4th George Olah Conference

XX Conference of the George Olah Doctoral School

26 September 2022

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4th George Olah Conference

26 September 2022

Program

EVENT VENUE: BME CHC14

Online streaming (only morning sessions): YouTube

8^{30} **Opening – Prof Dr. László Poppe**

ORAL PRESENTATIONS

Chairman: **Prof Dr. László Poppe**

8^{35}-9^{05} **Dr. Brigitta Nagy** – Mathematical modeling for modernizing the development and quality assurance of pharmaceuticals – Invited lecturer, George Olah Prize winner in 2021

9^{05}-9^{35} **Dr. Antal Kováts** – Industrial research and academic cooperation at Furukawa Electric Institute of Technology – Invited lecturer from Furukawa Electric Institute of Technology

9^{35}-9^{55} **Dr. Zsolt Rapi** – Carbohydrate-based crown ethers – Invited lecturer from the Department of Organic Chemistry and Technology

9^{55}-10^{15} **Dr. Viktória Feigl** – Re-use of bauxite residue: 15 years of research at BME – Invited lecturer from the Department of Applied Biotechnology and Food Science

10^{15}-10^{40} **Coffee Break**

Chairman: **Prof Dr. László Nyulászi**

10^{40}-11^{00} **Prof. Dr. Krisztina László Nagyné** – Carbon beyond adsorption– Invited lecturer from the Department of Physical Chemistry and Materials Science

11^{00}-11^{20} **Dr. Lajos Höfler** – Investigating Electrochemical Devices in the 21st Century: Experimental Approaches and Machine Learning Methods – Invited lecturer from the Department of Inorganic and Analytical Chemistry

11^{20}-11^{40} **Dr. Róbert Kun** – Supercritical carbon dioxide assisted synthesis of ultra-stable sulfur/carbon composite cathodes for Li-S batteries – Invited lecturer from the Department of Chemical and Environmental Process Engineering

11^{40}-12^{25} **Prof. Dr. Hansjörg Grützmacher** – Functional groups for organophosphorus chemistry – Invited lecturer from Eidgenössische Technische Hochschule, Zürich, Deputy head of Laboratory of Inorganic Chemistry

12^{25}-14^{00} Break

14^{00}-15^{00} Poster session – 3rd floor

Jury: Dr. László Hegedűs, Dr. Mónika Molnár, Dr. Benjámin Gyarmati

P01	Samantha Kathiuska Samaniego Andrade	Effect of GO dopping on N, S co-doped carrageenan-based porous carbon.
P02	Niloofar Bayat	Synthesis and characterization of some metal complexes: ammine complexes of cobalt
P03	Vajk Farkas	Biodegradable polymer synthesis via acyclic diene metathesis (ADMET) polymerization
P04	Hamsasew Hankebo Lemago	Fabrication and characterization of ZnO and ZnO-Al_2O_3 composites inverse opals by thermal and plasma-assisted ALD for photocatalysis
P05	Bettina Rávai	Multicomponent reaction of isatins, beta-ketophosphonates and primary amines
P06	Bence András Sármezey	Tunable thermoresponsive behavior of N,N'-diethylacrylamide and poly(ethylene glycol)acrylate and poly(ethylene glycol)methacrylate based copolymers
P07	Gergely Solymosi	Towards accurate control of surface charge of gold nanoporous membranes through covalent surface modification
P08	Kármen Szabó	Synthesis of potentionally biologically active acyclic aminophosphonate derivatives
P09	Zsuzsanna Szalai	The synthesis of hydroxymethylene-bisphosphonate derivates and their rearranged products by the Pudovik reaction
P10	Lan Yi	Drug formulation by electrospinning fibers from water soluble polymers: encapsulation and drug release
P11	Ábel Zsubrits	Investigation of the electrochemical ferrate synthesis: comparison of pure iron and white cast iron electrodes
P12	Amer Aljamal	The utilisation of phytic acid as a reactive flame retardant in a fully biobased waterborne epoxy system
P13	Réka Babai	Maintenance of genomic integrity in the malaria parasite Plasmodium falciparum

P14	Marcell Bohus	Atomic layer deposition surface-modified carbon nanosphere and carbon nanopowder nanofluids for thermal conductivity enhancement
P15	Balázs Decsi	Investigation of the biomimetic oxidation of Chloroquine in continuous flow mode
P16	Kata Enikő Decsov	Silica-based microfibrous structures for the flame retardancy of poly(lactic acid)
P17	Júlia Domján	Stability study of infliximab in electrospun and liquid formulations containing HPβCD
P18	Milán Ferdinánd	A novel approach to the impact modification of PLA
P19	Eszter Holub	Effects of thymidylate synthase inhibitors on cell cycle and cell viability
P20	Koppány László Majzinger	Effect of HHP treatment on the quality characteristics of mangalica flesh and bacon
P21	Reem Mourad	Studying the changes in probiotics fermented egg white drink during storage time
P22	Zoé Sára Tóth	Examination of structural basis of proteinaceous *M. tuberculosis* dUTPase inhibition
P23	Zalán István Várady	Investigation of rheological properties and thermal conductivity of SiO_2-TiO_2 composite nanofluids prepared by atomic layer deposition
P24	Dorottya Vaskó	Development of inline monitoring technology for diagnostic protein purification and filtration

STUDENTS' ORAL PRESENTATIONS

Section A – CH201

Chairman: Prof Dr. Miklós Kubinyi

15^{00}-15^{15} **Aiman Aitkazina** – Synthesis of novel sulfur-containing amphiphilic polymer conetworks

15^{15}-15^{30} **Andor Vancza** – Studying the ultrafast dynamics of Fe(II) coordination complexes

15^{30}-15^{45} **Daniel Karajz** – Photocatalytic photonic inverse opals crystals

15^{45}-16^{00} **Sarah Morais Bezerra** – Reaction mediated quantum bit generation in silicon carbide

Section B – CH308

Chairman: **Prof Dr. Béla Pukánszky**

15^{00}-15^{15} **Álmos Botond Orosz** – Population balance based modeling of diastereomeric salt crystallization process of pregabalin tartrate

15^{15}-15^{30} **Dóra Fecske** – Amphiphilic ABA triblock copolymers as self-assembling drug delivery systems with extraordinarily high solubilization capacity

15^{30}-15^{45} **Jonathan Wavomba Mtogo** – Comparison of extractive distillation and pressure-swing distillation for tetrahydrofuran dewatering: energy and controllability

15^{45}-16^{00} **Petra Záhonyi** – Continuous integrated production of glucose granules with enhanced flowability and tabletability

16^{00}-16^{20} Coffee Break

Section A – CH201

Chairman: **Prof. Dr. Krisztina László Nagyné**

16^{20}-16^{35} **Anna Petróczy** – Synthesis and characterization of polystyrene-l-poly(dimethylsiloxane) conetworks

16^{35}-16^{50} **Daniel Janos Incze** – Mycotoxin inactivating enzymes as feed additives

16^{50}-17^{05} **Nikolett Nagy** – Discovery of novel isoforms of the human DUT gene

17^{05}-17^{20} **József Kozma** – Solid-contact ion-selective electrodes based on redox-functionalized carbon nanotubes for improved potential and batch-to-batch reproducibility

Section B – CH308

Chairman: **Prof Dr. Alfréd Kállay-Menyhárd**

16^{20}-16^{35} **Mihály Mátyás Rudolf** – Synthesis and properties of spinel nanocrystals with X-ray excited optical luminescence

16^{35}-16^{50} **Áron Bajcsi** – New types of nanohybrids based on polymer conetworks

16^{50}-17^{05} **Ali O. Imarah** – Development of new enzyme-coated magnetic nanoparticle (MNP)-based bioreactors

17^{05}-17^{20} **Zsófia Bognár** – In situ silver nanoparticle coating of virions for quantification at single virus level

17^{35} Closing – CH201 – Prof Dr. László Nyulászi

ABSTRACTS

ORAL PRESENTATIONS – MORNING SESSIONS

MATHEMATICAL MODELING FOR MODERNIZING THE DEVELOPMENT AND QUALITY ASSURANCE OF PHARMACEUTICALS

Brigitta Nagy[1*], Botond Szilágyi[2], Dorián László Galata[1], Attila Farkas[1], Zsombor Kristóf Nagy[1], György Marosi[1]

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In the new century, the Industry 4.0. concept started to transform the manufacturing industries, fueled by digitalization, automation, and the tremendous amount of data collected during the processes. It has also brought a paradigm shift in the pharmaceutical industry, aiming for more efficient and agile drug development and manufacturing, supported by the Quality by Design (QbD), Process Analytical Technology (PAT), and Real-time Release Testing (RTRT) regulatory frameworks[1]. These new concepts require implementing several modern techniques, such as big data analytics, artificial intelligence, and digital twins, leading to the ever-increasing importance of mathematical modeling[2].

This talk will provide an overview of possible approaches and applications of mechanistic (first principles) and empirical (data-based) mathematical models. First, the development of a digital twin is presented to analyze the system-wide performance of the continuous manufacturing of acetylsalicylic acid (ASA) based on population balance modeling (PBM). Second, mechanistic (PBM), and empirical (artificial neural network, ANN) models were developed to predict the quality (e.g., in vitro dissolution) of the ASA final formulations (tablets, capsules) based on non-destructive NIR- and Raman-spectroscopic measurements. In this way, the RTRT of the products could be achieved. The results showed that mathematical modeling could play an essential role in supporting the development and quality assurance of pharmaceuticals throughout the manufacturing process.

This work is supported by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences and the ÚNKP-22-5 New National Excellence Program of the Ministry for Innovation and Technology from the source of the National, Research, Development and Innovation Fund.

[1] Rantanen, J., Khinast, J. *J. Pharm. Sci.* **2015**, 104, 3612-3638.
[2] Arden, N.S., et al. Int. J. Pharm. **2021**, 602, 120554

INDUSTRIAL RESEARCH AND ACADEMIC COOPERATION AT FURUKAWA ELECTRIC INSTITUTE OF TECHNOLOGY

Antal Kovats*; [1]

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How can an industrial company cooperate with academic partners?

This presentation will introduce the Furukawa Electric company: a Japanese company with wide range of business. It will be explained how the company organizes its R&D globally. The special requirements of industrial and academic research will be discussed.

The difference in research topic selection and project initialization will be explained with some examples. Although the way of conducting research have a lot of similarities the motivation is usually very different. I present the four strategies that can be used to help a firm grow and also analyzes the risk associated with each strategy.

Then I will show the cooperation examples between Budapest University of Technolgy and Economics and Furukawa Electric Institute of Technology (FETI).

It will include treatment of polypropylene sheets with a superhydrophobic surface made with a phase separation method. As another example material simulations related to clusters for CO2 activation will be explained. It was done in cooperation funded by the KU Leuven–Budapest University of Technology and Economics joint research funding (CELSA) and the European Union's Horizon 2020 research and innovation program(CATCHY).

CARBOHYDRATE-BASED CROWN ETHERS

Zsolt Rapi*

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The most modern, most economical and easiest way to prepare pure enantiomers is the asymmetric synthesis in the presence of chiral auxiliaries or chiral catalysts. Chiral crown ethers are a special type of chiral catalysts that can be used under phase transfer conditions and are capable of inducing asymmetric induction. By asymmetric phase transfer catalysis, chiral epoxides, Michael adducts, cyclopropane derivatives, phosphonates, fluorinated compounds, etc. can be synthesized which are potentially biologically active substances or intermediates. It has been found that the type of the monosaccharide, the substituents on the sugar unit and the side arm on the crown ring, have significant influence on both the yield and the enantioselectivity. It has been proven that the most efficient catalysts are monoaza-15-crown-5 type macrocycles annulated to a monosaccharide unit and incorporating a side arm on the nitrogen with three carbon atom. Therefore, this structural motif was retained and several derivatives of these macrocycles have been synthesized in our research group. A few representatives of the monosaccharide-based crown ethers induced a considerable asymmetric induction in certain reactions (in liquid-liquid and solid-liquid systems). In each asymmetric reaction, different catalysts showed the best results, however, crown compounds incorporating a D-glucose, or a D-galactose moiety proved to be the most efficient catalysts. A $(CH_2)_3OH$ substituent on the nitrogen atom resulted in the best enantioselectivity in the liquid–liquid reactions, while in solid–liquid systems, $(CH_2)_3OCH_3$ and 2-(3,4-dimethoxyphenyl)ethyl groups also enhanced the asymmetric induction. [1]

[1] Orbán, I.; Bakó, P.; Rapi, Zs. *Chemistry* **2021**, *3*, 550-577.

RE-USE OF BAUXITE RESIDUE: 15 YEARS OF RESEARCH AT BME

Viktória Feigl

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Bauxite residue (or red mud) is a solid waste produced during alumina extraction from bauxite ores. Bauxite residue has highly alkaline characteristics and a high sodium content (as the Bayer-process applies digestion with hot sodium hydroxide), small particle size, and contains several elements: Fe, Al, Ti, Si, Ca, Na as main components, nutrients (P) and economically valuable critical raw materials (CRMs) (Sc, Ga, Cr) and rare earth elements (REEs). Bauxite residue (BR) is deposited in large quantities (est. 2.7 billion t) worldwide, posing potential risks to the environment and humans, therefore, novel technologies for its re-use are needed. These technologies may focus on BR reuse in construction (as the component of cement), chemical industry (as a catalyst), mineral processing (as a source of valuable elements) and in environmental applications (adsorbent of water and soil pollutants or soil amendment for degraded or low-quality soils) (review: Ujaczki *et al*., 2019).

The Research Group of Environmental Biotechnology started to apply bauxite residue as a chemical stabilizer for toxic metals and metalloids (Cd, Zn, Pb, As) in contaminated soils and mine wastes several years ago. The chemical, microbiological and ecotoxicological analysis results during the laboratory-scale microcosm studies demonstrated the efficiency of the Hungarian BR immobilizing metals. Later, BR was applied to improve low-quality sandy soils and in municipal landfill cover systems as a component of the cover material. The changes in the soil microbial characteristics after BR amendments were studied in detail, and the microbial activity enhancing effects of the BR were confirmed in addition to other positive effects on the soil's physical and chemical characteristics. The group assessed the environmental impacts of the 2010 Ajka BR catastrophe, where the flood affected several hectares of soil and surface water sediment. Based on the performed studies, it was recommended that a maximum of 5 w/w% BR can be mixed into the soils in the affected area.

Lately, research has focused on the extraction of REEs (included on the list of CRMs by the EU) from BR. A pilot plant was developed in Greece to extract Sc from BR. The plant applies extraction by sulphuric acid at elevated temperatures, followed by a solvent-impregnated resin step. The environmental sustainability of the technology was assessed by ecotoxicological testing according to the green toxicology concept. Other novel methodologies include bioleaching of BR by acid-producing fungi (e.g. *Penicillium* sp.) or autotrophic iron oxidizers (e.g. *Acidithiobacillus* sp.). The future of bauxite residue re-utilization lies in achieving complex, zero-waste and environmentally sustainable technologies.

Acknowledgement: The author is thankful to all co-authors in her bauxite residue related publications, especially Éva Ujaczki, Mónika Molnár, Emese Vaszita, Katalin Gruiz, Orsolya Klebercz, Will Mayes, Markus Lenz and Efthymios Balomenos. The research was funded by various national and international project funds enlisted in the presentation.

Reference: Ujaczki, *et. al.* (2018). Reusing bauxite residues: benefits beyond (critical raw) material recovery. Journal of Chemical Technology & Biotechnology, 93 (9), 2498-2510.

CARBON BEYOND ADSORPTION

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Porous carbon materials have been associated with adsorption processes since their early application in Ancient Egypt. It was in the late 1980s when the up to then neglected importance of carbon surface chemistry was first analyzed in depth, as earlier neither the surface area nor the pore structure were sufficient to explain many of the properties of carbon-supported catalysts [1]. By today porous carbon materials are extensively used as electrodes in energy storage and conversion applications also taking advantage to the electrocatalytic activity of the tailor made surface chemistry.

The electrocatalytic processes on plain carbon may be too slow for practical applications, e.g., in oxygen reduction reaction on fuel cell cathodes:

I. 4-electron pathway: $O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$

II. 2-electron pathway: $O_2 + 2H^+ + 2e^- \rightarrow 2H_2O_2$

$H_2O_2 + 2H^+ + 2e^- \rightarrow 2H_2O$

The discrepancy can be efficiently bridged by Pt loading, which – on the other hand – is an economic obstacle to commerciale these devices. Incorporation of heteroatoms (N, S) and/or conductive carbon nanoparticles offers an alternative route to overcome this challenge, as they act ass extra active sites [2, 3].

The cooperative effect of graphene and heteroatom doping on the electrochemical behavior of well characterized carbon aerogels will be discussed [3, 4].

[1] Voitko, K.; Tóth, A.; Demianenko, E.; Dobos, F.; Berke, B.; Bakalinska, O.; Grebenyuk, A.; Tombácz, E.; Kuts, V.; Tarasenko, Y.; Kartel, M.; László, K. *J. Coll. Interface Sci.* **2015**, *437,* 283–290.

[2] Seredych, M.; László, K.; Bandosz T.J. *ChemCatChem* **2015**, *7(18)* SI 2924-2931.

[3] Nagy, B,; Bakos, I.; Bertóti, I.; Domán, A.; Menyhárd, A.; Mohai, M.; László, K. *Carbon* **2018**,*139*, 872-879.

[4] Andrade, S.K.S. et al: *in preparation*

INVESTIGATING ELECTROCHEMICAL DEVICES IN THE 21ST CENTURY: EXPERIMENTAL APPROACHES AND MACHINE LEARNING METHODS

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Experimental investigation of electrochemical devices (e.g., sensors and batteries) has long relied on laborious experiments, including performing large numbers of electrochemical tests in various combinations. A data-driven approach can drastically reduce the time and effort needed to test various device setups with little prior knowledge about the underlying physical mechanisms. By learning the relevant characteristics from existing experimental data, one can find promising arrangements for future experimental testing. In the past few years, a great number of different methods were applied to simulate the operation of electrochemical devices. Machine learning methods, on the other hand, were successfully applied to many other scientific areas to analyze large amounts of experimental data and find predictive relations among parameters and the performance of electrochemical devices.

When we have a sufficiently sophisticated theoretical model of a system, we can use the device's experimental response to an external stimulus to assess the most essential kinetic and thermodynamic parameters that govern their behavior. In many cases, this can be accomplished by using a simplified model – or even an explicit equation – and fitting it to the experimental data. However, in a large number of situations, simplified models are inadequate. For example, the electrochemical response of many electrochemical devices, such as the complex impedance of a sensor or charging-discharging of a battery, is governed by a complex interaction of the electric field and the diffusing-migrating species. The time-dependent response is not well-described by a simple equation. For these situations, we must resort to more sophisticated models, such as finite element numerical simulations.

Unfortunately, the simulation time of finite element models is on the order of several minutes, which can make the parameter estimation, where thousands of simulations are required, impractical. We have developed a fast method for speeding up the simulation of the electrochemical response in highly nonlinear and time-dependent systems to make parameter estimation feasible. We replace finite element simulations with supervised machine learning algorithms that can provide results six orders of magnitude faster. Two types of algorithms are presented. Feedforward deep neural networks are black-box machine learning models, so exact knowledge of the internal mechanism and reasons behind the output of the network is not accessible to us. However, it is possible to use white-box machine learning models that provide results that are understandable for experts. Symbolic regression – an accurate white-box machine learning technique – automates the process of finding human-readable symbolic expressions that match the observed data. Combining experimental and simulation/machine learning methods in a way that helps both, in turn, provides an ideal and fast feedback cycle, allows to explore a variety of experimental scenarios with reduced experimental costs and can also lead to more accurate theoretical models.

SUPERCRITICAL CARBON DIOXIDE ASSISTED SYNTHESIS OF ULTRA-STABLE SULFUR/CARBON COMPOSITE CATHODES FOR LI-S BATTERIES

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** Corresponding author:* *kun.robert@ttk.hu, kun.robert@vbk.bme.hu*

In this work, we report a simple, rapid, and green route allowing efficient impregnation of sulfur into highly porous and layered structured reduced graphene oxide (rGO) matrix using supercritical carbon dioxide (SC-CO_2) medium to fabricate rGO/Sulfur composite cathode (rGO-S-SCC) for Li-S batteries. Compared to the conventional synthesis techniques involving toxic solvents, the exploitation of nontoxic SC-CO_2 with hybrid properties of "gas-like" and "liquid-like" have unparalleled merits. SC-CO_2 can synchronously tune the layered/porous structure of rGO matrices, rendering plenty of storage space for small sulfur allotropes. SC-CO_2 being a promising hydrophobic solvent with appreciable density guarantees effective Sulfur dissolution at the molecular level and its gas-like diffusivity and viscosity facilitate diffusion and permeation of the dissolved Sulfur into the depth of micropores and mesopores of rGO much rapidly and efficiently. This creates intimate contact of Sulfur with rGO interlayers leading to enhanced electrical conductivity, guaranteeing precise sulfur content, uniform sulfur distribution, and high sulfur utilization efficiency. Utilizing this strategy benefits from the ease in product separation, non-toxicity, non-flammability, recyclability, and the liquid waste problem can also be minimized. The electrochemical performance tests of the prepared cell with RGO-S-SCC cathode, Li metal anode, and 1 M LiTFSi in DME and DOL (1:1 volume ratio) electrolyte showed remarkable initial specific discharge capacity of 991 mAh/g at 0.1 A g^{-1} with a capacity retention of 93.7% even after 200 charge-discharge cycles. The coloumbic efficiency of the cell was maintained at approximately 99% even after prolonged cycling. Through this work, we believe that exploiting SC-CO_2 technology can realize highly efficient sulfur transfer and precise microstructure regulation of S/C composite cathodes for Li-S batteries. This relatively new and facile approach provides new insight into the rational design and controllable synthesis of carbon/Sulfur composite cathodes for Li-S batteries with captivating lithium storage performance.

FUNCTIONAL GROUPS FOR ORGANOPHOSPHORUS CHEMISTRY

Hansjörg Grützmacher

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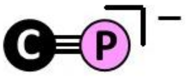
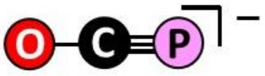
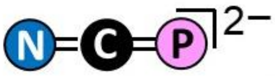
From the elements C,H,N,O the realm of organic chemistry is built and their combination leads to an endless array of molecules. A set of very well established functional groups allows organic chemists to synthesize these conveniently. In main group element chemistry, a very different situation is met and the mutual substitution of "homologous" elements - like nitrogen for phosphorus - looks simple only on paper. The lecture will give an overview on our efforts to generate new functional groups such as cyaphide, phosphaethynolate, or phosphacarbodiimide (as analogues of $[CN]^{-}$, $[OCN]^{-}$, or $[CN_2]^{2-}$). Not surprisingly, everything turned out differently than one thought. But some of these "funny" molecules help to solve fundamental problems in chemistry, such as the mutual conversion of cluster into planar aromatic compounds, while others like bis(acyl)phosphanes assist in the solution of practical problems.



CYAPHIDE



PHOSPHAETHYNOLATE



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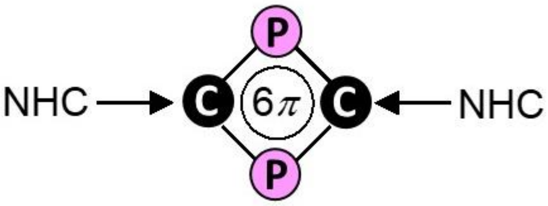
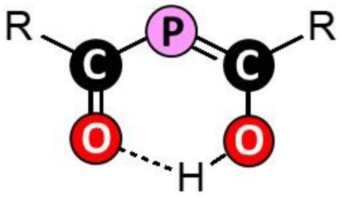
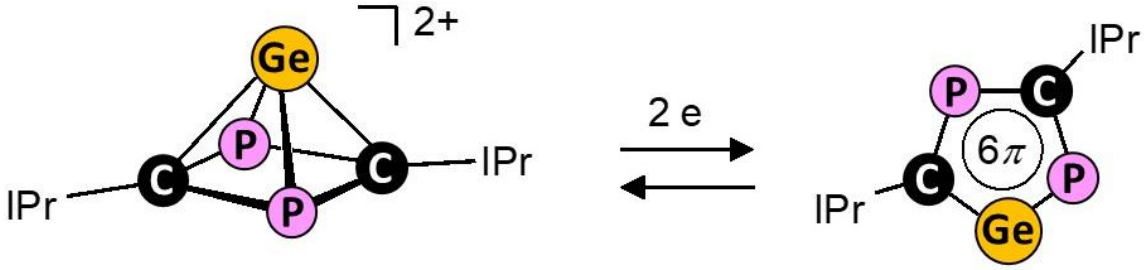


DICARBONDIPHOSPHIDE



BISACYLPHOSPHANE



GERMADIPHOSPHAPYRAMIDANE

DIPHOSPHAGERMOLIDE

ABSTRACTS

ORAL PRESENTATIONS – AFTERNOON SESSIONS

SYNTHESIS OF NOVEL SULFUR-CONTAINING AMPHIPHILIC POLYMER CONETWORKS

Aiman Aitkazina[1,2], Ákos Szabó[1], Béla Iván[1]

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[2] Hevesy György PhD School of Chemistry, Eötvös Loránd University
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In the past few years, sulfur-containing polymers have gained increased interest due to their advantageous properties which make them useful for a wide range of applications. Due to their versatile properties, both chemical and physical, sulfur-containing polymers have been investigated as sensors, controlled drug release matrices, and as new biomaterials.

The main purpose of our research is the systematic investigation of a series of novel classes of amphiphilic polymer conetworks (APCNs) based on polymers with sulfur-containing polymer component. Figure 1 shows the schematic representation of amphiphilic polymer conetworks (APCNs), which are composed of both hydrophilic and hydrophobic polymer chains linked by covalent bond to each other. In the course of our investigations, a special acrylate-telechelic P(DODT-*co*-PEGDA) copolymer was used as macrocrosslinker in the polymerization of the other monomer, methyl acrylate or styrene.

The P(DODT-*co*-PEGDA) copolymer was synthesized by simultaneous Michael-type addition of thiols and double bonds and oxidative coupling of thiols leading to disulfides.[1] This type of reaction shows the features of green chemistry, because of the convenient reaction conditions, that is, ambient temperature and pressure.

The synthesis of the conetworks was achieved by the free radical copolymerization of the P(DODT-co-PEGDA) macrocrosslinker with the comonomer, either methyl acrylate (MA) or styrene. Five different conetworks were synthesized successfully by this method with systematically varying the P(DODT-*co*-PEGDA) copolymer content. Then, the samples went through drying, and their characterization was carried out.

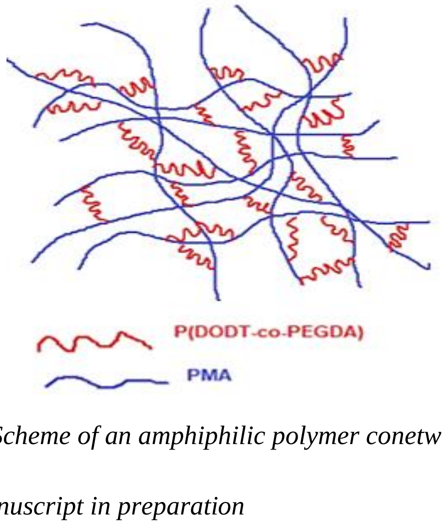

Figure 1. Scheme of an amphiphilic polymer conetwork

[1] Szabó, Á.; Szarka, Gy.; Iván, B. *manuscript in preparation*

NEW TYPES OF NANOHYBRIDS BASED ON POLYMER CONETWORKS

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Amphiphilic conetworks (APCN) are composed of immiscible hydrophilic and hydrophobic polymer chains covalently linked to each other. These materials are not soluble in any solvents but swell in both hydrophobic and hydrophilic media. Due to the covalent bonds, large scale phase separation is prevented, consequently nanophase separation takes place between the immiscible components.

During our research, methacrylate-telechelic polyisobutylene (MA-PIB-MA) crosslinker was applied as the hydrophobic component of the planned amphiphilic conetworks. This was copolymerized with N,N-dimethylacrylamide (DMAAm) to obtain the conetworks. Several APCNs were synthesized with systematically varied compositions. The gel fraction was high (>90%) in every cases. Gold nanoparticles were incorporated into the obtained APCNs by several methods. The effect between the applied methods, both in terms of reduction and the properties of the resulting nanoparticles, was investigated. The catalytic properties of the obtained conetwork-gold nanohybrids were tested in the reduction of 4-nitrophenol. The reduction was followed by UV-Vis spectroscopy between 200 and 600 nm. Our measurements showed that these gold containing nanohybrids have catalytic effect in the investigated reaction. Furthermore, it can be concluded that the composition of the APCNs also affect the catalytic efficiency. The reusability and recyclability of the obtained nanohybrids were also proved by our experiments.

Acknowledgments

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REACTION MEDIATED QUANTUM BIT GENERATION IN SILICON CARBIDE

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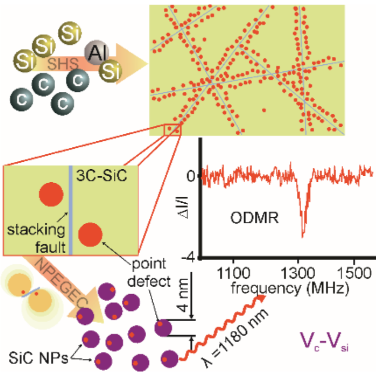
Bulk silicon carbide (SiC) is a wide band gap semiconductor that has useful properties like oxidation resistance, high thermal conductivity, stability and high wear resistance[1]. When this material is reduced to nanosized crystals, new attributes tend to appear because of quantum confinement effect. One of the applications for these NPs is to use them as quantum bits (qubits) by adding different types of defects to the structure, for example, silicon vacancy, carbon vacancy, and divacancy[2].

Vacancy generation, however, is not an easy task, especially in nanoparticles. A well-accepted method is the interaction of the host matrix (i.e., SiC) with high-energy particles, neutrons, ions, or electrons to knock out one or more atoms and subsequent annealing to create the desired vacancy. Such a reaction, however, destroys the crystallinity of the matrix and creates numerous unwanted defects too.

Despite of its extreme stability, SiC can react at high temperatures. We studied the formation of defects by the reaction of SiC and aluminum (Al). Al reacts faster with Si than C of the SiC crystal which can be harnessed to generate Si vacancies.

The paramagnetic defects and color centers formed by our synthesis method were analyzed by electron spin resonance and photoluminescence techniques. We found that the reaction of SiC with aluminum differs in SiC crystal growth and post reactions.



Scheme 1. The complex interaction between SiC and Al.

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IN SITU SILVER NANOPARTICLE COATING OF VIRIONS FOR QUANTIFICATION AT SINGLE VIRUS LEVEL

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In situ labelling and encapsulation of biological entities may provide a versatile approach to modulate their functionality and facilitate their detection at single particle level. [1]

We introduced a novel virus metallization approach based on in situ coating of viruses in solution with silver nanoparticles (AgNP) in a two-step synthetic process, based on the surface activation with a tannic acid – Sn (II) coordination complex, which subsequently induces silver ion (I) reduction. [2] The metalic coating on the virus surface opens the opportunity for electrochemical quantification of the AgNP-tagged viruses by nano-impact electrochemistry on a microelectrode with single particle sensitivity, i.e. enable the detection of particles otherwise undetectable. We showed that the silver coating of the virus particles impacting the electrode can be oxidized to produce distinct current peaks the frequency of which show a linear correlation with the virus count. The proof of the concept was done with inactivated Influenza A (H3N2) viruses resulting in their quantitation down to the femtomolar concentrations (ca. $5 \cdot 10^7$ particles mL^{-1}) using 50 s counting sequences.

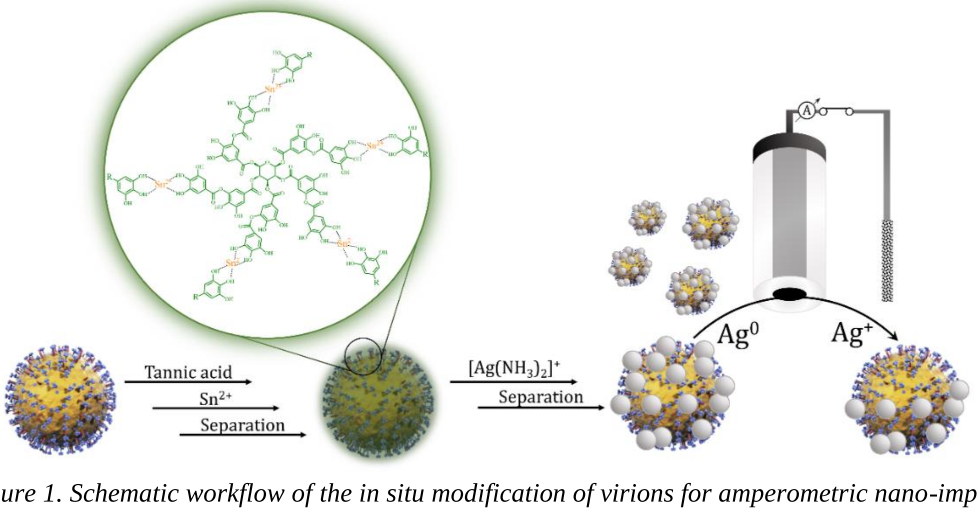

Figure 1. Schematic workflow of the in situ modification of virions for amperometric nano-impact measurements.

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AMPHIPHILIC ABA TRIBLOCK COPOLYMERS AS SELF-ASSEMBLING DRUG DELIVERY SYSTEMS WITH EXTRAORDINARILY HIGH SOLUBILIZATION CAPACITY

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Synthesis, self-assembling and drug delivery properties of biocompatible hydrophilic hyperbranched polyglycerol (HbPG) and hydrophobic poly(tetrahydrofuran) (PTHF) based amphiphilic ABA triblock copolymers and their applicability for drug encapsulation and delivery of hydrophobic drugs were investigated. Block copolymers with varying hydrophilic to hydrophobic ratios composed of different molecular weights of the hydrophilic HbPG blocks were successfully synthesized using amine-telechelic PTHF macroinitiators of three different average molar mass. Above the critical micelle concentration (*cmc*), the ABA triblock copolymers self-assemble into nanosized micelles which can be used for drug encapsulation and delivery of hydrophobic drugs to improve the water solubility and the bioavailability of such agents. The *cmc* values of the synthesized triblock copolymers were very low and changed in accordance with the inner PTHF molecular weight. Furthermore, DLS results proved the formation of nanosized micelles above the *cmc* values. Curcumin, which is a natural anticancer agent with very low water solubility, was used as a model drug to prove the potential application of the self-assembled triblock copolymer micelles as encapsulation and delivery nanocompartments. It was found that the micelles of the prepared triblock copolymers can encapsulate three order of times more curcumin than its water solubility, and the encapsulated drug content can be controlled by the composition of the triblock copolymers, mainly by the molar mass of the inner PTHF block and the concentration of their solutions as well. Stability measurements of the curcumin loaded micelles showed that the size and the curcumin content of the micelles were almost constant even after a week. Sustained drug release of the triblock copolymer micelles was obtained, which can be controlled by the hydrophobic/hydrophilic ratio and the concentration of the encapsulated drug. *In vitro* bioactivity studies of the curcumin loaded micelles were also implemented on U-87 glioblastoma cell line and an optimal composition of the triblock copolymer was found, which show good cellular uptake without toxicity. In summary, the prepared ABA triblock copolymers are promising candidates as advanced drug solubilization and delivery systems.

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DEVELOPMENT OF NEW ENZYME-COATED MAGNETIC NANOPARTICLE (MNP)-BASED BIOREACTORS

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This work aims to show the development and comparison of new bioreactors based on enzyme-coated magnetic nanoparticles (MNP). The enzymes attached covalently to MNPs were a lipase from *Candida antarctica* (CaLB) and an aspartate ammonia-lyase from *Pseudomonas fluorescens* (PfAAL). The surface of the core MNPs was modified with a silica shell and with a mixed function layer being appropriate for enzyme binding.[1,2] The resulting MNP-biocatalysts were tested in three different systems (batch mode, continuous flow static magnetic field (CFSMF), and continuous flow agitation magnetic field (CFAMF) created by 3D printing. First, two kinds of batch mode devices with external magnetic agitation were created. The first design applied two permanent magnets at two opposite sides of a vial with alternating movement along an x-axis direction (XM), while the second design used two permanent magnets rotating around the y-axis of the vial (RM). The effective specific enzyme activity of AAL-MNPs in the traditional shake vial method was compared with the new designs. The next CFSMF design comprised a polytetrafluoroethylene tube (PTFE) and small permanent magnets (6 for the single layer and 12 for the double layer versions) generating magnetic field within the PTFE tube to anchor the biocatalysts. The specific activity was compared in single layers and double layers setup. The third CFAMF mode uses the same principle as the first batch mode version for moving two permanent magnets at two opposite sides around a PTFE tube during the fluid flow into two designs (XM-AFR, RM-AFR).

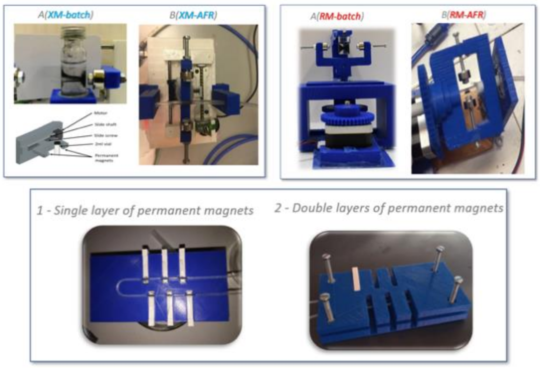

Figure 1. microreactors for different reaction modes.

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MYCOTOXIN INACTIVATING ENZYMES AS FEED ADDITIVES

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Fumonisins are one of the most prevalent mycotoxins produced by certain Fusarium species, that contaminate crops globally, predominantly corn. The most important and prominent substance of the family is Fumonisin B1 (FB1). FB1 inhibits ceramide synthase, an important enzyme of sphingolipid biosynthesis in mammals. The altered sphingolipid metabolism can lead to different serious adverse health effects in humans and animals, therefore crops contaminated with high levels of FB1 should be removed from the food or feed chain. Physical or chemical decontamination of crops is often not effective enough, however, enzymatic detoxification can be a solution to the problem. Fumonisin esterases cleave the two tricarballylic acid groups of FB1, leading to partially and fully hydrolysed FB1 (pHFB1 and HFB1, respectively) (Figure 1) [1]. These metabolites don't inhibit ceramide synthase, therefore possess significantly lower toxicity [2]. Fumonisin esterases are excellent candidates for food or feed additives against FB1 contamination, however, the kinetics and mechanism of these enzymes are not well characterized yet. The aim of the study is to understand the detailed enzymatic mechanism of two of these biocatalysts, to fine-tune already existing products. For that reason, the enzymes were expressed in Pichia pastoris expression system, and kinetic constants were evaluated, with both FB1 and pHFB1 as substrate. It was found that fumonisin esterases selectively produce one of the two possible pHFB1 (Figure 1), and the two enzymes significantly differ in their affinity towards pHFB1. We proposed a reaction mechanism based on our results, although further structure analyses are necessary.

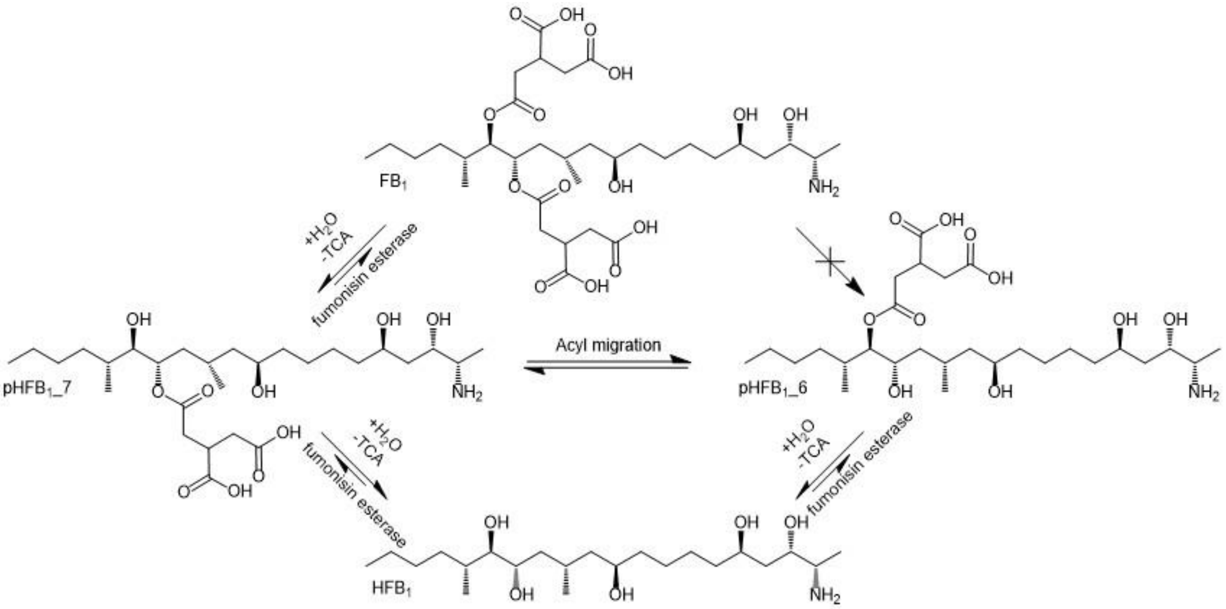

Figure 1. Degradation of Fumonisin B1 by fumonisin esterase

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PHOTOCATALYTIC PHOTONIC INVERSE OPALS CRYSTALS

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Inverse opal photonic crystals have a unique, porous structure which provides a large surface area and interesting optical abilities, like photonic band gap and the "slow" photon effect [1,2]. Special properties of this crystals make the material a candidate for a various applications: sensors, optoelectronics and photocatalysis to name a few [3,4]. The study of opals is also important since it's our template for the final product and has a large impact on it's properties [5].

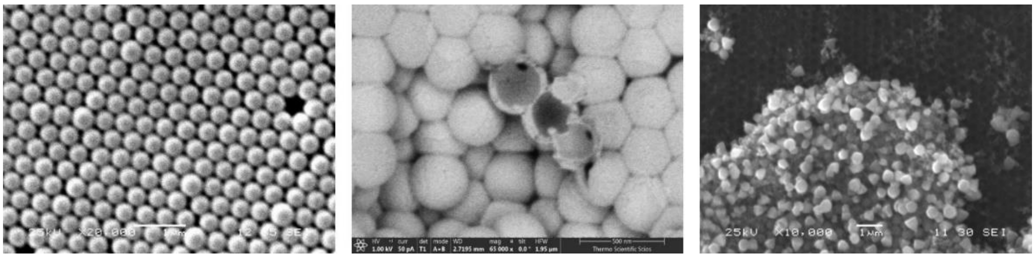

Figure 1. SEM image of polystyrene opal crystal (left), FIB-SEM image of TiO_2 inverse opal (middle) and ZnO inverse opal with nanorods (right).

In this study, I would like to summerize my research of opals and inverse opals. In details this consist of the optical properties of opals made from different sized spheres, combining different sized spheres to opal. The inverse opal studies were done with the aim of the modification of the photonic band gap, what material or structural change has an effect on it. With that in mind, inverse opals with different wall thickness were made by atomic layer deposition (ALD), hierarchical structure of inverse opal and nanorodds were synthesized and currently inverse opals using two different materials are under characterization.

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SOLID-CONTACT ION-SELECTIVE ELECTRODES BASED ON REDOX-FUNCTIONALIZED CARBON NANOTUBES FOR IMPROVED POTENTIAL AND BATCH-TO-BATCH REPRODUCIBILITY

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Solid-contact ion-selective electrodes (SCISEs) have long been the focus of interest during the development of low-cost, compact, miniaturized chemical sensors.[1] Most typically, different electrically conducting polymers and high surface area carbon materials (e.g., carbon nanotubes, graphene, carbon black etc.) have been tested as solid-contacts. However, the need persists for the appropriate material to enable a reliable large-scale fabrication process that provides sensors with excellent potential reproducibility and stability before SCISEs can be widely commercialized as ready-to-use wearable sensors in medical or sport devices with minimal maintenance.[2]

Here, we introduce redox-functionalized multi-walled carbon nanotubes (MWCNTs) as a novel solid-contact type that combines the advantageous properties of purely capacitive materials and redox-couples.[3] To introduce the redox-active functional group we modified MWCNTs with either ferrocene (Fc) or (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO), and used the thus formed material as solid-contact in K^+-ISEs as proof of concept. We applied different approaches (polarization, short-circuiting) to improve the potential reproducibility and stability of the SCISEs. Our investigation has shown that the presence of the redox group enables the E^0 adjustment via pre-polarization before the functionalized MWCNTs are applied as a solid-contact on the substrate electrode, making any subsequent potential improvement step after ISE fabrication unnecessary. The process not only improved the potential reproducibility for a single set of electrodes (SD=0.43 mV for n=6) but proved to provide excellent batch-to-batch E^0 reproducibility as well (SD= 2.13 mV for three batches of 6 electrodes based on TEMPO-MWCNT solid-contact) with a span of one year between the first and the last batch. The manufactured K^+-SCISEs showed excellent potentiometric response and selectivity with no sensitivity to ambient gases (O_2, CO_2) and light and also without any sign of an aqueous layer formation.

ACKNOWLEDGMENT
This research was funded by the National Research, Development, and Innovation Fund of Hungary under Grant TKP2021-EGA-02. Further support was received from National Research, Development and Innovation Fund through ÚNKP-21-3 New National Excellence Program of the Ministry for Innovation and Technology.

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COMPARISON OF EXTRACTIVE DISTILLATION AND PRESSURE-SWING DISTILLATION FOR TETRAHYDROFURAN DEWATERING: ENERGY AND CONTROLLABILITY

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The efficient separation of azeotropic mixtures is a difficult problem and there are different alternatives for such purposes. The extractive distillation and the pressure swing distillation are two competing alternatives. These two alternatives are studied and compared from energy consumption and controllability points of view. The two alternatives are modelled with Aspen Plus. The results of the optimized solutions are compared to obtain efficient help for process design activity.

As far as the energy consumption is concerned, being in agreement with other studies and mixtures[1], the extractive distillation needs less energy than the pressure swing distillation. However, the pressure swing distillation offers an automatic energy-integration option[2]. The condenser of the high-pressure column and the reboiler of the low-pressure column can be matched. Such an energy integration makes the pressure swing distillation competitive.

The controllability study is an integral part of chemical process design. Aspen Plus, Control Design Interface and Matlab are used to determine dynamic controllability indices in the function of the frequency. The indices are aggregated in a desirability function. The results are compared to obtain efficient help for process design activity.

The pressure swing distillation shows better controllability features than those of the extractive distillation. It can be explained that in the case of extractive distillation a third compound, the extractive agent is applied in the system. This third compound eliminates the azeotrope but makes the system more complex. As manipulated variables, the reflux ratios and/or the reboiler heat loads are selected and investigated. The alternatives studied show worse controllability features if the product purity requirement is close to the pure products. Such phenomenon can be observed also in the case of high purity fractionators.

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DISCOVERY OF NOVEL ISOFORMS OF THE HUMAN DUT GENE

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Maintaining the genomic integrity is of utmost importance, therefore in mammalian cells most of the enzymes responsible for DNA repair have many isoforms. The dUTPase enzyme contributes to the safe-guarding mechanisms against uracil incorporation into DNA by catalysing the hydrolysis of dUTP to dUMP [1]. In eukaryotic organisms the dUTPase enzyme is encoded by the *DUT* gene and is also shown in the literature to have a nuclear (DUT-N) and a mitochondrial (DUT-M) isoform with cognate localization signals [2,3]. Here we identified two additional isoforms; DUT-3 without any localization signal and DUT-4 with the same nuclear localization signal as DUT-N. Based on an RT-qPCR method for simultaneous isoform-specific quantification we analysed the relative expression patterns in 20 human cell lines of highly different origins. We found that the DUT-N isoform is expressed by far at the highest level, followed by the DUT-M and the DUT-3 isoform. A strong correlation between expression levels of DUT-M and DUT-3 suggests that these two isoforms may share the same promoter. We analysed the effect of serum starvation on the expression of dUTPase isoforms and found that the mRNA levels of DUT-N decreased in A-549 and MDA-MB-231 cells, but not in HeLa cells. Surprisingly, upon serum starvation DUT-M and DUT-3 showed a significant increase in the expression, while the expression level of the DUT-4 isoform did not show any changes. Our results indicate that the cellular dUTPase supply may also be provided in the cytoplasm, and starvation stress induced expression changes are cell line dependent. Nonetheless, the dUTPase repertoire in human cells is more extended than thought before and it includes four isoforms under the regulation of three different promoters.

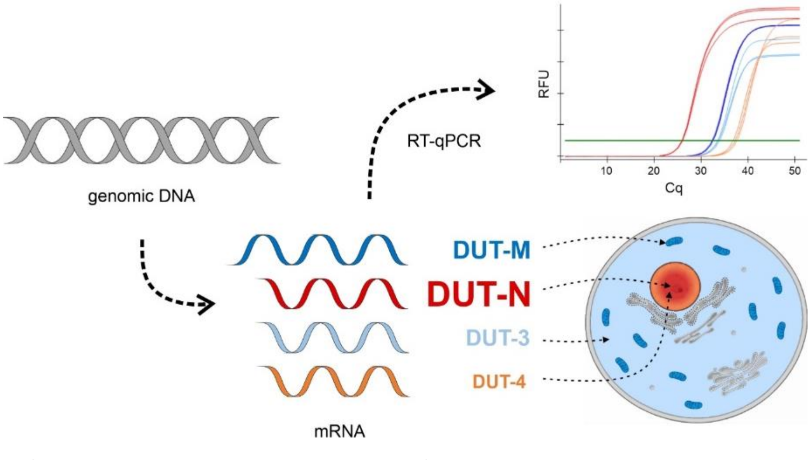

Figure 1. Schematic figure illustrating the main aspects of this study and the hypothetical cellular localisation of the dUTPase isoforms. The font size of the name of the isoforms corresponds to their relative expression levels.

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POPULATION BALANCE BASED MODELING OF DIASTEREOMERIC SALT CRYSTALLIZATION PROCESS OF PREGABALIN TARTRATE

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Since the biological activity of enantiomers may significantly differ, the presence of the undesired enantiomer even in minute quantities may be unacceptable. Therefore, ensuring the optical purity of active ingredients is crucial in the pharmaceutical industry. There are several examples for techniques aiming to obtain homochiral product quality such as: chiral chromatography, preferential crystallization of enantiomers, diastereomeric salt crystallization etc.[1] The latter is a widely used method due to its wide-scale applicability, which relies on selective crystallization of the desired diastereomeric salt that contains solely the enantiomer of interest. Crystallization engineering can be applied to alter the crystal size and shape in order to enhance the downstream operations e.g., filtration but also to maximize the yield and productivity of the process. Population balance modeling (PBM) enables to simulate the dynamics of particle systems, to optimize crystallization process parameters, and to achieve robust and precise process control.[2] PB equations (PBEs) were successfully applied in related areas, such as preferential crystallization of enantiomers.[3] When dealing with complex nonlinear and competitive sub-processes as nucleation, growth and agglomeration of particles, the ability of executing in-silico simulations to find optimal operating conditions becomes highly advantageous. Custom PBMs were intensively developed since early 60's when the concept was introduced, which activity was predominantly happening in academic research groups. Recently, the pharmaceutical industry has started to adopt crystallization modelling tools, mainly via specific software tools such as the DynoChem® and gCrystal®.

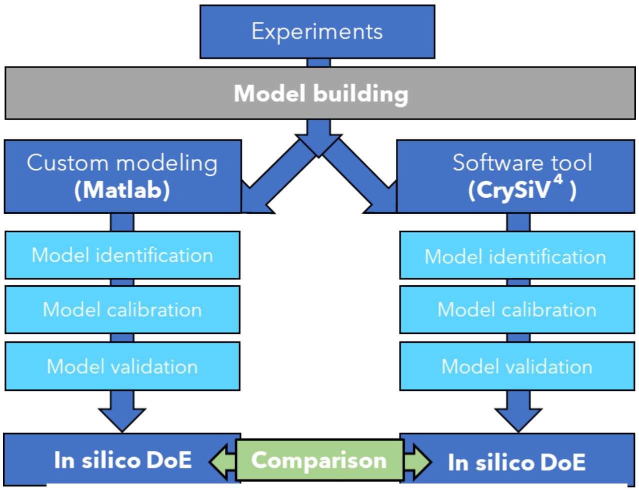

Figure 1. Summary of the work

The goal of this study is to present and compare the PBM based crystallization model development and in-silico analysis using the academic approach (custom PBM development and calibration) as well as the CrySiV software tool, which was co-developed by some of the co-authors of this study.[4] The case study involves the diastereomer salts of pregabalin, an anticonvulsant and anxiolytic drug substance.

This research was supported by Hungarian National Scientific Research Fund (OTKA) grant FK-138475.

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SYNTHESIS AND CHARACTERIZATION OF POLYSTYRENE-*l*-POLY(DIMETHYLSILOXANE) POLYMER CONETWORKS

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Nowadays, significant attention is paid to polymer conetworks which contain immiscible, covalently bonded polymer chains. Their beneficial properties derive from their special structure, where different, immiscible polymer chains form a cocontinuous nanophase separated morphology. Polystyrene-*l*-poly(dimethylsiloxane) (PSt-*l*-PDMS) and polystyrene-*l*-poly(dimethylsiloxane)/divinylbenzene (PSt-*l*-PDMS/DVB) polymer conetworks were synthesized by free radical copolymerization with a broad range of composition. For the synthesis, methacryloxypropyl-telechelic poly(dimethylsiloxane)s (MA-PDMS-MA) were used as crosslinkers with various number average molecular weights. Conetwork samples with different St and DVB ratios were prepared with constant PDMS content, and also with fixed St and DVB ratios having various PDMS contents as well. The syntheses were successful with high gel fraction values of around 90% in all cases. The composition of the resulting polymer conetworks were determined by elemental analysis which are in good agreement with the feed ratios. The structure of the PSt-*l*-PDMS and PSt-*l*-PDMS/DVB polymer conetworks were investigated by Small Angle X-ray Scattering (SAXS) and Atomic Force Microscopy (AFM). Both SAXS and AFM indicates nanophase separated structure, and the AFM shows also cocontinuous (bicontinuous) morphology. SAXS measurements indicate composition dependent d-spacing. In the PSt-*l*-PDMS and PSt-*l*-PDMS/DVB polymer conetworks, the two polymer components can be selectively swollen in n-hexane and 1-nitropropane which also confirms the phase separated structure. The Differential Scanning Calorimetry (DSC) measurements resulted in an unexpected phenomenon. Instead of two glass transition temperatures (T_g) of PDMS and PSt, only the T_g of the PDMS was observed. The T_g of the polystyrene component cannot be detected by DSC. The cocontinuous nanophase separated morphology of the PSt-*l*-PDMS/DVB conetworks provides several special application possibilities ranging from new material structures with unique properties to nanophasic catalyst supports etc.

Acknowledgments
This work was supported by the National Research, Development and Innovation Office, Hungary (NN129366 and K135946).

SYNTHESIS AND PROPERTIES OF SPINEL NANOCRYSTALS WITH X-RAY EXCITED OPTICAL LUMINESCENCE

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Spinel nanocrystals are promising in various optical applications due to their wide band gap and thermal- and chemical stability. These applications include background-free deep-tissue bioimaging, and photodynamic or photon-induced therapy. To avoid the autofluorescence of the body's tissues, the injected nanoprobe's emission needs to be in the near- or infrared range. The chromium-doped zinc-gallate (ZGO:Cr or ZGC) spinel nanocrystals have a strong and long-lasting emission of around 700 nm and can be excited by X-ray, which can make this material promising for these applications[1].

Several research works have enhanced the emission intensity of ZGC nanocrystals or lengthened the luminescence lifetime by using different syntheses, adding extra semiconductor materials, or co-doping with an additional emission center.

In our research work, we improved the intensity of the emission by adding SiC nanoparticles to the system or annealing the hydrothermally synthesized nanocrystals at different temperatures[2]. The results showed that these treatments were increasing the emission by an order of magnitude and differences were observed in the luminescence behavior of the material between the UV- and the X-ray irradiation.

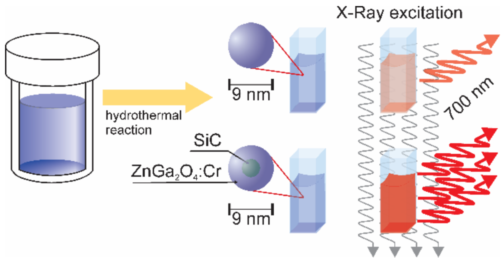

Figure 1. Schematic figure of the emission enhancemet by adding SiC nanoparticles.

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STUDYING THE ULTRAFAST DYNAMICS OF Fe(II) COORDINATION COMPLEXES

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Transition-metal complexes and systems based on them are promising candidates for various molecular devices. Our research group at the Wigner Research Centre for Physics mainly studies complexes of the terpyridine ligand, and among those, the focus of this presentation will be the $[Fe(terpy)_2]^{2+}$ system. This system is interesting, because these complexes switch to a quintet excited state through multiple intermediate states, when excited optically. The magnetic properties of this metastable quintet state differ from the singlet ground state. These complexes can be employed in molecular switches if the stability of the excited state can be significantly increased under standard conditions.

Our research group has previously shown that modifying the terpyridine ligand in the 4' position with various functional groups can increase or decrease the excited state quintet lifetime, depending on the electron donating or withdrawing characteristics of the substituent. Our group has also shown that these changes can be predicted with good accuracy via affordable DFT-based calculations.[1]

In this work I will discuss the effects of the modification of the terpyridine ligand in the 5,5" positions, with regard to the excited-state quintet lifetime. The measurement of the lifetimes was carried out with Transient Optical Absorption Spectroscopy, the results of which I will be presenting here. I will also compare the results with the calculations carried out by our group.

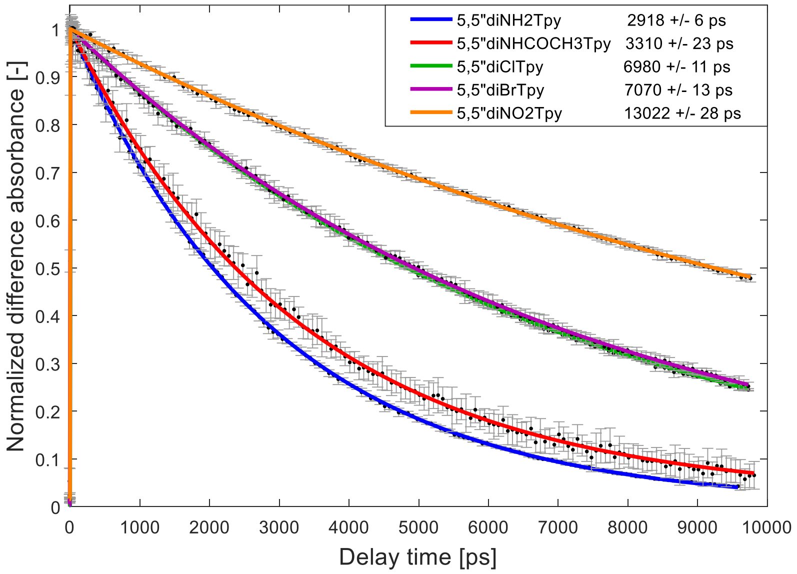

Figure 1. Quintet lifetimes of $[Fe(terpy\text{-}5,5''\text{-}diX)_2](BF_4)_2$ complexes in MeCN

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CONTINUOUS INTEGRATED PRODUCTION OF GLUCOSE GRANULES WITH ENHANCED FLOWABILITY AND TABLETABILITY

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Glucose is a widely used ingredient of the food and pharmaceutical industry (in the latter mostly as excipient but in some cases also as active ingredient).[1] However, the application of industrially crystallized glucose in solid dosage forms is challenged by its poor flowability and tabletability. These powder characteristics are usually improved by granulation, mostly carried out in batch production.[2] A continuous alternative with numerous benefits, the twin screw granulation (TSG) might be suitable for this purpose; therefore, the main goal of the research was to develop an integrated continuous technology based on TSG. A completely continuous manufacturing line (including feeding, granulation, drying and milling) was developed and the different production steps were examined and synchronized with each other.

Our line was supplemented with near-infrared spectroscopy used as a process analytical tool to monitor the moisture content of the milled granules in real-time. The flowability and tabletability of the powder improved significantly, and tablets with acceptable breaking force could be prepared from the granules. The developed continuous line can be easily installed into the industrial solid glucose production process resulting in pure glucose granules with adequate flow properties and tabletability in a simple, continuous and efficient way.

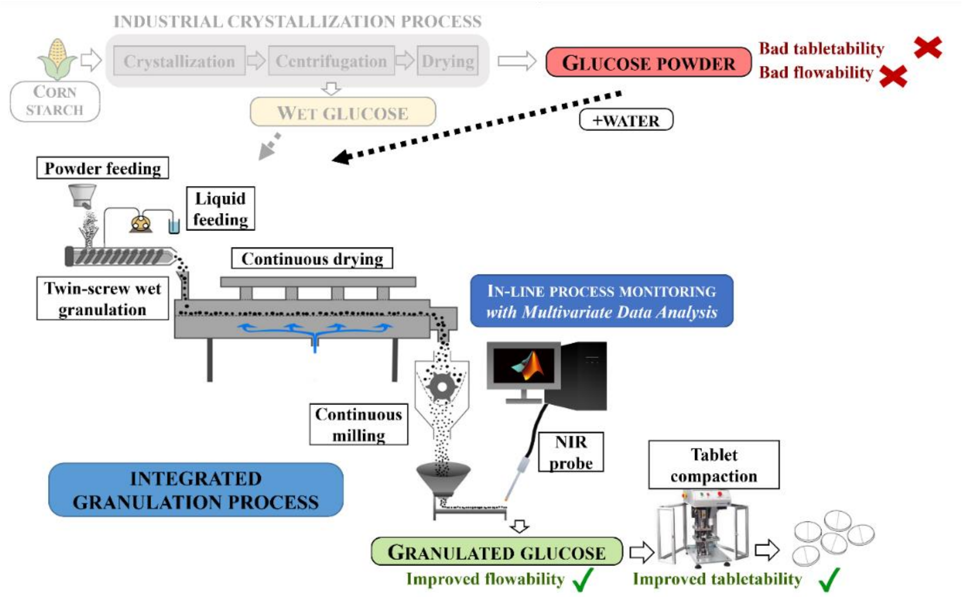

Figure 1. The continuous manufacturing line, developed to improve the flowability and tabletability of glucose.

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ABSTRACTS

POSTER PRESENTATIONS

THE UTILISATION OF PHYTIC ACID AS A REACTIVE FLAME RETARDANT IN A FULLY BIOBASED WATERBORNE EPOXY SYSTEM

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Epoxy resins have been used recently in different fields including composites, coatings, electronics, transportation and many other industries. However, maintaining the outstanding properties of their products while adapting the environmentally benign movement in the industry, is one of the main challenges for industry and academia [1].

Phosphorus-containing compounds present a good alternative to the halogen-containing flame retardants (FRs) to reduce the flamability of epoxy resins. P-containing groups can be part of the epoxy monomer or the curing agent as reactive FRs. Phytic acid (PA) has attracted some attraction to be used as FRs due to its high P-content (28%) [2].

This study aims to reach excellent FR properties by using phytic acid as a reactive flame retardant for sorbitol-based epoxy monomer (SPE) to form a fully biobased waterborne epoxy system. Ammonium polyphosphate (APP) were added also to form an intumescent FR system. The results of limiting oxygen index (LOI) and UL94 flammability tests showed better flame retardant properties and higher LOI via the addition of APP. The thermogravimetric analysis (TGA) measurements showed a relatively high char residual char weight which increased by increasing APP content. The charring effect of PA and APP was confirmed further by mass loss calorimetry (MLC), and the protective char not only reduced the heat release rate (HRR), but also reduced the thermal transition within the char, which was investigated by measuring the temperature on the back surface of a coated steel plates.

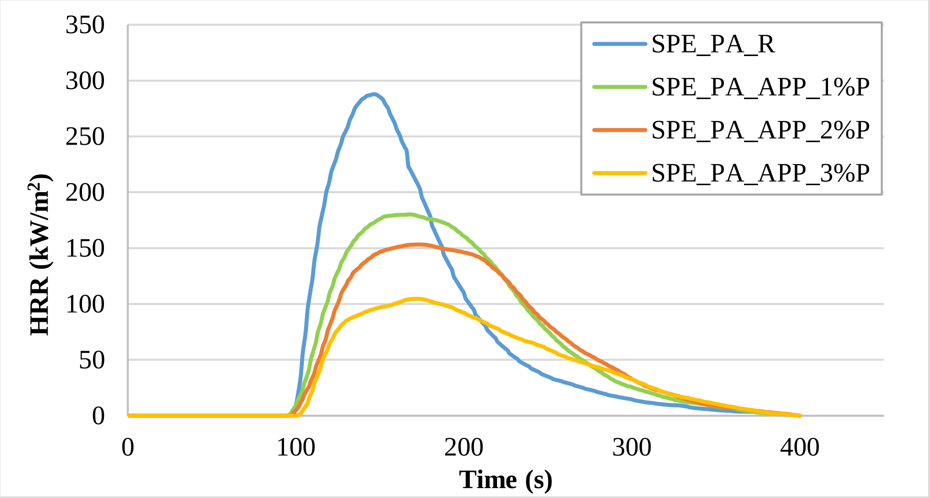

Figure 1. Heat release rate (HRR) curves of SPE-PA reference and APP cntaining samples

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EFFECT OF GO DOPING ON N, S CO-DOPED CARRAGEENAN BASED POROUS CARBON

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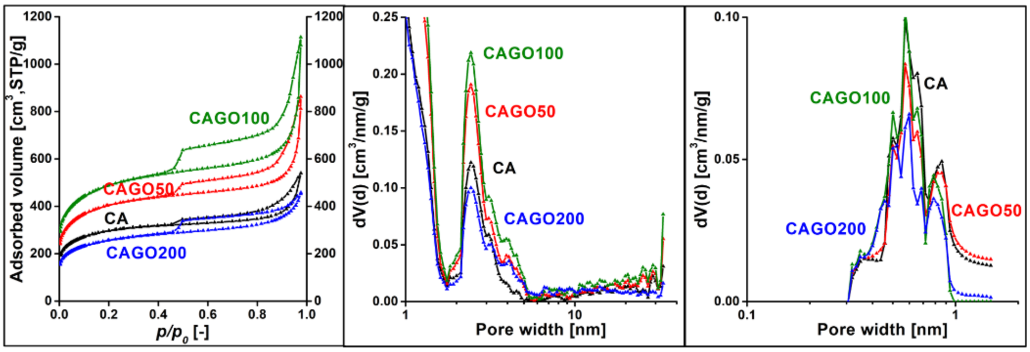
Carrageenan is a natural polysaccharide (sulfated polygalactan) extracted from red seaweeds with a content of 25% - 30% ester-sulfate groups. The sugar units in the chemical structure, sulfur content and the associated mineral content jointly determine the properties of carrageenan and the carbon materials derived from it [1]. Incorporating N atoms into high surface area carbon materials has proved to significantly increase their electrocatalytic activity [2], so adding a suitable N source in the synthesis of porous carbons is an excellent doping strategy. The synergistic effect of heteroatoms doping, creation of defects, and a hierarchical porous structure effectively contribute to enhance the physical chemical properties of carbon materials increasing their potential for green applications such as electrocatalysis and gas separation. In our work, the intrinsic S content of carrageenan works as self-dopant while N-doping results from the addition of urea during synthesis. The mineral content in carrageenan serves as template to develop the porous structure through acid washing and thermal treatment while defects are also created. The final product is a metal-free porous carbon to be used first as electrode in oxygen reduction reaction (ORR), and second as adsorbent in biogas upgrading (separation of CO_2 from CH_4) [3]. To enhance its performance, we must increase the electric and thermal conductivity of the carbon. To achieve this, graphene oxide (GO) is added in the reaction mixture to be incorporated into the carbon framework and be reduced later to graphene-like layers under thermal treatment. This should enhance the physical-chemical properties of the porous carbon and its performance in the above-mentioned applications.



(a) (b) (c)

Figure 1. a) N_2 adsorption/desorption isotherms; b) QSDFT pore size distribution functions, slit/cylinder geometry; c) CO_2 pore size distribution functions

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MAINTENANCE OF GENOMIC INTEGRITY IN THE MALARIA PARASITE PLASMODIUM FALCIPARUM

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Understanding and characterizing the molecular background of the maintenance of genomic integrity might be a major factor in comprehending the exceptional ability of the malaria parasite, *Plasmodium falciparum* to adapt at a fast pace to antimalarials. A balanced nucleotide pool is an essential factor for high-fidelity replication. The lack of detailed studies on deoxynucleotide-triphosphate (dNTP) pools in various intraerythrocytic stages of *Plasmodium falciparum* motivated our present study. Here, we focused on the building blocks of DNA and utilized an EvaGreen-based dNTP incorporation assay[1] to successfully measure the relative ratio of dNTPs in every intraerythrocytic stage and in WR99210 treated trophozoites. Our findings show that the ratio of dNTPs in the ring-stage parasites significantly differs from the more mature trophozoite and schizont stages. We were also able to detect dGTP levels that have never been shown before and found it to be the least abundant dNTP in all stages. Treatment with WR99210, a TS-DHFR inhibitor[2], not only affected dTTP levels, but also dGTP levels, despite it being a purine nucleotide. Results from our studies might assist in a better understanding of genome integrity mechanisms and may potentially lead to novel drug development aspects involving purine and pyrimidine metabolic targets.

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SYNTHESIS AND CHARACTERIZATION OF SOME METAL COMPLEXES: AMMINE COMPLEXES OF COBALT

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In the current study, some ammine complexes of cobalt including: Co $(NH_3)_6Cl_3$, $Co(NH_3)_6Br_3$, $Co(NH_3)_6(ClO4)_3$, $Co(NH_3)_6(MnO_4)_3$ were successfully synthesized and characterized by x-ray powder diffraction (XRD), Fourier transform infrared (FTIR) and Raman spectroscopy (Figure1). By confirming the purity, these complexes, are used for further new compounds synthesizes.

In addition, the constituents of prepared $[Co(NH_3)_6]Cl\ (ClO_4)_2$ were analyzed by some classical analytical methods such as gravimetric and titrimetric analysis. In a short description, for the cobalt content, the salt was decomposed using acid sulphuric and then heat treatment process applied to separate the cobalt. NH_3 determination accomplished using a strong base to distil ammonia off the salt solution and then measured by titrimetric method. Cl content was precipitated and measured as AgCl. Finally, ClO_4 measurement achieved using strong KOH and precipitating as $KClO_4$. [1,2]

In the recent study, to synthesize a new compound, there have been some trials on preparing and characterization of $Na[Co(NH_3)_6]Cl_2.2MnO_4$. This complex basically forms by reaction between $Co(NH_3)_6Cl_3$ and $NaMnO_4$ solution. On the last attempt, manganese determination carried out using nitric acid and concentrated ammonia followed by a heat treatment.

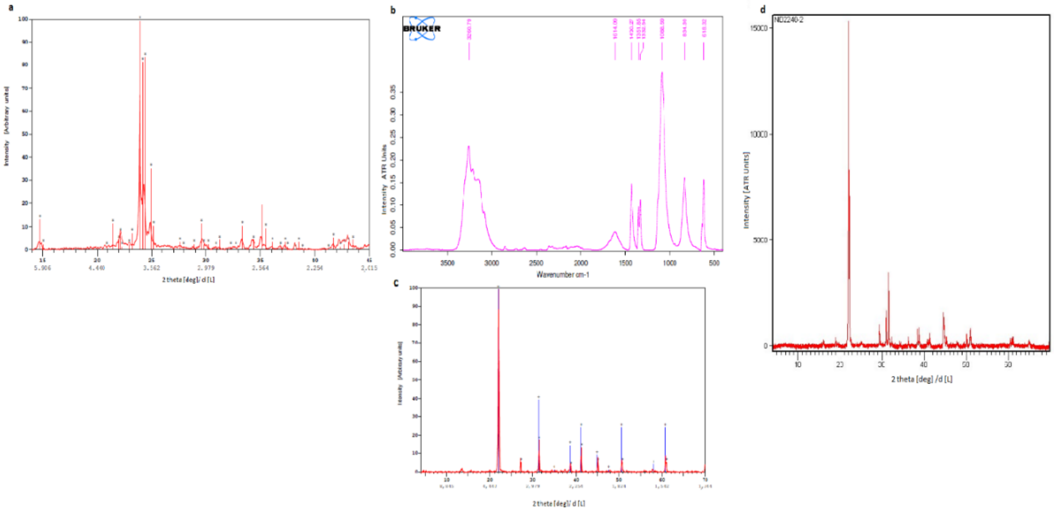

Figure1: (a) XRD of $Co(NH_3)_6Br_3$, (b) IR spectroscopy and (C) XRD of $Co(NH_3)_6(ClO_4)_3$, (d) XRD of $Co(NH_3)_6(MnO_4)_3$

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ATOMIC LAYER DEPOSITION SURFACE-MODIFIED CARBON NANOSPHERE AND CARBON NANOPOWDER NANOFLUIDS FOR THERMAL CONDUCTIVITY ENHANCEMENT

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Nanofluids are phase colloids with a special application as a workfluid with enhanced thermal conductivity. Nanofluids have numerous applications as a work fluid in heat exchangers and solar thermal collectors[1].

In our research we worked with nanostructures new to the field of nanofluids. Carbon nanosphere (CNS) and carbon nanopowder (CNP) were coated with a thin film of TiO_2 with the utilization of atomic layer deposition createing core-shell nanostructures (indexed with "ALD" marking). We confirmed the existance of the metal-oxide layer and studied the nanoparticles with numerous characterization methods, such as SEM/TEM, EDX, FTIR, Raman spectroscopy, TG/DTA and XRD.

Based on a previous research 1:5 EtOH and ethylene-glycol was used as a base fluid for the CNS_{ALD} and CNP_{ALD} nanofluids respectively[2]. Nanofluids with the oncentrations of 0.5, 1.0 and 1.5 vol% were prepared. The nanofluids viscosity, stability and thermal conductivity were examined. In Figure 1. the thermal conductivity enhancement of each nanofluid are shown. The CNS_{ALD} nanofluids show a nearly constant enhancement, which is strictly concentration dependent. On the contrary the CNP_{ALD} nanofluids thermal conductivity enhancement depends not only on the concetration, but also on the temperature. According to this, the use of CNS_{ALD} nanofluids are better at lower temperatures (20-40 °C) while on higher temperatures (40-60 °C) CNP_{ALD} nanofluids are advised, with higher thermal stability.

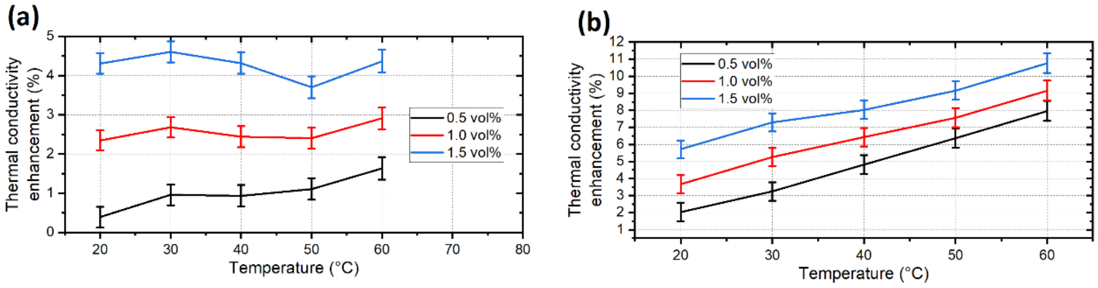

Figure 1. Thermal conductivity enhancement of (a) CNS_{ALD} and (b) CNP_{ALD} nanofluids

[1] S. U. S. Choi and J. A. Eastman, "*Enhancing thermal conductivity of fluids with nanoparticles*," in ASME International Mechanical Engineering Congress & Exposition, **1995**.

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INVESTIGATION OF THE BIOMIMETIC OXIDATION OF CHLOROQUINE IN CONTINUOUS FLOW MODE

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Chloroquine, an originally antimalarial drug, aroused high interest during the rise of Covid-19 pandemic. Based on previous experiences, next to antimalarial, chloroquine has antiviral effect too and was used successfully to treat SARS in 2004. Thus chloroquine was used as an experimental treatment to alleviate the symptoms and accelerate the recovery process from the Covid-19 disease in the first half of 2020.

Chloroquine is metabolized partially in the liver, giving the major metabolite desethylchloroquine. This liver based reaction is found to be catalyzed by the Cytochrome P450 (CYP450) enzyme family. The operation of the CYP450 enzymes can be modelled using synthetic metalloporphyrins and organic or inorganic oxygen donors.

Metalloporphyrins were found to be sensitive to oxidative stress in homogeneous conditions. Their stability can be improved by immobilization on the surface of solid supporters. Next to the stability improvement it introduces other advantages, like the easy sepration (filtration or magnetic separation) and reusability of the catalyst.

In my work I investigated the biomimetic oxidation of chloroquine. I compared three different settings (homogeneous batch, heterogeneous bach and heterogeneous continuous flow) for the biomimetic oxidation of chloroquine. The effect of the distance between the supporter and the catalyst was investigated using different length linkers in heterogeneous and continuous flow mode. Also the effect of the temperature on the continuous flow reaction was investigated. The major metabolite of chloroquine was identified and isolated from the biomimetic reactions.

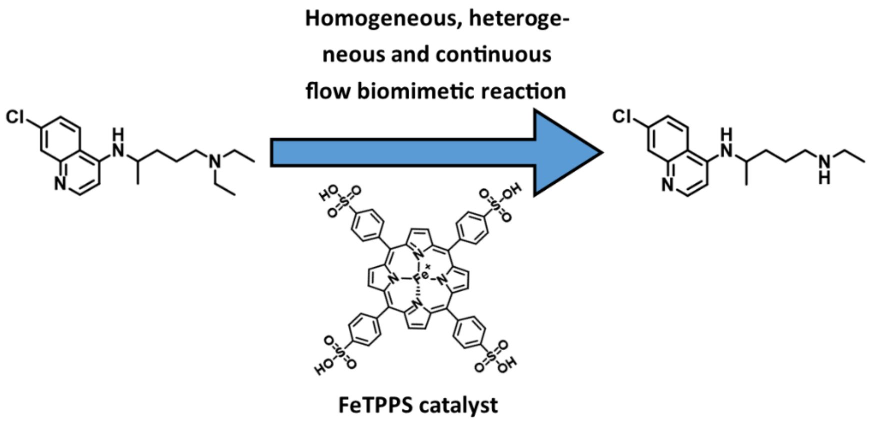

Figure 1. Biomimetic oxidation of chloroquine

SILICA-BASED MICROFIBROUS STRUCTURES FOR THE FLAME RETARDANCY OF POLY(LACTIC ACID)

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Silane-based reactive surface modification of natural fibres is generally performed to improve the fibre-matrix interaction in polymeric composites. Surface treatment of reinforcing natural fibres was also found to effectively promote the charring and improve the fire resistance of intumescent flame retardant (IFR) systems.[1] Nevertheless, various forms of silica-based additives have proven synergistic efficacy in phosphorus-based flame retardant systems. In this study, neat silica microfibers and silane-treated polysaccharide microfibers were prepared using a solvent-based high-speed electrospinning technique and then applied as potential synergists in the IFR system besides ammonium polyphosphate to obtain flame retarded poly(lactic acid) composites. The effect of the silica microfibres, differing in dimensions and chemical composition, was comprehensively investigated based on morphological, spectroscopic and thermal analyses, flammability (cone calorimetry, LOI, UL-94) and mechanical testing of the composites.

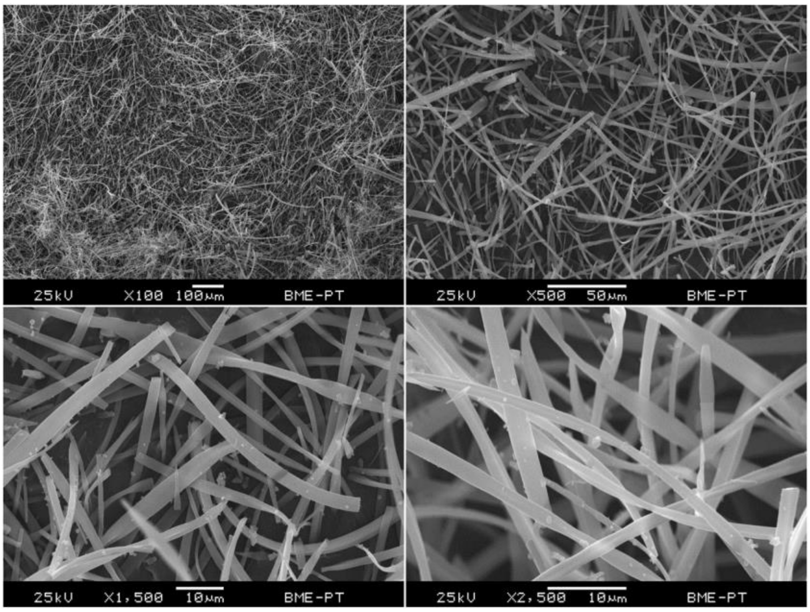

Figure 1. Electronmicroscopic images of the electrospun silica nanofibres

[1] K. Bocz, B. Szolnoki, A. Marosi, T. Tábi, M. Wladyka-Przybylak, and G. Marosi, "Flax fibre reinforced PLA/TPS biocomposites flame retarded with multifunctional additive system," **2014** *Polym Degrad Stab*, vol. 106, pp. 63–73.

STABILITY STUDY OF INFLIXIMAB IN ELECTROSPUN AND LIQUID FORMULATIONS CONTAINING HP-β-CD

Julia Domjan[1*]; Edit Hirsch[1]; Panna Vass; Sune K. Andersen[2]; Tamás Vigh[2];
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Liquid drug products involve the advantages of low cost, fast development process and convenient preparation for administration.[1] However, in the presence of water, sensitive biomolecules can undergo a multitude of physical and chemical degradation pathways. Thus, eliminating water through drying can be an alternative route to improve stability and extend shelf life. Furthermore, solid formulations enable decreased storage space resulting in simpler packaging and transportation. At the same time, the lack of efficient and gentle drying technologies poses a significant challenge to the production of solid bioformulations. Electrospinning (ES) can be considered a new and innovative technology in the field of pharmaceutical manufacturing that enables a gentle and fast drying. The most significant advantage of the ES compared to the currently used freeze- and spray drying is that the process can be implemented without applying heat treatment.[2]

The aim of this research was to evaluate the stability of infliximab in liquid and solid formulations containing 2-hydroxypropyl-beta-cyclodextrin (HP-β-CD). Cyclodextrins (CDs), as widely used excipients in pharmaceutical formulations, have been shown to be able to increase the conformational stability of therapeutic proteins in both liquid and dried formulations.[3] Besides that, CDs are capable of self-assembly in high concentrated solutions and several investigations have successfully applied them as a non-polymeric matrix system to fabricate CD-based nanofibers by electrospinning technology.[4] Scaled-up high-speed electrospinning (HSES) technology was used for the production of solid electrospun formulations, where HP-β-CD was applied as the matrix system. The stability of infliximab was evaluated for six months in electrospun formulation stored at -18°C, 4°C, and 25°C with controlled relative humidity (11%, 33% and 50%). In addition, aqueous solutions containing infliximab were prepared using HP-β-CD at concentrations of 1, 10, and 62 w/w%. Different analytical methods (SEC, SDS-PAGE, DLS, UV) were applied to compare the effect of HP-β-CD in liquid and dried states. Based on the results, infliximab showed much greater stability in fibrous material than in liquid formulations. However, the relative monomer content was very similar for samples stored at low (-18°C, 4°C) and at 25°C representing a potentially high tolerance for room-temperature storage. In the case of aqueous solutions, the increasing HP-β-CD content had a significant positive effect on preserving the long-term stability of the sensitive infliximab.

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BIODEGRADABLE POLYMER SYNTHESIS VIA ACYCLIC DIENE METATHESIS (ADMET) POLYMERIZATION

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During this work we investigated ruthenium-based olefin metathesis catalysts activity and efficiency in acyclic diene metathesis (ADMET) polymerization of diallylesters. Commercially available first-generation Grubbs catalyst (G1) had already investigated in the literature, Ben-Haida and his co-workers reported that in the case of diallylterephtalate G1 was able to reach high polymerization degree (PD) of 45 with molecular weight (M_w) of 39,1 *kDa* and polydispersity (PDI) of 2,14. In the case of diallyladipate G1 showed significantly lower activity with PD of 3, M_w of 0.7, and PDI of 1,16.[1] Recently polybuthylene adipate terephthalate (PBAT) and polybuthylenesuccinate (PBS) gain more and more attention as alternative biodegradable polymers for polypropylene (PP) and low-density polyethylene (LDPE).[2,3] These polymers can be synthetized via acyclic diene metathesis reaction (ADMET) with olefin metathesis catalysts. Newly synthesized cyclic alkyl amino carbene (CAAC) catalyst proofed to be most efficient catalayst when the polymerization was carried out in bulk with mechanical stirring at 75°C with 0.5 mol% catalyst load. Advance polymer chromatography (APC) analysis showed acceptable molecular weight of the synthesized polymer. The unsaturated polymer can be hydrogenated at high pressure (20 bar) and high temperature(100°C) using 10 % palladium on carbon.

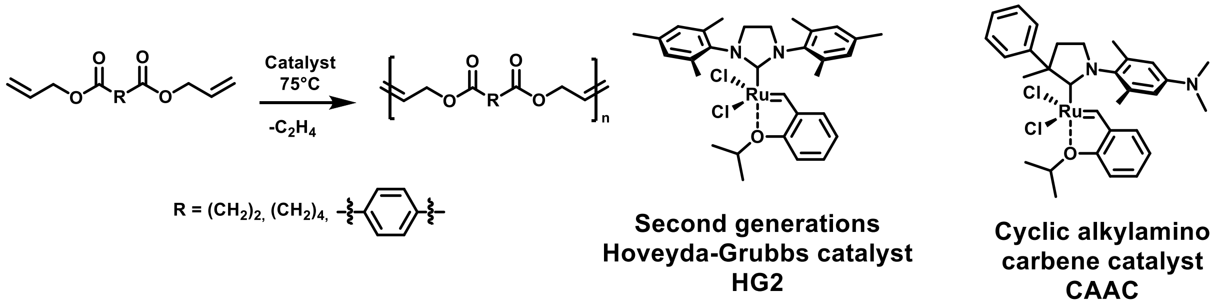

Figure 1. Polymerization of diallylesters and applied olefin metathesis catalysts.

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A NOVEL APPROACH TO THE IMPACT MODIFICATION OF PLA

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PLA is a promising candidate for the replacement of the traditional commodity polymers derived from petrochemical resources. Unfortunately, the neat PLA is very brittle thus hindering its widespread application, especially in the engineering field. Numerous attempts have been made to impact modify the polymer but none of them were truly successful. The extent of improvement in impact strength very often does not meet the expectations and/or another important property deteriorates due to modification. In order to overcome the problem, the concept of adding synthetic polymer fibers for impact modification was applied to PLA in the present study. Two polymer fibers, poly(ethylene terephthalate) (PET) and poly(vinyl alcohol) (PVA) were used for the purpose, while wood flour, a natural reinforcement was added as reference. The results proved that the proposed approach works very well. Polymer fibers increase stiffness to some extent and impact resistance considerably. The impact modification efficiency of the fibers is retained even at low temperature, -20 °C. The improvement in fracture resistance is the result of fiber related local processes. Plastic deformation of PLA initiated by debonding and the fracture of PVA fibers consume a considerable amount of energy thus increasing impact strength. The property combination of PLA/PVA fiber composites with 5 GPa stiffness and 15 kJ/m^2 impact resistance is exceptionally good for engineering applications.

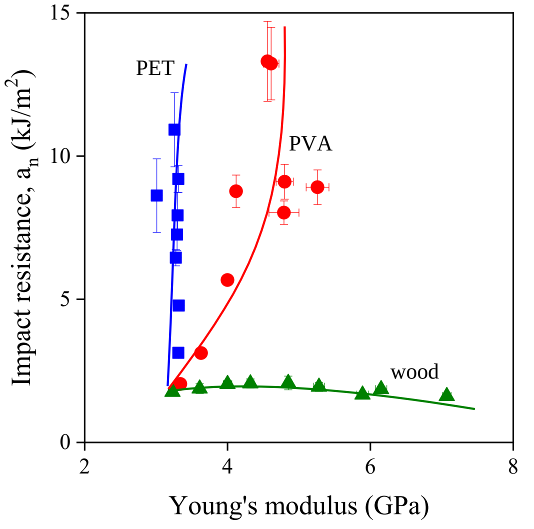

Figure 1. Notched Charpy impact resistance plotted against the Young's modulus of PLA composites.

EFFECTS OF THYMIDYLATE SYNTHASE INHIBITORS ON CELL CYCLE AND CELL VIABILITY

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Thymidylate synthase (TS) inhibitors are widely used in chemotherapeutic treatments, especially for colorectal cancer. By inhibiting TS, the dTTP precursor dTMP cannot be formed. This way these drugs efficiently perturb the dUTP/dTTP ratio of the cellular pool, and the DNA polymerases can more frequently incorporate uracil into the DNA. Under such conditions, uracil-DNA repair pathways turn into hyperactivate futile cycles, leading to cell cycle arrest and finally cell death.

We have been studying the effects of the base analogue 5-fluoro-2'-deoxyuridine (5FdUR) and the antifolate raltitrexed (RTX), two TS inhibitors widely used in cancer treatment. 5FdUR forms stable complex with TS and methyl-tetrahydrofolate [1], while RTX competitively inhibits the enzyme [2]. We had already seen in our U-DNA-Seq data that these drugs lead to somewhat different genomic uracil pattern despite inhibiting the same target.[3] To better describe other possible differences, we investigated the effect of the two TS inhibitors on the cell cycle and cell viability in a time- and dose-dependent way. We could see that the cell cycle arrest happens already within the first 24 h of treatments. However, at this timepoint there were no drastic changes in the cell viability yet (Figure). After 40 h, both drugs except the lowest applied concentrations caused decrease of cell viability. In the case of the lowest applied drug concentration for both TS inhibitors the cells viability stayed almost the same as the un-treated control (NT) all along the treatment. Interestingly there is a change in the tendency of the cytotoxicity of 5FdUR when applied in the highest concentration which cannot be observed in the case of RTX treatment. This might mean that some mechanisms get induced in this concentration of 5FdUR which is working against cell death.

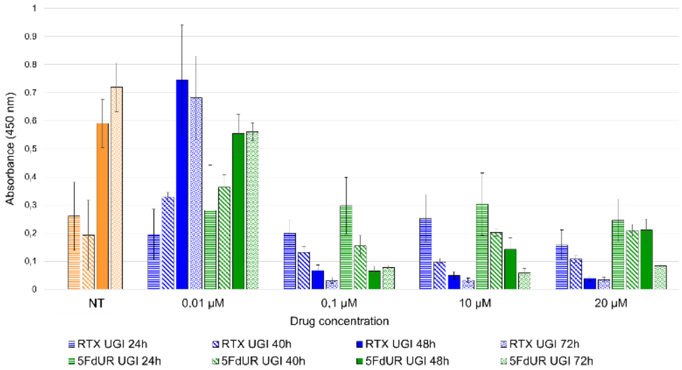

Figure: The effects of the applied TS inhibitors on cell viability depend on the drug concentration and the duration of the treatment.

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FABRICATION AND CHARACTERIZATION OF ZNO AND ZNO-AL$_2$O$_3$ COMPOSITE INVERSE OPALS BY THERMAL AND PLASMA-ASSISTED ALD FOR PHOTOCATALYSIS

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In this study, ZnO and ZnO-Al$_2$O$_3$ composites inverse opal (IO) were successfully synthesized from 600 nm diameter polystyrene (PS) colloid opal crystal templates using thermal and plasma-assisted ALD techniques. ZnO was filled in the pores of the templates by ALD and the template was removed at a higher temperature to achieve ZnO IO. The extra Al$_2$O$_3$ layers were grown on the surface of IO through either thermal or plasma-assisted ALD techniques. SEM-EDX, XRD, Raman, TG-DTA, and UV Vis spectroscopy were used to study morphology, composition, structure, and optical and thermal properties of the samples. SEM-EDX, Raman, and XRD results confirmed the visible microporous crystalline hexagonal wurtzite structure of the IO and its additional Al$_2$O$_3$ ALD coated layers as well. The UV-Vis results revealed that strong absorption bands were detected both in the UV and vis regions including increased visible absorption due to slow photons in the photonic crystals for all specimens, which is very important for photocatalysis.

The photocatalytic activity was investigated by the degradation of MB dye in the presence of UV light irradiation. The photocatalytic degradation efficiency (%) of pure ZnO IO (57.27%), Al$_2$O$_3$-ZnO thermal (68.27%), and Al$_2$O$_3$-ZnO plasma (46.12%) ALD samples. The results confirmed that the Al$_2$O$_3$-ZnO thermal composite sample exhibited enhanced photocatalytic activity compared to pure ZnO and ZnO-Al$_2$O$_3$ plasma composite samples.

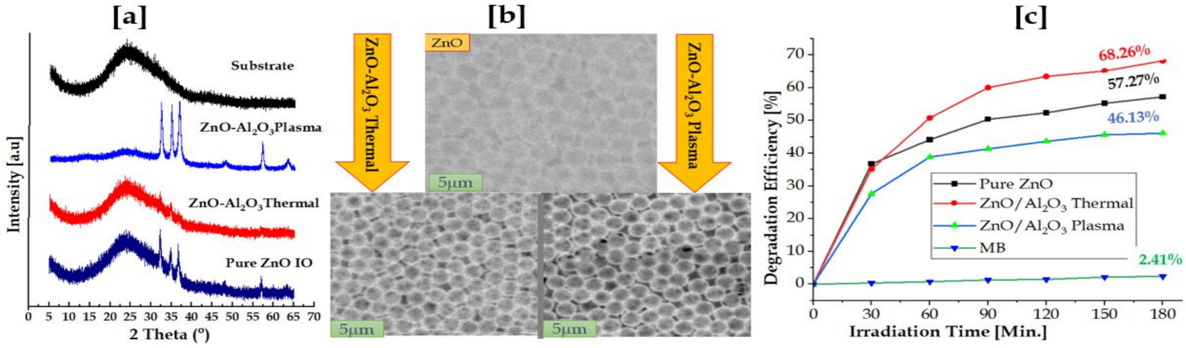

Figure 1: (a) XRD (b) SEM images (c) Photodegradation efficiency in %

EFFECT OF HIGH HYDROSTATIC PRESSURE TREATMENT ON THE QUALITY CHARACTERISTICS OF MANGALICA FLESH AND BACON

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Food industry is facing increased consumer expectations, so permanent innovation has a major role to play. Consumers want both enjoyable and nutritious, aesthetic, preservative-free and affordable products at the same time. High hydrostatic pressure treatment can provide a suitable solution to meet all these requirements, but it is also worth investigating the possible side effects caused by the pressure. The preservative process can catalyze certain chemical and biochemical reactions that can lead to color and structure defects.[1]

To perform the experiment, pre-chilled, vacuum-packed mangalica meat and bacon were used, which, after the proper preparation, were subjected to a hydrostatic preservation process of 200. 400 and 600 MPa for 2 minutes. After the treatment, a storage test was performed, which was continued for five weeks.

Investigating the physical properties, in the case of color, the change was clearly visible. As the pressure increased, the value of the brightness factor also increased so the flesh got faded. However the correlation between the change in texture and the applied pressure was not so obvious. 200 MPa had a tenderizing effect on the meat, 400 and 600 MPa resulted in hardening of the texture. All these findings apply only to the meat, the properties of the bacon have only been modified to a minimal extent. The pH value of the samples did not significantly change from the initial values as a result of the treatment. The biggest difference was seen during the storage in the case of pieces not subjected to hydrostatic pressure. The process increased the loss during roasting but the amount of pressure did not affect the rate of reduction. Evaluating the microbiological results the opposite conclusion was drawn because the 600 MPa pressure had orders of magnitude higher germ-killing effect than the 200 MPa.

Based on the results, the conclusion was made that meats preserved with high hydrostatic pressure are not suitable to be sold at meat counters. Although the pressure of 200 MPa does not change the color of the product to such an extent that it would cause disgust in consumers, it does not have an adequate lethal effect on microorganisms either. The products subjected to pressure treatment of 400 and 600 MPa can be used in the catering system and can also serve as raw materials for the livestock product industry.

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MULTICOMPONENT REACTION OF ISATINS, β-KETOPHOSPHONATES AND PRIMARY AMINES

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Nitrogen heterocycles are essential in several fields of life, as they can be found in many biomolecules, pharmaceuticals, as well as in agrochemicals and dyes.[1] Spirooxindoles, as key members of *N*-heterocycles, show antitumor, antiviral, antimicrobial and antifungal activites.[2] 1,4-Dihydropyridines, another significant family of compounds, also exhibit various biological activities, such as calcium channel blockers, antitumor and analgesic drugs.[3] Due to the features of these compounds, spirooxindole dihydropyridines can be considered as interesting candidates in the drug discovery.

During our research work, our aim was to study the three-component reaction of isatins, β-ketophosphonates and various primary amines to synthesize new, biologically active spirooxindole dihydropyridines. First, a model reaction was studied and optimized in respect of the molar ratio of the starting materials, heating mode, catalyst, solvent, temperature and reaction time. After that, the reaction was carried out with further isatin derivatives (6-chloroisatin or *N*-methylisatin), various primary amines (isopropylamine, cyclohexylamine, benzylamine, aniline, ethanolamine), as well as with dimethyl (2-oxopropyl)phosphonate. Altogether, 10 new spirooxindol dihydropyridine bisphosphonates were synthesized and fully characterized by ^{31}P, ^{13}C and ^{1}H NMR spectroscopy, as well as by HRMS data.

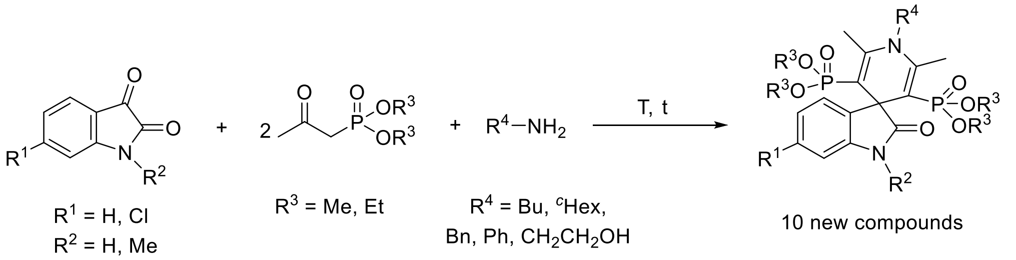

Figure 1. Synthesis of spirooxindole dihydropyridine derivatives

Our further aim is to study the *in vitro* cytotoxicity and antibacterial activity of the products synthesized and investigation of their complexation with cylodextrins, which focuses on how to increase their water solubility and optimize their physical chemical properties.

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TUNABLE THERMORESPONSIVE BEHAVIOR OF N,N'-DIETHYLACRYLAMIDE AND POLY(ETHYLENE GLYCOL) ACRYLATE AND POLY(ETHYLENE GLYCOL) METHACRYLATE BASED COPOLYMERS

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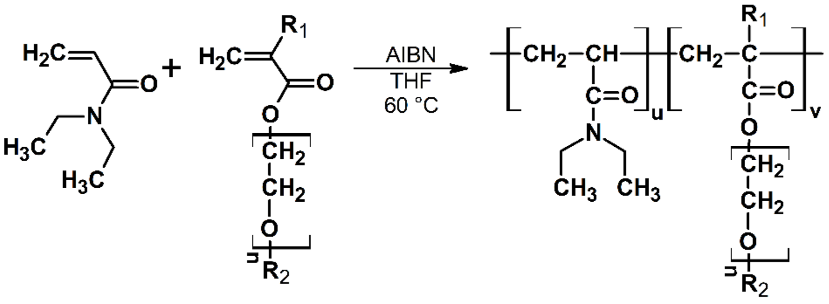

O/P(EG)	R_1	R_2	n
DEGEEA	H	CH_2-CH_3	2
mPEGA-480	H	CH_3	9
mPEGA-640	H	CH_3	13
mPEGMA-300	CH_3	CH_3	4
mPEGMA-500	CH_3	CH_3	9
mPEGMA-1100	CH_3	CH_3	23

Figure 1. Synthesis of copolymers based on N,N'-diethylacrylamide and various poly(ethylene glycol) acrylates and methacrylates.

Copolymers based on N,N'-diethylacrylamide (DEAAm) and poly(ethylene glycol) (meth)acrylates (PEG(M)A) with different comonomer ratios and various ethylene glycol repeating units from 2 up to 23 were synthetized by free radical copolymerization. The GPC results show that the molecular weight of the produced copolymers is in the range of 3000-6000 g/mol with acceptable polydispersity indices typical for free radical polymerization. The composition of the copolymers was determined by ^{1}H NMR spectroscopy. The thermoresponsive behavior of the produced copolymers was investigated by turbidity measurements with UV-Vis spectroscopy. Based on the performed systematic investigation, the effect of the philicity of the pendant PEG-chain and the composition of the copolymers on the critical solution temperature (CST) of the copolymers based on DEAAm and PEG(M)A have been revealed. The results show a clear correlation between the number of repeating units of the pendant PEG chain, the composition of the copolymers and the critical solution temperature. Based on the equation describing this correlation, the CST of the DEAAm and PEG(M)A based copolymers can be estimated or the required composition can be defined easily for the designing and preparing DEAAm-PEG(M)A copolymers with desired CST values.

TOWARDS ACCURATE CONTROL OF SURFACE CHARGE OF GOLD NANOPOROUS MEMBRANES THROUGH COVALENT SURFACE MODIFICATION

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Gold nanoporous membranes[1] with controlled surface charge could have applications for ion sensing[2-3], separations and liquid junctions[4]. By modifying the gold surface with thiol-derivatized ion-exchangers, a wide range of surface charges can be conferred to the membrane. To improve control over the modification process, we introduce kinetically controlled surface modification with real-time potentiometric monitoring. We show that by using low concentrations of the thiol-derivatized functional molecules and continuous monitoring enhanced control over surface charge can be achieved.

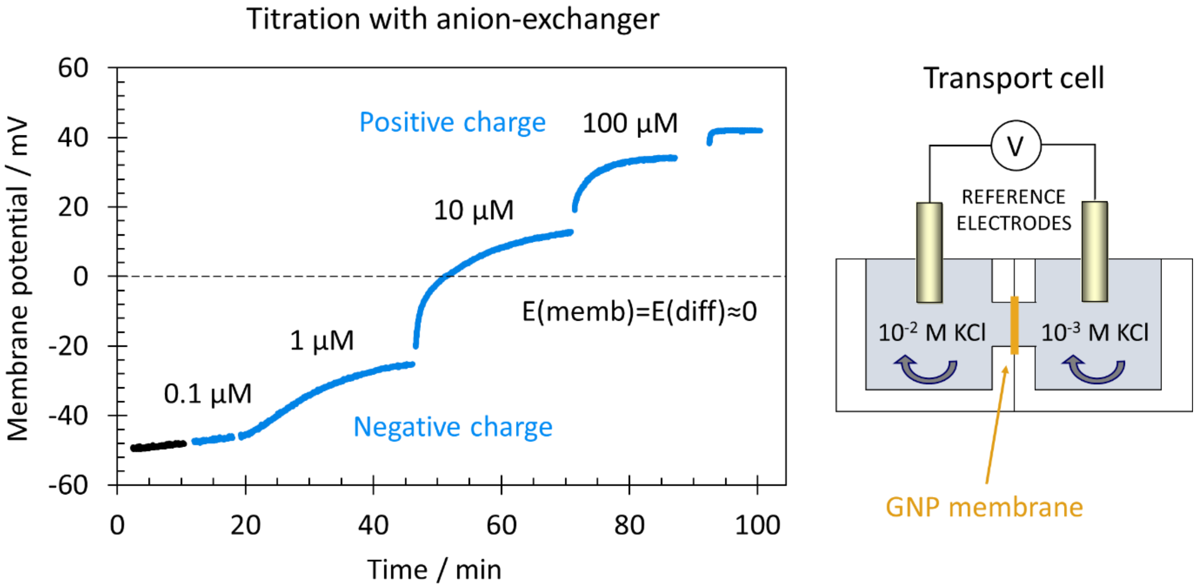

Figure 1. Titration curve and measurement setup of
kinetically controlled surface modification with real-time potentiometric monitoring.

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SYNTHESIS OF POTENTIONALLY BIOLOGICALLY ACTIVE ACYCLIC AND CYCLIC AMINOPHOSPHONATE DERIVATIVES

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Organophosphorus compounds play an important role in several fields of life, such as in organic and medicinal chemistry, as well as in agriculture or plastic industry.[1] α-Aminophosphonates are one of the most important family of compounds within organophosphorus derivatives due to their versatile biological activity [2]

During our research work, our aim was to synthesize novel acyclic and cyclic aminophosphonate and aminophosphine oxide derivatives by the Kabachnik-Fields reaction of 2-alkynylbenzaldehydes, primary amines and dialkyl phospites or secondary phosphine oxides. In addition, our aim was also study the *in vitro* cyctotoxycity of the compounds synthesized *(Figure 1)*.

First, a model reaction was studied and optimized for the synthesis of acyclic, as well as for cyclic aminophosponates in respect of the heating mode, catalyst, solvent, temperature and reaction time. After that, the three-component reactions were extended for substitueted 2-alkynylbenzaldehydes, various aliphatic or aromatic amines and P-reagents. Altogether, 42 new aminoposphonate and aminophosphine oxide derivatives were prepared in good to high yields and fully characterized.

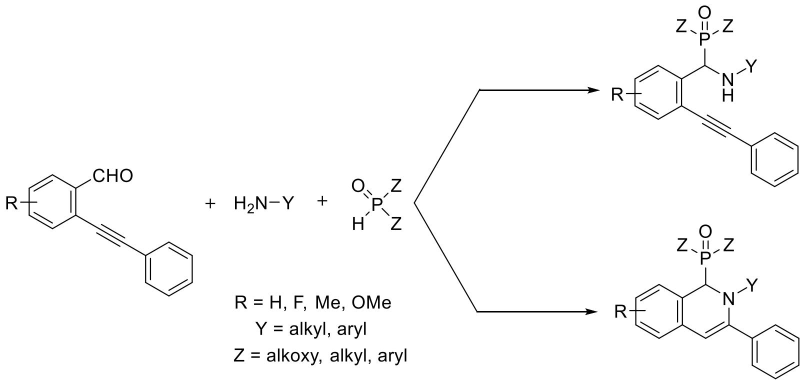

Figure 1. Kabachnik-Fields reaction of 2-alkynylbenzaldehydes, primary amines and >P(O)H reagents

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Köszönetnyílvánítás: A kutatás a Nemzeti Kutatási és Fejlesztési Hivatal FK123961 sz. páylázat támogatásával készült.

THE SYNTHESIS OF HYDROXY-METHYLENEBISPHOSPHONATE DERIVATES AND THEIR REARRANGED PRODUCTS BY THE PUDOVIK REACTION

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Hydroxymethylene bisphosphonic (dronic) acid derivatives are of importance due to their beneficial effect in the treatment of bone diseases [1,2]. Their synthesis, starting from the corresponding substituted acetic acid and phosphorus trichloride/phosphorous acid, was thoroughly investigated [1,3,4]. Another approach is the Pudovik reaction, which involves the addition of dialkyl phosphites onto the carbonyl carbon of oxo compounds, such as aldehydes and ketones [5,6].

The reaction of diethyl α-oxoethylphosphonate and diethyl α-oxobenzylphosphonate with diethyl phosphite, dimethyl phosphite, and diphenylphosphine oxide affords, depending on the substrates and conditions (nature and quantity of the amine catalyst, temperature, and solvent), the Pudovik adduct and/or the corresponding >P(O)–CH–O–P(O)< rearranged product (**Figure 1.**). The nature of the substituent on the central carbon atom (methyl or phenyl group) influences the inclination for the rearrangement. The asymmetric products (adducts or rearranged species) with different P(O)Y functions (Y =RO or Ph) exhibit interesting NMR features. [7]

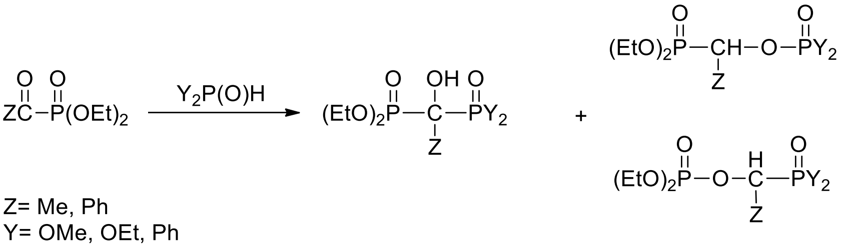

Figure 1.

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EXAMINATION OF STRUCTURAL BASIS OF PROTEINACEOUS *M. TUBERCULOSIS* DUTPASE INHIBITION

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The dUTPase enzyme has an important role in several species in keeping genome integrity. The decrease in dUTPase activity can indirectly lead to DNA double strand brakes and to cell death.[1] This process can be used in defence against different human pathogens, like *M. tuberculosis*, if the inhibitor molecule has an effect only on (myco)bacterial dUTPase. A Staphylococcal Pathogenity Island repressor protein, $\text{Stl}_{\text{SaPIbov1}}$(Stl) is able to interact with dUTPases from several species, and in most of the cases protein Stl is capable of inhibiting the dUTPase activity, but with various efficiency.[2,3] This difference gives us an opportunity to design species-specific Stl based dUTPase inhibitors. However, the design of inhibitors also requires knowledge about the emerging interactions between Stl and dUTPases as well as the differencies between the interactions that occur in different complexes.

Our aim was to understand the interaction between the *M. tuberculosis* dUTPase (MTB DUT) and a truncated version of protein Stl (Stl^{STOP}). In order to find out whether the MTB DUT specific loop has a role in the interaction with protein Stl, we also examined the delta loop version of MTB DUT (MTB $\text{DUT}^{\text{dloop}}$) enzyme.

The structure of the protein complexes and the MTB $\text{DUT}^{\text{dloop}}$ enzyme were examined using X-ray diffraction measurement at Elettra synchroton light source. Steady state activity and Bio-layer interferometry measurements were performed in favor of the investigation of the inhibitory effect of the Stl^{STOP} mutant and the analysis of the protein-protein binding kinetics.

According to these measurements the truncated version of protein Stl possesses lower inhibitory effect, than the full length protein. The structural model of MTB $\text{DUT}^{\text{dloop}}$ enzyme reveals that the loop plays an important role in the stabilization of the C-terminal arm of MTB DUT enzyme. The comparison of the stuctural models of the MTB DUT-StlSTOP complex with complexes emerging between truncated versions of protein Stl and dUTPases from other species may allow us to design mycobateria-specific Stl based inhibitors with introduction of adequate mutations.

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INVESTIGATION OF RHEOLOGICAL PROPERTIES AND THERMAL CONDUCTIVITY OF SiO_2-TiO_2 COMPOSITE NANOFLUIDS PREPARED BY ATOMIC LAYER DEPOSITION

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Nanofluids are dispersions where the aim of adding solid particles is improve the thermal properties (such as heat capacity, thermal conductivity) of the basefluid. Adding solid particles to a fluid implies increasing viscosity, so this is the second most important property of the nanofluid.

The goal of my investigation is to obtain more efficient nanofluids using ALD (atomic layer deposition) modified particles. The original nanoparticles were amorphous SiO_2 particles with an average diameter of 10-20 nm. On these particles we applied 410 ALD cycles of $TiCl_4$ and H_2O precursors at 108°C. An amorphous TiO_2 layer is expected at this temperature, but it was undetectable in IR-spectrum due to the small amount of TiO_2. The TiO_2 layer on the surface was detected by TEM and EDS. 0.5, 1.0, 1.5 vol% of pure SiO_2 or composite particles were dispersed in 1:1 ethylene glycol: water mixture to acquire information on the effect of thin TiO_2 covering. The stability of the different nanofluids was checked by zeta potential measurements. The rheological properties of the different nanofluids were measured by a rotation viscosimeter. Both kinds of nanoparticles increased the viscosity but in a different extent. The composite particles have a lower viscosity rising effect than the simple ones. Parts c and d of Figure 1 represent the thermal conductivity of different nanofluids. It is clearly seen; composite particles increase thermal conductivity more efficiently. Although composite nanofluids are more expensive than simple ones, they can be efficient in producing better heat transfer fluids.

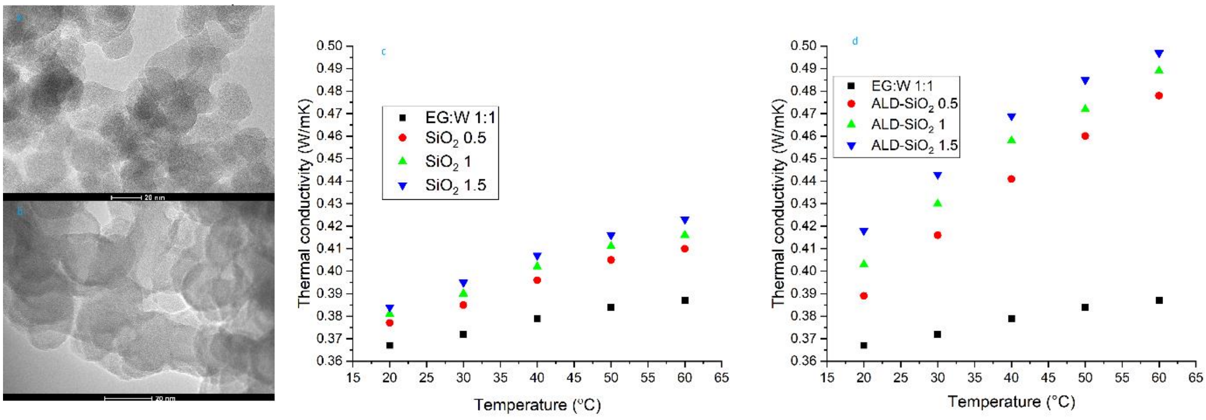

Figure 1. .TEM pictures about the simple (a) and the composite (b) nanoparticles and thermal conductivity of the simple SiO_2 (c) and the composite (d) nanofluids

DEVELOPMENT OF INLINE MONITORING TECHNOLOGY FOR DIAGNOSTIC PROTEIN PURIFICATION AND FILTRATION

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Proteins can be produced by mammalian cells, resulting a supernatant that also contains cells, cell debris, and other impurities. One of the main steps in the purification process is affinity chromatography, which removes most impurities. However, the protein must be purified in additional steps, besides, buffer exchanged and concentrated, preferably.

For this purpose, due to their low operating costs, membrane-type filter units are used, in which the material flow is introduced parallel to the membrane surface. This so-called tangential flow filtration (TFF) works advantageously under mild operating conditions (low pressure and temperature) and has high performance, why it is widely used for filtration with aggregation-prone macromolecules. During the filtration step, the concentration of the protein and the contamination are critical parameters, thus continuous inline monitoring of these quantities can be valuable and necessary.

The model protein was the receptor-binding domain (RBD) of SARS-CoV-2 virus, which plays an important role in determining the antibody level cause by COVID-19 disease in the human body. During affinity chromatographic purification, the RBD protein is contaminated with imidazole. Imidazole causes acute toxicity, skin corrosion, and serious eye damage in the human body. Therefore, its removal is necessary in the next steps.

The aim was to develop a process analytical technology for the filtration step of protein purification. It was found that the imidazole concentration can be determined with Raman and near-infrared (NIR) spectroscopy. Calibration models were successfully developed for the monitoring of imidazole concentration using multivariate data analysis methods. The implementation of inline monitoring technology for the exchange of the imidazole-containing solution buffer was well traced and automated, thus it makes the process efficient and robust.

DRUG FORMULATION BY ELECTROSPINNING FIBERS FROM WATER SOLUBLE POLYMERS: ENCAPSULATION AND DRUG RELEASE

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Electrospun fibers containing Levocetirizine, a BCS III drug, were prepared from three water soluble polymers, hydroxypropyl-methyl-cellulose (HPMC), polyvinyl-pyrrolidone (PVP) and polyvinyl-alcohol (PVA). Fiber spinning technology was optimized for each polymer separately. The polymers contained 10 wt % of the active component. The otherwise crystalline drug was homogenously distributed within the fibers in the amorphous form. The solubility of the drug in the polymers used is limited, maximum 2.0 wt%, but very large in most of the solvents used for fiber spinning. The size distribution of HPMC fibers is large, while fibers prepared from the other two polymers have quite uniform diameter. Most of the drug is located within the fibers, probably as separate phase; encapsulation efficiency proved to be 80-90 %. The kinetics of drug release was evaluated quantitatively by the Noyes-Whitney model. The same amount of drug is released into the surrounding media almost independently of the type of polymer and pH. The rate of release, however, changed in a much wider range; the rate constant of release varied between 0.1 and 0.9 min^{-1}. Consequently, the selection of the carrier polymer allows the adjustment of release rate according to requirements thus justifying the use of electrospun fibers as carrier materials for levocetirizine.

INVESTIGATION OF THE ELECTROCHEMICAL FERRATE SYNTHESIS: COMPARISON OF PURE IRON AND WHITE CAST IRON ELECTRODES

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Ferrate salts are little-known materials consisting of ferrate ions, which is the +6 oxidation state of iron. Due to the highly oxidized form of the ferrates, they are potent oxidant reagents. Their oxidation capability makes them suitable in many areas, most of all in water treatment. Besides their extraordinary oxidation power, the reduction product of ferrate ion is ferric iron, which is a non-toxic chemical, making ferrate an environmentally friendly oxidant.

There are three main ways for ferrate synthesis, of which the electrochemical ferrate synthesis may be the most favorable due to the simple execution, and lack of expensive chemical reagents. The electrochemical ferrate synthesis is mostly carried out through the anodic dissolution of an Iron-containing electrode in highly alkaline media. Despite the great interest in electrochemical ferrate synthesis, there are several contradictions in the literature concerning the optimum conditions and no clear information on the exact mechanism of the process. This can be explained by the lack of appropriate apparatus for the adequate investigation of the system.

The comparative study of two iron-containing electrodes, used for electrochemical ferrate synthesis was executed. The results of the Cyclic Voltammetric (CV) measurements show a considerable difference in the suitability of the two electrodes, suggesting the White Cast Iron (WCI) to be preferred compared to the high purity iron. Dual Dynamic Voltammetry (DDV), a unique experimental method for a Rotating Ring Disk electrode (RRDE) setup, is used to clearly determine an optimum potential region for the ferrate synthesis. It also confirms that the WCI electrode is superior to the pure iron. These results, combined with the results of Electrochemical Impedance Spectroscopic (EIS) measurements clarify the different mechanisms of ferrate production concerning the two electrodes. The different time-dependence of the processes has been found to be the crucial point. Using high-purity iron, the electrode quickly reaches a relatively stable state, causing the processes to converge at a constant rate. However, using WCI the electrode surface does not seem to converge, causing the high time-dependence of the processes. These behaviors can be explained by the different structures of the two materials, and the different changes in the surface structure during the ferrate production.