genetically determined and variations at the molecular level can modulate the response to external/internal stimuli affecting thus phenotype of the disease [2,3]. In our research, we investigated the circadian pattern of time of onset in acute myocardial infarction and acute heart failure and its influence on clinical parameters. Further, we analyzed effect of chronotype (determined by functional polymorphism VNTR in *Period3* gene) on basic characteristics of myocardial infarction [4]. In both studied groups we described significant 24h rhythmicity in time-of-onset, especially in men. The most significant rhythm in acute heart failure was observed in the subgroup of younger patients < 70 years and in patients with low oxygen saturation < 85% at the time of onset. Analyses for relation of AHF onset with 30-day mortality revealed a significant pattern with an increase in mortality in patients with AHF onset during the daytime (7 am - 7 pm). By analyzing genetically determined chronotype in acute myocardial infarction, we revealed that homozygosity for longer variant *Period3*^{5/5} shows reduction in circadian activity. This variant *Per3*^{5/5}, which represent extreme morning chronotype, was further associated with higher levels of interleukin-6 (IL-6), B-type natriuretic peptide (BNP) and lower vitamin A levels. Our results indicate that time of onset of acute heart failure and myocardial infarction and diurnal preference is associated with differences in clinical parameters and severity of disease.

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L31: Comparison of capillary electrophoresis and isothermal titration calorimetry for determination of the binding constant

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The binding constant is commonly used to describe the strength of binding between ligands (drugs) and protein. The strength of the interaction has a significant effect on the biological activity of the drug, and knowledge of the nature and extent of drug-protein binding can help us to understand the pharmacokinetics and pharmacodynamics of a drug [1].

Both the capillary electrophoresis (CE) and the isothermal titration calorimetry (ITC) measure the affinity of binding partners in their native states without immobilization or labelling of the interacting partners. What is more the investigated interactions takes place in a solution, which can simulated physiological conditions. Whereas ITC has a problem with large sample consumption and estimation of weak affinity interactions [2], the advantage of CE is very low sample consumption and a high resolution and also it does not require the highly purified samples.

The main objective of this study was to compare both these methodological approaches for the study of drug-protein interaction. The couple of diclofenac and HSA was chosen as a model system.

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L32: Fluorescence study of systems with native hyaluronan and hydrophobic solutes treated by drying method

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Biopolymer hyaluronan is qualified as essential for vertebrates. Therefore it is widely used in medical industry. It perfectly fulfils the requirements of carrier systems in drug delivery medicine. Native unmodified hyaluronan has hydrophilic character and strong hygroscopic behavior. Due to these facts it organizes molecules of water along his chain. Hyaluronan chain contains also "hydrophobic patches" but they are inaccessible because of the configuration and water package. Majority of utilized or potential cytostatic drugs have hydrophobic character and hence they does not interact with the hyaluronan without any support.

In this work we used drying method to remove water package from the hyaluronan chain. This step opens up the binding sites on the chain which are ordinarily protected. As model of hydrophobic substances fluorescence probes were used. Efficiency of creation of the interaction was studied by fluorescence spectroscopy – steady state and time-resolved. As probe with specific properties, which provides information about polarity of microenvironment, the pyrene was chosen.

Both fluorescence methods yielded results of which the method appears to be successful. Data obtained from these measurements showed, that pyrene in the solution of hyaluronan was transferred from polar environment to nonpolar after application of our drying method.

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L33: Regulation of microRNA expression based on their common factors and properties

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MicroRNAs (miRNAs) are lately very popular class small non-coding RNAs. They are known to regulate a large portion of protein coding genes and are involved in both physiological and pathological processes. This regulation is mostly based on complementarity pairing between miRNA and mRNA 3' UTR through a so-called seed sequence (nucleotides 2-8 in a miRNA mature sequence). Life of miRNA starts in a form of long primary transcript which is cut into a shorter precursor sequence (pre-miRNA), exported from a nucleus, cleaved and further processed into a final form - mature miRNA. Interesting is, that the level of pri-miRNA is not equal to the level of mature miRNA [1-2]. As much as we know about the influence of miRNAs on a gene expression, we know very little about regulation of microRNAs expression itself.

In this work we explored how the miRNA expression can be regulated. The latest miRNA database (miRBase v. 21 [3]) contains 1,881 human pre-miRNAs and it is very unlikely each of these miRNAs have separate mechanism that regulates the expression. Therefore, we focused on miRNAs which show similar expression patterns and explored their common properties. The preliminary bioinformatics analysis showed interesting results pointing out the evolution conservation of miRNAs as well as features that most likely influence the regulation of miRNAs expression. This includes basic properties of miRNAs, such as stability, as well as a possibility of miRNA-protein cooperation or binding. Although the results seem promising they have to be confirmed in a wet lab.

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L34: Novel method for conformational sampling of biomacromolecules using molecular dynamics simulations

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Many biological phenomena like allosteric regulation, protein folding or unfolding, enzyme catalysis, substrate recognition and binding, etc. strongly rely upon conformational transitions [1,2]. Thus, when modeling such phenomena it is essential to be able to simulate conformational transitions. Conformational sampling refers to the degree to which biologically and statistically relevant molecular conformations have been attained during the course of a given simulation. Several techniques with the purpose of enhancing conformational sampling have been published and implemented in modern molecular modeling software [2,3]. However, these are not really feasible for studying large conformational changes in biomacromolecules.

In this contribution, we propose a conformational sampling approach which relies on the well-established technique of classical molecular dynamics. The goal of the approach is to generate biologically relevant conformations for biomacromolecules, using minimal computational effort. Here, we describe the concept of the approach, and then assess the variability of the resulting conformations for an ion transporting protein [4].

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L35: Possible use of urinary miRNA as potential biomarkers of urothelial carcinoma

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Urothelial cell carcinoma (UCC) is the second most common urologic malignancy. The majority (90-95%) occurs in the bladder, is characterized by high rate of recurrence and its incidence increases every year. WHO classification divides these carcinomas into two groups: non-invasive (80%) and invasive urothelial carcinoma. At the moment the most used and important method for diagnostics and long-term surveillance is cystoscopy. This approach is very invasive, mainly in cases of repetitive cystoscopy to determine the tumor progression. As non-invasive and specific marker the urine cytology of exfoliated cells is used, although this method fails to detect low-grade tumors with high sensitivity. For these reasons, many new urine-based tests have been developed, yet there is no sensitive enough biomarker available for early detection of relapse, which appears in 70% of non-invasive urothelial carcinomas. As very promising biomarkers of urothelial carcinoma of the bladder seem to be urinary miRNA, which exhibit high stability and good analytical properties.

Using Affymetrix miRNA microarrays expression profiles of 1733 miRNA in urine supernatant were analyzed. The group of samples consisted of 16 patients diagnosed with UCC, 17 healthy controls, 10 patients diagnosed with renal cell carcinoma (RCC) and 4 patients with urinary tract infection. Validation part of the study was performed on a new group of 80 patients using qRT-PCR, which further confirmed the ability of these miRNA to distinguish urothelial carcinoma of the bladder.

Our results show, that urinary miRNA have the potential to be used as a new group of non-invasive diagnostic biomarkers.

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L36: Glycoprofiling of prostate specific antigen by impedimetric and piezoelectric biosensing

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Alterations of glycosylation are frequently accompanied by pathological processes, tumor metastasis and disease development in a human body [1,2]. Hence, aberrant glycan moieties of glycoproteins are becoming an appropriate diagnostic tool for early-stage cancer detection. A fabrication of ultrasensitive impedimetric and piezoelectric biosensors suitable for glycoprofiling of cancer biomarker is discussed here. In this study we present a sandwich platform based on covalent antibody immobilization with further incubation with a blocking agent (gelatin) to avoid non-specific interactions. In the following step an incubation of prostate specific antigen (PSA) was performed with a final lectin glyco-recognition. The fabricated biosensor was measured by electrochemical impedance spectroscopy (EIS) with quartz crystal microbalance (QCM) verification. Furthermore, an efficiency of blocking agent was examined with human serum albumin (HSA) as a negative control. Such biosensors with nano-scale patterning protocol have a great potential for sensitivity enhancement of biomarker discovery and even for future cancer diagnostics applications [3].

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L37: *COBLL1* as a survival predictor in chronic lymphocytic leukaemia patients

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Chronic lymphocytic leukaemia patients are stratified into two prognostic groups according to their mutated (M-CLL, indolent course) or unmutated (U-CLL, aggressive course) IGHV. CLL cells are also characteristic by upregulated expression of a transmembrane tyrosine-protein kinase (ROR1), a member of Wnt/planar cell polarity (PCP) pathway, which influences migration and chemotaxis of CLL. We have identified Cordon-bleu protein-like 1 (*COBLL1*) as a ROR1 binding partner using mass spectrometry of CLL samples and confirmed the binding by immunoprecipitation of HEK293 cells transfected with *COBLL1* and ROR1 vectors. Subsequently, we explored *COBLL1* expression in 174 previously untreated patients (82 U-CLL, 92 M-CLL). *COBLL1* expression was upregulated in M-CLL ($p < 0.0001$, Mann-Whitney test). Intriguingly, in U-CLL it showed a bimodal pattern; the U-CLL *COBLL1*-high patients had shorter overall survival than the U-CLL *COBLL1*-low patients (medians 75 vs. 207 months, $p = 0.0037$, Mantle-Cox test). Also, the migration of U-CLL *COBLL1*-high cells towards chemokines CCL19 and CXCL12 was enhanced compared to M-CLL and U-CLL *COBLL1*-low cells. Therefore, *COBLL1* expression in CLL cells identifies a novel subgroup with inferior prognosis within U-CLL patients. Their short survival can be caused by deregulated Wnt/PCP pathway.

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L38: Anatomy of protein channels

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Ligand-accessible channels are indispensable for a huge variety of cell-life processes. They enable passage of substrate/product compounds to/from the interaction (active) site in case this site is deeply buried within the protein structure. Physicochemical properties of these channels such as polarity, hydrophathy, charge, or bending and radius greatly influence the specificity and selectivity of chemical reactions. Therefore, precise detection and especially characterization of their properties is of a main interest of many researchers involved in rationalizing their roles in enzymatic reactions. Such knowledge can be directly utilized in drug design, rational design of enzymes and other biotechnological application.

We carried out PDB-wide analysis of ligand-accessible channels leading to the buried ligands both to the protein structure, so as to the active sites of enzymes. Properties and specificities of individual channel classes, with respect to the ligand type, are discussed and statistically evaluated. We found out that the average composition of channels significantly differs from the average composition of proteins, their surface or core. The overall chemical properties of channels also differ among individual channel classes. For the analysis we utilized a successor of the tool well-received by a scientific community for identification of channels MOLE 2.0. The tool is available as a standalone application and plugins for popular molecular-browsers free of charge at <http://mole.chemi.muni.cz>, or as web-service (<http://mole.upol.cz>).

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L39: Diversity of *Cryptosporidium* of wild rodents genus *Rattus* in the Czech Republic, Slovakia and Kenya

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Cryptosporidium rat genotypes I-IV, *C. parvum*, *C. suis*-like, *C. scrofarum*, *C. tyzzeri* and *C. muris* were described in wild rats before using molecular techniques. In our research we collected samples of rat faeces from 36 locations in Czech Republic, three locations in Slovakia and three locations in Kenya. We tested these samples by molecular and microscopical methods. There were not any *Cryptosporidium* positives from 46 samples from Slovakia and 31 samples from Kenya. We tested 233 samples from all over the Czech Republic and there were 24 (10.30%) positives for *Cryptosporidium*. None of the positive rodents had diarrhoea. Intensity of infection was microscopically determined in 6 cases ranging from 2×10^3 – 4×10^5 OPG. Phylogenetic analyses based on sequences of genes encoding small subunit rRNA, actin and *Cryptosporidium* oocyst wall protein revealed that 18 (7.72%) wild living rats in the Czech Republic had *Cryptosporidium* genotype I, 2 (0.86%) had genotype IV, 1 (0.43%) had *Cryptosporidium* genotype II and 1 (0.43%) had *C. andersoni*. *Cryptosporidium andersoni* could not be simply passed through rats GIT accidentally by cross-contamination because those animals were from inside husbandry held and strictly closed for three years. It is first finding of *C. andersoni* in genus *Rattus*. In oposite of our expectations we didn't find any other species or genotypes of *Cryptosporidium* including *C. muris*.

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L40: Immobilized cytochrome P450 2C9 microreactor: a promising tool in hits' and leads' screening.

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Cytochromes P450 (CYP), a superfamily of hepatic enzymes, play a key role in drug metabolism and therefore assays describing interaction between a new drug and these enzymes are integral part of preclinical phase of a new drug development. In principal these assays demand for high throughput and cost effectiveness. Immobilization of such enzymes can offer a number of desirable features, including improved enzyme stability and repeated use. Immobilized enzyme microreactors (IMERs) therefore represent a promising tool for high throughput screening.

In this work we present an IMER based on CYP 2C9 isoform representing approximately 20 % of all CYP in human liver while being responsible for metabolizing over 10 % of commonly prescribed drugs. This IMER was integrated into capillary which further improves IMER features due to miniscule sample consumption; only tens of nanoliters of sample are consumed per analysis, and enabling rapid quantification by the means of capillary electrophoresis. Using this instrument a kinetic and inhibition study was performed, deploying diclofenac as a model substrate and sulfaphenazole as a model inhibitor. All kinetic and inhibition parameters were acquired and showed good correlation with literature. On the other hand a broadly used model for determination of the reactants' effective concentration, the Hagen-Poiseuille law, showed some major discrepancies and therefore an adjusted model for concentration profile modeling is presented as well.

L41: The effect of ZAP-70 on adaptor molecule involved in microenvironmental interactions of malignant B cells

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The microenvironment of bone marrow and lymph nodes plays a crucial role in pathogenesis of chronic lymphocytic leukemia (CLL) by providing supportive signals to malignant B cells via adhesion, chemokines and B cell receptor (BCR). The ZAP-70 protein supports these interactions in CLL; however, the mechanism of its function has not yet been well established. We observed that ZAP-70 directly affects the expression and function of an adaptor molecule involved in PI3K/BCR signalling, as the high-level expression of ZAP-70 positively correlates with the amount of this adaptor molecule in CLL cells ($n=37$, $P=0.0003$). Our immunoprecipitation experiments demonstrate the existence of a yet unknown complex of ZAP-70 and this adaptor molecule from IRS1-like multisubstrate docking protein family. Additionally, high expression of the complex upregulates the level of phospho-AKT ($P=0.04$), a key component in PI3K/BCR signalling. High-level of the studied molecule also facilitates the migration of malignant B cells towards stromal cells in the Transwell assay ($P=0.02$). Altogether, we identified a novel partner of ZAP-70, which expression of affects BCR signalling and the migration of malignant B cells into the supportive microenvironment.

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L42: How to use lectin microarray in medicine

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Lectin microarray is used for detection of glycan structures that are bound to different molecules and substrates such as protein, lipids, cell walls as well as in biological material, including stem cells, tissue, viruses, microorganism, sera, etc. Changes in glycosylation are associated with physiological and pathophysiological changes. The lectin – glycoconjugate interaction is usually multivalent and complex and there is a need to be studied thoroughly to understand it and utilize lectin and glycan biorecognition for development for e.g. diagnostics tools. We used microarray to study the interactions between glycostructures and lectins. Lectin microarray to perform study of bioanalytical use of lectin – glycoproteins interactions for biological, medical and pharmaceutical applications [1]. We used for measuring samples from people with rheumatoid arthritis, systemic sclerosis, colorectal cancer and many others [2,3].

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L43: Barrier properties of natural biopolymers studied by innovative diffusion techniques

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One of the most important gaps in the knowledge of biopolymers is the study on their reactivity. The reactivity and barrier properties of natural biopolymers were studied by interactions with basic organic dyes (Methylene Blue) by diffusion techniques (non-stationary diffusion and diffusion cell) in hydrogel medium (agarose). The reactivity and barrier properties of chosen studied materials were compared by determination of fundamental diffusion parameters (effective diffusion coefficients, break-through time and sorption capacity). Developed methods together with classical sorption experiments represent a universal reactivity-mapping tool for study on reactivity various natural substances. The universality of developed methods was tested on systems with natural biopolymers (chitosan, sodium alginate, hyaluronic acid) and supramolecular compounds (humic acids). The influence of basic physical-chemical conditions (pH, ionic strength, temperature, concentration, modification of studied materials, etc.) of the systems containing natural substances can be studied easily at laboratory conditions and this is one of the greatest advantages of developed methods.

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L44: Early inflammatory response in rat brain after subarachnoid haemorrhage

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Inflammation represents an important part of the pathophysiology of subarachnoid haemorrhage (SAH). Major effectors of early response including proinflammatory cytokines and adhesive molecules can contribute to severity of disease. The aim of this study was to determine character of the early inflammatory response in rat brain after subarachnoid haemorrhage (SAH). In the group of 55 animals (sham, light SAK, severe SAK; 4h and 8h after surgery) mRNA expression from brain tissue and serum levels (IL-6, IL-1beta, IL-10, TNF alpha, ICAM1, VCAM1) were measured. Expression levels of IL-6, IL-1beta and TN alpha was significantly increased at the site of haemorrhage in the group of heavy SAH compared to sham groups. Moreover, levels of ICAM-1 were increased at the site of haemorrhage exclusively in the group of heavy SAK 4 hours after surgery. In the case of brain area which is not in direct contact with haemorrhage an increased expression of TNF alpha and ICAM1 in the group of heavy SAH (4h) versus sham (4h) was observed. Serum levels showed no differences between experimental groups in any of the monitored parameters. A severe form of SAH is associated with activation of the early inflammatory response in the brain tissue predominantly in the affected area. Our results indicate that the activation of inflammation after SAH is demonstrable even in areas which are not primarily adjacent to the site of haemorrhage. This data point toward the global activation of inflammation in the brain tissue.

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L45: To decipher the possible presence of auxin transport machinery in chloroplast

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Environmental stresses adversely affect plant growth and development leading to worldwide yield losses. The plant hormone and signaling molecule auxin is a key player in plant development and plays an important role in plant stress responses. Lesser photosynthesis is partially responsible for some of the observed symptoms in stress adapted plants. This symptoms such as growth retardation, reduced metabolism and increased antioxidant activities helps to maximize plant survival. Auxin modifies chloroplast structure, chlorophyll synthesis, nuclear photosynthetic genes expression, and chloroplast transcription in response to environmental changes [1]. Thus auxin could hypothetically affect the remodeling of the photosynthetic apparatus to minimize photo oxidative damage induced upon stress [1]. Reciprocally, chloroplasts synthesize tryptophan-derived precursors for IAA biosynthesis and in some plants can actively biosynthesize auxin [1]. Moreover, recently chloroplast redox state was shown to modulate auxin homeostasis [2]. These data show that there is a strong connection between chloroplast processes and auxin homeostasis. However, the connection between auxin and photosynthesis is rarely described.

To investigate whether the Arabidopsis chloroplast can transport auxin, chloroplast localized putative auxin transporters were selected. *In silico* promoter gene analysis shows that our target genes share some similarities with the promoters of ATP Binding Cassette auxin transporters. Auxin transport machinery in chloroplasts will be studied using a novel ratiometric auxin biosensor [3]. Owing to the vital importance of photosynthesis for plant growth and survival, understanding how chloroplast and auxin metabolism are interconnected will bring novel insights into plant stress biology applicable to improve the performance of crops under field conditions.

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L46: Identification of genes regulating plant meiosis by suppressor screen in *Arabidopsis thaliana*

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Meiosis is a specialized cell division that halves number of chromosomes and gives rise to haploid gametes. The goal of my PhD project is to elucidate the regulation of meiosis in plants. Previous studies in our lab revealed that the SMG7 gene in model plant *Arabidopsis thaliana* is involved in regulating RNA stability and in reproduction. Inactivation of SMG7 leads to sexual sterility caused by an atypical arrest of meiotic division in anaphase II, likely through interference with the core cell cycle regulators. I want to identify new genes regulating meiotic cell division via a suppressor screen to search for *smg7* mutant lines with increased fertility. Applying an EMS treatment on a mild fertility mutant of *smg7*, we have phenotypically identified a large number of such candidate lines and we are currently mapping the causative mutations in selected lines using genome wide next generation sequencing. We have already identified several candidate genes, which we validate using a set of genotyping techniques for detecting single nucleotide polymorphisms (High-Resolution-Melting/HRM and Derived-Cleaved-Amplified-Polymorphic-Sequences/dCAPS). Once candidates are validated I will proceed with the phenotypic analysis and in depth functional characterization of identified genes. This will include a number of microscopy techniques that map the cellular localization of mutant proteins and help describe the meiotic division in mutant plants, as well as other biochemical techniques, which depend on the nature of the selected candidate protein.



L47: Mutations in the *TP53* gene show features of somatic hypermutation process with prominent difference between *IGHV* mutated and unmutated chronic lymphocytic leukemia

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Background: Introducing somatic hypermutations (SHM) into immunoglobulin genes is a physiological process during antibody maturation. SHM introduction is a two-step process; the first step involves deamination of cytosine to uracil by Activation-Induced (Cytidine) Deaminase (AID). During the second step, uracil is removed and error-prone DNA polymerases (mainly polymerase ϵ) are recruited to fill the gap. AID's off-targeting may result in mutations in nonimmunoglobulin genes, including tumor suppressor gene *TP53*. **Aims:** We explored the *TP53* mutation patterns with regards to SHM features emphasizing in differences between mutations occurring in *IGHV* unmutated (U-CLL) and *IGHV* mutated (M-CLL) patient groups.

Methods: We used the set of 121 mutations found in M-CLL cases and 343 mutations detected in U-CLL patients by Illumina ultra-deep Next Generation Sequencing with high sensitivity (0.2%).

Results: We found a mutations overrepresentation in GNW motif (typical for AID activity) in U-CLL (14.58% vs. 6.61% in M-CLL; $P=0.025$). Contrarily, mutations detected in M-CLL cases showed features of targeting by polymerase ϵ : prevalence of mutations in WA/TW motifs (40.5% vs. 23.91% in U-CLL; $P<0.0001$) with strand bias favoring WA observed in both groups, but extremely prominent in M-CLL (23.5 fold in M-CLL vs. 4.37 fold in U-CLL; $P=0.014$).

Conclusion: We documented significantly different patterns of *TP53* mutations in U-CLL vs. M-CLL. Mutations detected in U-CLL showed the features corresponding to the first step of SHM process: deamination by AID. In contrast, spectra of mutations detected in M-CLL cases suggested the more prominent involvement of polymerase ϵ during the second SHM step.



L48: The study of humic acid interactions via ITC

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There are various modelling systems including the Isothermal titration calorimetry to study interactions between ligand and molecule to describe the strength of bond with selected ligand acting in modelling system.

Isothermal titration calorimetry is used to describe and characterize intermolecular interactions and recognition of reactions happening in studied system with excellent sensibility. It's huge advantage is that it is possible to estimate the level of affinity of studied ligand to the substance.

Major components of the organic matter in soil and water are humic substances. These compounds are basically organic polymers, therefore their complexity and structure reveal is needed, as their use and impact on soil quality is of huge interest. In the soil, these substances are highly chemically reactive with respect to biodegradation. There is also a huge impact on nutrients availability when these substances are presented in the soil used for harvesting variety of crops.

The higher the importance of the presence of humic substances is revealed, the bigger effort is done to understand their behavior in the systems and to describe the humic substances with appropriate definable systems to obtain basic chemical experience describing the behavior of humic acids in the complex natural systems. This work discuss uses of ITC in humic research.

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L49: Lectin-based microarray for protein glycosylation analysis

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The glycosylation of proteins is one of the most important co-translational and post-translational events. Various structures of glycans have diverse functional roles in many specific biological functions. Quality and quantity of glycosylation as well as changes in glycan structures can serve as important biomarkers signaling onset and course of many diseases such as cancer, neurodegenerative diseases, AIDS and many others. Thus glycoprofiling could be used as a tool for early diagnosis. The aim of this work is to develop and apply lectin-based microarray assay for quantification and glycoprofiling of glycoproteins. Here we presented glycoprotein microarray technology using multiple lectin-based, biotin-streptavidin detection scheme. Selective detection of glycan structure was made possible by employing multiple lectins to screen glycoprotein standards. We glycoprofiled fetuin, asialofetuin, transferrin and invertase and evaluated analytical characteristics as limit of detection and sensitivity of the assays.

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Material science and physics

Students' abstracts



Mo1: Dynamic focus in e-beam lithography

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Magnetic objective lenses in e-beam lithography systems create the image of the beam crossover (or the aperture for shaped-beam systems) on the substrate only on the optical axis, i.e. without deflection. The deflected beam, due to field curvature, is focused above the substrate. This aberration can be compensated by adding a small fast lens to the optical column to dynamically adjust the focal length for all deflections. We are currently evaluating and optimizing the use of such dynamic focus lenses. Our design uses the optical column of the e-beam lithography system BS600 designed by the Institute of Scientific Instruments, Academy of Sciences of the Czech Republic. Our results can, however, be accommodated to commercially available e-beam lithography systems.

We are evaluating the use of both electrostatic and magnetic dynamic focus lenses. To minimize optical aberrations and the influence on beam rotation, we are looking at several placements of the dynamic focus lens, such as inside the objective lens or in the last condenser lens.



Mo2: Characterization of deposition of thin films by magnetron sputtering excited by high power pulse

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High power impulse magnetron sputtering (HiPIMS) is a newly developed technique of physical vapor deposition (PVD). It is characterized by very high peak power density, pulse frequencies from 1 to 1000 Hz and pulse widths from 50 to 500 microseconds [1].

The main advantage in comparison with DC sputtering is a metal ion density higher than 10^{18} m^{-3} . However the process of high power pulse sputtering shows lower deposition rate as DC sputtering, the structures of thin films have promising qualities for industrial and medical usage.

The aim of this work was to set suitable experimental parameters of the deposition process primary. Secondary to compare these two techniques in difference structural quality of deposited nanocomposite formed by carbide crystallites embedded in amorphous carbon matrix.

In our planar magnetron system we used Ti target for deposition of metal particles, different acetylene flows (from 1 to 5 sccm) for carbon matrix. Working gas pressure in chamber was around 1 Pa. We controlled the process with the power of constant value of 1255 kW. The pulsed plasma was produce with a 30 Hz repetition rate and pulse width was 400 microseconds. Prepared samples were subsequently analyzed by scanning electron microscopy, optical microscopy and x-ray diffractometry.

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Mo3: Titanium oxide based anode materials for li-ion batteries

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Chemical and thermal stability are the key bottlenecks of conventional graphite anodes used in the li-ion batteries today. Graphitic materials are the most common anode active materials mostly due to their high specific capacity and relatively low cost. On the other hand, drawbacks like low stability of solid electrolyte interface layer protecting it from spontaneous reaction with electrolyte and the risk of thermal runaway are more and more evident with rising of interest in electro mobility and EV.

One of the most promising successors in the field of lithium anode active materials is the group of ceramic materials based on titanium oxide. Their thermal and chemical stability is incomparable with graphitic materials – they are almost inert and due to higher operation voltage they do not suffer from irreversible capacity loss as a result of SEI layer formation.

This work deals with structural and electrochemical characterisation of spinel $\text{Li}_4\text{Ti}_5\text{O}_{12}$ and TiO_2 nanostructured anode active materials for lithium-ion batteries. Electrochemical characterization by cyclic voltammetry, galvanostatic cycling, electrochemical impedance spectroscopy and rate capability was made and physical characterization by XRD and SEM is provided.



Mo4: Electrical characterisation of PEDOT:PSS for sensing applications

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The modern electronic industry is constantly searching for novel materials and processing methods. That could bring new devices with potentially new parameters. One of the new direction of electronics involves devices based on organic polymers (OP). PEDOT:PSS (poly(3,4-ethylenedioxythiophene) and poly(4-styrenesulfonate)) with H₂O as a pristine solvent is optically transparent, well spin-coated, and a hole transport material. The PEDOT:PSS has been widely used as an antistatic coating material, as electrodes for capacitors or photodiodes, and as a hole transport layer of organic LED [1].

In this study, we investigate electric behavior of spin coated PEDOT:PSS. The PEDOT:PSS layer is coated on glass substrate with ITO (Indium-Tin-Oxide) different interdigital structure. We have fabricated these structures by photolithographic technique and next etching processes. Coating processes of the PEDOT:PSS had to be proceeded in inert atmosphere because the PEDOT:PSS is a high downgrading material, especially when affected to humidity. We have done A-V characteristics and EIS (Electro Impedance Spectroscopy) measurement by using our probe station. Measured substrates were put into a special case with inert atmosphere as well. The results from measurement could be used for basic settings of sensor.

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Mos: Structural coloration of butterfly wings

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Some colors in living world are caused by structure of material [1]. The one chemical color surface could be bright and iridescent or dim and dull. The natural photonic structures have remarkable properties [1, 2] and are the source of inspiration and of great interest as template material for photonic devices design. The wings of two different colors were studied by atomic force microscopy. The analyzed data showed similarities for the same color places of the different species wings. The topography of the blue butterfly wing is shown in the picture 1.

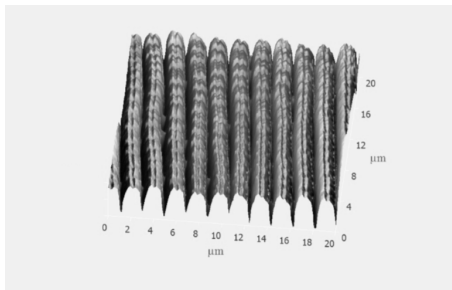


Fig.1. AFM image of the butterfly wing [3]

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Mo6: Study of background contribution in spectroscopic ellipsometry of biomolecules under SPR condition

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Determination of the properties of a thin (multi)layer on a substrate with complicated structure is a challenging task in spectroscopic ellipsometry (SE). Mathematically, the contribution of the substrate (including the optical path of the equipment) cannot be separated from the sample measurement in a straightforward way, but only when the structure of the substrate (geometry of its layers and optical constants for each layer) is fully known in advance. In addition, to reach the detection limits needed for liquid measurements of biomolecules in physiological concentrations, the surface plasmon must be involved in the total internal reflection configuration (TIRE); even then, the spectrum is dominated by the background structure of the plasmonic resonance (SPR) with only a small contribution from the measured (bio)molecules. In this paper we propose a simple method, based on difference spectra, which allows us to work directly with the signal from the layer of interest. This method works well even if changes in spectra are very small in comparison with the background signal. We demonstrate the method on TIRE measurement of bovine albumin (BSA) immobilization over a gold SPR chip via sequence of self-assembled monolayers (SAMs). Using the difference spectra allows us to determine properties of the growing albumin layer in detail without explicit knowledge of the sample substrate parameters. This is very useful under SPR setting when especially the information on properties of the crucial SPR gold layer is only available with large uncertainties.

Mo7: Endocyted gold-nanoparticles in intact-cell mass spectrometry

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Gold nanoparticles (AuNPs) were recently reported to increase ionization of biomolecules in Matrix-Assisted Laser Desorption Ionization Time-Of-Flight (MALDI-TOF) Mass Spectrometry (MS) of complex biological samples, such as cells and tissues.[1,2] In this setup, the matrix-sample mixture is enriched with AuNPs of various size and geometry that most probably enhance distribution of laser energy throughout the sample and facilitate ionization and/or quantum nano-plasmons effects during the process of measurements. We asked, whether AuNPs endocytosed by cultured cells can enhance subsequent MS analysis. In this work, we treated HEK293 cells with either polyhedral or flower-like AuNPs or left them untreated and cultured them overnight. Then the cells were washed, harvested, mixed with matrix and directly analyzed by MS. Both the polyhedral and flower-like AuNPs were massively endocytosed by HEK293 cells. The mass spectra acquired from intact cells containing endocytosed AuNPs showed an increase of intensity of specific peaks. Interestingly, mass spectra generated from intact cells containing polyhedral or flower-like AuNPs showed differences in m/z or intensity values, suggesting selective effect of AuNPs structure on cell targets. The endocytosed nanoparticles can interact with various components of cellular metabolism. The interactions of AuNPs with biomolecular pool in living cells can therefore extend the analytical approaches such as MALDI, SALDI (Surface Assisted Laser Desorption Ionization) or NALDI (Nano Particles Assisted Laser Desorption Ionization) used in intact cell MS.

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Mo8: Gas sensor based on MEMS cantilever resonator

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The aim of this work is about fabrication of MEMS gas sensor based on resonance cantilever beam. Cantilever will exploit piezoelectric effect; frequency of oscillation is measured with change of load of cantilever. Loading of cantilever is dependent on molecules bind on active layer which could be realized by using polymers, carbon nanotubes, etc. Sensor will be created as sandwich structure with silicon oxide passivation layer. Bottom electrode will be made from titanium. It is very important to reach required crystallographic structure of piezoelectric aluminum nitride layer with c-axis orientation which is in the middle of electrodes. This crystallographic structure is affected by crystallographic structure of titanium layer. Top electrode will be fabricated from gold. Width of cantilever beam will be in range from 50 μm to 200 μm and length will be in range from 100 μm to 800 μm with thickness about 2.5 μm . These dimensions will be optimized to find ideal resonance of cantilever. MEMS gas sensors can achieve very sensitive detection limit (several ppm) and very fast response (hundreds of milliseconds).

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Mog: All-dry processed organic solar cell structures

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Zinc phthalocyanine (ZnPc) and Diphenyl-Diketo-Pyrrolopyrroles (DPP) thin films were vacuum deposited onto ITO covered substrates. Aluminum top electrode was also deposited in vacuum onto the organic films (OF). As a result solar cell structures of type ITO|OF|Al was produced in all-dry process avoiding the solvent usage.

The device parameters were estimated by a measurement of current-voltage characteristics in dark and under illumination of white light produced by solar simulator according to standard AM 1.5.

It was found that the photovoltaic properties of the samples depend on the conditions for deposition of the top Al electrodes. The increased substrate temperature during the electrode deposition resulted in a worsening of the photoelectrical properties. Optimal conditions for electrode deposition were established, which allows reproducible samples to be prepared. Under these conditions a clear diode dark current characteristics with a diode rectification ratio of 1×10^5 was obtained. Under light exposure the open circuit voltage of 0.7 V was observed and the photocurrent increases more than 5 orders of magnitude.

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M10: Retinoic acid analysis by mass spectrometry

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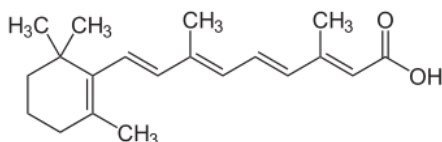
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Retinoic acid (RA) is a vitamin A (retinol)-derived, small lipophilic molecule, involved in cell proliferation, differentiation or histogenesis, with important clinical applications, e.g. in leukemia treatment.

In this work, we analysed retinoic acid by Laser Desorption Ionization (LDI), Surface Assisted Laser Desorption Ionization (SALDI) or Matrix Assisted Laser Desorption Time Of Flight Mass spectrometry (MALDI TOF MS). A formation of cation radical $RA^{\cdot+}$ using LDI or the protonated form $RA.H^+$ in MALDI was observed. In addition, we developed and optimized SALDI of RA using various forms of gold nano-particles [1]. Applying SALDI or combination of nano-particles and common matrices (SALDI-MALDI) allowed a highly sensitive determination of RA. In summary, determination of RA by MS was optimized, allowing for subsequent studies in cells or tissues.



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M11: Microstructural changes of titanium diboride by addition of Ta and Ni dopants

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Materials predetermined for high temperature applications are usually based on the ceramics which possess extremely low fracture resistance due to an inherent brittleness. The possible way how to change this limitation can be optimisation of the microstructure, i.e., grain arrangement and inter-grain bonding as is successfully used in silicon nitride. The weak point in such materials is usually lower temperature resistance of the phase forming inter-grain interface, therefore the application of silicon nitride is limited to the temperatures around 1000°C. On the contrary, titanium diboride can serve up to 2000°C and the limitation is in processing side where solid state sintering is demanding and requires higher sintering temperatures leading in extreme grain growth. In addition, when liquid phase sintering is applied the high temperature properties are limited by this phase. The aim of this work was to describe in detail microstructural development when combination of used dopants can form high temperature resistant solid solution. Microstructural changes of pure titanium diboride doped by various amounts of nickel and tantalum were investigated using ceramographic methods supplemented by elemental SEM microanalysis and X-ray analysis. Materials used in this study were prepared by the standard and the rapid hot-pressing method at temperatures around 2000°C. The effect of processing route applied as well as the effect of selected metallic elements was studied from the grain growth and a porosity development point of view. The link between resulting microstructure and basic mechanical properties was found and positive influence of dopants was determined.



M12: Electron beam lithography of graphene Hall-bar for micro-contacting

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Hall-bar like structures are widely used for measuring electrical transport properties of materials with two-dimensional electron gas, for example graphene. They allow us to measure the x and y component of conductivity separately, therefore making the measurement of Hall resistance, electron mobility and Shubnikov-de Haas oscillations possible.

Graphene is prepared using a chemical vapor deposition (CVD) technique and transferred on top of prefabricated titanium/gold conductive contacts on top of silicon wafer with 280 nm of silicon thermal oxide. Since the graphene layer does not come in the shape of the Hall-bar it has to be modified using electron beam lithography (EBL) and plasma etching.

Electron beam lithography starts with spin coating a trilayer of electron resists (2 positive, 1 negative). The first positive resist used is PMMA 50K A3 to minimize unwanted residues left on the surface of graphene, followed by PMMA 495K A4 as a protection for the first layer from the developer and the last layer is the negative resist HSQ 6%.

Lithography is done on Tescan Mira3 + Raith, the HSQ layer is exposed to the electron beam, developed in TMAH(aq), and then used as a plasma etching mask of the PMMA and graphene layer.

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M13: Hydrochemical evaluation of groundwater in Wadi El Natrun area, Egypt

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Groundwater is the main source for water supply in Wadi El-Natrun area. Wadi El-Natrun area is an elongate sandy depression located in the northeastern part of the Western Desert of Egypt. Hydrogeochemical characteristics of groundwater in Wadi El Natrun area have been investigated to identify the distributions of groundwater geochemistry and the hydrogeochemical evolution pattern in the area. Groundwater samples from 55 different wells were analysed for their physical and chemical properties. Results reveal that the water is alkaline on account high pH values. The study also reveals saltwater contamination as Chloride contents in some boreholes are up to 710.00mg/l. Piper trilinear diagram was plotted based on the results of the analysis for separating the different water types for wells. Groundwater of the Pliocene aquifer is dominated by NaCl and Na₂SO₄ water types. Groundwater is suitable for irrigation and most of them are free from residual sodium carbonate(RSC) which reflects good quality and is suitable for using in irrigation for all types of soils. Concerning the origin of the groundwater in the area of study, it is mainly has meteoric origin and the main mechanism that controls the chemical composition of groundwater is the evaporation- fractional crystallization process. Besides providing an assessment of the hydrogeochemistry of and possible controls, this study has shown that, groundwater quality problems in the study area are traceable to the lack of consistent efforts to squarely address the problems, hence the need for a regular groundwater quality monitoring and effective management strategies in the area.



M14: Improvement in the quality of graphene synthesized by chemical vapor deposition

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Graphene is a carbon allotrope with many promising application related properties. Nowadays is graphene commonly synthesized by chemical vapor deposition (CVD) (in high temperature) on copper foil using hydrocarbon (methane) as source of carbon atoms.

There are two main advantage in using copper foil for the graphene synthesis: growth of graphene on copper is (because the mechanism of catalytic decomposition of hydrocarbon on the surface) self-limited and the copper substrates are also very cheap in comparison with alternatives.

However graphene samples prepared by CVD on copper foil usually exhibit poor structural quality in comparison with samples prepared by the mechanical cleavage. The aim of this work was to adjust experimental parameters of the deposition process in order to improve structural quality of deposited graphene layer. We used two types of the 25 micrometer thin copper foil during deposition with different purity (99.8% and 99.999%) as catalyst and methane as precursor. Copper foil was heated in hydrogen atmosphere before the deposition in order to reduce native oxide layer on the surface. Depositions were carried out in the electrical heated laboratory furnace pumped down with rotary pump. Temperature during pretreatment and during deposition was 1000°C. Prepared samples were subsequently analyzed by optical microscopy, scanning electron microscopy and Raman spectroscopy.

M15: Ageing of epoxies with nano fillers

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Epoxies with microfillers are now widely used in the electrical engineering industry as insulation in electrical machines and devices and at other places [1], [2]. In order to improve insulating properties of epoxy composites plans are in place to start using nanofiller which would better hinder tree discharge to prevent breakdown. However, due to the large amount of interface these materials are assumed that the aging brings about a rapid degradation of their improved properties.

The aim of the investigation was a comparison of behaviour of epoxies without insulation fillers and with nanofillers, SiO_2 and TiO_2 . The subjects of the comparison are dielectric spectra before, during and after ageing of 5000 hours. For ease of identification and evaluation, the results were fitted using Havriliak – Negami (HN) equation. Results of the HN equation fitting were further analyzed using Arrhenius and Vogel – Fulcher – Tammann equations.

Results achieved so far show that the chosen ageing, i.e. at 200 °C for 5000 hours did not result in a significant change of the dielectric spectrum. Therefore, the concerns expressed in [3], which concern the accelerated degradation due to the presence of nanocomposites, on the basis of this research appear to be unjustified.

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M16: The use of flower-like gold nanoparticles in time-of-flight mass spectrometry

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Various types of gold nanoparticles (AuNPs) represent promising tools in many biomedical applications.[1,2] Here we report the first use of flower-like (FL) AuNPs as a mediator enhancing ionization in mass spectrometry (MS) of biomolecules. The main objective was to determine the effect of FL AuNPs on the ionization of biomolecules by surface assisted and matrix assisted laser desorption ionization (SALDI and MALDI) MS with time-of-flight analyzer. FL AuNPs alone or combined with cyano-4-hydroxycinnamic acid (CHCA) for MS measurement of peptides (500-3500 m/z) were used. The comparison with classical CHCA matrix shows that FL AuNPs increase the ionization ($\sim 7.5\times$) of peptides both alone and in combination with CHCA matrix. For ionization of higher mass peptides/proteins and those from mouse embryonic fibroblast (MEF) cells, FL AuNPs combined with CHCA and sinapinic acid (SA) were used. The signal of peptide/protein peaks (3600-17000 m/z) was up to $2\times$ higher with using FL AuNPs enriched CHCA matrix than using conventional CHCA matrix. The signal of MEF cells profile peaks (4000-20000 m/z) was $2\times$ higher when using FL AuNPs combined with sinapinic acid (SA) as compared to SA matrix alone. In addition, gold clusters generated from FL AuNPs provide suitable internal calibration standard for MS analysis of peptides. In conclusion, FL AuNPs are capable of efficient improving of MS detection of peptides/proteins and their use may contribute to mass spectrometry based proteomics of biomolecules.

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M17: Effect of pretreatment parameters on the anodizing behaviour of Al foils in citric acid electrolytes

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Nanoporous anodic alumina films grown in citric acid electrolytes at potentials exceeding 300V are of considerable interest both for applications in electronics and as models for studying film formation at frontier conditions [1]. However, a reproducible anodic process for steady-state alumina growth at moderate current densities remains a challenge due to the difficulty to reveal and maintain the right balance between the technological, electrical and electrolytic conditions for anodizing and pre-anodizing treatments. Here we demonstrate the impact of important surface finishing techniques for Al foils, such as annealing and electropolishing, on the pore nucleation and growth during galvanostatic anodization in citric acid electrolytes.

It was revealed that the self-organized pore formation is strictly dependent upon the anodizing setup, the surface morphology and crystalline structure of aluminium foils, which are affected by the conditions of high temperature annealing and electropolishing pretreatments. The optimized process parameters give microscopically flat sample surfaces, without the usual textures of nanometre dimensions [2], which plays a role in the electrochemical behaviour of Al and its response to further anodizing.

The new knowledge gained in this work is useful for creating advanced processes for growing well-distanced, individual or multiplied nanopores, grouped in a customary way, with and without applying an external technique, for templated formation of metal-oxide nanostructures.

Acknowledgement: This work was supported by GA ČR grant no. 14-29531S.

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M18: Nanoparticle induced changes in rheological behavior of polystyrene solutions under LAOS

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Polymer nanocomposites represent a group of nano-structured materials which offer a possibility to reach a substantial enhancement of properties at very small loadings compared to classical composites. According to the simulations, there are four basic spatial organization states of nanoparticles in polymer matrix. [1] Despite the growing interest in this field, fundamental understanding is lacking and the application approach usually remains rather semi-empirical.

It was the aim of this study to investigate the influence of nanoparticles on polystyrene (PS) solutions. Polyhedral oligomeric silsesquioxanes (POSS) were chosen as a model filler because of its well-defined structure and the possibility to tune the interaction strength by choosing the organic substituents on the POSS cage. High-affine octaphenyl-POSS (OP-POSS) and low-affine octamethyl-POSS (OM-POSS) were utilized. Three distinct regions were found under large amplitude oscillation shear (LAOS) in the range of strain amplitude between 0.01-5 000 %. In the middle-strain region, low concentrations of OP-POSS introduced strain overshoot whereas OM-POSS and high concentrations of OP-POSS remained rather uninvolved. We expect that the overshoot is caused by formation of though structures where the attractive particles could be involved but only in sufficiently low concentrations because the particles are prone to form aggregates at higher concentrations.

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M19: Electrochemical preparation and characterization of tantalum layers

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Electrodeposition (ED) of tantalum metal onto thin Au layers sputtered on a sital substrate was investigated in ionic liquid (IL) 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl) imide, ([BMP]Tf₂N) (Solvionic, 99.9%), containing 0.5 mol dm⁻³ TaF₅ (Alfa Aesar, 99.9 %) and 0.5 mol dm⁻³ LiF (Alfa Aesar, 99.99%) in inert atmosphere with oxygen and humidity less than 20 ppm.

We searched for an electric potential of tantalum (V) to metallic tantalum reduction by cyclic voltammetry, followed by potentiostatic electrodeposition on the Au films at -1.1 V at working temperature of 200°C. The electrodeposited layers were analyzed by scanning electron microscopy and energy dispersive X-ray analysis.

Although the process of tantalum electrodeposition has been reported in previous studies [1], our approach is expected to be advantageous for nanostructured Ta ED, especially for creating 3-dimensional nanofilms for a wide range of potential applications, including capacitors, sensors, switching devices, memristors. A totally electrochemistry-based process, implying electrodeposition and anodization, will be developed for forming metal/oxide interfaces based on tantalum or other refractory and valve metals and oxides. Following the approach described in Ref. [2], electrochemical doping of Ta/Ta₂O₅ nanodeposits could be another option worth investigating in future works.

Acknowledgement: Research leading to these results was supported in part by project CZ.1.07/2.3.00/30.0039 and by GAČR grant no. 14-29531S.

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M2o: Generation of gold clusters by laser desorption ionization from various sources

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Gold nanoparticles (AuNPs) are of particular importance because of their applications in diagnostics and biomedicine [1-3], in calibration of mass spectra, as matrix in MALDI, for the determination of small organic molecules and biopolymers, as drug carriers, in photothermal cancer therapy, enhancement of visual tissue analysis etc. Aim of this work is to compare distribution of gold clusters generated from commercial AuNPs, polyhedral AuNPs prepared by reduction from auric acid and Au-FeNPs prepared by the reduction of auric acid using stainless steel as reducing agent. Laser Desorption Ionization (LDI) TOF MS of various AuNPs produce single charged Au_m^\pm clusters with different distribution. Next, some of the analyzed AuNPs enhanced MS of various biomolecules providing in parallel precise calibration standard *in situ*. The applications of AuNPs and LDI-derived Au_m^\pm clusters in state-of-the-art MS are discussed.

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M21: The influence of various additives and admixtures on the mechanical properties of alkali-activated slag mortars

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Alkali-activated slag (AAS) binder is obtained by a manufacturing process less energy-intensive than Portland cement and involves lower greenhouse gases emission. AAS belongs to prospective materials in the field of Civil Engineering. But AAS has also disadvantage - high drying shrinkage which impedes its application as a construction material. Therefore, chemical admixtures, mineral additives and other materials are used as additives in AAS system aiming to modify and improve some properties of this system. This paper presents laboratory study on the mechanical properties of AAS mortars with addition of various mineral and polymer admixtures such as fly ash and microspheres, carboxymethyl cellulose (CMC), hydroxypropyl methyl cellulose (HPMC), polyvinyl alcohol (PVA) and others.

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M22: Using the analytical centrifuge to characterize of magnetic nanoparticles

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Magnetic Fe_3O_4 nanoparticles were prepared by co-precipitation method according to the literature [1]. Prepared Fe_3O_4 nanoparticles were dispersed in water solution of surfactant. The dispersion system was characterized by the analytical centrifuge LUMiSizer (LUM, Germany).

The separation process of the magnetic nanoparticle dispersion was characterized by the very polydisperse sedimentation (no sharp front) of particles with relatively narrow particle size distribution of fine particles which move with different speed. This type of sedimentation points out colloidal stable dispersions against particle aggregation. Prior to separation, particle concentration was equally distributed along the complete sample length, i.e. transmission was constant at a low level (first transmission profile with the lowest transmission). During sedimentation, the concentration of particles decreased in the region of meniscus and transmission increased. The last profile (highest transmission) indicated that the smallest particles were not yet fully separated out from the supernatant within the applied centrifugation time. Only the very small sediment was observed due to a dense packing of particles characteristic for colloidal stable systems with the repulsive particle-particle interaction. This technique was also used to determine the nanoparticle hydrodynamic density and particle size distribution.

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M23: Numerical simulations of low-temperature plasmas with biomedical applications

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Atmospheric-pressure low-temperature laboratory plasmas have been recently utilized in a number of promising biomedical applications. These applications are either direct, such as surface sterilisation or wound healing, or indirect, such as production of nanoparticles for various biomedical diagnostic techniques.

However, to properly describe the processes taking place in these plasmas, one has to account for their non-equilibrium nature, (the temperatures of various particle species generally differ), the large number of plasma chemical reactions and the strong coupling of the gas flow, the electric field and the chemistry. This usually requires sophisticated numerical modelling.

This contribution presents two numerical models of low-temperature plasmas. The first describes the gas dynamics, mixing and the electromagnetic field in a microwave plasma torch used for magnetic nanoparticle synthesis. The other is an afterglow model of a high-frequency plasma jet used for surface sterilisation. The results of the models are compared with plasma diagnostics (Thomson scattering, Rayleigh scattering) and correlated with biomedical experiments carried out at the University of Notre Dame (*E.Coli* inactivation by plasma, inducing apoptosis in cancer cells).

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M24: Composition induced changes in optical response of Si-doped titanium dioxide

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TiO₂ thin films are good candidates for designing optical integrated waveguides or optical devices such as filters or resonators due to their high refractive index and low absorption in the visible range. However, they grow in columnar structure and have a relatively low band gap. Mixed Ti_xSi_yO_z materials open new possibilities in overcoming some of the limitations imposed by TiO₂ material.

In the present work, the variation of Si_xTi_{1-x}O₂ optical constants caused by changed Si concentration are examined by employing Density Functional Theory. Special Quasirandom Structures method is used to generate structural models of Si_xTi_{1-x}O₂ disordered solid solutions for anatase and rutile phases. These initial supercells are structurally optimized (i.e. optimized with respect to the cell shape, size, and atomic positions) using the Vienna *Ab initio* Simulation Package. *Ab initio* Molecular Dynamics approach (“simulated annealing”) is used to generate structural models of amorphous phase. Optical constants of the resulting structures are calculated by the linearized augmented plane wave method as implemented in the Wienzk code together with the recently developed modified Becke-Johnson exchange-correlation potential allowing precise prediction of electronic structure and band gap.

The calculated dielectric function is compared to the experimental data obtained by fitting the optical measurements (ellipsometry, spectrophotometry) carried out on TiO₂ and Ti_xSi_yO_z films prepared by plasma enhanced chemical vapor deposition.

M25: Response of PMMA to simultaneous static and dynamic loading near glass transition

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Discovering the relationship between nano scale segmental dynamics and macro scale mechanical properties of polymer glasses is challenging fundamental scientific problem with extreme technological importance. Deformation behavior of polymer glasses is closely connected to their segment scale relaxation behavior. However, a microscopic theory unambiguously relating nano scale segmental dynamics and packing to the macro scale deformation behavior in glass forming polymers has not been developed, yet. Understanding of the structure-property-function connection could lead to assignment of molecular processes to individual regimes of mechanical response and to better understanding of relaxation behavior of polymer glasses. This could lead to prediction and tailoring of properties of these materials.

Experimental technique combining static and oscillatory mechanical excitations can provide unique data for testing validity of theoretical models of polymer glasses. The experimental set up used here can be considered a non-isothermal creep with superimposed oscillatory small amplitude deformation. The small vibrations force the pre-strained segment scale structures in the supercooled liquid to adapt with temperature accelerating this process. Here, the response of PMMA was investigated by simultaneously applying static and oscillatory load over a wide interval of temperature, frequency and static load. As the result, we found two molecular mechanisms governing two modes of deformation behavior. Different frequency dependences and activation energies of the α -relaxation at T_g and α' -relaxation above the T_g suggested different microscopic processes involved. Based on the experimental evidence, we propose that the α' -relaxation is caused by the intermolecular segment scale process involved in strain hardening.



M26: Separation and detection of bioconjugated QDs in microfluidic devices using capillary electrophoresis

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Semiconductor nanocrystals, also known as quantum dots (QDs), are nanoscale inorganic particles, and have been attract a lot of attention due to their unique optic and electronic properties [1]. One of the most important characteristic is their bioconjugation with different biological materials such as protein, peptides and nucleic acid [2]. Due to very diverse and numerous applications, it is really important to make a tool for precise and controlled detection of QDs. In this study, we investigate on-a-chip detection and separation of QDs. Separation is done by capillary electrophoresis using high voltage and as a carrier fluid, different buffers. Detection is done using UV filter and photodetector including high voltage photomultiplier. In first step mold, microchannels width of 50 μm was made using silicon wafer and photolithography. Next, mixture of the PDMS was completely degassed and pours onto the wafer mold to create transparent, flexible chip. Our first results showed that this method can be used to detected QDs, and separate QDs of different size as well as separate QDs bioconjugated with different biological material. Capillary electrophoresis is powerful separation technique that has been very useful in the analysis of biological material. What characterize this method are simplicity, short analysis time, small sample and reagent requirements, high separation efficient.

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M27: Hydrophilic-like gel-templated porous gold structures

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Surface morphology is a critical parameter influencing the performance of electrodes in electrochemistry. One of the most common ways is the use of a template with a desired 3D structure. Gelatin was previously tested for templating of nanoparticle growth in the solution [i,ii] or for fabrication of sponge-like materials in gel [iii]. Gelatin gel can be hardened to build more rigid structure [iv] in comparison with agarose. We have tested two novel protocols for preparing porous layers. Electrochemical deposition of gold in the gel does not complement the gel structure, but the gel has a strong influence to layer formation. Agarose gel does not have strong mechanical resistance and tertiary structure is broken by forces of growing crystals resulting in large dendrites. In case of gelatin, degree of hardening determine type of structure and its substructure. Electrodeposition in gelatin is the most promising method and resulting structures can be changed in wide range by processing parameters.

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M28: Ion exchange membrane with antimicrobial effect

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The aim of work is to prepare ion exchange membrane with antimicrobial effect used in food industry for filtration of milk. The main problem is to eliminate bacteria from family Enterobacteriaceae such as *E. coli* or *S. aureus* from milk which degrade filtration process and lifetime of membrane by congesting and also contamination of milk can rapidly increase which is unacceptable for final consumers. In this study, antimicrobial effect of membrane will be achieved by utilizing silver nanoparticles prepared by various chemical techniques in colloidal state which brings a big advantage of tailoring properties of nanoparticles (size, shape, optical properties) during the preparation process. The second crucial task is to bind nanoparticles onto surface of polymeric ion exchange membrane. These bonds should be as strong as possible, thus covalent, to avoid contamination of milk by silver nanoparticles which brings another problem; toxicity of nanoparticles. As the mechanism of antibacterial effect of silver nanoparticles is still not clearly known for most of the mammals so consequences of proceeding contamination cannot be predicted properly. Therefore, test of toxicity (MTT test) needs to be done before being applied for milk filtration. Another task is to study growth and adhesion of bacteria on surface polymeric membrane (polypropylene, polybutylene) under various conditions such as temperature or electric field for their effective degradation. In final step, the effectivity and electrochemical function of such modified membrane has to be tested.

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M29: Novel hydrogels based on natural polysaccharide Gum Karaya for soft tissue regeneration

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Natural polysaccharides are biodegradable, freely available, relatively cheap and nontoxic materials. They are widely used in food and pharmaceutical industry. Moreover, polysaccharide based hydrogels are promising for use in medicine. They provide moist environment which stimulates faster wound healing. Hydrogels can be utilized as wound dressing for soft tissue regeneration (e.g. skin burns or ulcers). Gum Karaya (GK) is a natural polysaccharide obtained from *Sterculia urens* tree. GK is anionic polysaccharide containing β -D-galactose, L-rhamnose, β -D-glucuronic acid and D-galacturonic acid. Natural GK is partially acetylated high molecular weight polymer ($M_w \approx 9$ mil Da) insoluble in water. On the other hand, GK is biodegradable and cheap having high swelling and retention capacity, high viscosity and inherent antimicrobial activity. Therefore, GK has good potential to be utilized in medicine. [1 2] The objective of this study is preparation a soluble sample of GK by alkali treatment followed by designing new procedure for GK hydrogel preparation meeting properties of wound healing coverings. Prepared samples were, characterized by SEM, FTIR, NMR, TGA, DSC and rheological evaluated.

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M30: TiO₂ surfaces for photocatalytic degradation of organic pollutants

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Highly ordered TiO₂ nanostructures have great potential as superior photocatalyst due to their valuable surface area, low cost, transparency, chemical stability and nontoxicity. However the activity of pure TiO₂ is only in UV region. This work presents titanium dioxide nanostructured surfaces prepared by anodic oxidation in organic electrolytes containing ammonium fluoride. This method is very cheap, fast, reproducible, and easily tunable. Two approaches were used for fabrication, one-step and two-step anodization of titanium layer, the second one with ultrasonic treatment. The morphology of anodized TiO₂ nanostructures was characterized by scanning electron microscopy (SEM). The obtained TiO₂ surfaces have unique nanoporous structure, with high surface area and ordered configuration. The first nanoporous layer can act as protective layer for underneath nanostructures or as stable matrix for supporting oD metallic nanoparticles in order improve photocatalytic efficiency in the VIS region. According to SEM, TiO₂ nanoporous film was almost two times higher (about 2 μm) than original Ti layer. More TiO₂ material leads to increase of charge-carriers photogeneration, which is important for intended degradation of resistant organic pollutants from water and wastewater [1,2].

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M31: Detection of separating defects during FDM 3D printing

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This paper is dealing with online optical detection of very common failures happening during 3D printing technology called Fused Deposition Modeling (FDM) by using CCD camera.

Additive manufacturing like FDM is mostly used in automatic system designs without persistent supervision of operator. However, these days are under automated control effectors of printer's nozzle and stepping motors but no during-process quality inspection is used. This means that 3D printing is without feed-back control – when a print get defect and starts to distinguish from a print model the printer cannot recognize. That might cause higher time and money losses compared to early detection.

This project uses CCD camera to obtain a bitmap of a print and applies advanced computer vision techniques on it. When a layer is finished the surface of a print is analyzed and the program delivers deviation of separating material laying above its fundament. Then a simple AI determines whether the process shall be stopped or not or whether an operator shall be informed. This depends on cross-section, used material (like ABS, PLA, etc.), actual layer count, temperature and other parameters of printed material which may influence whether is still possible that printer's hot nozzle may "repair" previous separating layer or not.

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M32: Structural properties of Ge microcrystals on Si investigated by X-ray diffraction

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Monolithical integration of different material layers is increasingly required during fabrication process of modern semiconducting optical and electronical devices. Keeping heteroepitaxial structures defect free however becomes complicated, when lattice parameters and thermal expansion coefficients of used materials are mismatched. Misfit and threading dislocations arise from the interfaces where lattice parameters do not match and different thermal expansion coefficients cause wafer bowing and cracks when temperature of heterostructure changes.

These fabrication obstacles can be prevented by replacing the flat substrate by the one patterned into a periodic array of pillars [1]. The high growth rate deposition on these pillars forms completely relaxed, separated microcrystals where the defects are localized only in a small area around the interface with substrate [2]. The crystals can be grown up to height of several tens of micrometers with space filling up to 96 % [1].

In this work, we have studied several samples of Ge microcrystals deposited on Si substrates with different patterning geometry by high-resolution x-ray diffraction technique using reciprocal space mapping and by scanning electron microscopy. As a result, we have discussed dependency of Ge layers crystal quality, obtained as diffraction peak width, on the Si substrate structure parameters.

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M33: Optical chemodosimeter sensor for determination of organic molecules having thiol group

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Analysis of biologically important molecules having thiol group is important task that requires development of fast, inexpensive and practical method for their determination [1].

The azodyes are widely utilized chromogenic and fluorogenic reagents for determination of various metal ions. Unfortunately, the determination of metal ions is in some cases hampered by the presence of interfering anions and organic molecules, which impact the change in color/fluorescence of the dye-metal complex. This apparent liability can, however, can be used for determination of some these analytes. We found that the changes in optical properties of metal-reagent complexes in aqueous solution due to a ligand substitution reaction are sufficient to establish optical chemodosimeter sensor for analysis of some organic molecules having thiol group.

Acknowledgement: The research was supported by EU program (project CEITEC CZ.1.05/1.1.0/02.0068).

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M34: Calcium partially stabilized ZrO₂ ceramics nanocrystals

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Zirconia ceramics have several advantages over other bioceramic materials, due to the transformation toughening mechanisms acting in their microstructure, which can impart the components made out of them very interesting mechanical properties. The Y₂O₃ partially stabilized zirconia (Y-PSZ) is the most typical and the most often studied. However by substitution of Y³⁺ ions with biogenous Ca²⁺ ions we can achieve more biologically active material while maintaining similar mechanical properties.

The aim of this study is to prepare a nanocrystalline partially CaO-stabilized ZrO₂ (Ca-PSZ) and to find the proper molar concentration of Ca²⁺ ions and calcination temperature for the highest content of tetragonal phase in Ca-PSZ system using the sol-gel method. By varying the calcium molar concentration (2.5, 5, 11, 17, 18.5 and 50 %_{mol}) and calcination temperature (700 – 1200 °C) the percentual amount of crystalline phases (monoclinic, cubic, and tetragonal) varied, as was observed using the XRD analysis. Morphology and the chemical composition of the product were studied by the SEM/EDX analysis and the surface area was determined by the BET analysis. Then the hydrothermal reaction of 5%_{mol} Ca-PSZ was done. By the XRD analysis the amount of amorphous and crystalline phase as well as the composition of the crystalline phase, were determined.

M35: Preparation of magnetic nano-sized iron oxide particles

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Powder catalysts are of great advance over the world due to the high surface area, considering the kinetics proceeds through heterogenous phase boundary catalysis. Formation of nano-sized iron oxide particles such as maghemite $\gamma\text{-Fe}_2\text{O}_3$, hematite $\alpha\text{-Fe}_2\text{O}_3$ and magnetite Fe_3O_4 is of great interest for their multiply use in industrial applications such as; medicine, catalysis, sensors, memory devices and electronics. Among many advantageous properties of these nanoparticles such as high surface volume, ease of surface modification and adsorption, the magnetization plays significant role in their application.

Previously many synthetic methods for preparation of tailored particles of iron oxide were developed including coprecipitation, microemulsion, laser pyrolysis and hydrothermal synthesis. Among them, coprecipitation of ferrous and ferric salts in water solutions is very common and easy way to produce quite uniformed particles. As coprecipitation is kinetically driven process, the control of produced iron oxide and size distribution is of great interest, resulting in examination of many kinds of ferrous and ferric salts for formation of magnetic iron oxide particles.

This work discuss simple one-step precipitation method for magnetic iron oxide production from solution of Mohric salt $(\text{NH}_4)_2\text{Fe}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ in order to evaluate the composition of prepared iron oxide variety due to the pH in which precipitation occurred.

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M36: Physical Vapour Deposition of As-Te glass layers and Mass Spectrometry analysis

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The aim of this work is to introduce the preparation and analysis of chalcogenide glass thin films. Chalcogenide glasses show remarkable optical or physico-chemical properties and are finding applications in electronics, computer technology, optoelectronics, optical modulation, energy generation, and optical sensors. Arsenic tellurium glassy layers were prepared via Physical Vapour Deposition (PVD) – thermal evaporation from As-Te mixtures [1]. Interaction of tellurium with arsenic was studied via laser ablation synthesis using Laser Desorption Ionisation Time of Flight Mass Spectrometry (LDI TOF MS) which has a high potential for generation of new compounds. Clusters of As-Te were generated using nitrogen laser while stoichiometry of As_mTe_n was determined via analysis of isotopic envelopes and computer modeling. Scanning Electron Microscope (SEM) was used for characterization the topology of deposited layers and Energy Dispersive X-ray spectroscopy (EDX) was used for evaluation the distribution of arsenic and tellurium in layer. Laser ablation synthesis with LDI TOF MS shows formation of As_mTe_n clusters. Distribution of arsenic and tellurium in cross section of layer was homogenous. New As-Te glass layers were manufactured and analyzed. Determined stoichiometry of As-Te clusters might inspire the development of new chalcogenide materials.

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M37: Optical modeling of bulk-heterojunction organic solar cells based on squaraine dye as electron donor

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Recently, the organic photovoltaic (OPV) cells based on low molecular weight semiconductors are a subject of continuously growing interest as promising low-cost alternative of Si-solar cells, which are currently dominating the market. Despite the significant progress, attained in the last few years, the efficiency of light conversion into electricity in a single device remains considerably lower than this of their inorganic counterparts. Obviously, much effort is still needed to achieve tangible progress in the basic understanding of the processes determining the generation of photovoltaic energy in OPV devices, in the synthesis of new materials and the development of advanced concepts for their design.

In the present work a symmetrical n-hexyl substituted squaraine dye, labeled as Sq1, was synthesized by optimizing a method, proposed recently in the literature. The structure and electronic properties of the dye were studied by means of density functional theory calculations. Further, optical modeling based on transfer matrix method was performed to predict and improve the photovoltaic performance of a bulk heterojunction (BHJ) cell with active layer from a solid-state blend of Sq1 and the PC₆₁BM acceptor. The influence of inserted PEDOT:PSS hole transporting layer as well as optical spacers from ZnO and C₆₀ layers on the optical performance of the model OPVs was also studied. On the basis of the results obtained the perspective for application of the synthesized squaraine dye as electron donating component of active layers in real OPV devices has been discussed.



M38: Early inflammatory response in rat brain after subarachnoid haemorrhage

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Laser Desorption Ionisation Time Of Flight Mass Spectrometry (LDI TOFMS) was applied for (i) laser ablation synthesis and (ii) to elucidate structure of chalcogenides via analysis of clusters formed via LDI of chalcogenide glasses. E.g., nanogold-Te nano-composite was found as a suitable precursor for laser ablation generation of new gold tellurides [1].

On the other hand, the clusters generated via LDI from chalcogenide glasses, especially from Ge-As-Te and Ge-Sb-Se systems, possess to a certain extend part of the original structure - the following bonds were identified in the structures: Ge-As, Ge-Sb, Ge-Se, Ge-Te, As-Te, Sb-Se, Sb-Sb, Se-Se, and Te-Te [2,3]. Concluding, LDI TOFMS is destructive technique but it was proved that it is useful tool for structure elucidation of this kind of inorganic materials.

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M39: The influence of ionic strength on aggregation of mixed liposomal system with polyelectrolyte

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Hyaluronic acid is biocompatible and biodegradable polysaccharides composed of alternating disaccharide units with inter glycosidic linkage [1].

By mixing of biocompatible zwitterionic phospholipid with cationic lipid we get composite structures with improved mechanical stability [2] which could be utilized in interactions with polyelectrolyte.

This work is based on studying of formation of mixed liposomal systems and of interactions of these mixed systems with hyaluronic acid in water and physiological solution.

Systems were studied using fluorescence spectroscopy. Pyrene was utilized as a fluorescence probe because of its sensitivity to polarity of the local environment [3]. The decrease of pyrene emission polarity index was monitored with increasing concentration of lipid mixture. Critical aggregation concentration was obtained, suggesting the formation of aggregates or a change of an aggregate character.

Two mixtures with different ratio of phospholipid and cationic lipid were studied. In all cases, the addition of hyaluronan caused the precipitate formation and the increase of ionic strength influenced the value of critical aggregation concentration.

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M40: Synthesis of carbon nanosheets using microwave plasma torch at atmospheric pressure

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Graphene and graphene related materials are rapidly progressing field in many areas of basic and applied research. In our work we study possibilities of synthesis of graphene nanosheets consisting of 1 or several graphene layers with rectangular shape and typical size of hundreds of nanometers by hydrocarbon (ethanol, toluene) precursor disintegration in microwave torch discharge (2.45 GHz, 140-350 W) while applying atmospheric pressure conditions. Hydrocarbon precursor is introduced by carried gas (argon, 700-2800 sccm), in given, center or outer, channel of our nozzle. The torch discharge is ignited in argon (250-1000 sccm) flowing through the central channel. The plasma torch system is enclosed in quartz tube (8 cm diameter, 20 cm length) with flanges. The synthesized material is collected on single, four or six silicon substrates (depending on the top flange configuration) located below the top flange or from the tube wall. The deposition process (discharge power, gas flows, substrate temperature) is investigated with aim to obtain maximum amount of single layer graphene. Such prepared samples are analyzed by scanning and transmission electron microscopy, Raman spectroscopy and energy-dispersive X-ray spectroscopy (EDX). The discharge was examined using optical emission spectroscopy.

M41: Biofeedback and modern imaging methods for rehabilitation

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Nowadays, assessment of functional changes of human musculoskeletal system is based primarily on subjective evaluation of physiotherapists, orthopaedist and rehabilitation specialists. Expert community lacks appropriate objective methods for quantification of functional changes such as muscular imbalance or uncoordinated posture of a body segment. Specialists also lack a possibility to objectively assess effects of targeted rehabilitation. Since it is impossible to objectively evaluate positive changes of conservative therapy, arthroscopic surgery is oftentimes performed, irreversibly disrupting surrounding tissues. Besides the direct invasive intervention in the integrity of the body segment, there are other disadvantages of surgical intervention: the surgery itself is expensive and time demanding, and convalescence of patients is long.

Thus our goal is creation of new possibilities of non-invasive diagnostics of ankle-joint and in-depth assessment of functional posture of extremities in static posture, potentially in dynamic posture too.

Basic requirement is establishment of external referential points on the lower extremity. Mutual spatial arrangement of these points will provide predictive value about the position of internal structure. Such referential points will be recorded by modern imaging sensors. One of the possible suitable sensors is Kinect One from Microsoft. Contrary to common colour cameras, Kinect One allows in-depth 3D sensing of the scene which enables high quality reconstruction of the scanned part of the patient's body, especially more faithful kinematic bone model. Compared to other typically used optical proximity sensors, Kinect One is cheaper while providing sufficient parameters important for the given application (space as well as length resolution, framerate, latency, etc.).



M42: Preparation of conductive microcontacts

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Preparation of conductive contacts (electrodes) in huge amount is crucial for the development of solar cells and sensors. An example could be a matrix of gold electrodes ($500 \times 4000 \mu\text{m}^2$) for solar cells on a SiO_2/Si wafer for chip expander contacting. We have tried three approaches for preparing this type of electrodes. The first method was Electron beam lithography (EBL). Due to the beam spot size in the nanometre region EBL is inappropriate for microcontacts preparation (time consuming approach) [1]. The second method was the UV Lithography approach with a special mask with an anti-reflex coating layer. A disadvantage of this method is the starting price of the mask with the anti-reflex layer starting from 400 €. This method is very useful for mass production but not for prototyping due to the fixed design of the mask. The last method was direct UV laser writing [2]. This approach allows designing and redesigning electrodes very fast because masks are not needed. Other advantages are the speed of lithography (usually 20x faster than EBL) and the preparation of UV lithography masks for mass production of contacts for lower price than 400 €. At the end the direct UV laser lithography approach was the most suitable for developing of conductive contacts. We are currently using this approach for developing contacts for our Schottky solar cells and sensors.

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M43: Modeling of EDLC supercapacitors for on-body biosensor systems powering

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Standalone sensor systems, especially on-body biosensor networks, have to be powered by small, unobtrusive and maintenance free power sources. An energy harvesting power sources which collect energy from the environment should be used for this purpose. For energy accumulation, special types of energy storage components should be used. Electric double layer capacitors (EDLC) are well suited for long term and low power energy storage. The EDLC supercapacitors are designed as high power density energy storages. Due to this fact, they have unique electrical characteristics which are different from other capacitors. Novel models, characterization techniques and simulation of the EDLC supercapacitor behavior are discussed in this work. A standard parallel RC equivalent circuit is usually used for EDLCs modelling. A series-parallel equivalent circuit was studied in our work as an alternative model. This model precisely respects physical behavior of the real EDLCs but it is more difficult to be calculated than the parallel model. We have used analytical mathematical methods against the numerical methods for complex description of the equivalent circuit. Hereby, the inner behavior of the EDLC should be studied from the results of calculated equations. The results of the calculations were used for simulation model design. This model was simulated in SPICE environment and results were compared with characteristics measured on the real device samples. The comparison showed the acceptable approximation of the real EDLC characteristics by four-stage equivalent circuit.

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M44: Effects of crack-flanks roughness in the vicinity of crack front

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Present studies in linear-elastic or elastic-plastic fracture mechanics are mostly aimed at idealized crack geometry - crack surfaces are ideally planar or kinked on the macro-scale. This study is focused on numerical modeling of cracks with imperfections on the crack surfaces and on the crack front on the micro-scale level for pure shear loading (remote mode II) in Compact-Tension-Shear (CTS) specimen which is commonly used for experiments under shear loading [1,2]. The real crack surface mostly contains micro-deviations which represent either rough crack surfaces and rough crack fronts (both in the direction and normal to the macroscopic crack plane) or kinked crack [1]. These small changes in shape of crack faces have in some cases influence on the fracture parameters. This influence is based on the shape of crack front and crack surfaces and on the magnitude of their roughness. Numerical calculations in this work showed that the remote pure mode II loading applied on CTS specimen results to local mixed mode I+II+III loading at the tortuous crack front. The global ratio of values of stress intensity factors (SIFs) was still very close to pure mode II loading but local presence of mode I loading caused a local crack closure or opening which may have impact on the crack driving force.

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M45: Short fiber reinforced thermoplastic composites

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Polymer composites are one of the most progressive and performing materials born in past century with wide sphere of applications. They are based on polymer matrix and different kind of reinforcement and they considerably overcome the properties of neat polymers. Their mechanical properties are strictly driven by structure and mechanical properties of components [1]. Traditional manufacturing technologies are employed to fabricate composite parts with sufficient short and economical production cycle. In this work, simple melt mixing and further compression molding was used to fabricate composites. Amorphous thermoplastic polymers - PMMA and PC were used as matrix and short glass, carbon and novel PBO (poly(*p*-phenylene-2,6-benzobisoxazole)) fibers were used as reinforcement. Mechanical properties of composites were determined by tensile test and influence of fiber volume fraction, orientation and length on the tensile modulus, strength and strain was investigated. Significant enhancement of stiffness and strength was achieved by addition of glass and carbon fibers. Addition of PBO fibers had negligible effect on mechanical properties caused by poor adhesion and creating of fiber bundles. Experimentally measured data of tensile modulus were compared with Halpin-Tsai model, with the respect to the decrease of fiber length, showing fair good match for low fiber contents. Scanning electron microscopy was employed for observation of structure that showed weak adhesion and increasing number of transversely oriented fibers at higher fiber volume fractions.

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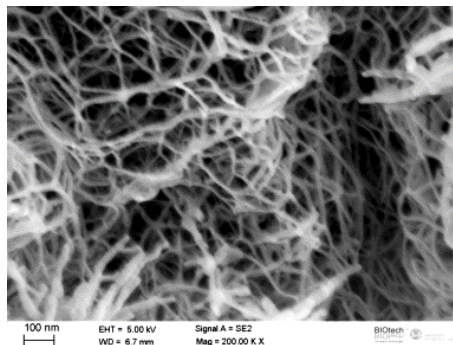
M46: New atellocollagen processing method and preparation of collagen gels

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Atellocollagen is a nonimmunogenic material widely used in medicine and Tissue Engineering. It is usually dissolved by acid and quickly neutralized by buffer and base which induce gel formation. These gels contain fibers few hundreds nanometers thick, which makes the gel partly cloudy. This work introduces continuous dissolution and neutralization process which forms fully transparent gels with much smaller fiber sizes. We demonstrate that our process does not disrupt secondary structure of collagen (SDS-PAGE, Circular Dichroism), extent of swelling was characterized by rheology and SEM was used for gel morphology imaging.



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