

Chemistry Physics and Biology of Colloids and Interfaces

06-10 June 2022 Eger, Hungary



BOOK OF ABSTRACTS

	Monday 06. June	Tuesday 07. June	Wednesday 08. June	Thursday 09. June	Friday 10. June
8.30-9.00		OPENING			
9.00-9.30		Jungwirth	Hafeli	Vancso	Boda
9.00-9.50					Fábián
9.50-10.10		Benková	Voniatis	Csicsor	S. Nagy
10.10-10.30		László	Idrissi	Árok	Juhász
10.30-11.00		Coffee break	Coffee break	Coffee break	Coffee break
11.00-11.20			Bilous	Szilágyi	
11.20-11.40		Ohta	Horváth	Jorge	Dinnyés
11.40-12.00		Juriga	Novák	Novikau	
12.00-12.20		Szabó I.	Illés	Kéri	Ádám
12.20-12.40		Farah	Kuznetsov	Szabó T.	Csontos
12.40-13.00		Tóth	Kovács	Ender	CLOSING
13.00-13.15					
13.15-14.30		Lunch	Lunch	Lunch	Lunch
14.30-15.20		Salvati	Dellago	Nenes	
15.20-15.50		Coffee break	Coffee break	Coffee break	
15.50-16.20			Puskas	Balbisi	
16.20-16.40			Kantorovich	Szóri	
16.40-17.00			Pázmány	Sarkadi	
17.00-17.20			Bóna		
17.20-18.00		POSTER SESSION			
18.00-18.30					
18.30-19.00	Backus				
19.00-19.20					
19.20-21.30	GET TOGETHER PARTY	Wine tasting (optional)		CONFERENCE DINNER	
21.30-22.00					

Conference Program

Monday, 6 June

Session 1 (chair: Pál Jedlovsky):

18.30-19.20: **Ellen Backus** (Vienna, Austria): *Water at interfaces: from wetting to atmospheric chemistry*

19.00-21.00: Welcome reception

Tuesday, 7 June

08.30-09.00: Conference opening

Session 2 (chair: Miguel Jorge):

09.00-09.50: **Pavel Jungwirth** (Prague, Czech Republic): *Electrons in liquid ammonia and in water: from blue electrolytes to golden metals*

09.50-10.10: **Zuzana Benková** (Bratislava, Slovakia): *Molecular dynamics simulations of interactions of SARS-CoV-2 spike protein with graphene during initial stage of adsorption*

10.10-10.30: **Krisztina László** (Budapest, Hungary): *Chemical stability of graphene oxide in aqueous suspensions*

10.30-11.10: Coffee break

Session 3 (chair: Abdenacer Idrissi):

11.10-11.40: **Makoto Ohta** (Sendai, Japan): *Flow chamber for evaluation of Endothelial cell adhesion on stent struts*

11.40-12.00: **Dávid Juriga** (Budapest, Hungary): *Application of poly(aspartamides) in drug delivery*

12.00-12.20: **István Szabó** (Gödöllő, Hungary): *Observing long term bacterial colonization of polypropylene microplastics in a freshwater lake by optical and molecular methods*

12.20-12.40: **Shereen Farah** (Budapest, Hungary): *Long-term aging of concentrated aqueous graphene oxide suspension seen by various analytical techniques*

12.40-13.00: **Krisztina Tóth** (Budapest, Hungary): *Nanofibrous biocompatible polymer-based drug-delivery implants*

13.00-14.30: Lunch

Session 4 (chair: István Szilágyi):

- 14.30-15.20: **Anna Salvati** (Groningen, the Netherlands): *Dissecting how cells internalize and process nano-sized drug carriers for nanomedicine applications*
- 15.20-15.50: Coffee break
- 15.50-18.30: POSTER SESSION
- 19.00-22.00: Wine tasting (optional event)

Wednesday, 8 June

Session 5 (chair: Milán Szőri):

- 09.00-09.50: **Urs Hafeli** (Vancouver, Canada): *Targeting Rheumatoid Arthritis Using Nanomedicines*
- 09.50-10.10: **Constantinos Voniatis** (Budapest, Hungary): *Polysuccinimide/Polycaprolactone composite meshes for surgical tissue engineering*
- 10.10-10.30: **Abdenacer Idrissi** (Lille, France): *Local structure in mixtures of ionic liquid with molecular solvent*
- 10.30-11.00: Coffee break

Session 6 (chair: Etelka Tombácz):

- 11.00-11.20: **Oksana Bilous** (Vienna, Austria): *Field-induced structural transitions in magnetic granulate*
- 11.20-11.40: **Barnabás Horváth** (Veszprém, Hungary): *Nonlinear dynamic susceptibility of magnetic fluids in symmetry breaking dc magnetic fields*
- 11.40-12.00: **Levente Novák** (Debrecen, Hungary): *Paramagnetic metal chelates of polycarboxylamino-type macromolecules: high relaxivity complexes without coordinated inner sphere water?*
- 12.00-12.20: **Erzsébet Illés** (Szeged, Hungary): *Biocompatible folate targeted cobalt ferrite nanoparticles for magnetic hyperthermia*
- 12.20-12.40: **Andrey Kuznetsov** (Vienna, Austria): *Magnetic and structural equilibrium properties of multicore nanoparticle suspensions and bimodal ferrofluids*
- 12.40-13.00: **Nikoletta Kovács** (Nagykanizsa, Hungary): *Glyphosate/AMPA adsorption on magnetite: measure the trace amounts and separate simply*
- 13.00-14.30: Lunch

Session 7 (chair: Zuzana Benková):

- 14.30-15.20: **Cristoph Dellago** (Vienna, Austria): *Simulating bulk and interfacial water with neural network potentials*
- 15.20-15.50: Coffee break
- 15.50-16.20: **Judit Puskas** (Wooster, USA): *Synthesis and characterization of folate-targeted monodisperse PEG-based conjugates made by chemo-enzymatic methods for cancer diagnosis and treatment*
- 16.20-16.40: **Sofia Kantorovich** (Vienna, Austria): *Magneto-rheology of clusters formed by magnetic polymers*
- 16.40-17.00: **Rita Pázmány** (Budapest, Hungary): *Ultrasound induced, easy-to-store porous poly(aspartic acid) based electrospun scaffolds*
- 17.00-17.20: **Áron Bóna** (Nagykanizsa, Hungary): *The effect of annealing and layer numbers on the ion exchange capacity of polyelectrolyte multilayer nanofiltration membranes*

Thursday, 9 June

Session 8 (chair: Tamás Szabó):

- 09.00-09.50: **Julius G. Vancso** (Enschede, the Netherlands): *Marine biofouling: The surface science challenge and some lessons to learn*
- 09.50-10.10: **Attila Csicsor** (Szeged, Hungary): *Antioxidant effect of humic substances: an overview*
- 10.10-10.30: **Zsófia Árok** (Szeged, Hungary): *Effect of brine salinity on the solution properties of polymers for enhanced oil recovery*
- 10.30-11.00: Coffee break

Session 9 (chair: Krisztina László):

- 11.00-11.20: **István Szilágyi** (Szeged, Hungary): *Heteroaggregation of nanozymes and latex particles for highly stable antioxidant colloids*
- 11.20-11.40: **Miguel Jorge** (Glasgow, UK): *Sticky-MARTINI – a reactive coarse-grained model for self-assembly in materials synthesis*
- 11.40-12.00: **Ivan Novikau** (Vienna, Austria): *Behavior of a magnetic nanogel in a shear flow*
- 12.00-12.20: **Mónika Kéri** (Debrecen, Hungary): *Application of NMR relaxation methods for colloids and interfaces*
- 12.20-12.40: **Tamás Szabó** (Szeged, Hungary): *Removal of caine anesthetics from water, saline solutions and model wastewaters using nanofiltration membranes*
- 12.40-13.00: **Ferenc Ender** (Budapest, Hungary): *Development of laboratory electrospinning as a tool for the entrapment of biomolecules*
- 13.00-14.30: Lunch

Session 10 (chair: Dezső Boda):

- 14.30-15.20: **Athanasios Nenes** (Lausanne, Switzerland): *The importance of aerosol acidity and its impacts*
- 15.20-16.00: Coffee break
- 16.00-16.20: **Mirjam Balbisi** (Budapest, Hungary): *Computer simulation investigation of the adsorption of acetamide under atmospheric and interstellar conditions*
- 16.20-16.40: **Milán Szőri** (Miskolc, Hungary): *Molecular simulation of the passive membrane penetration by the products of the CO₂ and 1,3-butadiene reaction for a greener technology*
- 16.40-17.00: **Zsófia Sarkadi** (Veszprém, Hungary): *Scaling in uniformly charged and bipolar nanopores through a modified Dukhin number*

Friday, 10 June

Session 11 (chair: István Bányai):

- 09.00-09.30: **Dezső Boda** (Veszprém, Hungary): *Physics, Chemistry, Biology, and Beyond: A Complex Systems Perspective*
- 09.30-09.50: **Balázs Fábrián** (Frankfurt am Main, Germany): *Martini Cholesterol gives membranes the chills – and what you can do about it*
- 09.50-10.10: **Krisztina S. Nagy** (Budapest, Hungary): *Development of poly(aspartic acid) based hydrogels for tissue engineering purposes*
- 10.10-10.30: **Ákos Juhász** (Budapest, Hungary): *Characterizing 3D biodegradable artificial matrices*
- 10.30-11.10: Coffee break

Session 12 (chair: Angéla Jedlovszky-Hajdú):

- 11.10-12.00: **András Dinnyés** (Gödöllő, Hungary): *Human induced pluripotent stem cell-derived cardiomyocyte maturation on elastic bioactive electrospun materials to obtain an adult heart organotypic model*
- 12.00-12.20: **Péter Ádám** (Budapest, Hungary): *Space tests of porous aluminum oxide insulation fibers*
- 12.20-12.40: **Máté Csontos** (Debrecen, Hungary): *Study of bentonite hydration by NMR relaxometry and chemometrics*
- 12.40-13.00 Conference closing
- 13.00-14.30: Lunch

List of Posters

1. **Mónika Bak** (Budapest, Hungary): *Building a solid-like layer on the interface of two immiscible liquids using a polyelectrolyte and an opposite charged conventional surfactant*
2. **Diána Balogh-Weiser** (Budapest, Hungary): *Development of nanostructured biomimetic catalysts for the investigation of drug metabolism*
3. **Katalin Bere** (Szeged, Hungary): *Modelling the colloidal behavior of nano-sized particles in natural waters*
4. **Áron Bóna** (Nagykanizsa, Hungary): *The Effect of Surfactants on Polyelectrolyte Multilayer Nanofiltration Membranes*
5. **Bálint Budavári** (Budapest, Hungary): *Preparation and characterization of liposomal corticosteroids*
6. **Attila Csicsor** (Szeged, Hungary): *Impact of humic substances on the living organisms*
7. **Jennifer N. Enemmoh** (Leeds, UK): *Heavy-metal-removal-using-combined-Clinoptilolite-ion-exchange-and-co-precipitation-coagulation-techniques*
8. **Sándor Guba** (Veszprém, Hungary): *Determination of intrinsic loss power of magnetic fluid with differential thermometric system*
9. **Anna Harsányi** (Budapest, Hungary): *Preparation of highly fluorescent soft nanoparticles for bioimaging applications*
10. **Zoltán Horváth** (Budapest, Hungary): *Zn-loaded nanofiber based wound dressings*
11. **Tomáš Hrivnák** (Bratislava, Slovakia): *Atomistic and coarse-grained molecular dynamics study of self-diffusion of poly(alkyl acrylate) chains in melt*
12. **Ákos Juhász** (Budapest, Hungary): *Mechanical testing of nanofiber matrices with an affordable rupture detection system*
13. **Edit Kaszab** (Gödöllő, Hungary): *The potential role of antibiotic resistant environmental Pseudomonas species in microplastic colonization*
14. **Gábor Koplányi** (Budapest, Hungary): *Functionalized nanoparticles for efficient isolation and immobilization of a recombinant transaminase*
15. **Nikoletta Kovács** (Nagykanizsa, Hungary) *High-sensitivity analytical methods supporting the evaluation of adsorption studies*
16. **Patrik Kula** (Prague, Czech Republic): *The shape of near-critical interfaces*
17. **Sándor Mester** (Zalaegerszeg, Hungary): *Polarizabilities and electric field induced forces in periodic two-component linear dielectric sphere chains*
18. **Roland Nagy** (Zalaegerszeg, Hungary): *Investigation of the sedimentation characterization of magnetorheological fluids*
19. **Mónika Nanys** (Budapest, Hungary): *Biodegradable, three-dimensional fiber structures created by electrospinning – the effect of humidity*
20. **Dávid Nyul** (Debrecen, Hungary): *The effect of ionic liquid on the morphology and surface character of carbon aerogels seen by NMR*

21. **Veronika Pálos** (Budapest, Hungary): *Optimization and potential medical application of fibrous structures made of polysuccinimide / inorganic salt mixture*
22. **Vanda Papp** (Debrecen, Hungary): *NMR characterization of cement binders related to the radioactive waste conditioning*
23. **Kadosa Sajdik** (Szeged, Hungary): *Monitoring the effect of pH and ionic strength on the interaction between Bovine Serum albumin molecules and graphene oxide nanosheets*
24. **Evelin Sánta-Bell** (Budapest, Hungary): *Stabilization of selectively complexed His-tagged enzymes on magnetic nanoparticles*
25. **Gergely Stankovits** (Budapest, Hungary): *The contribution of mucin in the in vitro mucoadhesion measured on hydrogel substrates*
26. **Gergő D. Tóth** (Budapest, Hungary): *Formulation of Lipases into Polymer Nanofibers for Pancreatin Replacement Therapies*
27. **Ildikó Y. Tóth** (Szeged, Hungary): *Solvent specific evaporation from CNT buckypapers with different functionalization*
28. **Mónika Valiskó** (Veszprém, Hungary): *A scaling parameter for selectivity in the infinitely long nanopore limit: extension to multivalent electrolytes*
29. **Viktória Varga** (Szeged, Hungary): *Preparation, characterization and stability of magnetite nanoflowers*
30. **Constantinos Voniatis** (Budapest, Hungary): *Application differences of liquid and gel alcohol based handrubs formulations*

Invited lectures

Water at interfaces: from wetting to atmospheric chemistry

E.H.G. Backus¹

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ABSTRACT

Aqueous interfaces are not only fundamentally interesting, but also play important roles in for example wetting, electrochemistry, and atmospheric chemistry. Studying just the interfacial molecules is very challenging as often a macroscopic amount of water is present and solutes are not solely located at the interface. By using the surface-specific technique, sum frequency generation spectroscopy (SFG), we can selectively probe the interfacial molecules by obtaining the vibrational spectrum of just the interfacial layer.

In the first part of the talk we will focus on understanding certain aspects of wetting. The contact angle of a polystyrene/polyacrylic acid (PS/PAA) film is higher before exposure to water than after wetting. By monitoring with SFG the characteristic vibration of the PS moiety at 3050 cm^{-1} , we can show that the polymer film restructures upon wetting. Only after annealing the polymer film, the intensity of the PS band recovers proving the reversibility of the process [1].

In the second part of the talk we will shift towards atmospheric chemistry. Pyruvic acid is an important intermediate in several metabolic relevant processes and also in the environment. Its acid/base behavior, especially at interfaces, is relevant for understanding the chemical interaction of organic matter in oceans and atmospheric aerosols, where reaction rates and product distributions change due to different pH conditions, e.g. chemical processing and molecule transport. Using SFG we determine the dissociation of pyruvic acid at the air/water interface by probing the COO^- and COOH vibrations of the carboxylic acid groups. For comparison to the protonation state in bulk, infrared bulk measurements utilizing ATR spectroscopy are performed. We observe that the carboxylic acid group of pyruvic acid deprotonates at a higher pH value at the surface than in the bulk [2]. The different protonation states can have an impact on the conformation and functioning of molecules on the aqueous surface and an influence on the environment and biologically relevant reaction processes.

REFERENCES

- [1] Li, X.; Encheva, E.; Butt, H.-J.; Backus E. H. G.; Berger, R., "Adaptation and Recovery of a Styrene-Acrylic Acid Copolymer Surface to Water", *Macromol. Rapid Commun.* **2100733**, (2022).
- [2] Lesnicki, D.; Wank, V.; Cyran, J. D.; Backus E. H. G.; Sulpizi, M., "Lower degree of dissociation of pyruvic acid at water surface than in bulk", *Phys. Chem. Chem. Phys.* accepted (2022)

Simulating bulk and interfacial water with neural network potentials

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ABSTRACT

The strong, directed network of hydrogen bonds of water lies at the heart of its rich phase diagram and numerous anomalous properties and is responsible for the peculiar structure of its liquid/vapor interface. Detailed insights into the molecular structure and dynamics of bulk and interfacial water have been gleaned from first principles simulations, which provide an unbiased description of water at the atomic level and yield information on the underlying molecular forces. However, the computational cost of such simulations is still daunting, particularly for interfacial systems that require relatively large system sizes as they suffer from finite size effects more than bulk systems. Recently, artificial neural networks have been proposed to overcome these limitations, yielding the accuracy of first principles simulations at a fraction of their computational cost. In this talk, I will report on the structural and thermodynamic properties of bulk water and ice [1, 2] as well as of the water/vapor interface [3] obtained using a neural network potential. In particular, I will discuss the liquid/vapor coexistence curve and its size dependence as well as the structure of the interface in terms of density profiles and molecular orientations. I will also discuss results obtained for bulk water with a neural network potential including accurate long-range interactions and charge transfer [4].

REFERENCES

- [1] Morawietz, T.; Singraber, A.; Dellago, C.; Behler, J.; „How van der Waals interactions determine the unique properties of water“, Proc. Natl. Acad. Sci. USA **113**, 8368-8373 (2016).
- [2] Cheng, B.; Engel, E. A.; Behler, J.; Dellago, C.; Ceriotti, M.; “Ab initio thermodynamics of liquid and solid water” , Proc. Natl. Acad. Sci. USA **116**, 1110-1115 (2019).
- [3] Wohlfahrt, O.; Dellago, C.; Sega, M.; „*Ab initio* structure and thermodynamics of the RPBE-D3 water/vapor interface by neural-network molecular dynamics“, J. Chem. Phys. **153**, 144710 (2020).
- [4] Tsz Wai, K.; Finkler, J. A.; Goedecker, S.; Behler, J.; “A fourth-generation high-dimensional neural network potential with accurate electrostatics including non-local charge transfer“, Nature Comm. **12**, 398 (2021).

Human induced pluripotent stem cell-derived cardiomyocyte maturation on elastic bioactive electrospun materials to obtain an adult heart organotypic model

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ABSTRACT

Human induced pluripotent stem cell-derived cardiomyocytes (hiPSC-CMs) are human-relevant cardiac disease models, and an emerging platform for *in vitro* drug and chemical toxicology replacing animal models (3Rs). The commercially available hiPSC-CMs, however currently limited in their applicability due to the lack of full adult-like maturity. The EU H2020 EMAPS-Cardio project attempts to develop a superior maturation system for hiPSC-CMs by applying complex materials mimicking extracellular scaffolds. We developed a cardiac differentiation protocol from hiPSCs to induce CM development, resulting in beating clusters of hiPSC-CMs carrying the characteristic features of human fetal CMs, which need to be stimulated further to attain an adult-like CM phenotype. In order to obtain that goal, a complex, multi-approach system is being developed. One of the key components are elastic electrospun materials. These bioactive scaffolds serve as a surface for the cells to grow on and as an extracellular matrix, which is crucial for the maturation of hiPSC-CMs. Several potential materials (silk fibroin, PCL-gelatin composites, PLCL, etc.) are being tested in different fibre morphologies (nanofibrous vs. microfibrous) and orientations (aligned vs random). Bioactive molecules, promoting hiPSC-CM maturation are encapsulated in the optimized scaffolds, with the needed elastic modulus and elastic limit. Besides encapsulating hydrophilic molecules, the use of liposomes, niosomes or micelles is tested as carriers of hydrophobic compounds. The spontaneously beating CMs are cultured on the various electrospun scaffolds inside a meso-fluidic bioreactor to provide the substantial stimuli needed for CM maturation (electrical, mechanical, biochemical, topological) in a controlled environment. Overall, progress is promising towards the ultimate goal of building a more accurate human adult cardiac organotypic model with a high translational value for drug development and toxicology.

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Targeting rheumatoid arthritis using nanomedicines

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ABSTRACT

Inflammatory arthritis is a group of diseases characterized by inflammation of the joints and often other tissues including rheumatoid arthritis. Rheumatoid arthritis (RA) patients are frequently prescribed anti-arthritic drugs including nonsteroidal anti-inflammatory drugs, glucocorticoids, disease-modifying anti-rheumatic drugs and biologics, or combinations thereof. Many patients fail to respond satisfactorily to these treatments because only a small percentage of the dose reaches the target. In addition, many patients experience serious side effects. Improving the uptake of the existing drugs in the joints might reduce the dosing frequency and increase therapeutic effects with less toxicity.

Herein we report a theranostic nanomedicine prodrug with long circulation time and sustained release of the drug in the inflamed joints. Pharmacokinetics studies using radiolabelling techniques and SPECT/CT imaging showed that the theranostic nanomedicine approach delivers higher concentrations of anti-arthritic drugs to inflamed joints than has previously been possible, despite lower and less frequent drug doses (**Figure 1**). The efficacy of the prodrugs was established in the same mouse RA model and compared to the free drug given in the same form and timing as is currently administered to patients. *In vitro* stability measurements of the prodrugs in human synovial fluid from rheumatoid arthritis patients help to better understand the impact of the local environment of an inflamed joint and how that influences drug release.

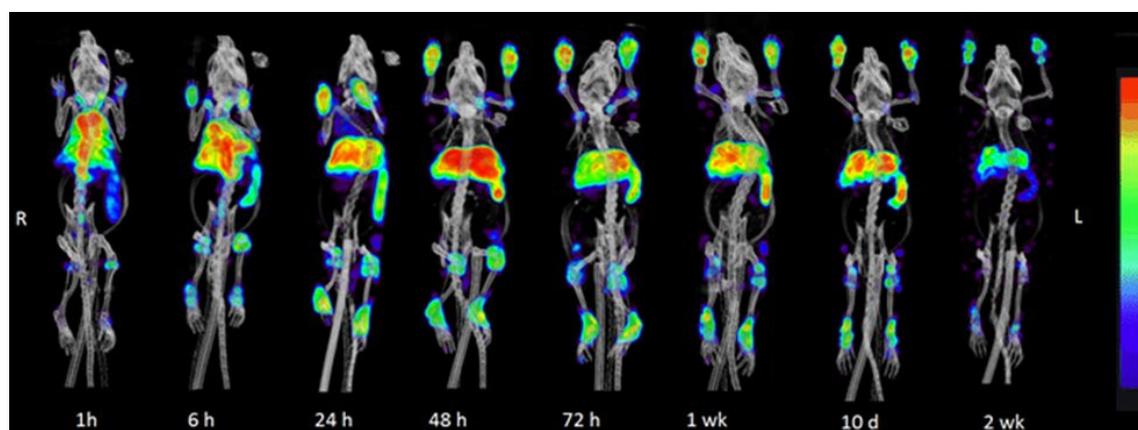


Figure 1. Radiolabelled targeted theranostic nanomedicine biodistribution in an RA model.

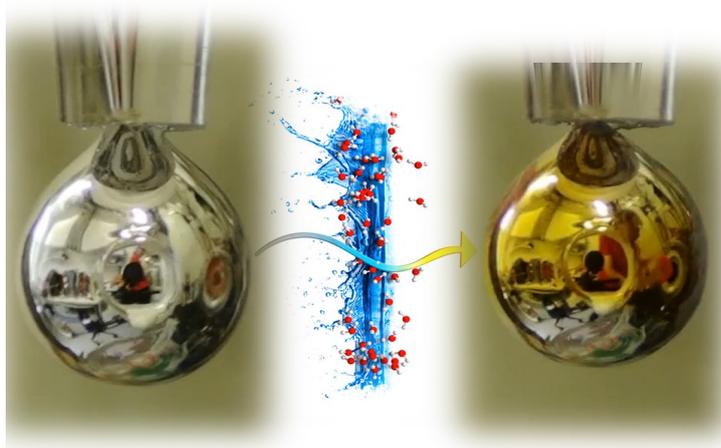
Electrons in liquid ammonia and in water: from blue electrolytes to golden metals

Pavel Jungwirth

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ABSTRACT

It would be exciting to have water with metallic properties; however, attempts to convert pure water from a perfect insulator into a metal by pressurizing the system remain in the realm of science fiction. This is because the estimated required pressure of 48 Mbar is an order of magnitude higher than what is accessible in the laboratory nowadays and may only exist in cores of large planets or stars. In this talk, we show that a metallic aqueous solution can be prepared by massively doping water by electrons liberated from alkali metals. Note that metallic solutions of liquid ammonia have been known for decades. However, it is a textbook knowledge that dissolution of alkali metals in water leads to an explosive chemical reaction, thus only low (sub-metallic) electron concentrations have been prepared so far. We have now found a way around the explosive chemistry by adsorbing water vapor at a pressure of about 10^{-4} mbar onto a train of liquid sodium-potassium alloy drops ejected from a nozzle into a vacuum chamber. This leads to a formation – on the surface of the alkali metal drop – of a thin transient gold-colored layer of water doped with $\sim 5 \times 10^{21}$ electrons/cm³, the metallic character of which is visible by naked eye and demonstrated by a combination of optical reflection and synchrotron x-ray photoelectron spectroscopies.



REFERENCES

- [1] Mason P.E., Schewe Ch.H., Buttersack T., Košťál V., Vitek M., McMullen R.S., Ali H., Trinter F., Lee Ch., Neumark D.M., Thürmer S., Seidel R., Winter B., Bradforth S.E., Jungwirth P.: Spectroscopic Evidence for a Gold-Coloured Metallic Water Solution. *Nature* **595** (2021) 673.
- [2] Buttersack T., Mason P.E., McMullen R.S., Schewe C., Martínek T., Březina K., Crhan M., Gomez A., Hein D., Wartner G., Seidel R., Ali H., Thürmer S., Maršálek O., Winter B., Bradforth S.E., Jungwirth P.: Photoelectron spectra of alkali metal–ammonia microjets: From blue electrolyte to bronze metal. *Science* **368** (2020) 1086.

The importance of aerosol acidity and its impacts

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ABSTRACT

Human activities profoundly alter the composition of the atmosphere, leading to a cascade of effects on climate, ecosystems and human health. Atmospheric particulate matter, or aerosols, play a central role in all these changes; they affect climate by modulating the Earth's energy balance, clouds and precipitation; they contain toxic compounds which upon inhalation cause millions of premature deaths every year. The same particles also contain substances that act as nutrients when deposited in ecosystems, which in turn can affect their productivity and global biogeochemical cycles. Knowledge of the levels and drivers of aerosol acidity (pH) is critical for understanding the processes that determine aerosol concentrations, chemical composition, toxicity and nutrient bioavailability. Despite its importance, aerosol pH remains poorly constrained because a practical method of direct measurement is currently not available.

This talk will focus on recent advances in constraining in-situ particle pH from the thermodynamic analysis of aerosol and gas-phase composition, and show that strong acidity (pH of 0 to 3) is ubiquitous in global aerosol. The strong acidity is caused by the large difference in volatility between sulfate (the main acidic compound, which resides completely in the aerosol phase), and ammonia (the main neutralizing agent, which partitions between aerosol and gas-phase). This counterintuitive, but thermodynamically consistent result, explains why for example aerosol acidity in the southeastern United States or in South Europe has not substantially changed over the past few decades, despite continuous reduction in sulfates and a constant ammonia background.

We then discuss under which conditions substantial changes in aerosol acidity changes occur with a focus on its impact on the solubilization of trace metals, deposition of reactive nitrogen, and responses of PM to aerosol precursors (especially those conditions that can lead to intense haze episodes). We conclude with providing outlooks for the future and emphasizing the usefulness of using aerosol pH as a fundamental property for understanding aerosol state, and formulating policy.

Dissecting how cells internalize and process nano-sized drug carriers for nanomedicine applications

A. Salvati¹

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ABSTRACT

Nano-sized materials are used in nanomedicine to deliver drugs more efficiently to their site of action. In order to improve their efficacy, a better understanding of how cells interact with nano-sized materials is required. Within this context, our research is focused on characterizing the molecular details of the early interactions of nano-sized materials at the cell membrane, and the subsequent mechanisms of uptake and intracellular trafficking.

To this aim, we use fluorescence imaging in live cells and a method based on organelle flow cytometry which we have recently developed to determine nanoparticle intracellular trafficking.[1] We then combine classic transport studies with inhibitors and RNA interference to genetic screening and proteomic-based methods to characterize the mechanisms by which nanoparticles are internalized by cells.

We show that the corona molecules adsorbing on the nanoparticle surface once applied in serum can interact with specific cell receptors, and in this way they also affect the mechanism cells use for their internalization.[2] Thus, by correlating corona composition and uptake by cells, corona proteins promoting or reducing uptake can be identified.[3] Finally, we found that even when interacting with specific receptors, nanoparticles may be internalized by cells via different mechanisms than what it is usually observed for their endogenous ligands.[2,4]

Our findings highlight the importance of understanding how cells interact with and process nano-sized materials, in order to be able to design nanomedicine with improved efficacy.

REFERENCES

- [1] Garcia Romeu et al, Time- and Space-Resolved Flow-Cytometry of Cell Organelles to Quantify Nanoparticle Uptake and Intracellular Trafficking by Cells, *Small* **17**, 34, 2100887, (2021)
- [2] Francia et al, Corona Composition Can Affect the Mechanisms Cells Use to Internalize Nanoparticles, *ACS nano* **13** (10), 11107, (2019).
- [3] Aliyandi et al, Correlating Corona Composition and Cell Uptake to Identify Proteins Affecting Nanoparticle Entry into Endothelial Cells, *ACS Biomater. Sci. Eng.* **7**, 12, 5573, (2021).
- [4] Francia et al, Mechanisms of Uptake and Membrane Curvature Generation for the Internalization of Silica Nanoparticles by Cells, *Nano Letters* **22**, 7, 3118 (2022).

Marine biofouling: The surface science challenge and some lessons to learn

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ABSTRACT

The audience is invited to join the speaker on a journey aiming at the surface science challenge of biointerfaces and related interactions with biological systems. First we shall discuss surface characterization with relevance to materials use in marine environments. Combatting marine biofouling, i.e. the undesirable accumulation of organisms on objects immersed in seawater, is a grand technological challenge. If progress is to be made in this field, a better understanding and control of the adsorption of adhesion proteins and proteinaceous macromolecules across the length scales are needed. The three key parameters that govern biomaterial accumulation encompass the surface mechanics, the morphology and the chemical composition (including charge) of surfaces. In systematic studies of marine fouling it is difficult to separate the effects of these three parameters and study them independently. Thus first we shall introduce designer model substrates prepared from polyelectrolytes using the layer-by-layer (LbL) assembly approach that allowed us to independently study and characterize the effect of surface charge on protein adhesion without altering other structural characteristics. We will show how molecular scale AFM based force spectroscopy experiments enable the determination of surface isoelectric point values of selected proteins, including adhesion proteins that are responsible for marine barnacle cyprid larva attachment to surfaces. Our LbL studies further confirmed the dominating role of electrostatic forces in the adhesion of marine attachment proteins. In fibroblast cell and bacteria adhesion tests, similar trends (high adhesion on positively charged surfaces, but much lower on neutral and negatively charged surfaces) were observed because the fibroblast cell and bacterial surfaces studied possess negative potentials. We will then focus on mechanical characterization of bacteria employing AFM, and assessment of their conditions with respect to live or death, as well as their adhesion to synthetic substrates, by using AFM based quantitative nanomechanics. To this end, we designed and prepared PDMS surfaces by varying their surface modulus of elasticity, but not changing their surface chemistry, or topology. We show then the effect of surface modulus, providing a critical modulus value approximately equal to bacterial moduli as a condition for stable attachment.

As the performance of bioadhesives often surpasses their synthetic counterparts, lessons can be learned also for preparing medical and technical adhesives using results obtained in biofouling studies. For example, it has been known that polydopamines (PDA) are responsible for the high performance of marine mussel adhesion. In a synthetic study we prepared biomimetic PDA copolymers with side chain grafts that allowed facile chemical attachment to the copolymer backbone to obtain macromolecular bottlebrushes. While PDA is a strong adhering molecule even to polyethylene (PE), side chain grafts of fouling resistant chains such as poly(oligo(ethylene glycol)methacrylate) provided clear antifouling performance also for PE. We have used such PDA based polymers also in aerospace applications bonding titania and high temperature resistant polymers. Regarding fiber adhesion in these composites, we shall elucidate single fiber adhesion characterization approaches using model matrix polymers and titania wires.

Keynote lectures

Physics, chemistry, biology, and beyond: a complex systems perspective

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ABSTRACT

Complex systems are composed of a large number of interacting components (agents). From the zillions of micro-level individual behaviors of these agents, a macro-level behavior of the whole system emerges. This phenomenon is coined as emergence. Physical and chemical systems are composed of molecules whose behavior produces measurable properties on the macro level. These systems are called complex physical systems (CPS). In biological and social systems, the agents can be macromolecules, cells, organs, organisms, individuals, or social groups. In these systems, called complex adaptive systems (CAS), the behavior of agents can be described by rules [1]. The main difference between CPS and CAS is that the rules governing the behavior of molecules do not change in time (they are the laws of nature), while the rules governing agents' behaviors in CAS can change via the mechanisms of evolution, adaptation, learning, creativity, and social innovation. Feedback loops exist in the system through which the agents can gain information about the consequences of their actions. The vertical hierarchical structure of complex systems makes it possible to model the systems on the microscopic level and simulate the emergent macro-level properties. In CPS these simulations (molecular dynamics and Monte Carlo) work on the basis of a well-founded theory: statistical mechanics. It is based on ergodicity that ensures the existence of equilibrium and reproducible experiments. In CAS the space of possible to-be-explored states is huge and complexity increases during time. Often, only a single historical time exists. Still, modeling and simulations of CAS is possible: this is called agent-based modeling. By modeling the rules and feedback loops of the CAS, we can build a bottom-up understanding of the studied phenomena.

REFERENCES

- [1] D. Boda. "*Complexity in Nature and Society. From Dancing Molecules to Collapsing Societies*". Kőszeg, Hungary (2020). ISBN 978-615-5742-19-4

Flow chamber for evaluation of Endothelial cell adhesion on stent struts

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ABSTRACT

A stent placement is a medical device for expansion of stenotic artery or for flow diversion of intracranial aneurysm. The stent struts are left on arterial walls, and especially touching with endothelial cells (ECs) and exposed on blood flow. After treatment, the ECs are expected to cover on the struts called endothelialization (EN) to avoid the reaction by the body for a strange material. Therefore, the quick EN is a key factor to the success of stent placement and the surface treatment of strut is an attractive method for the quick EN. One way for the screening test for EN was to put ECs on the material in the culture medium and the check the behaviors of ECs. However, the lack of flow leads the lack of stress to ECs from the flow.

We proposed a flow chamber for ECs adhesion on struts[1]. Confluent ECs on the bottom of chamber is exposed to culture media flowing with parallel. The wall shear stress (WSS) of 2Pa is generated on the ECs by the flow. In our study, one or two straight stent strut [2] was placed on the ECs, respectively and the behaviors of ECs were observed with optical microscope after 24 hours exposure by the flow. The surface struts were treated with anodization developed by Ohtsu et al[3]. The flow pattern and WSS was simulated using Computational Fluid Dynamics (CFD). The observations show the number of ECs on the back flow side of strut is larger than the proximal side. The density of ECs around 2 mm behind the stent strut position are higher than other places. The position is consistent with WSS. In conclusion, the use of flow chamber will reveal the effects of surface treatment and the shape of struts on EN under flow exposure.

REFERENCES

- [1] Anzai, H.; Watanabe, T.; Han, X.; Putra, N.K.; Wang, Z.; Kobayashi, H.; Ohta, M., "Endothelial Cell Distributions and Migration under Conditions of Flow Shear Stress around a Stent Wire", *Technology and Health Care*, vol. **28**, 345-354 (2020)
- [2] Wang, Z.; Putra, N.K.; Anzai, H.; Ohta, M., "Endothelial Cell Distribution After Flow Exposure With Two Stent Struts Placed in Different Angles", *Frontiers in Physiology*, vol. 12, 733547 (2022)
- [3] Yamasaki, K.; Taniho, H.; Tate, K.; Ohtsu, N., "Electrolyte effect in pulsed anodization of NiTi alloy to form a Ni-free oxide layer", *Surface and Coatings Technology*, vol. 417, 127221(2021)

Synthesis and characterization of folate-targeted monodisperse PEG-based conjugates made by chemo-enzymatic methods for cancer diagnosis and treatment

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ABSTRACT

This lecture focuses on the synthesis and characterization of new bivalent folate-targeted PEGylated doxorubicin (FA₂-dPEG-DOX₂) made by modular chemo-enzymatic processes using *Candida antarctica* lipase B (CALB) as biocatalyst. The synthetic strategies can be found in details in [1-3]. The modular approach with enzyme catalysis leads to selectivity, full conversion and high yield, and no transition metal catalyst residues. Unique features are the use of monodisperse PEG (dPEG) and the synthesis of FA-SH yielding exclusive γ -conjugation of folic acid (FA). In comparison, conjugates in the literature use the activated ester method to attach FA to polymers that gives a mixture of products that need to be purified to separate the biologically active γ -conjugate. DOX fluoresces in the red so it has dual properties as both a diagnostic and therapeutic agent, and it does not interfere with live tissue fluorescence. Flow cytometry analysis showed that at 10 μ M concentration, both free DOX and FA₂-dPEG-DOX₂ would be taken up by 99.9% of triple-negative breast cancer cells in 2 h. Fluorescence was detected for 5 days after injecting FA₂-dPEG-DOX₂ into mice. Preliminary results showed that intra-tumoral injection seemed to delay tumor growth more than intravenous delivery [4].

REFERENCES

- [1] Puskas, J. E.; Sen, M. Y. US 8,710,156, **2014**
- [2] Puskas J. E.; Sen, M. Y. US 9,885,070, **2018**
- [3] Puskas, J. E.; Molnar, K.; Krisch, E., "Toward the Effective Synthesis of Bivalent Folate-Targeted PEGylated Cancer Diagnostic and Therapeutic Agents Using Chemo-Enzymatic Processes", *Journal of Molecular Liquids* **310.**, 113218–113227 (2020)
- [4] Nagy, K. S.; Toth, K.; Pallinger, E.; Takacs, A.; Kohidai, L.; Jedlovszky-Hajdu, A.; Mathe, D.; Kovacs, N.; Veres, D. S.; Szigeti, K.; Molnar, K.; Krisch, E.; Puskas, J. E.; "Folate-Targeted Monodisperse PEG-Based Conjugates Made by Chemo-Enzymatic Methods for Cancer Diagnosis and Treatment", *International Journal of Molecular Science* **22.**, 10347 (2021)

Oral contributions

Space tests of porous aluminum oxide insulation fibers

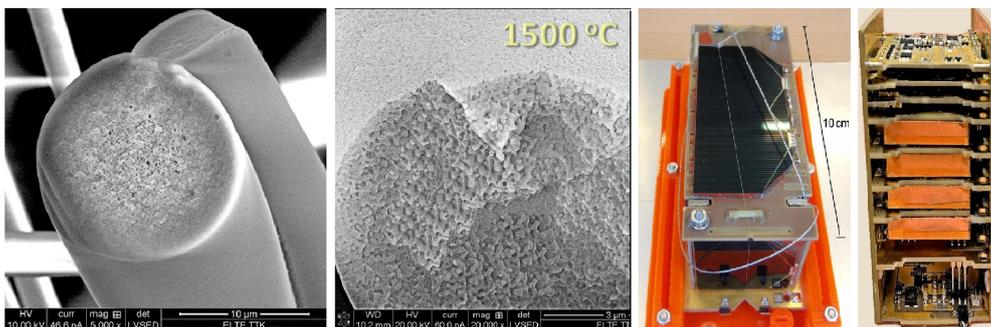
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ABSTRACT

The aim of this present work was to develop a new, low-cost sol gel synthesis route to produce porous aluminum oxide thermal insulation fibers to high temperature application [1]. The ultralight alumina ceramic fibers were produced by a new solution method and electro spinning technique [2]. The Al_2O_3 fibers can be characterized by $0.035\text{-}0.037 \text{ W} \cdot \text{mK}^{-1}$ thermal conductivity, good flexibility, and excellent heat resistance. The porous fibrous structure is reminded up to $1600 \text{ }^\circ\text{C}$. One of their applications is the insulation of space vehicles, like satellites. This study extended to check the fibers during the lunch and in the conditions of space by a satellite test.

The porous aluminum oxide fibers were tested by means of ATL-1 satellite. The ATL-1 mission was started at 2019.12.06 when the satellite was delivered to a 390 km high Solar Synchronize Orbital as a payload of Rocket Lab's Electron rocket from New Zealand. During the experiment the insulation character of Al_2O_3 fibers has slightly changed during near 10 months demonstrating the stability of the fibers even in extreme fast changing conditions. The Al_2O_3 fibrous insulation material showed nearly 20% less temperature fluctuation compared to the well-known Kapton-foil, which was used as a reference. Finally, the only 1 mm layer thick Al_2O_3 fibrous could show better than 20% thermal insulation capacity, than Kapton-foil.



REFERENCES

- [1] P. Ádám, O. Temesi, Z. Dankházy, C. Voniatis, J. Rohonczy, K. Sinkó, Various colloid systems for drawing of aluminum oxide fibers, *Ceramics International* **48** 5499-5508, (2022)
- [2] Sinkó, K, Temesi, O., Ádám, P., Nagy, A.: Process for the production of 100% alumina, porous, fibrous material. Hungarian Patent **P2100158** (2021)

Effect of brine salinity on the solution properties of polymers for enhanced oil recovery

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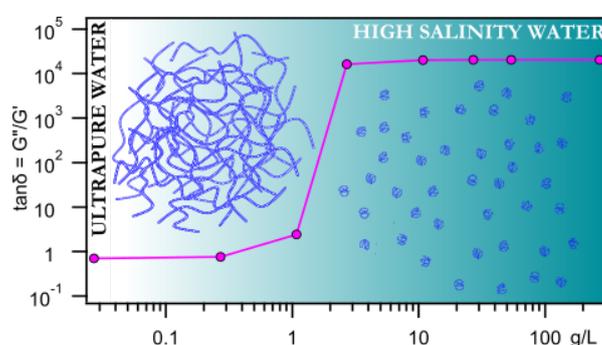
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ABSTRACT

Partially hydrolysed polyacrylamide (HPAM) and ATBS (2-acrylamido-tertiary-butyl sulfonic acid) based polymers are widely applied to recover residual oil from reservoirs during polymer flooding processes in enhanced oil recovery (EOR). Although this technique showed good efficiency in oil fields of mild environmental conditions, harsh circumstances, such as elevated temperature and high salinity, may adversely affect the performance of the polymers. In the present research, physico-chemical features of Flopaam 3630 and Flopaam AN125SH were investigated at different salt concentrations. The possible intermolecular interactions between the polymer chains were explored by rheology in both rotational and oscillatory modes under different experimental conditions. It was shown that the rheological properties of the polymer solutions change significantly around 1 g/L salinity. Accordingly, the observed pseudoplastic behaviour indicated remarkable intermolecular interactions below this threshold value, while tendencies in the parameters of the flow curves as well as in the storage and loss modulus clearly confirmed the breakup of such a coherent (gel-like) structure above 1 g/L salt concentration (see figure below). Therefore, the solution behaviour of these polymers could be described by considering the presence of individual macromolecule chains without formation of gel structure at elevated salt levels. These results were further underpinned in modulated 3D cross-correlation light scattering and electrokinetic measurements performed at different salt levels. The above findings provide valuable information for the applicability of the Flopaam 3630 and the Flopaam AN125SH polymers during EOR processes in oil reservoirs of various salinity.



ABSTRACT

This work was financially supported by the GINOP-2.3.4-15-2020-00006 project.

Computer simulation investigation of the adsorption of acetamide under atmospheric and interstellar conditions

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ABSTRACT

Acetamide is not only released into the atmosphere from natural sources, but its large-scale industrial use also results in its atmospheric emission. The main atmospheric sink of acetamide is its oxidation, however, other atmospheric fates are also plausible. In wet deposition, acetamide can be captured by ice grains through adsorption. Thus, we investigated the adsorption of acetamide at the surface of crystalline (I_h) and low density amorphous (LDA) ices by performing a set of grand canonical Monte Carlo simulations at the tropospheric temperature of 200 K. Besides calculating the adsorption isotherms, we also characterised the energetics of the adsorption and the orientational preferences of the first layer molecules. We demonstrated that at low enough surface concentrations, the adsorbed acetamide molecules prefer to lay parallel with the ice surface. With increasing surface coverage, acetamide molecules preferentially stay perpendicular to the surface, pointing by the CH_3 group straight away from the ice phase, typically forming 2 H-bonds with each other and 2 with the surface waters. Finally, after the appearance of outer layer acetamide molecules, first layer molecules prefer to form 3 H-bonds with their acetamide neighbours and only 1 with the surface waters.

As acetamide has been detected in a relatively large amount in space as well, we extended our study by performing grand canonical Monte Carlo simulations at 50 and 100 K on LDA ice, which are more characteristic of typical domains of the interstellar medium. We found that the relative importance of the acetamide–acetamide H-bonds with respect to the acetamide–water ones increases with decreasing temperature. As a result of it, the saturated monolayer, which is stable in a broad range of chemical potentials at 200 K, shrinks with decreasing temperature, and, eventually, vanishes at 50 K, while multilayer adsorption becomes more and more pronounced at the lower temperatures. Furthermore, our results suggest that non-negligible acetamide adsorption might occur on LDA surfaces at low enough temperature (i.e., 50 K and below), thus, the interstellar formation of peptide chains through acetamide molecules might well be a plausible process in the cold domains of the interstellar medium; however, it is rather unlikely in the higher temperature domains.

Molecular dynamics simulations of interactions of SARS-CoV-2 spike protein with graphene during initial stage of adsorption

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ABSTRACT

The interactions of SARS-CoV-2 virus with the cells or surfaces is governed by the protruding spike protein [1,2], which is responsible for the infection of susceptible cells through its interaction with the ACE2 enzyme. The formation of a stable complex with the ACE2 receptor and consequent cell infection is only feasible if the spike glycoprotein trimer adopts an open conformation. Materials based on graphene are often employed in protection against viruses and even in deactivation of viruses. In the present study, the structural changes of non-glycosylated monomer (S-protein) and glycosylated receptor binding domain (RBD) of the spike glycoprotein trimer triggered by their adsorption onto graphene at the initial stage are investigated by means of atomistic molecular dynamics simulations. The S-protein becomes more prolate after its fast adsorption on graphene. RBD of S-protein appears to be the most rigid fragment and upon adsorption, its rigidity is enhanced. During adsorption, new internal hydrogen bonds are formed at the expense of hydrogen bonds between the S-protein and water molecules. In the initial phase, the secondary structure of the RBD fragment specifically interacting with ACE2 receptor is not affected during the adsorption onto the graphene.

ACKNOWLEDGEMENTS

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REFERENCES

- [1] Wu, F.; Zhao, S.; Yu, B.; Chen Y.-M.; Wang, W.; Song Z.-G.; Hu, Y.; Tao, Z.-W.; Tian, J.-H.; Pei, Y.-Y.; Yuan, M.-L.; Zhang, Y.-L.; Dai, F.-H.; Liu, Y.; Wang, Q.-M.; Zheng, J.-J.; Xu, L.; Holmes, E. C.; Zhang, Y.-Z., "A new coronavirus associated with human respiratory disease in China", *Nature* **579**, 265-269, (2020).
- [2] Walls, A. C.; Park, Y.; Tortorici, M. A.; Wall, A.; McGuire, A. T.; Velesler, D., "Structure, Function, and Antigenicity of the SARS-CoV-2 Spike Protein", *Cell* **180**, 281-292, (2020).

Field-induced structural transitions in magnetic granulate

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ABSTRACT

In nature, structural and phase transitions are significant and lead to drastic changes in material macroscopic properties. The underlying mechanisms, time and length scales of those transitions might differ depending on the material. At the beginning of 2000, for dynamically asymmetric mixtures, containing a fast and a slow component, a new type of viscoelastic phase separation (VPS) was proposed by Hajime Tanaka [1]. This transition goes in two steps: first, the slow component forms open networks that dynamically evolves in time (viscous phase); second, the networks collapse into compact aggregates/droplets (elastic phase). As for any new phenomena, the question arose for VPS, whether it is scalable to system of larger sizes and whether it is universal. Recently, we showed that a Tanaka-like transition takes place on a millimeter scale in a shaken mixture of steel and glass spheres, *i.e.* in a so-called ferrogranulate [2]. In the experiment, a flat vessel filled with a mixture of magnetized steel beads and glass beads is vibrated with high frequency to preserve a gas phase. Next, it is quenched, and the agglomeration of magnetic spheres is followed optically. The experiment is accompanied by molecular dynamics computer simulations, where the complex magnetization of the macroscopic steel beads is modelled in a simple Stockmayer approach [2].

Using the magnetic nature of the slow steel component, in our work, we put forward a hypothesis: an applied magnetic field can alter the VPS and force the structural transitions in ferrogranulate to follow a different scenario, depending on the field direction/intensity. We find that if the field is aligned parallel to the vessel plane, chains and elongated clusters parallel to the field are favored. Vertical connecting structures tend to be suppressed, leading to the unknotting of the networks, which are observed at zero field [3]. Importantly, we show that moderate field strengths lead to larger clusters at intermediate time intervals than in the case of weak and strong fields. Moreover, the latter tend to limit the overall growth of the clusters at longer time scales. Suppose the field is aligned perpendicular to the layer plane. In that case, instead, we see that there is a critical ratio between the applied field and the granulate temperature at which clusters get disintegrated entirely. The slow component assumes a hexatic phase in which the distance between steel beads is maximized.

Not only is the ferrogranulate a fascinating system to investigate Tanaka-like transitions at a convenient scale, but elucidation of the mechanisms in ferromagnetic granulate could deepen our understanding of such versatile processes as sedimentation in magnetorheology or the early stage of planet formation.

REFERENCES

- [1] Tanaka, H., "Viscoelastic phase separation", *J. Phys.: Cond. Mat.* **12**, R207, (2000).
- [2] Kögel, A.; Sánchez, P. A.; Maretzki, R.; Dumont, T.; Pyanzina, E. S.; Kantorovich, S. S., & Richter, R., "Coarsening dynamics of ferromagnetic granular networks – experimental results and simulations", *Soft Matter* **14(6)**, 1001, (2018).
- [3] Sánchez, P. A.; Miller, J.; Kantorovich S. S.; Richter R., "Unknotting of quasi-two-dimensional ferrogranular networks by in-plane homogeneous magnetic fields", *J. Magn. Magn. Mater.* **499**, 166182, (2020).

The effect of annealing and layer numbers on the ion exchange capacity of polyelectrolyte multilayer nanofiltration membranes

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ABSTRACT

The Layer-by-Layer (LbL) assembly method to build NF membranes on UF and MF substrates has become a staple in membrane fabrication technology, leading to highly selective and robust membranes [1]. By controlling the synthesis parameters, the selectivity and permeability of these membranes can be fine-tuned to a high degree. The polyelectrolyte anions and cations bind together with Coulomb bonds in these membranes to form a dense active layer, however some charges remain unbound, which leads to ion exchange sites. The ion exchange capacity of these membranes can have a significant effect on the measured salt rejections (by conductivity) in some circumstances, which can lead to the distortion of the experimental results. The ion exchange capacity is affected not just by the amount of pure water used for washing the membranes, but also the annealing time in pure water.

REFERENCES

- [1] Sewerin, T., Elshof, M.G., Matencio, S., Boerrigter, M., Yu, J., de Grooth, J., “Advances and Applications of Hollow Fiber Nanofiltration Membranes: A Review.”, *Membranes* 11, 890-924 (2021)

Antioxidant effect of humic substances: an overview

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ABSTRACT

The major population of Hungary suffers from one of the diseases related to free radicals (diseases of civilization, obesity, cardiovascular, etc.). Berries have become a major player in a number of related research papers. What other options do we have, what other substances in nature may still have high antioxidant content? It could be humic substances (HS) and their components, which play a crucial role in the development of their antioxidant effect, both qualitatively and quantitatively. The aim of the research is to compare the antioxidant properties of humic acids with already well-known antioxidants like ascorbic acid, gallic acid and trolox.

HS are chemically ill-defined natural organic colloids made up of decomposition products of plant-derived biomass, in a process called humification [1]. They are heterogeneous, redox-active organic macromolecules with distinct electron-donating properties. HS behaves as free radical scavengers and they have antioxidant properties based on their phenolic and polyphenolic hydroxyl groups. [2]

In the lecture I will present the different antioxidant test methods (total phenol, DPPH, CUPRAC) used to examine the antioxidant capacity of different humic substance fractions (Humic acid: HA, Fulvic acid: FA, Himatomelanin acid: HY) and the official samples of the International Humic Substances Society. ESR spectra of selected samples were also recorded to measure free electron contents for estimating their electron capture capability.

Based on the total phenol analysis the HA has the most of the phenolic groups. The HY acid is located in the middle and FA has the fewest phenolic groups. The results suggest that the studied HS are likely to have an antioxidant effect. From the DPPH data it can be concluded that the self-made humic materials have antioxidant properties because they definitely inhibited the decomposition of the DPPH radicals. The results from the CUPRAC test also pointed that the HS have a good antioxidant properties. The measured free electron contents also support it.

REFERENCES

- [1] Stevenson, F. J. Humus Chemistry: Genesis, Composition, Reactions, Wiley & Sons, New York, 188-210, 1994 ISBN 0471594741
- [2] Seyda K. et al, "Determination of total antioxidant capacity of humic acids using CUPRAC, Folin–Ciocalteu, noble metal nanoparticle- and solid–liquid extraction-based methods" Talanta Volume 153, 120-129, 2016

Study of bentonite hydration by NMR relaxometry and chemometrics

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ABSTRACT

One of the key features of clay minerals which makes them potential engineered barriers is the swelling. During hydration the clay mineral expands, and many physical properties will change by the change of its pore structure.

In this study, water transverse T_2 relaxation decays were recorded by time-domain NMR relaxometry in permanent gradient magnetic field at different water-bentonite ratios and different different Na-bentonite/Ca-bentonit ratios. The number of the relaxing components (water protons) and the value of the relaxation times depend on numerous effects, but on the other hand, monitoring the change of this values can give us information about the hydration state of the bentonites.

The other huge advantage of the permanent gradient probehead, the NMR-MOUSE (Mobile Universal Surface Explorer) is the moveability – in two sense: the mobility of the water protons can be determined, and the probehead can be moved practically to anywhere. Since one of the applications of the bentonites is the usage as engineered barriers, the possibility of the on-field measurements can be very helpful.

NMR relaxometry makes possible to determine also the Na/Ca ratio in the clay minerals. The convenient evaluation method for relaxometry data is the Multi Exponential Relaxation Analysis (MERA). This regularization of the relaxation decay allows us to obtain the relaxation time distribution. However this method is quite time consuming, and at some cases –especially at low Echo-times – mathematical artifacts appear and make the analysis even more difficult. Multivariate data analysis provides a powerful tool to build a soft-sensor model for predicting the the clay mineral mixture composition or the mixture hydration state.

[1] W.F. Bradly, R.E. Grim, G.K. Clarck, “A Study of the Behavior of Montmorillonite upon Wetting”, Zeitschrift für Kristallographie **97**, 260–270, 1937

[2] C.Y. Lee, R.T. Thompson, F. S. Prato, D. E. Goldhawk, N. Gelman, “Investigating the Relationship between Transverse Relaxation Rate (R2) and Interecho Time in MagA-Expressing, Iron-Labeled Cells”, Molecular Imaging **14** 551-560, 2015

[3] I. Ardelean, R. Kimmich, “Principles and Unconventional Aspects of NMR Diffusometry”, Annual Report on NMR Spectroscopy **49**, 44-115, 2003

Development of laboratory electrospinning as a tool for the entrapment of biomolecules

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ABSTRACT

Electrospinning is a promising tool for production of polymer nanofibers, providing innovative matrices for the entrapment of various biomolecules such as cells, cell organelles, enzymes, proteins or antibodies. [1] In the process of electrospinning polymer precursor (containing the targeted biomolecules) held by its surface tension at the end of a capillary is continuously subjected to electrostatic field. By the selection of polymers excipients, a favorable chemo-structural environment can be ensured for the biomolecule, which is one the most critical issue during the immobilization procedure. On the other hand, the finetuning of the electrospinning conditions (applied voltage of electrostatic field and precursor feeding, construction and geometrical characteristic of the spinning cabinet etc.) are also influence the properties and quality of the nanofibrous product. Our several studies showed that by the rational design and optimization of precursors and electrospinning process, wild type and engineered recombinant enzymes can be successfully entrapped in polymer nanofibers. The nanofibrous biocatalyst could be efficiently applied for various type of synthetic biotransformation for the production of chiral compounds with pharmaceutical relevance. [2] In addition, enzyme loaded nanofibers as an alternative therapeutic formula with enhanced activity and stability opened the opportunity in the development of novel enzyme replacement therapies. [2,3]

REFERENCES

- [1] Balogh-Weiser, D.; Németh, C.; Ender, F.; Gyarmati, B.; Szilágyi A.; Poppe, L, "Electrospun nanofibers for entrapment of biomolecules", *IntecOpen*, 135-147, (2018).
- [2] Koplányi, G.; Sánta-Bell, E.; Molnár, Z.; Tóth, G.D.; Józó, M.; Szilágyi A.; Ender, F.; Pukánszky, B.; Vértessy, G.B.; Poppe, L.; Balogh-Weiser, D, "Entrapment of Phenylalanine Ammonia-Lyase in Nanofibrous Polylactic Acid Matrices by Emulsion Electrospinning", *Catalysts*, **11**, 1149, (2021).
- [3] Tóth, G.D.; Kazsoki, A.; Gyarmati, B.; Szilágyi, A.; Vasvári, G.; Katona, G.; Sente, L.; Zelkó, R.; Poppe, L.; Balogh-Weiser D.; Balogh, G.T, "Nanofibrous Formulation of Cyclodextrin Stabilized Lipases for Efficient Pancreatin Replacement Therapies", *Pharmaceutics*, **13**, 972, (2021).

MARTINI cholesterol gives membranes the chills – and what you can do about it

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ABSTRACT

Cellular membranes consist of hundreds of different lipid species and exhibit lateral inhomogeneities and membrane domains with specific biophysical properties. Coarse-grained molecular dynamics simulations of membranes containing a ternary mixture of phospholipids with high and low melting temperature and cholesterol [1] provide a minimal model to study the separation of liquid-ordered (L_o) and liquid-disordered (L_d) phases. However, we recently uncovered the presence of artificial temperature gradients in simulations of phase separating ternary lipid mixtures using the popular Martini force field [2]. We traced the origin of this artifact to the presence cholesterol, whose planarity is maintained with constrained dynamics as implemented in the linear constraint solver LINCS [3]. Incomplete numerical solutions to the constraint equations for typical integration time steps result in artificial cooling of cholesterol, which in turn impacts phase separation and other membrane properties. Here, we use rigid body mechanics to construct *equimomental systems* [4] of particles to optimize the constrained “scaffold” of cholesterol. Our optimized cholesterol topology reproduces the properties of the original model under strict LINCS settings and/or small simulation time steps, that is, in the absence of temperature gradients. Importantly, the optimized model does not develop temperature gradients even at less strict LINCS settings and larger time steps. The optimized model is computationally less expensive than the original model combined with strict LINCS settings, and the comparison is even more favorable when other constrained moieties are present that do not require such vigorous constraining.

REFERENCES

- [1] Heberle, F. A.; Feigenson, G. W., “Phase Separation in Lipid Membranes”, *Cold Spring Harbor Perspectives in Biology* **3(4)**, a004630 (2011)
- [2] Thallmair, S.; Javanainen, M.; Fábíán, B.; Martinez-Seara, H.; Marrink, S. J., “Nonconverged Constraints Cause artificial Temperature Gradients in Lipid Bilayer Simulations”, *The Journal of Physical Chemistry B*, **125**, 9573-9546 (2021)
- [3] Hess, B., “P-LINCS: A Parallel Linear Constraint Solver for Molecular Simulation”, *Journal of Chemical Theory and Computation*, **4**, 116-122 (2008)
- [4] Laus, L.P.; Selig, J. M., “Rigid body dynamics using equimomental systems of point-masses”, *Acta Mechanica*, **231**, 221-236 (2020)

Long-term aging of concentrated aqueous graphene oxide suspension seen by various analytical techniques

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ABSTRACT

Nowadays, graphene oxide (GO) is commercialized in suspended form, because techniques such as direct ink writing, 3D printing, film casting, wet spinning require GO dispersions. However, nanoparticle suspensions may tend to aggregate and/or gelate. These changes may influence the chemistry and morphology of these suspensions and thus their application potential.

Three aqueous GO suspensions of 10 mg/mL were obtained by an improved Hummers' method^[1] within 1 year time gap between each (0 y, 1 y and 2 y). The aging of these suspensions was

followed by various techniques^[2]. Herein we report the results of Raman spectroscopy, XPS and laser particle size analysis. The particle size distribution curves reveal the aggregation of the particles. After 2 years storage, the size of the largest particles increases from about 68 μm to 300 μm . From Raman spectra the intensities of the D (structural disorder) and G (sp^2 building blocks) bands of the first order and the 2D (graphitic order) of the second order regions were used to follow the changing in the GO suspensions. The systematic increase of the intensity ratios I_D/I_G (Figure 1) and the I_{2D}/I_G , implies a slow oxidation process of the most upper GO sheets making them more vulnerable to be peeled off.

The oxidation process was also corroborated by XPS in which the O/C atomic ratio increased from 0.33 to 0.49 after 2 years storage, while the shearing off was confirmed by independent methods.

ACKNOWLEDGMENTS

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REFERENCES

- [1] Marcano, D.C.; Kosynkin, D.V.; Berlin, J.M.; Sinitskii, A.; Sun, Z.; Slesarev, A.; Alemany, L.B.; Lu, W.; Tour, J.M. Improved synthesis of graphene oxide, *ACS Nano*, 2010, 4, 4806–4814.
- [2] Gyarmati B.; Farah S.; Farkas A.; Sáfrán G.; Voelker-Pop LM.; László K.; Long-Term Aging of Concentrated Aqueous Graphene Oxide Suspensions Seen by Rheology and Raman Spectroscopy, *Nanomaterials*, 2022, 12:916.

Nonlinear dynamic susceptibility of magnetic fluids in symmetry breaking dc magnetic fields

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ABSTRACT

The nonlinear contribution to the dynamic magnetic susceptibility of magnetic fluids – which are colloidal dispersions of magnetic nanoparticles (MNPs) – becomes significant in several practical applications, such as magnetic hyperthermia, and magnetic particle imaging. In these applications the magnetic behavior determines the response of the fluids under an external magnetic field. Theoretical models are essential tools to predict the magnetic properties, and to help design optimized and well-suited MNPs for practical uses. Ranging from the simple theory given by Langevin for the collection of noninteracting magnetic dipoles, through different mean-field models to include the effect of dipole-dipole interactions, to the solution of the Fokker-Planck-Brown equation numerous theoretical approaches are available to describe the magnetic properties of an ensemble of MNPs. In one of our recent works [1], we proposed an expansion method within the framework of mean spherical approximation (MSA) to calculate the nonlinear susceptibilities of magnetic fluids. The method uses the field expansion of magnetization, while the frequency dependence of the higher order susceptibilities is treated based on the Debye relaxation of magnetic dipoles. The theory was successfully applied under weak fields to determine the magnetic field strength and frequency dependence of the linear and nonlinear susceptibility components up to the 4th harmonic relevant for magnetic fluids. Here we build upon those results and extend the expansion based MSA model to cover the case when a symmetry breaking dc magnetic field is superimposed on the ac field. We investigate the magnetic field strength and frequency dependence of the magnitude of the even and odd harmonic susceptibilities. Under an applied dc field not just the even components are present, but the odd ones also appear due to symmetry reasons.

REFERENCES

[1] Horváth, B.; Decsi, P.; Szalai, I., “Nonlinear contributions to the dynamic magnetic susceptibility of magnetic fluids”, *Journal of Molecular Liquids*, 119279, (2022). In press

Local structure in mixtures of ionic liquid with molecular solvent

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ABSTRACT

Ionic liquids (IL), being low-temperature melts by their nature, are of considerable scientific interest due to a number of their unique properties. The practical application of ILs, especially in electrochemistry, has significantly expanded due to the use of mixtures with molecular solvents of various natures. A detailed microscopic description of the local structure in such systems, depending on the nature of its constituent components and the composition of the mixture, remains an urgent problem of modern chemistry of liquid state. In this chapter, we review the results obtained by vibration spectroscopy and NMR chemical shift on the variations in microscopic structure as a function of mixture composition. The most significant changes in the ^1H chemical shift occur at low ionic liquid content. Dilution and stacking interactions between the cation rings induce negative variation of the ^1H relative chemical shift. As the solvent and the ions can establish hydrogen bond interactions, when these interactions are weaker, almost equal or higher than the interionic interactions, this results in negative, almost equal to zero or positive values of the relative chemical shift, respectively. We also used molecular dynamic simulation and the nearest neighbor approach to calculate radial distribution and spatial radial distribution functions, and to define two statistical distance descriptors of the hydrogen bond structure C-H... X (X being atom of either the anion or of the solvent) to characterize the local structure around the C-H bond of the cation. The mole fraction dependence of these statistical properties, calculated by taking into account only the nearest neighbor, correlates consistently with spectroscopic data. Indeed, these descriptors are relatively unaffected in the ionic liquid mole fraction (x_{IL}) range between 1.0 and 0.3, while with further decrease of x_{IL} a large effect on these descriptors, is observed. These changes are compatible with the physical picture that the solvent molecules compete with the anions to occupy positions close to the hydrogen atoms of cation ring.

REFERENCES

- [1] B. A. Marekha, V . Koverga, N. Maity, A. Juhasz, F. A. Miannay, A. Inkol, T. Takamuku, P. Jedlovsky, O. N. Kalugin, and A. Idrissi "Local Structure in Mixtures of Ionic Liquid with Molecular Solvent: Vibration Spectroscopy, NMR and Molecular Dynamics Simulation" *Molecular Basics of Liquids and Liquid-Based Materials* 289-334, Springer, Singapore (2021) (<https://doi.org/10.1007/978-981-16-5395-7-10>)

Biocompatible folate targeted cobalt ferrite nanoparticles for magnetic hyperthermia

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ABSTRACT

The capability of magnetic nanoparticles (NPs) to release heat in alternating magnetic field, i.e., magnetic hyperthermia, is a very interesting property for medical application. Here we report the effect of cobalt content on magnetic properties and hyperthermic efficiency of spinel ferrites with various composition. Eight $\text{Co}_x\text{Fe}_{3-x}\text{O}_4$ samples were synthesized by alkaline coprecipitation with $x=0-1$ cobalt content. The average size determined by light scattering was ~ 45 nm for magnetite, while Co-ferrites showed larger hydrodynamic diameter (65-160 nm). The pH-dependent surface charging characterized by electrophoretic light scattering revealed, that pure magnetite has an IEP about $\text{pH}\sim 8$, but with increasing Co-content the pH_{IEP} shifted to more acidic values ~ 6.5 . Based on magnetic measurements performed by SQUID at 5 and 300 K and calorimetric studies carried out at various frequencies (252-808 kHz) and at different field strengths (50-300 G) three samples (the pure MNP and Co-ferrite and one sample with 25 % theoretical cobalt content) were chosen to coat with a new PEG containing polysaccharide type copolymer anchored with folate side chain. Magnetization measurements and hyperthermia tests showed that the presence of the polymer layer on the particle's surface do not change their characteristics significantly, only a slight decrease in saturation magnetization and SAR values were observed. Although a moderate reduction was detected in viability for 48 h incubation for each bare nanoparticles in the case of all 4 cancer cell lines (human colon cancer (HCT116), human breast adenocarcinoma (MCF7), human normal bronchial epithelial (16HBE) and human dermal fibroblast (HDFa)) used, the reduced viability could not be observed for FA-INU-PEG coated samples, the values did not change neither after 24 h nor 48 hours.

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REFERENCES

[1] Scialabba, C.; Puleio, R.; Peddis, D.; Varvaro, G.; Calandra, P.; Cassata, G.; Cicero, L.; Licciardi, M.; Giammona, G., Folate targeted coated SPIONs as efficient tool for MRI, Nano Res., pp 1-16. (2017).

Sticky-MARTINI – a reactive coarse-grained model for self-assembly in materials synthesis

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ABSTRACT

Reflecting recent developments in computer hardware and algorithms, computer simulations have been increasingly employed, with remarkable success, to study the phase behaviour and synthesis mechanisms of porous materials. The main challenge, however, is that such processes involve multiple physical phenomena – self-assembly, chemical reactions, phase separation, electrostatic interactions – taking place over a wide range of time and length scales. In particular, the ability to simultaneously describe mesoscale self-assembly processes and chemical reactions has remained an elusive goal. Typically, highly coarse-grained (CG) classical models are required to describe mesophase self-assembly [1], while describing chemical reactions usually relies on computationally expensive and/or parameter-rich approaches such as Quantum Mechanical calculations, kinetic Monte Carlo or reactive force fields that are restricted to small system sizes and short times [2]. In this work, we bridge this gap and propose a new molecular modelling paradigm to describe silica polymerization reactions in aqueous solutions at conditions that are representative of realistic experimental processes like biosilicification or porous silica synthesis – i.e. at close to ambient temperatures and over a wide range of pH. The key innovation is to describe the Si-O-Si chemical bond formation and breakage process through a continuous potential with a balance between attractive and repulsive interactions between suitably placed virtual sites and “sticky” particles – hence the name “Sticky-MARTINI” [3]. The simplicity of the model, its applicability in standard parallelized molecular dynamics codes, and its compatibility with the widely used MARTINI coarse-grained force field [4] allows for the study of systems containing millions of atoms over microsecond time scales using an explicit solvent formalism.

REFERENCES

- [1] M. Jorge, *et al. Mol. Simul.* **44**, 435–452 (2018).
- [2] S. M. Auerbach, W. Fan, P. A. Monson, *Int. Rev. Phys. Chem.* **34**, 35–70 (2015).
- [3] A. Carvalho, *et al. npj Comput. Mater.* **8**, 49 (2022).
- [4] S. J. Marrink, *et al. J. Phys. Chem. B* **111**, 7812–7824 (2007).

Characterizing 3D biodegradable artificial matrices

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ABSTRACT

Polymers are widely used in our everyday life, as well as for medical or pharmaceutical purposes. For that reason, natural and biocompatible polymers are getting more and more attention to use them in a harmless way. Technological advances made it possible to create micro-, and nanofiber based artificial matrices from these polymers to be used for simple filtration systems or mimic the extracellular matrix (ECM). These matrices look very close to ECM and can act like a scaffold for cell cultures as well. One of the methods to create fibers is the electrospinning technique. Varying the electrospinning parameters, we can influence the properties as well, to fine tune the system for a desirable outcome. To create a high porosity fibrous mesh for culturing cells in a suitable three-dimensional way, we need to step forward from conventional electrospinning.

Our aim was to create and characterize 3D fiber structures from Poly(succinimide) with the help of electrospinning. Therefore, the effect of the presence of different inorganic salts (LiCl, MgCl₂, CaCl₂) and the effect of humidity on the fiber structures were investigated. By adding salt to the polymer solutions, the weight percent needed to create homogenous fibers were decreased along with the fiber diameter (from 25 to 20w/w%). The conductivity and infrared spectra of salt-solvent, polymer solution and the fibers were measured. Increasing the amount of CaCl₂ increased the tensile strength as well. A critical humidity level was defined as a threshold to create 3D fiber structures. The fiber diameter and surface roughness were analyzed and observed with the help of Scanning Electron Microscopy.

REFERENCES

[1] Juhász, A. G., Molnár, K., Idrissi, A., & Jedlovsky-Hajdú, A. (2020). Salt induced fluffy structured electrospun fibrous matrix. *Journal of Molecular Liquids*, 312, 113478.

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Application of poly(aspartamides) in drug delivery

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ABSTRACT

Polymers show very unique physical properties compared to small molecular compounds or inorganic nanoparticles, therefore they can be widely used in the pharmaceutical industry. Applications of different both natural and synthetic polymers in drug delivery are still one of the most researched areas in the pharmaceutical field. Polymers can be used to improve the solubility and bioavailability of drug molecules, protect the drug from deactivation, carry the drug into a specific organ, and build up nanocarrier systems, that can provide new strategies in drug therapies. Since the chemical structure and molecular weight have a high influence on the physical properties and also biocompatibility of the polymer molecules, therefore polymers with variable chemical structures have been getting more and more attention in the last decade.

Poly(succinimide) (PSI), the anhydrous form of poly(aspartic acid) (PASP), and poly(aspartamide) derivatives made from PSI belong to the previously mentioned group of polymers. The chemical structure of poly(aspartamide) can be tailored for the final application by easy chemical reactions, therefore the number of research papers have been increased significantly in the last few years in the medical and pharmaceutical fields^{1,2}. Through chemical modifications, the physical parameters such as solubility, biodegradability, and biocompatibility can be altered. Moreover, drug molecules and biological molecules can be covalently attached to the polymer to form polymer-drug conjugates. In this talk, I would like to present the latest results related to poly(aspartamides) and provide examples from our research for the different applications of poly(aspartamides) in drug delivery.

REFERENCES

- (1) Yavvari, P. S.; Awasthi, A. K.; Sharma, A.; Bajaj, A.; Srivastava, A. *J. Mater. Chem. B* **2019**, 7 (13), 2102–2122.
- (2) Adelnia, H.; Tran, H. D. N.; Little, P. J.; Blakey, I.; Ta, H. T. *ACS Biomater. Sci. Eng.* **2021**.

Magneto-rheology of clusters formed by magnetic polymers

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ABSTRACT

The idea of creating magnetically controllable colloids whose rheological properties can be finely tuned on the nano- or micro-scale has caused a lot of experimental and theoretical effort. The latter resulted in systems whose building blocks are ranging between single magnetic nanoparticles to complexes of such nanoparticles bound together by various mechanisms. The binding can be either chemical or physical, reversible or not.

One way to create a system that is physically bound is to let the precrosslinked supracolloidal magnetic polymers (SMPs) to cluster due to both magnetic and Van-der-Waals-type forces. The topology of the SMPs in this case can be used to tune both magnetic and rheological properties of the resulting clusters as we show in this work.

We employ Molecular Dynamics computer simulations coupled with explicit solvent modelled by Lattice-Boltzmann approach in order to model the behaviour of the clusters formed by chains, rings, X and Y shaped SMPs in a shear flow with externally applied magnetic field. We find that the shear stabilises the shape of the clusters not letting them extend in the direction of the field and disintegrate. The stabilising effect is particularly strong for clusters made of linear SMPs. Independently from the field strength and direction clusters are involved into rotational motion accompanied by periodic shape changes with frequencies defined by the SMP topology.

Application of NMR relaxation methods for colloids and interfaces

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ABSTRACT

The relaxation was in focus of the nuclear magnetic resonance (NMR) from the very beginning of its history even if the great success of high resolution, multidimensional, chemical shift-based NMR time to time overshadowed it. NMR relaxometry is a powerful tool to study the motion, phase transition and sorption of liquids on solid surfaces in non-invasive way. In this lecture we present our recent results by means of low-field (cheap) NMR relaxometry, NMR cryoporometry and diffusometry on macromolecules, colloid dispersions and porous solids.

Liquid-state NMR does not see the measured nucleus if it goes to solid state, therefore the melting and freezing process will be followed by quantitative NMR. In colloid size pores the phase-transfer temperature depends on the surface-to-volume ratio. By NMR cryoporometry we show the cavities in PAMAM dendrimer macromolecules, furthermore the shape and pore size distributions in wet aerogels. [1,2]

Based on low-field NMR relaxometry we can determine the mechanism of wetting of solid surfaces. The wetting mechanism can be correlated to the hydrophilic character of the surfaces of carbon aerogels. [2]

NMR diffusometry refers to the mobility of liquids in porous systems. It is very important data for applications and also can give information about the maximum volume of loaded water. By means of diffusometry we determined the steric stabilization mode of gold nanoparticles, as well as the hydration number and the exact hydrodynamic size of PAMAM dendrimers. [1-4]

REFERENCES

- [1] Kéri, M., Peng, C., Shi, X., Bányai.: "NMR characterization of PAMAM-G5.NH₂ entrapped atomic and molecular assemblies" *J. Phys. Chem. B* **119**, 3312-3319 (2015)
- [2] Kéri, M., Nyul, D., László K., Novák, L., Bányai.: "Interaction of resorcinol-formaldehyde carbon aerogels with water: A comprehensive NMR study" *Carbon* **189** 57-70 (2022)
- [3] Bányai, I.; Kéri, M., Nagy, Z., Berka, M., Balogh, L.P.: "Self-diffusion of water and poly(amidoamine) dendrimers in dilute aqueous solutions", *Soft Matter* **9**, 1645-1655 (2012).
- [4] Kéri, M., Nagy, Z., Novák, L., Szarvas, E., Balogh, L.P., Bányai, I.: "Beware of phosphate: evidence of specific dendrimer-phosphate interactions" *Phys. Chem. Chem Phys.* **19**, 11540-11548 (2017)

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Glyphosate/AMPA adsorption on magnetite: measure the trace amounts and separate simply

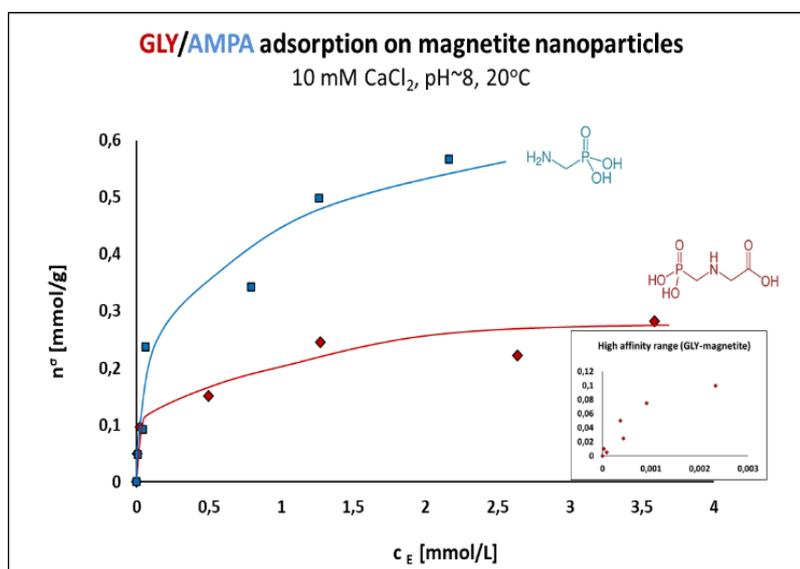
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ABSTRACT

Although WHO classifies glyphosate (GLY) as probably carcinogenic to humans (Group 2A), GLY-based formulations are today's most frequently used herbicides worldwide. GLY has already been restricted or banned in several countries, because of its environmental toxicity (e.g. endocrine disrupting activity). In soils, microbial decomposition of GLY produces aminomethylphosphonic acid (AMPA), as main metabolite. Magnetite nanoparticles (MNPs) show relatively high adsorption capacity towards GLY and can easily be separated from water due to their magnetic properties [1]. In this work the adsorption of GLY and AMPA on MNPs was studied. Trace quantification of the adsorbed amounts was carried out by UPLC-MS/MS. Adsorption conditions were determined considering quick separation possibilities and environmental relevancies. The pH- and ionic strength-dependent surface charge states of MNPs were determined in a previous study [2]. Present zeta potential and dynamic light scattering measurements revealed the effect of Ca^{2+} ions and pH on the aggregation of MNP.

RESULTS The maximum adsorption capacity of MNPs was ~34 mg/g and ~56 mg/g (~0.2 mmol/g and ~0.5 mmol/g) for GLY and AMPA, respectively. Assuming a specific surface area of 100 m²/g, the average number of GLY and AMPA molecules adsorbed on MNPs surface was calculated to 1.2 and 3 molecules per nm². These values align well with the available ≡Fe-OH of ~5 per nm².



The high-affinity binding is of environmental importance; however, the complete depletion of glyphosate is only apparent, as measured by UPLC-MS/MS (see $c_e < 0.5$ ppm in Fig. inserted).

REFERENCES

- [1] H. Park *et al.*, "Magnetite nanoparticles as efficient materials for removal of glyphosate from water," *Nat. Sustain.*, vol. 3, no. 2, pp. 129–135, Feb. 2020.
- [2] I. Y. Tóth *et al.*, "Designed polyelectrolyte shell on magnetite nanocore for dilution-resistant biocompatible magnetic fluids," *Langmuir*, vol. 28, no. 48, pp. 16638–16646, 2012.

Magnetic and structural equilibrium properties of multicore nanoparticle suspensions and bimodal ferrofluids

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ABSTRACT

Magnetic multicore nanoparticles (MMNPs) are dense clusters of single-domain magnetic nanocrystals embedded in a rigid non-magnetic matrix. In this work, we combine Langevin dynamics simulations and statistical theory of dipolar systems to study equilibrium properties of a weakly concentrated suspension of MMNPs. We model MMNPs as spherical impenetrable particles filled randomly and uniformly with spherical magnetic grains. Each grain has a magnetic moment of constant magnitude which can freely rotate under the action of applied magnetic fields and thermal fluctuations. All grains interact with each other via the dipole-dipole interaction potential. The system is subjected to a uniform magnetic field and maintained at a constant temperature. Simulation results demonstrate that equilibrium magnetic properties of the suspension depend crucially on the dipolar coupling constant $\lambda = \mu^2/\sigma^3 k_B T$ (μ is the grain magnetic moment, σ is its diameter). Increasing λ leads to a non-linear increase in the suspension initial magnetic susceptibility. For small and moderate values of λ , this behavior can be accurately described theoretically, but at $\lambda \sim 10$ the theory strongly underestimates numerical results. At non-zero field, the discrepancies between theory and simulations arise even at smaller dipolar constants. We interpret the anomalous magnetic response as a result of self-aggregation processes in the ensemble of MMNPs. For $\lambda < 10$, magnetic interactions between superparamagnetic MMNPs in zero-field are insignificant and do not lead to the formation of aggregates. However, in large enough fields chain-like structures can be observed. It is shown based on a systematic cluster analysis of the simulation data that MMNPs constituting these structures are magnetized by the field much stronger than isolated ones.

Additionally, we present numerical and theoretical results on the equilibrium properties of a “bimodal ferrofluid”, i.e. a mixture of MMNPs and single-core magnetic nanoparticles (SMNP). At large fields, a special self-assembly scenario known as “haloing” takes place in this system: smaller SMNPs grow on the poles of MMNPs, forming dense shells or “halos”. The effect of haloing on the system magnetization curve is analyzed.

ACKNOWLEDGEMENT

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Chemical stability of graphene oxide in aqueous suspensions

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ABSTRACT

For many years graphene oxide (GO) has been mainly considered as an intermediate of wet chemical graphene production. Today, however, graphene oxide itself has gained its own well-deserved recognition and its application potential is continuously expanding.

In GO – water colloid system a microstructure develops as long and short range, permanent and induced interactions evolve between the hydrated particles, hindered or fostered by the presence of water molecules [1]. Meanwhile these interactions may result in chemisorption and the oxidative alteration of the particles.

The results of XPS and acid/base potentiometric titrations will be shown and discussed in order

to demonstrate the chemical changes (Fig. 1). It is proposed that these changes are related to a slow oxidation process that occurs in the acidic aqueous medium during long-term storage. These observations draw attention to the role of storage time in the performance of such GO suspensions that must be considered in processing technologies and applications.

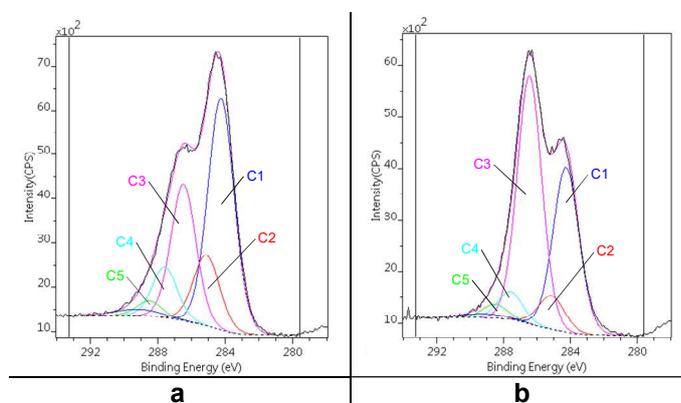


Fig. 1. C1s envelop of the XPS spectra

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REFERENCES

[1] Gyarmati B.; Farah S.; Farkas A.; Sáfrán G.; Voelker-Pop LM.; László K.; “Long-Term Aging of Concentrated Aqueous Graphene Oxide Suspensions Seen by Rheology and Raman Spectroscopy”, *Nanomaterials* **12**, 916 (2022).

Development of poly(aspartic acid) based hydrogels for tissue engineering purposes

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ABSTRACT

Tissue engineering applies proper combination of cells, scaffold materials and bioactive molecules for regeneration of diseased or injured tissues. The most important criteria for scaffolds: biocompatibility, biodegradability and 3D structure mimicking the natural environment of the cells, i.e. the extracellular matrix. Amino acid based hydrogels fulfill these requirements.

The aim of our study was to develop poly(aspartic acid) (PASP) based hydrogel scaffolds that can provide ideal conditions for cell survival, adhesion, proliferation and also migration.

In order to prepare biocompatible hydrogels, PASP was crosslinked with natural amines: diaminobutane or cystamine alone or in combination, and in some cases disulfide bridges were cleaved to thiol groups. During the first experiments, the effect of different types and densities of crosslinking on cell viability was assessed. In the second round, PASP gels with different thiol group densities were synthesized. Finally, in the third experimental series, dopamine-modified thiolated PASP gels were fabricated. For cell viability tests, the WST-1 proliferation reagent was used. Cell morphology was monitored under a phase contrast microscope. Three-dimensional cell distribution in the gels was visualized by two photon microscopy.

Our results revealed that PASP gels with double crosslinking and increased hardness were suitable for cell adhesion. The highest cell viability was obtained on the thiolated gels. Higher densities of free thiol groups in the gels facilitated increased cell proliferation. Modification of the thiolated PASP gels with dopamine permitted enhanced three-dimensional cell migration.

In conclusion, poly(aspartic acid) based thiolated hydrogels support survival, adhesion, proliferation, as well as migration of human cells. Therefore, these gels are promising candidates for application as scaffold materials in tissue engineering.

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REFERENCES

- [1] Juriga D., Nagy K., Jedlovsky-Hajdú A., Perczel-Kovács K., Chen Y. M., Varga G., Zrínyi M., "Biodegradation and Osteosarcoma Cell Cultivation on Poly(aspartic acid) Based Hydrogels", *ACS Appl. Mater. Interfaces*. **8.**, 23463-23476 (2016)
- [2] Hegedűs O., Juriga D., Sipos E., Voniatis C., Juhász Á., Idrissi A., Zrínyi M., Varga G., Jedlovsky-Hajdú A., S. Nagy K., "Free thiol groups on poly(aspartamide) based hydrogels facilitate tooth-derived progenitor cell proliferation and differentiation" *PLoS One* **14.**, e0226363, (2019)
- [3] Juriga D., Kálmán, E. É., Tóth K., Barczikai D., Szöllősi D., Földes A., Varga G., Zrínyi M., Jedlovsky-Hajdú A., S. Nagy K., "Analysis of Three-Dimensional Cell Migration on Dopamine-Modified Poly(aspartic acid)-Based Hydrogels", *Gels* **8.**, 65, (2022).

Paramagnetic metal chelates of polycarboxylamino-type macromolecules: high relaxivity complexes without coordinated inner sphere water?

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ABSTRACT

It is known that paramagnetic metal ion complexes of large macromolecular ligands efficiently shorten the magnetic relaxation time of water protons. Besides the fast exchange between water directly coordinated to the metal ion and bulk water, the slow tumbling motion of the macromolecule contributes significantly to the effect observed [1]. There are several attempts at gaining benefit from this phenomenon, mostly by grafting well-known (and well characterized) metal chelates onto large carrier macromolecules (“platforms”). We opted to take a different way by synthesizing these platforms first and characterize them as well as their metal chelates afterwards. Starting from commercial polyethyleneimine, through derivatives carboxymethylated to different extent, we obtained several Gd(III) and Mn(II) metal chelates which possess relaxivities surpassing that of Gd(III) and Mn(II) aquo complexes in the whole pH range studied. Similar complexes based on copolymers of glycidyl methacrylate and hydroxyethyl methacrylate functionalized with iminodiacetic acid were also prepared. In each case studied, the relaxivities stood high even at high donor atom to metal ratios and under conditions where the presence of inner sphere coordinated water is unlikely. We attribute their efficiency to the highly hydrated state of the macromolecular platform allowing the effect of the paramagnetic ion to manifest onto the hydration layer water molecules without direct coordination. Such metal chelates should present a lesser risk to leach potentially toxic metal ions from the macromolecular complex compared to those containing inner sphere coordinated water.

REFERENCES

[1] Tóth, É.; Helm L.; Merbach A. E., “Relaxivity of MRI contrast agents”, *Topics Curr. Chem.* **221.**, 62–101 (2002)

Behavior of a magnetic nanogel in a shear flow

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ABSTRACT

Magnetic nanogels (MNG) -- soft colloids made of polymer matrix with embedded in them magnetic nanoparticles (MNPs) -- are promising magneto-controllable drug carriers. In order to develop this potential, one needs to study MNG's behavior in various microfluidic systems, one of which can be modelled as a channel with a given flow. At the same time, MNG motion can be governed by an external magnetic field. Thus, a clear understanding of the interplay between magnetic and hydrodynamic influence on MNGs dynamics will be an essential step to facilitate their usage in targeted drug delivery.

Considering the size of the MNG and typical time and velocity scales involved in their nanofluidics, experimental characterisation of the system is challenging. In this work [1], we perform molecular dynamics (MD) simulations combined with the Lattice-Boltzmann (LB) scheme aiming at describing the impact of the shear rate on the shape, magnetic structure and motion of an MNG.

We find that in a shear flow, the centre of mass of an MNG tends to be in the centre of a channel and to move, preserving the distance to both walls. The MNG monomers along with translation are involved in two more types of motion, they rotate around the centre of mass and oscillate with respect to the latter. It results in synchronised tumbling and wobbling of the whole MNG accompanied by its volume oscillates. The fact, the MNG is a highly compressible and permeable for the carrier liquid. It makes its behaviour different from a simple droplet in an emulsion. We show that the volume oscillations and rotations are two faces of the same periodic process whose frequency is a growing function of the shear rate. We find that the stronger magnetic interactions between MNPs are, the higher is the frequency of this complex oscillatory motion, and the lower is its amplitude. Finally, we show that the oscillations of the volume lead to the periodic changes in MNG magnetic energy.

REFERENCES

[1] Ivan S. Novikau, Ekaterina V. Novak, Elena S. Pyanzina, Sofia S. Kantorovich, "Behaviour of a magnetic nanogel in a shear flow", *Journal of Molecular Liquids*, Volume 346, 2022

Ultrasound induced, easy-to-store porous poly(aspartic acid) based electrospun scaffolds

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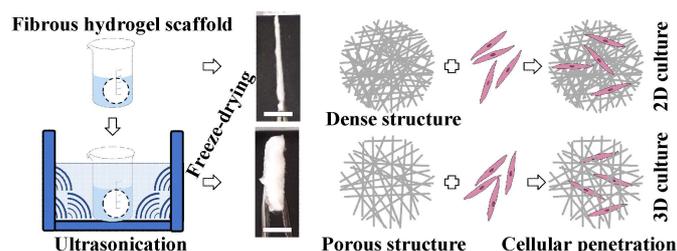
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ABSTRACT

The aim of tissue engineering is to develop methods to restore, maintain or improve tissue functions. To imitate the fibrous structure of the native extracellular matrix, the electrospinning technique is widely used. However, the dense packing of fibers results in small pores and hereby the inhibition of cellular penetration.

In our research [1], we used biocompatible and biodegradable poly(aspartic acid) based fibrous hydrogel scaffolds to enhance the cell infiltration using ultrasonication (US). The US can enlarge the space between the fibers in the scaffold and create a 3D structure based on the thickness increase of the samples. A freeze-drying process was also introduced to prevent the scaffolds from degradation and create an easy-to-store sample beyond the US treatment. After all these treatments, the scaffold's specific load capacity was $0.11 \pm 0.01 \text{ Nm}^2/\text{g}$ which did not change after a rehydration cycle. The elongation break became almost two times higher than before the US treatment. The enhanced cellular penetration was visualized by multiphoton microscopy.

In summary, we were able to overcome the major limitation of conventional electrospun scaffolds regarding their application in tissue engineering. We also improved the storing conditions of fibrous hydrogel scaffolds and extend their shelf life without degradation.



This work was supported by the National Research, Development, and Innovation Office (NKFIH FK137749), and by the Higher Education Institutional Excellence Program of the Ministry for Innovation and Technology in Hungary, within the framework of the Therapeutic Development thematic program of the Semmelweis University (TKP2021-EGA-23).

REFERENCES

- [1] R. Pázmány, K.S. Nagy, Á. Zsembery, A. Jedlovszky, Ultrasound induced, easy-to-store porous poly (amino acid) based electrospun scaffolds, J. Mol. Liq. 359 (2022).

Scaling in uniformly charged and bipolar nanopores through a modified Dukhin number

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ABSTRACT

Nanopores are nanoscale channels embedded in a membrane providing a controlled transport of ions between the two bulk phases on the two sides of the membrane. The nanopore's radius, R , is in the nanometer range, comparable to the Debye length, λ_D . Charge patterns are deposited on the inner wall of the nanopore providing different output signals for different input parameters. The relation of the input and output signals defines the device function. In the case of a uniformly charged nanopore, the device function is selectivity.

Scaling of the selectivity of the nanopore means that selectivity is a unique smooth and monotonic function of a well-defined scaling parameter. The nanopore's input parameters are used to create the scaling parameter. We showed [1] that the Dukhin number defined for 1:1 electrolytes as $Du = \sigma / eRc$, where σ is the surface charge density and c is the electrolyte concentration. This equation can be transformed into the form $Du = \sigma 8\pi l_B \lambda_D^2 / eR$, where l_B is the Bjerrum length. We show that Du is a suitable scaling parameter for the nanotube limit, i.e., for the infinitely long nanopore ($H \rightarrow \infty$, where H is the length of the pore). For the nanohole limit ($H \rightarrow 0$), we introduced [2] the modified Dukhin number defined as $mDu = Du(H/\lambda_D)$ and showed that it is an appropriate scaling parameter. A mixed scaling parameter can be used in between. We also showed that mDu is a good scaling parameter for the bipolar nanopore where the device function is rectification [3].

We use simple models based on the implicit-solvent model of electrolytes and study those models with the Nernst-Planck transport equation coupled either to the Local Equilibrium Monte Carlo method or the Poisson-Boltzmann theory.

REFERENCES

- [1] Zs. Sarkadi, D. Fertig, M. Valiskó, D. Boda. "The Dukhin number as a scaling parameter for selectivity in the infinitely long nanopore limit: extension to multivalent electrolytes." *J. Mol. Liq.* **357**, 119072 (2022).
- [2] Zs. Sarkadi, D. Fertig, Z. Ható, M. Valiskó, D. Boda. "From nanotubes to nanoholes: scaling of selectivity in uniformly charged nanopores through the Dukhin number for 1:1 electrolytes." *J. Chem. Phys.* **154**, 154704 (2021).
- [3] D. Fertig, Zs. Sarkadi, M. Valiskó, D. Boda. "Scaling for rectification of bipolar nanopores as a function of a modified Dukhin number: the case of 1:1 electrolytes." *Mol. Sim.* **48**, 43-56 (2022).

Observing long term bacterial colonization of polypropylene microplastics in a freshwater lake by optical and molecular methods

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ABSTRACT

Bacterial colonization of microplastic surfaces in freshwater might alter the physicochemical properties of the plastic surfaces, these changes are better to be investigated in the long term perspective. In this study, self-designed plastic colonizers (Al-Omari et al., 2021) filled with polypropylene plastic straws cut into less than 5-mm small pieces were incubated in a freshwater lake in Vácszentlászló, Hungary (47°33'37.0"N, 19°33'09.4"E) The incubation period was fourteen months starting from April 2019 till June 2020. A plastic colonizer was collected every month together with one surrounding water sample. Water and the polypropylene associated bacterial community of these samples were analyzed by Illumina 16S rDNA amplicon sequencing. An analytical sampling of the lake water was also made during our study. Not only general water quality analyses were made but the concentration of heavy metals, pesticides and pharmaceutical residuals were also measured.

The plastic associated bacterial communities were described on the different taxonomic levels. In the first month, the water associated community was dominated by *Proteobacteria* followed by *Cyanobacteria*. Whereas the polypropylene associated community was dominated by *Proteobacteria* followed by *Bacteroidetes* and *Actinobacteria*. With time the bacterial composition on polypropylene surface, in terms of phylum level, has been changed, especially when compared with the water community. In addition to that scanning electron microscopy (SEM), FTIR and Raman spectroscopy were used to study the physicochemical changes of the incubated microplastic surfaces due to bacterial colonization. Although the chemical composition of PP was nearly without any traces of ageing in spectra, various changes in surface morphology were observed, which could have a significant influence on the physical properties of microplastics and their interaction with the environment. It is strengthening that the morphological parameters of these surfaces are very important to better understand the colonization of plastic sphere niche (Dabrowska et al, 2021).

REFERENCES

[1] Szabó, I., Al-Omari, J., Szerdahelyi, G.S. Milán Farkas, Yazid Al-Omari, Péter Márton Szabó, Rózsa Sebők, Jeffrey Griffiths, Balázs Kriszt & Sándor Szoboszlai "In Situ Investigation of Plastic-Associated Bacterial Communities in a Freshwater Lake of Hungary". *Water Air and Soil*

Removal of caine anesthetics from water, saline solutions and model wastewaters using nanofiltration membranes

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ABSTRACT

The caine drugs such as lidocaine and procaine carry the important function of anaesthesia. They have their own structures separate from the ecgonine nucleus of cocaine and its derivatives and are different both pharmacodynamically and pharmacokinetically, as well as legally, from cocaine. A handful of caine drugs are still in considerable biomedical use and constitute potential and real environmental pollution in wastewater or drinkwater sources.

The aim of our study was to study the nanofiltration-assisted removal of 5 selected caine anaesthetics such as procaine and bupivacaine from three different types of water-based media: (i) pure water, (ii) electrolyte solutions containing monovalent ions and (iii) synthetic wastewaters representing the ionic composition of a typical natural freshwater. Tight and loose, polyamide-based nanofiltration membranes (NF90 and NF270) were used to reject the passage of drug molecules via their selective interfacial layer and concentrate their solutions. The rejection and flux changes of the membranes are evaluated and explained by several molecular properties such as charge and size of drug molecules and their molecular structure.

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Heteroaggregation of nanozymes and latex particles for highly stable antioxidant colloids

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ABSTRACT

Nanozymes are defined as nanomaterials of enzyme-like functions, which are capable to overcome the limitations of natural enzymes in biomedical or industrial catalytic applications. These limitations include cost, difficult storage, and high sensitivity to the environmental conditions and that highly efficient enzymes are often obtained from genetically modified species, which are being controlled by increasingly strict regulations. Although nanozymes became promising alternatives to native enzymes in the last decade, several related questions such as engineering substrate specificity, understanding catalytic mechanism, tuning interparticle interactions and studying degradation must be still addressed. The present research aims for the design of nanozyme-based composites from preparation through characterization to in-lab validation of their efficiency.

Prussian blue [1], manganese oxide [2] and ceria nanoparticles of suspected antioxidant activities were synthesized by hydrothermal processes resulting in one-phase materials of narrow size distribution, as determined by scattering (DLS), spectroscopy (XPS, UV-Vis) and microscopy (SEM, TEM, AFM) techniques. These nanomaterials were found to mimic the function of superoxide dismutase, catalase and peroxidase enzymes in biochemical tests, i.e., they have proven to act as antioxidant nanozymes.

To improve their limited colloidal stability, the nanozymes were aggregated with polystyrene latex particles using polyelectrolytes such as poly(diallyldimethylammonium chloride) for surface functionalization to adjust the charge balance during the heteroaggregation between the nanozymes and the latex. The obtained composites possessed excellent structural, colloidal, and functional stabilities confirming the advantages of the presence of the carrier latex particles. For instance, manganese oxide nanozyme-based composites showed both superoxide dismutase and catalase activities even at high temperature, where the natural enzymes quickly lose their activities [2].

REFERENCES

- [1] Alsharif, N. B.; Samu, G. F.; Sáringi, S.; Muráth, S.; Szilagyi, I., "A colloid approach to decorate latex particles with Prussian blue nanozymes", *J. Mol. Liq.* **309**, 113066, (2020).
- [2] Alsharif, N. B.; Bere, K.; Sáringi, S.; Samu, G. F.; Takács, D.; Hornok, V.; Szilagyi, I., "Design of hybrid biocatalysts by controlled heteroaggregation of manganese oxide and sulfate latex particles to combat reactive oxygen species", *J. Mater. Chem. B* **9**, 4929-4940, (2021).

Molecular simulation of the passive membrane penetration by the products of the CO₂ and 1,3-butadiene reaction for a greener technology

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ABSTRACT

To this day, over 350 000 chemicals and mixtures of chemicals are registered for production and use [1], which annual production rate exceeds 10⁸ tons. [2] While chemicals are essential to our life standard, a non-negligible portion of the produced substances is released into the environment due to their improper handling. Furthermore, production of these chemicals requires energy which generates a further increase in CO₂ emission and acceleration of the global warming.

On the other hand, the use of carbon dioxide in organic synthesis is a favored strategy for attenuating its rising atmospheric levels and satisfying modern energy requirements. One of the most promising reactions for this reason is the telomerisation of CO₂ with 1,3-butadiene which results in the synthesis of a highly functionalized δ -lactone, 3-ethylidene-6-vinyltetrahydro-2H-pyran-2-one (EVL), a promising platform molecule. Aside from EVL, several byproducts can form during this reaction such as acids lactones and covalent butadiene dimer (BDDI), of which properties and possible effects on biological systems are unknown to this day. In this work the membrane structure altering properties and passive membrane transport of these compounds is investigated by the means of molecular dynamics (MD) simulations and well-tempered metadynamics (WT-MD). In addition, the pure liquid densities and hydration free energies of these compounds are determined by using MD simulations and ab initio calculations.

REFERENCES

- [1] Wang, Z.; Walker, G. W.; Muir, D. C. G.; Nagatani-Yoshida, K. "Toward a Global Understanding of Chemical Pollution: A First Comprehensive Analysis of National and Regional Chemical Inventories", *Environ. Sci. Technol.*, **54**., 2575–2584, (2020).
[2] Sheldon, R. A. "The E Factor: Fifteen years on", *Green Chem.*, **9**., 1273–1283, (2007).

Nanofibrous biocompatible polymer-based drug-delivery implants

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ABSTRACT

Biocompatible polymers are frequently administered for biomedical purposes such as wound dressing, drug-delivery [1], implants, and scaffolds for tissue regeneration [2] as well. Biodegradable polymer based implants loaded with drug molecules can provide prolonged release of the drug therefore lower dose and administration can be achieved.

In this work, electrospun biocompatible polymer meshes (poly(vinyl alcohol) – PVA; polycaprolactone – PCL and poly(succinimide) – PSI) were investigated, that can attend to the normal metabolism of the human organism and cause no harm and inflammation after the administration. The solubility and the release kinetics of drugs can be tailored by choosing the appropriate polymers, solvents, drugs and the parameters during electrospinning. Regarding the drugs, doxorubicin (DOX) was applied as a chemotherapeutic agent and prednisone was used as an anti-inflammatory substance.

In the experiments, fiber diameter and morphology were determined by scanning electron microscopy, the drug-release at different pH (pH 6.5, 7.4) was investigated by UV-Vis spectrophotometry. The biocompatibility of the samples and the effect of the drugs were investigated through cell viability assay after 24 and 72 h on MDA-MB-231 cells. The internalization of DOX and PSI-DOX conjugates were investigated and proved by flow cytometry analysis.

By using different drug-containing polymers the release time (from days through weeks, and even to months) could be tailored. The IC₅₀ value for DOX was determined while the prednisone did not show cytotoxic effect in the investigated concentration range.

After further optimization, these tailored implants could be feasible for attenuation of bleeding and inflammation. Moreover, they might prevent the recurrence of cancer after tumor surgery, therefore they could provide potential support, or might substitution of the intravenous chemotherapy.

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REFERENCES

- [1] D. Juriga et al, “Kinetics of dopamine release from poly(aspartamide)-based prodrugs”, *Acta Biomater.* **76**, 225-238 (2018).
- [2] D. Juriga et al, “Analysis of Three-Dimensional Cell Migration on Dopamine-Modified Poly(aspartic acid)-Based Hydrogels”, *Gels* (Basel, Switzerland) **8(2)**, (2022).

Polysuccinimide/Polycaprolactone composite meshes for surgical tissue engineering

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ABSTRACT

Tissue engineering trends now move towards the fabrication of composite multi-functional materials aiming to tackle multiple problems at the same time. One of the most intriguing problems is tissue integration and especially integration of surgically implanted scaffolds. In this regard, our objective was fabricating electrospun poly(succinimide) (PSI) / polycaprolactone (PCL) composite meshes exhibiting enhanced tissue integration. PSI is an easily modifiable synthetic poly(amino acid) that is typically utilised as functionalization component. PCL on the other hand is a well-known polymer with excellent mechanical properties. Both polymers are biocompatible and biodegradable. While PCL typically takes 6 months to 2 years to fully biodegrade and thus tissue infiltration and incorporation of the system is slow and limited, PSI is rapidly degraded unless cross-linked by a chemical agent. In the current work two different nanofibrous meshes are presented by utilizing two different electrospinning configurations: a. Co-electrospun meshes and c. Blend electrospun meshes. Physico-chemical and mechanical characterization was performed as well as in vitro and in vivo investigations with fibroblast cell lines and small animals (Wistar Rats) respectively. PSI/ PCL meshes proved mechanically stronger as they exhibited almost double the loading capacities when compared to PSI only meshes. Wettability proved that addition of a PSI component will decrease the water contact angle. Meshes were found to be cyto and biocompatible with favourable cell adhesion properties. While each material has its own advantages, a composite mesh could provide further options in the wide and diverse application spectrum of electrospun fibrous membranes. Funding: EFOP-3.6.3-VEKOP-16-2017-00009,

REFERENCE

Constantinos Voniatis et al. Fabrication and characterisation of electrospun Polycaprolactone/Polysuccinimide composite meshes, Journal of Molecular Liquids, Volume 323, 115094, ISSN 0167-7322, 2021

Poster presentations

Building a solid-like layer on the interface of two immiscible liquids using a polyelectrolyte and an opposite charged conventional surfactant

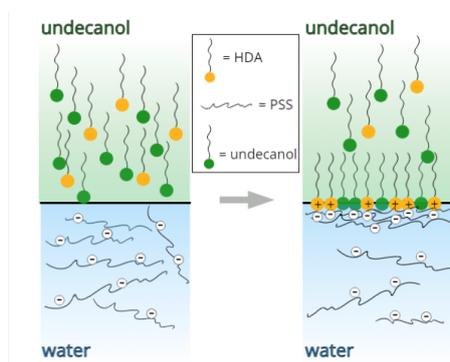
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ABSTRACT

One of the most exciting area of today nanoscience is related to the production and application of the so-called structured liquids. These nanosystems can be produced through interfacial assembly of a polyelectrolyte and a nanoparticle [1] or two polyelectrolytes [2] dissolved separately in an oil and water phase, which results in a solid-like layer on the surface of the two immiscible liquids. This phenomenon is of major interest in the scientific and industrial community due to their unique application possibilities, for which examples are biphasic catalysis, 3D printing or creating biomimetic materials. Conventional long carbon chained amphiphile surfactant molecules and linear polyelectrolytes were not considered robust enough to be able to be a part of building this kind of structure. In the present paper we have revealed this type of layer composed of a polyelectrolyte (poly(styrenesulfonate)) paired with a conventional alkyl chain-based surfactant (hexadecylamine) for the first time. The assembly occurs due to the opposite charge of the molecules, which requires appropriate composition and experimental conditions. Another remarkable novel aspect of our system is the strong solvent-dependent nature of the film suggesting the distinguished role of the solvent molecules participating in the process of the association. The phenomenon also influences the structure of the emulsions prepared at the same composition.



REFERENCES

- [1] Cui, M.; Emrick, T.; Russell, T. P., "Stabilizing Liquid Drops in Nonequilibrium Shapes by the Interfacial Jamming of Nanoparticles", *Science* **342(6157)**, 460–463, (2013)
- [2] Xu, R.; Liu, T.; Sun, H.; Wang, B.; Shi, S.; Russell, T. P., "Interfacial Assembly and Jamming of Polyelectrolyte Surfactants: A Simple Route to Print Liquids in Low Viscosity Solution", *ACS Applied Materials & Interfaces* **12 (15)**, 18116-18122, (2020)

Development of nanostructured biomimetic catalysts for the investigation of drug metabolism

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ABSTRACT

In vitro mimicking of drug metabolism is a key issue in early-stage of drug discovery. Synthetic metalloporphyrins show structural similarity with the hem type prosthetic group of cytochrome P450, which is the main hepatic enzyme in oxidative drug metabolism. Concerning technological and economical aspects and the poor stability of metalloporphyrin, their immobilization onto or into solid carriers can be promising solution. [1] This research presents a novel immobilized metalloporphyrin nanocomposite system and its potential use as biomimetic catalysts. A so-called 2nd generation immobilization procedure was developed combining two main steps (Fig.1). First, binding of metalloporphyrin onto functionalized magnetic iron-oxide nanoparticles is established, followed by entrapment the nanoparticles into poly(lactic acid) nanofibers by electrospinning technique. [2] Due to the synergistic morphological and chemo-structural advantages of the nanocarriers the biomimetic efficiency of the immobilized metalloporphyrin can be enhanced.

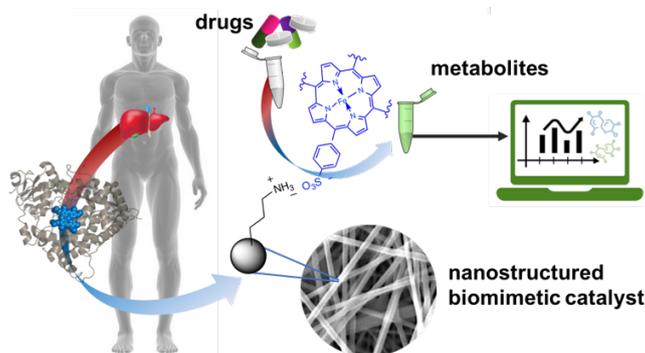


Fig1. Metalloporphyrin immobilized in nanostructured system and biomimetic catalyst for liver dependent drug metabolism.

REFERENCES

[1] Földi, T. et al., "Biomimetic Synthesis of Drug Metabolites in Batch and Continuous-Flow

Reactors", *Chemistry – A European Journal* **24**, 9385-9392, (2018).

[1] Balogh-Weiser, D. et al., "Magnetic Nanoparticles with Dual Surface Functions—Efficient Carriers for Metalloporphyrin-Catalyzed Drug Metabolite Synthesis in Batch and Continuous-Flow Reactors", *Nanomaterials* **10**, 2329, (2020).

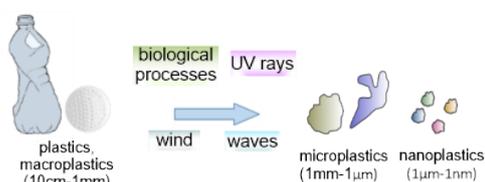
Modelling the colloidal behavior of nano-sized particles in natural waters

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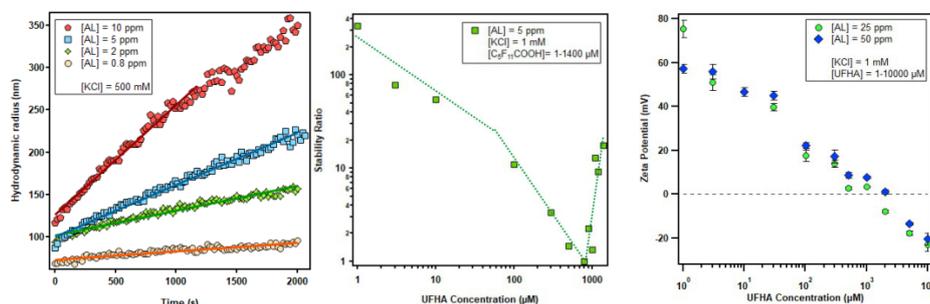
ABSTRACT

Nowadays the plastic pollution is one of the most worrying problem which affects the world. The biggest emission sources are land-based: in the largest proportion the industry, but the consumer society and the marine activity plays significant role too. The plastics in the nature are exposed several environmental effects which generates the erosion of these materials [1]. The fragmentation eventuates the formations of micro- and nanoplastics and the debris are reach the oceans and the seas via riverine transport [2].



exposed several environmental effects which generates the erosion of these materials [1]. The fragmentation eventuates the formations of micro- and nanoplastics and the debris are reach the oceans and the seas via riverine

transport [2]. During our project we are working with nano-sized amidine latex particles (ALPs) and perfluoric acids (PFAs). The colloidal behavior of the ALPs were studied at different ionic strengths. Thereafter the measurements were directed to the mixing of the positively-charged ALPs and the PFAs and mixing process induced the charge reversal of the ALPs with the increasing amount of the acid. Currently we are performing MS/MS analysis to identifying the potential fragments in the PFAs. Henceforth we would like to observe the toxicity of these materials. The aim of our research work is to find an operable method for the elimination of these materials from the natural waters.



REFERENCES

- [1] L. Wang, W-M. Wu, N.; S. Bolan, "Environmental fate, toxicity and risk management strategies of nanoplastics in the environment: Current status and future perspectives", **401**, (2021)
- [2] O. S. Alimi, J. F. Budarz. L.M. Hernandez, N. Tufenkji, "Microplastics and Nanoplastics in Aquatic Environments: Aggregation, Deposition, and Enhanced Contaminant Transport", **52**, 1704-1724, (2018)

The effect of surfactants on polyelectrolyte multilayer nanofiltration membranes

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ABSTRACT

The Layer-by-Layer (LbL) assembly method to build nanofiltration membranes on ultrafiltration and microfiltration membrane substrates has become a staple in membrane fabrication technology, leading to highly selective and robust membranes [1]. These membranes offer a powerful self-healing ability and high chemical stability: resistance to chlorine, a wide pH range and solvent resistance (if the supporting substrate allows this).

Conversely, a known downside of these membranes is that polyelectrolyte multilayers can be destabilized by very high salinity (above 2-3 mol/dm³) or by surfactants above their critical micellar concentration (CMC) [2]. However, effects at concentrations below CMC are unknown, although the usefulness of this information points beyond theoretical knowledge: the fouling resistant LbL membranes could be applied for various challenging separation tasks (e.g. industrial wastewater treatment, food industrial separations, etc.) where surfactants can be present in varying amounts.

By measuring the changes of the membrane properties (flux, rejection of various compounds) through progressively elevating the concentrations of different surfactants (cationic and anionic) on these membranes, we propose a hypothesis for the mechanism of the degradation process.

REFERENCES

- [1] Sewerin, T., Elshof, M.G., Matencio, S., Boerrigter, M., Yu, J., de Grooth, J., "Advances and Applications of Hollow Fiber Nanofiltration Membranes: A Review", *Membranes* 11, 890-924 (2021)
- [2] Ilyas, S., de Grooth, J., Nijmeijer, K., de Vos, W.M., „Multifunctional polyelectrolyte multilayers as nanofiltration membranes and as sacrificial layers for easy membrane cleaning”, *J. Colloid Interface Sci.* **446**, 386–393 (2015)

Preparation and characterization of liposomal corticosteroids

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ABSTRACT

Liposomes are nano-scale drug-delivery systems, which provide several advantages regarding biodistribution, absorption and controlled drug-release. Applying liposomal corticosteroids, the efficacy of several anti-inflammatory therapies can be improved. Our aim was to create small, unilamellar, corticosteroid-loaded liposomes which are able to release their entrapped drug at the typical temperature of inflamed tissues.

Using three kinds of phospholipids, liposome samples with two different constitutions were produced: type 1 consisted of dipalmitoyl-phosphatidylcholine (DPPC) and dimyristoyl-phosphatidylcholine (DMPC), while type 2 contained distearoyl-phosphatidylcholine (DSPC) as well. Prednisolone was added at 10 m/m% to both samples. For liposome preparation, thin layer hydration technique was used then extrusion was applied to reach 100 nm in diameter. The liposomes were stored at 3 different temperatures (4°C, 25°C, 37°C). The particle size-distribution was monitored by dynamic light scattering (DLS). The phase-transition temperature (T_c) was determined by differential scanning calorimetry (DSC). Drug-release was studied by dialysis at body temperature (37°C) and above T_c of liposomes (42°C) applying an UV-Vis spectrophotometer. In order to visualize the samples, atomic force microscopy (AFM) was used. According to the DLS measurements, the liposomes were stable for 1 year at 25°C and kept their hydrodynamic diameter around 100 nm suggesting that no aggregation occurred. The DSC results showed that both drug-free samples types had T_c between 40 and 41°C as well as the added prednisolone had no significant effect on T_c . The liposome samples were able to release their entrapped active agents within 5-6 hours at both temperatures. The AFM study confirmed the spherical shape and the size of the liposomes measured by DLS.

In conclusion, we could successfully prepare small unilamellar liposomes with 100 nm in diameter, which can be stored in a stable state for at least 1 year. The entrapped prednisolone can be released at inflamed body temperature in a few hours.

ACKNOWLEDGEMENT

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Impact of humic substances on the living organisms

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ABSTRACT

Humic substances (HS) are the most abundant natural organic matter on Earth. Humus is the most relevant decomposition product of living matter, so it is the most important media for the reproduction of the continental biomass.

In the humification process, plant residues parts that get into the soil are broken down by soil bacteria and fungi by means of their enzymes, so simple compounds (sugar, ammonia, etc.) are formed from carbohydrates, fats, proteins and lignin. They serve partly as food for the soil microbes and partly as a source in the formation of HS. Numerous confirmations have been obtained that they affect the growth processes in plants. For example, enhanced root formation accompanied by the development of the assimilation apparatus and increased growth of the aerial part. Protein metabolism is accelerated, which is accompanied by increased plant growth, decreased nitrate content in the finished product, and improves quality [1].

The latest studies and also my research showed that the HS has a good antioxidant effect. According to their chemical structure, they are polyhydroxy carboxylic acids with quinone and semiquinone groups. In some respects, they are similar to flavonoid phenols, in which the so-called flavone skeleton is polysubstituted by hydroxy groups. In addition to the well-known complex forming ability with essential metals and trace elements, the antioxidant properties of humic acids have already been demonstrated in a number of scientific publications. This is the reason why these materials are often used as dietary supplements [2].

They also have a good effect in the animal feeding industry like: boosting immune system anti-inflammatory activity and antiviral properties. The use of HS and related products in feed improves gut health for better nutrient utilization as well as improves the health status by working against pathogens by developing immunity. Routine use of HS in feed improves growth of broilers by increasing digestion of protein and trace element utilization [3].

REFERENCES

- [1] Olga Bezuglova and Aleksandr Klimenko, "Application of Humic Substances in Agricultural Industry", *Agronomy*, 12(3), 584; 2022
- [2] A. Csicsor. E. Tombácz, "Antioxidant effect of humic substances from Hungarian Leonardite" *Hungarian Journal of Industry and Chemistry* Vol. 50 No. 1, 2022
- [3] Islam K.M.S et al, "Humic Acid Substances in Animal Agriculture", *Pakistan Journal of Nutrition*, Volume: 4, 126-134, 2005

Heavy metal removal using combined Clinoptilolite ion exchange and co-precipitation coagulation techniques

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ABSTRACT

Liquid effluent containing heavy metal ions is one of the most significant environmental challenges the world is facing today, due to its high toxicity. The concerns for treatment are because the ions are not biodegradable and can accumulate into living organisms, causing various health effects and other problems in plants and animal life. Some of the most important contaminants are metal ions like lead. Inorganic Ion exchange is one of most widely used methods for the treatment of heavy metals, because of the high cation exchange capacity and low-cost commercial availability. However, exchange performance can be highly selective and negatively affected by other competing ions. Also, as most inorganic minerals exchange in surface sites, they are more effective when using smaller particles that are thus more difficult to dewater and separate. Therefore, in this study, fine Clinoptilolite was studied for the removal of various heavy metal ions from wastewater in combination with coagulant. Iron (oxy) hydroxide 'Fe(O)OH' co-precipitation was chosen for enhanced removal of the metal ions, due to its ability to co-crystallise multivalent cations, as well as to enmesh and separate the ion exchange resin. The combined Clinoptilolite -Fe(O)OH system showed a maximum percentage removal of Pb (II) as 100 % and 100% removal for Cu (II) at high 200 ppm doses. Due to the coagulation mechanisms, precipitated electronegative colloid particles become destabilized to attract ions of opposite charge (intraparticle Bridging) to form large aggregates by reduction of the electrostatic forces, which enmesh the fine negatively charged ion exchange. The result was enlarged flocs that had a significantly greater size and faster settling rate than either ion exchange or coagulant species alone. Analysis by analytical centrifuge also indicated lower compressional yield stress in the composite flocs, meaning they are more readily dewatered in downstream processing. Characterisation by XRD and SEM-EDS further inferred the flocs were homogenous, with the hydroxide crystal structure not affected by heavy metal adsorption. Overall, this work evidenced that coagulation combined with co-precipitation could be an effective and fast alternative process for removing lead and copper ions in wastewater.

Determination of intrinsic loss power of magnetic fluid with differential thermometric system

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ABSTRACT

In calorimetric measurement setups the direct temperature detection is one of the simplest ways to characterize the heating efficiency of magnetic fluids used in hyperthermia treatment [1]. The measurement of temperature increase under an alternating magnetic field requires a thermometric system immune to magnetic interference and to the self-heating of the sensor elements. In our double cell differential temperature measurement system [2] the disturbing effect of the magnetic field was compensated by detecting only a differential signal between the symmetric sides of two negative temperature coefficient (NTC) thermistors. The control measurements were made with an optical fiber thermometer. The performance of the system was evaluated based on acquiring the heating curves and determining the specific loss power (SLP) and therefore the intrinsic loss power (ILP) of the EMG700 ferrofluid at low frequency and field strength, where the conditions of the magnetic field met the Brezowich criterion [3]. The calculated SLP and ILP values were compared with numerical calculations. Based on our recent publication [4], we calculate the power loss from the magnetic properties of the fluid by an expansion method within the framework of mean spherical approximation (MSA).

REFERENCES

- [1] Papadopoulos, C., Efthimiadou, E.K., Pissas, M., Fuentes, D., Boukos, N., Psycharis, V., Kordas, G., Loukopoulos, V.C., Kagadis, G.C., "Magnetic fluid hyperthermia simulations in evaluation of SAR calculation methods", *Physica Medica*. **71**, 39–52. (2020)
- [2] Guba, S., Horváth, B., Molnár, G., Szalai, I., "A double cell differential thermometric system for specific loss power measurements in magnetic hyperthermia", *Measurement* **169**, 108652 (2021)
- [3] Dutz, S., Hergt, R., "Magnetic particle hyperthermia a promising tumour therapy?", *Nanotechnology* **25**, 452001 (2014)
- [4] Horváth, B.; Decsi, P.; Szalai, I., "Nonlinear contributions to the dynamic magnetic susceptibility of magnetic fluids", *Journal of Molecular Liquids*, 119279, (2022). In press

Preparation of highly fluorescent soft nanoparticles for bioimaging applications

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ABSTRACT

Highly fluorescent biocompatible dyes are required in several bioimaging and biosensing applications. While fluorescent proteins play an important role, their application may be limited by the fluorescence intensity of the individual protein. To overcome this barrier we developed a method to incorporate a large number of fluorescent proteins into a soft nanoparticle. This approach allows not only the significant increase of the fluorescent intensity from the volume of the nanogel bead but by the functionalization of the external shell of the nanogel particles their targeting can also be achieved. We present a simple approach for the preparation of Bovine Serum Albumine (BSA) functionalized poly(N-isopropylacrylamide) pNIPAM microgels, and demonstrate that the microgel bound protein can form red fluorescent complexes with Au(III) ions similarly to the free protein.

Zn-loaded nanofiber based wound dressings

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ABSTRACT

Today, there is still a need to treat some wounds (e.g. ulcerative wounds in diabetic patients) in addition to traditional single-function dressings. Multi-functional wound dressings, currently under research, should have antibacterial, drug delivery and fluid retention capabilities in addition to physical protection. Several sources in the literature report on the antibacterial effect of zinc-oxide nanoparticles (ZnONPs), attributed to the nanoparticles themselves and to the released Zn²⁺-ions. [1] Our goal was to prepare a polymer nanocomposite system containing ZnONPs and/or Zn-salts that could be developed into a potential multifunctional wound dressing.

The ZnONPs were prepared by spontaneous hydrolysis of Zn-salt dissolved in dimethylformamide (DMF) or dimethylsulfoxide (DMSO) solvents. [2] The ZnO sols were investigated by dynamic light scattering (DLS) and infrared spectroscopy (ATR-FTIR). Polysuccinimide (PSI) was synthesized in the laboratory and wound covers were prepared by electrospinning. In some cases, 7w% ZnCl₂ was added to the PSI/PSI-ZnO systems. The viscosity and conductivity of the solutions were determined, and the systems obtained by electrospinning were characterized by ATR-FTIR and scanning electron microscopy (SEM), and their mechanical strength was also investigated. The antibacterial activity of the nets was determined using *S. epidermidis*, *B. subtilis*, *P. aeruginosa* and *E. coli* bacteria.

We successfully prepared colloidal ZnO with particle size distributions between 100-200 nm (PDI 10%). The advantage of organic medium reactions is that they are also the solvents for electrospinning (DMF, DMSO), so that a one-pot synthesis can be performed. Colloidal ZnO particles were added to solutions containing PSI, and ZnCl₂ and perform smooth fibers with electrospinning yielded around 1000 nm fibres with mechanical properties approaching those of conventional gauze sheets. The antibacterial assays resulted in an inhibition zone for the discs containing ZnCl₂ and ZnONPs for 3 strains, which showed synergistic effects in some cases.

REFERENCES

- [1] Jin SE, Jin HE, *Nanomaterials* **11(2)**, 263, (2021)
- [2] Geonel Rodríguez-Gattorno et al., *J. Phys. Chem. B* **107**, 12597, (2003)

Atomistic and coarse-grained molecular dynamics study of self-diffusion of poly(alkyl acrylate) chains in melt

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ABSTRACT

By means of coarse-grained molecular dynamics simulations, the formation of active topological glass has been identified in a melt of circular polymer chains comprising a fragment with increased mobility [1]. This composition promotes the mutual entanglement of chains and induces vitrification. So far, the active topological glasses arising from a melt of circular chains have been the subject of computer simulation studies based on a physical coarse-grained model. The effort to bring these systems closer to reality relies on experimental syntheses of polymers with circular topology in which one block displays increased mobility. Poly(alkyl acrylate) chains appear to be suitable candidates for building such diblock circular polymer chains. Atomistic molecular dynamics simulations employing the OPLSAA force field are used to estimate the self-diffusion coefficients of different poly(alkyl acrylates) in order to distinguish their mobility in melts which, in turn, suggests the design of circular polymer chains composed of poly(alkyl acrylate) block with enhanced mobility. Since the molar mass of the investigated polymers is limited when the atomistic approach is considered, the coarse-grain MARTINI model has been developed, which allows the study of melts of poly(alkyl acrylate) chains with a backbone length above the entanglement length. In addition to the self-diffusion coefficients, the distributions of the end-to-end distance, radius of gyration, relaxation times, and averaged persistence length are calculated at the atomistic as well as coarse-grained level. The effect of alkyl substituents of poly(alkyl acrylates) and different temperatures on these properties is systematically scrutinized. Based on these results, the molecular dynamics simulations of a melt composed of circular diblock poly(alkyl acrylate) chains will be performed.

ACKNOWLEDGEMENTS

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REFERENCES

[1] Smrek, J.; Chubak, I.; Likos C. N.; Kremer, K., "Active topological glass", Nature Communications **11**, 26, (2020).

Mechanical testing of nanofiber matrices with an affordable rupture detection system

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ABSTRACT

Acoustic emission (AE) occurs in a solid material as elastic waves when the observed material is under stress resulting irreversible changes in its internal structure. Crack formation or plastic deformation, temperature changes or mechanical force can cause stress to the material. With the help of the electrospinning technique, one can create micro- and nanofiber structures which are becoming increasingly popular. These samples loosely structured porous materials have low mass and generally high mechanical strength. If the force at a given point exceeds a threshold value specific to the fiber, it will break. These individual ruptures appear on the mechanical curve, but the fibers are also displaced and straightened during the pulling process, and these can be also detected on the curve. To better understand these mechanisms, one should be able to separate ruptures and movements.

Our aim was to create an affordable non-invasive piezoelectric sensor to detect signals appearing after the ruptures. The sensor had to be amplified with an operational amplifier because the signal created by the piezo plate is very low. An Arduino UNO microcontroller is used to collect the signals and for the analog-digital conversion, then one can visualize the signals on the computer. Visualization and comparison with the mechanical curve implemented in Python programming language. To test the apparatus, a 3D printed model was used with ten thin fibers to be cracked with an Instron 5940 Mechanical Tester. Then electrospun meshes were characterized with this method as well. Our results show that it's possible to collect rupture data with the help of our affordable AE device without the need to apply the sensor to the electrospun meshes which will give better understanding of how the fibers are behaving over the course of mechanical testing.

ACKNOWLEDGEMENT

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The potential role of antibiotic resistant environmental *Pseudomonas* species in microplastic colonization

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ABSTRACT

Pseudomonas species are often found in locations associated with human activity [1], such as in surface waters under sewage load. The main characteristics of these species (virulence, antibiotic resistance, biofilm forming ability) make them a potential threat to environmental health. Sewage is not only the source of microbial contamination but a verified emitter of microplastic particles as well [2]. Microplastics serve as potential vectors for the spread of biofilm-forming microorganisms, but the ability of antibiotic-resistant *Pseudomonas* to adhere to plastic particles is not deeply investigated. Therefore, this research aimed to isolate and identify *Pseudomonas* sp. strains from surface water bodies located in the Balaton catchment area with and without sewage load to evaluate their potential role in microplastic colonization. In the summer period of 2021, 15 environmental *Pseudomonas* strains (belonging to species *P. cichori*, *P. pisciculturae*, *P. poae*, *P. putida*, *P. chloraphis*, *P. alloputida*, *P. mosselii*, *P. synxantha*, and *P. asplenii*) were isolated and identified with 16S rRNA sequencing. Five of them showed multidrug-resistant phenotype: resistance was detectable against Carbapenems (imipenem, meropenem doripenem), ciprofloxacin, colistin, ceftazidime, cefepime, and piperacillin. The plastic adherence of the isolated strains proved that four examined *Pseudomonas* strains were moderate, and one was a strong biofilm producer on a polystyrene surface. Only one multidrug-resistant strain showed adherence to PS. Based on our results, further investigations need to evaluate the adherence of environmental *Pseudomonas* to the commonly detectable plastic materials (PE, PET, PP, PVC) to get a reliable picture of their role in the plastisphere.

ACKNOWLEDGEMENTS

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REFERENCES

- [1] Crone, S., Vives-Flórez, M., Kvich, L., et al., The environmental occurrence of *Pseudomonas aeruginosa*. APMIS **128.**, 220–31. (2020)
[2] Waldschläger, K., Lechthaler, S., Stauch, G., Schüttrumpf, H., The way of microplastic through the environment – Application of the source-pathway-receptor model (review). Science of The Total Environment, **713.**, 136584. (2020)

Functionalized nanoparticles for efficient isolation and immobilization of a recombinant transaminase

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ABSTRACT

In recent years, the application of the ω -transaminases has gained interests as promising biocatalysts that provides an environmentally friendly way to the synthesis of pharmaceutically relevant chiral amines with high stereoselectivity and catalytic turnover. [1] Simultaneously, heterologous expression systems and protein engineering strategies such as directed evolution and point mutations have made the high-level production of recombinant enzymes with improved performance and catalytic activity possible and tailored them to the desired process. The main focus of our research was to develop a proper method for the immobilization of the recombinant *Chromobacterium violaceum* transaminase (CvTA) expressed by *Escherichia coli* in a multistep process to create a novel nanofibrous composite biocatalyst. First the functionalized silica nanoparticles (fSNPs) were prepared with specific affinity linkers, that allowed the complexation of metal ions on the surface. Thus, the resulting nanocarrier systems became suitable for the selective isolation of the target CvTA enzymes labeled by histidine polypeptide tag from the highly complex cellular environment. [2] Then the primer CvTA-fSNPs biocatalysts were entrapped in polylactic acid (PLA) matrices by electrospinning technique resulting the desired nanofibrous composite structure. [3] The enzyme immobilization yield was fine-tuned and the CvTA-fSNPs loading in PLA nanofibers were systematically examined. Furthermore, the morphology of each biocatalyst, the effect of the immobilization parameters and the composition of nanocomposite system on the enzymatic activity were investigated.

REFERENCES

- [1] D Patil, M., Grogan, G., Bommaris, A., Yun, H., Recent advances in ω -transaminase-mediated biocatalysis for the enantioselective synthesis of chiral amines. *Catalysts* **8**, (2018).
- [2] Sánta-Bell, E., Molnár, Z., Varga, A., Nagy, F., Hornyánszky, G., Paizs, C., D. Balogh-Weiser, Poppe, L., "Fishing and Hunting"—Selective immobilization of a recombinant phenylalanine ammonia-lyase from fermentation media. *Molecules* **24**, (2019).
- [3] Koplányi, G., Sánta-Bell, E., Molnár, Z., Tóth, G. D., Józó, M., Szilágyi, A., Ender, F., Pukánszky, B., Vértessy, B.G., Poppe, L., D. Balogh-Weiser, Entrapment of Phenylalanine Ammonia-Lyase in Nanofibrous Polylactic Acid Matrices by Emulsion Electrospinning. *Catalysts* **11**, (2021).

High-sensitivity analytical methods supporting the evaluation of adsorption studies

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ABSTRACT

High-sensitivity analytical methods are essential for the proper evaluation of adsorption studies of water micropollutants. The quantification of the quasi zero equilibrium concentrations in the high-affinity range of most H-type isotherms is challenging by conventional analytical methods. Ultra performance liquid chromatography-tandem mass spectrometry (UPLC-MS/MS) is a suitable tool for the trace quantification of various analytes in complex matrices. A Waters ACQUITY UPLC H-Class System coupled with a Xevo TQ-S micro triple quadrupole mass spectrometer equipped with an electrospray ionization source (Figure 1) is employed in our Research Center to carry out high-sensitivity analysis of adsorption studies conducted with water contaminants of anthropogenic origin. After proper sample preparation, the targeted analysis of the water pollutants is possible at environmentally relevant, low ng/L (ppt) levels. The low LOQ (limit of quantification) values provide an opportunity to study the high-affinity range of H-type isotherms in detail. In the case of micropollutants, high sensitivity also facilitates improving the experimental design allowing performing adsorption experiments under environmentally relevant conditions.



Figure 2 Waters Acquity UPLC-TQS micro tandem quadrupole mass spectrometer

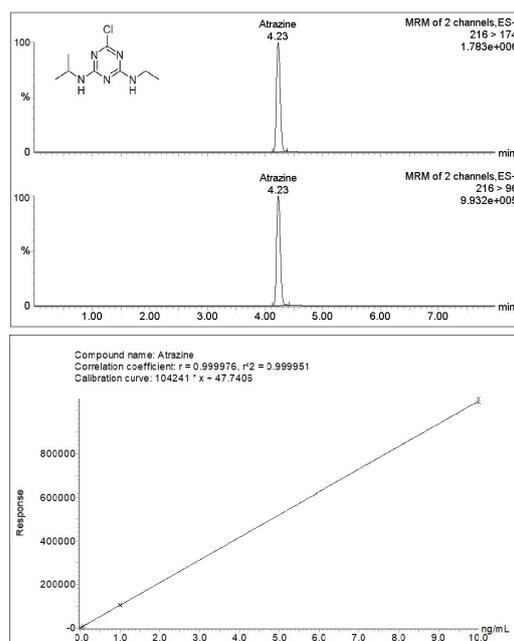


Figure 1 Chromatogram and calibration curve of atrazine (herbicide), limit of detection (S/N=5) 0.0069 ppb

The shape of near-critical interfaces

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ABSTRACT

Density profiles of liquid-vapor interfaces far from their critical points are readily measured by X-ray scattering experiments¹. The results are commonly interpreted in the context of capillary wave theory (CWT)². CWT describes the interface in terms of thermally activated capillary waves which corrugate an otherwise sharp surface. However, as one approaches the critical point of the liquid-vapor coexistence, the characteristic width of the interface increases along with a decrease in the surface tension which goes to zero at critical point. This behavior suggests the breakdown of CWT close to the critical point, which is usually remedied by combining CWT with the van der Waals theory of liquids. Here, we investigate the behavior of liquid-vapor interfaces close to their critical points, and the validity of CWT at high temperatures. To test the physical quality of the interface, we compare density profiles obtained from MD simulations of argon close its critical point to two reference systems. The first model is the CWT-predicted sharp surface, while the second one assumes an essentially flat region that continuously transitions between the liquid and vapor densities. We analyze the MD simulations by directly comparing them to the two model interfaces. For a thorough characterization of the interface, we compute the distributions and the normal-direction profiles of a range of quantities, such as the number of neighboring atoms within a certain radius, the Voronoi volume of the particles along with its asphericity and the GITIM surface⁴. According to our results, the surfaces $1-T/T_c = 0.013$ can still well be represented by a sharp, undulating surface, beyond which the distinction between the models becomes increasingly meaningless.

REFERENCES

- [1] Bu, W.; Kim, D.; Vaknin, D. "Density profiles of liquid/vapor interfaces away from their critical points." *The Journal of Physical Chemistry C* 2014, 118, 12405–12409.
- [2] Tarazona, P.; Chacón, E. "Monte Carlo intrinsic surfaces and density profiles for liquid surfaces." *Physical Review B* 2004, 70, 235407
- [3] Sides, S. W.; Grest, G. S.; Lacasse, M. D. "Capillary waves at liquid-vapor interfaces: A molecular dynamics simulation." *Physical Review E* 1999, 60, 6708
- [4] Sega, M.; Hantal, G. "Phase and interface determination in computer simulations of liquid mixtures with high partial miscibility." *Physical Chemistry Chemical Physics*, 19, 18968-18974.

Polarizabilities and electric field induced forces in periodic two-component linear dielectric sphere chains

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ABSTRACT

The electrorheological (ER) fluids are a type of intelligent materials and are gained by dispersing solid particles with dielectric permittivity ϵ_p in a fluid with dielectric permittivity $\epsilon_f < \epsilon_p$. The apparent viscosity of an ER fluid can be changed if an external electric field is applied to the fluid. The apparent viscosity increases, as the dispersed particles gain induced dipole moments, and form chain-like structures in the fluid, which act against any shearing motion. The fluids can be used in microfluidic chips, dampers, brakes, shock absorbers.

The forces acting between the particles in the chains under the influence of the electric field are described by Kim et al [1]. The formula defines the force in the case of uniform particle size. If there are at least two distinguished particle sizes, new formula is required for the acting forces.

The permittivity change of the fluid in a two-component periodic chain is described using the Clausius-Mosotti equation. We describe the local electric fields in the case of two one-component, and one bidisperse chains. New formulas for the forces acting in two-component periodic finite and infinite chains are given. The forces acting in chains with varied ratio of sizes of the two particles are also discussed. The calculations indicate the forces in the two-component chain are always smaller than the forces acting in the chain consisting only the larger particle.

REFERENCES

- [1] Kim, H. Y.; Sofo, J. O.; Velegol, D.; Cole, M. W. and Mukhopadhyay, G., "Static polarizabilities of dielectric nanoclusters", *Phys. Rev. A - At. Mol. Opt. Phys.* **72** 1-44, (2005).

Investigation of the sedimentation characterization of magnetorheological fluids

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ABSTRACT

Magnetorheological (MR) fluids can change their viscosity in external magnetic fields. MR fluids can be obtained by dispersing ferromagnetic particles with diameters from 1 μm to 100 μm in a fluid. The magnetic field induces a dipole moment in the dispersed particles, which causes them to organize themselves into chains, then columns, resulting in a magnitude increase in the viscosity of the fluid. This effect is used in mechanical engineering and mechatronics for vibration damping and shock absorption. [1]

If the particle size of the particles is not small enough, the dispersions will settle out over time. The operation of actuators based on magnetorheological fluids may be hindered by the loss of homogeneity of the dispersions due to sedimentation. In our work, we present a measurement and data acquisition system for MR fluid sedimentation operating in gravitational space. A simple theoretical description for the sedimentation is also given. [2]

The detector part based on the LVDT principle was used, which is moved along a vertically positioned glass tube by a linear unit, thus continuously scanning the sedimentation. The coupling between the detector coils being provided by the dispersed magnetic particles in the magnetorheological fluid. As the particles settle at the top of the liquid column, the coupling between the primary and secondary coils decreases so that the output voltage is proportional to the number of settled particles. Since the complete settling process can take several days, an automated system was developed.

With the completed measurement system, several measurements were performed. The MR fluid samples were made by Lord company with Fe microparticles and silicone oil carrier fluid. The samples had different apparent viscosities and densities, which provided a good basis for comparison and evaluation. The results are plotted in diagrams showing the continuous settling of the particles as a function of time and space.

REFERENCES

- [1] Jönkkäri, I.: "Rheological characterization of magnetorheological fluids", Tampere University of Technology, vol. 1566, pp. 3 - 6, (2018).
- [2] Takehito, K.; Takaya, K.; Isao, A.; Akio, I.: "Particle sedimentation in magnetorheological fluid and its effect", IEEE International Conference on Advanced Intelligent Mechatronics, (2017).

Biodegradable, three-dimensional fiber structures created by electrospinning – the effect of humidity

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ABSTRACT

Very thin, invisible to the eye, nano- and microfibers can be created through the technique called electrospinning. The formed fiber meshes are closely resembling the extracellular matrix (ECM) which is the non-cellular component present within all tissues and organs in the human body. Using the cells of a patient and engrafting them onto the created fiber structure, missing tissues can be replaced, and a quicker healing process of wounds can be assisted. However, if the pores are too small, the fibers are tightly packed, the cells cannot permeate into the material and reach their native form.

The aims of my work were to find the right salt and salt concentration for the increase of the pore size, creating three-dimensional structures, and observing the effects of humidity.

During the experiments I used different polysuccinimide (17-25 w/w %) and salt (3-7 w/w % CaCl_2 , MgCl_2 and LiCl) concentrations dissolved in dimethylformamide, and created solid polymer fibers with the help of an electrostatic field. At 20 w/w % polysuccinimide concentration we could form thinner fibers, reaching a closer resemblance to the extracellular matrix than at the tried and tested 25 w/w % the research group used before. Although beads appeared on the strings these disappeared with adding salt to the solution. For characterization we measured the FTIR spectrum, mechanical endurance, average fiber diameter of the fiber meshes and through these observed the effect of different percentage of humidity (27.4-60 %). It seems that we have found a minimum humidity level, 48 %, that is needed for forming three-dimensional structures with the use of salts, aiding the permeation of the cells into the material.

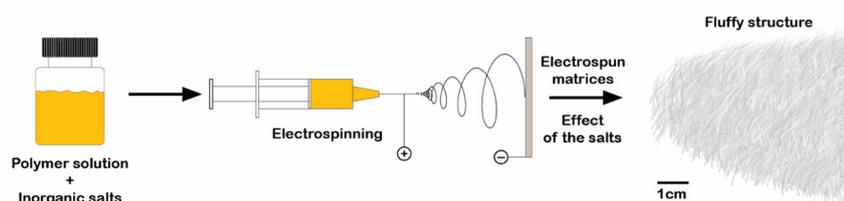


Figure 1.: Schematic of the electrospinning process, using inorganic salts¹

REFERENCES

[1] Ákos György Juhász; Kristóf Molnár; Abdenacer Idrissi; Angéla Jedlovszky-Hajdú, "Salt induced fluffy structured electrospun fibrous matrix", *Journal of Molecular Liquids* vol. **312**, 113478, (2020).

The effect of ionic liquid on the morphology and surface character of carbon aerogels seen by NMR

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ABSTRACT

Resorcinol-formaldehyde (RF) based carbon aerogels are widely used materials as catalyst, electrodes or adsorbents because of their high surface area, good electrical conductivity and tunable pore size. During the synthesis many factors can affect the resulting pore structure including the concentration and molar ratio of the reagents, the pH and the temperature. Beside the reaction conditions, porogens (solvents, additives, catalysts) have a crucial role in the resulting pore system. [1] Ionic liquids in the RF precursor solution can serve not only as a porogen, but as a template or a source of nitrogen or carbon. Recently the effect of several room temperature ionic liquids as co-solvent of water and their concentration was studied on the pore structure of the resorcinol-formaldehyde polymer and carbon aerogels. [2,3] The applied 1-ethyl-3-methylimidazolium ethyl sulphate ionic liquid mainly acted as a catalyst for the polymerization reaction, thus the pore morphology could be tuned by the water to IL ratio. The supramolecular system of water and IL also contributed to the formed aerogel texture.

Nuclear magnetic resonance (NMR) methods are well applicable for the characterization of porous materials like aerogels in wet state. With the use of NMR cryoporometry, relaxometry and diffusometry the whole wetting mechanism of carbon aerogels, from hydration to immersion can be described, and the differences in the hydration properties can also be pointed out. [4]

In our work, we used the mentioned NMR techniques to study the morphology of carbon aerogels, synthesized with changing IL/water ratio [3], in aqueous medium. It is confirmed that the pore size of the resulted carbon aerogels can be tailored by the IL/water ratio during the synthesis. Moreover, the IL modifies the hydration properties of the aerogels as well. The explanation is based on the high-field NMR analysis of the monomer/IL/water solutions.

REFERENCES

- [1] Mansour, F. R.; Waheed, S., Paull, B., Maya, F., "Porogens and porogen selection in the preparation of porous polymer monoliths", *J. Sep. Sci.* **43**, 56-69, (2020).
- [2] Nagy, B., Geissler, E. László, K., "Room temperature ionic liquids to tailor resorcinol – Formaldehyde polymer gels." *Microporous and Mesoporous Materials* **294**, 109888 (2019).
- [3] Nagy, B., Bakos, I., Geissler, E., László, K. "Water-Ionic Liquid Binary Mixture Tailored Resorcinol-Formaldehyde Carbon Aerogels without Added Catalyst." *Materials (Basel)*. **12** 4208
- [4] Kéri, M., Nyul, D., László K., Novák, L., Bányai.: "Interaction of resorcinol-formaldehyde carbon aerogels with water: A comprehensive NMR study" *Carbon* **189** 57-70 (2022)

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Optimization and potential medical application of fibrous structures made of polysuccinimide / inorganic salt mixture

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ABSTRACT

Due to its antibacterial effect, silver is increasingly being pushed out of medicine, and other ions with a similar effect are coming to the fore. Since silver ions have a significant toxic effect on microorganisms, it has been suggested that they may also be harmful to human cells.

The aim of my research is to create a two-component polymer network by electrospinning, which contains inorganic salts in addition to the polymer, which according to the literature, have antibacterial properties. If such a new type of biocompatible wound dressing could be created, not only would a mechanical barrier to infection be provided to severely damaged tissues, but due to the high water-binding capacity of the polymer, it could also provide a solution for dehydration that inhibits wound healing as well. Zinc and strontium ions, based on the literature, also have antibacterial activity against microorganisms.

The first step in my work was to synthesize the polymer, then mix it with the selected inorganic salts, and then optimize the electrospinning parameters. The inorganic salts used in the experiments were ZnCl₂, Zn(O₂CCH₃)₂, SrCl₂ and Sr(NO₃)₂. Next, the chemical and mechanical properties of the complete polymer networks were investigated by IR spectroscopy, SEM images, and their specific load capacity (mechanical characterization). In the next step, we investigated the dissolution of the different salts from the meshes in distilled water, then the antibacterial effect of polymer networks on four different application relevant bacterial strains was examined.

Based on IR spectroscopy, all the salts formed a physical bond with polysuccinimide, and the presence of the salts was provable, but there was no chemical bonding between the salts and the polymer. Scanning electron micrographs of polymer meshes containing various inorganic salts showed a big difference between the fiber diameters (240-500 nm). However, no significant difference was found in their mechanical properties (specific load capacity) except for the polymer mesh which contains SrCl₂ salt, which has larger specific load capacity value (0.19 Nm²/g), than the meshes containing other salts (0.05-0.09 Nm²/g). In antibacterial experiments, a fairly big, but not exactly clear zone appeared for the polymer containing ZnCl₂ and Zn(O₂CCH₃)₂ on the *B. subtilis*, and a smaller, but completely clear inhibition zone on *E. coli* and *P. aeruginosa* species containing Sr(NO₃)₂ salts in different concentration.

NMR characterization of cement binders related to the radioactive waste conditioning

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ABSTRACT

Radioactive wastes generated during the operation and decommissioning of a nuclear power plant and during various other uses of radioactive isotopes are usually immobilized in a binder depending on their level of hazard. The most common conditioning method for low and intermediate level wastes is cementation. The properties of cements can be improved by added components, like geopolymers or complexing agents, which also affect the porous structure. [1, 2] For the long-term safe disposal and the proper immobilization of the wastes, it is important to know the structural properties of these binders and their interaction with water.

In our study, we used liquid - state nuclear magnetic resonance (NMR) methods to identify the different pore types and determine the mobility of water in numerous cement matrices with different compositions (containing metakaolin, basic model solution, complexing agents and model ions). First, we determined the pore structure of the cement and metakaolin constituents by NMR relaxometry and cryoporometry, then compared them with the cement matrix containing both initial constituents to draw conclusion of their immobilization capability. We also investigated the effect of the possible application conditions on the pore structure of the binders, like the concentration of the complexing agents, the presence of model ions and the rehydration time. Information on the mobility and diffusion properties of water within the cement structure was obtained by H₂O - D₂O exchange diffusion technique. [3]

These results can greatly contribute to the development of matrix materials, effectively complement standard dissolution studies, and provide input to modeling processes.

REFERENCES

- [1] Bede, A.; Scurtu, A.; Ardelean, I., NMR relaxation of molecules confined inside the cement paste pores under partially saturated conditions. *Cement and Concrete Research* 89, 56-62 (2016).
- [2] Li, J. et al., Curing process and pore structure of metakaolin-based geopolymers: Liquid-state ¹H NMR investigation. *Cement and Concrete Research* 143, 106394 (2021).
- [3] M. Fleury, G. Berthe, T. Chevalier, Diffusion of water in industrial cement and concrete, *Magnetic Resonance Imaging* 56, 32–36, (2019).

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Monitoring the effect of pH and ionic strength on the interaction between Bovine Serum albumin molecules and graphene oxide nanosheets

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ABSTRACT

Recently, the scientific interest of graphene-based materials has been impressive, especially in the medical and pharmaceutical fields. This is no coincidence, as these materials, such as graphene oxide, are promising for medical applications due to their physicochemical properties, such as large specific surface area. Because of this it has huge importance to understand fundamentally the interaction between graphene oxide (GO) and the biomolecules, such as serum albumins. To our surprise, only a few articles [1][2] are available in the literature that specifically explore the exact types of interactions between bovine serum albumin and graphene oxide in detail including the quantitative characterization. Therefore, at the basic research level, we would like to provide a comprehensive explanation of the interaction effects between BSA and GO. The most common methods employed previously were UV-Vis spectrophotometry in the UV range, CD, SEM, and Fluorescence Quenching. These techniques such as CD provide useful information but some other approaches may reveal additional structural characteristics. For example, we also used UV-Vis spectrometry, but using the less misleading Biuret test in the Vis range. We also performed XRD measurements for the analysis of the intercalation of BSA molecules between the GO lamellae, a method we have not seen yet in the literature we reviewed so far. We also measured the zeta potential of the BSA/GO composite. These measurements were carried out at several pH-s and ionic strength, so we monitored the adsorption properties of GO, the desorption processes of BSA from GO, the size of this composite and the occurring intercalation in different conditions.

Acknowledgement:

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REFERENCES

- [1] H. Zhang, Changing the activities and structures of bovine serum albumin bound to graphene oxide, *Appl. Surf. Sci.*, 427, 1019-1029 (2018).
- [2] M. Šimšiková, Interaction of graphene oxide with albumins: Effect of size, pH, and T, *Arch. Biochem. Biophys.*, 593, 69-79 (2016).

Stabilization of selectively complexed His-tagged enzymes on magnetic nanoparticles

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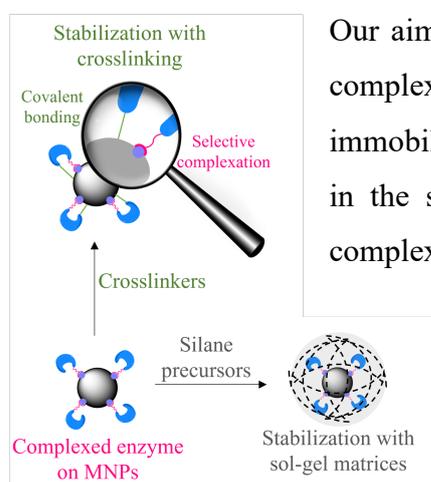
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ABSTRACT

Novel enzyme immobilization techniques are constantly emerged, due to the advantageous stability and catalytic properties of immobilized biocatalysts. In this work we focused on a selective method based on immobilized metal affinity chromatography (IMAC). IMAC mostly used for purification of histidine tagged enzyme, but in the last two decades it has been increasingly used for reversible one-step enzyme purification and immobilization [1]. Disadvantage of the reversible interaction over covalent immobilization is that enzyme leakage is more common phenomenon.



Our aim was to combine the fast and selective IMAC based complexation with a stabilization method in a two-step immobilization process. Metal chelating agents were formed in the surface of magnetic nanoparticles (MNPs) and after complexing Co^{2+} ions, histidine tagged phenylalanine ammonia-lyase and transaminase enzymes were attached to the surface. The stabilization of the MNPs-complexed enzymes was accomplished in two different ways. Covalent crosslinking was

performed via bisepoxides as a chemical stabilization. As a physical stabilization the enzyme complexed MNPs were embed in silica sol-gel matrices.

REFERENCES

[1] Sánta-Bell, E.; Kovács, N.K.; Alács, B.; Molnár Z; Hornyánszky, G., "Immobilization of Phenylalanine Ammonia-lyase via EDTA Based Metal Chelate Complexes – Optimization and Prospects", *Periodica Polytechnica Chemical Engineering* **65**, 308-319, (2021).

The contribution of mucin in the *in vitro* mucoadhesion measured on hydrogel substrates

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ABSTRACT

Mucoadhesive drug delivery systems are capable to adhere to the surface of mucosa and provide a prolonged drug release bypassing the first pass metabolism. The strength of adhesion is conventionally determined by tensile tests on animal tissues. However, the reproducibility of measurements is not always satisfactory [1]. Here we describe a semi-synthetic mucosa-mimetic material, which can be produced easily by the physical cross-linking of polyvinyl alcohol (PVA) containing the mucin protein (Mucin/PVA), which is the main component of the mucus covering the mucosal membranes [3]. Tensile test was used to determine the strength of adhesion using polymer tablets made of positively charged chitosan, negatively charged poly(acrylic acid) (PAA) and neutral hydroxypropylmethylcellulose (HPMC). Zeta potential of the polymers used and that of mucin is shown in Figure 1A. Chitosan as a positively charged polymer showed enhanced adhesion on Mucin/PVA substrate compared to mucin-free PVA (Figure 1B) showing the contribution of electrostatic interactions in mucoadhesion.

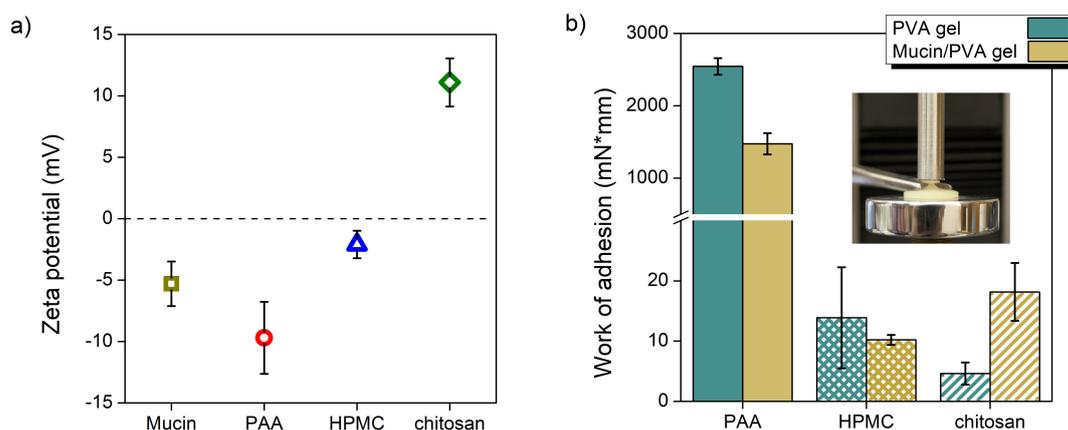


Figure 1 (a) Zeta potential of mucin dispersion and polymer solutions (b) adhesion measurements with polymer tablets comparing Mucin/PVA and mucin-free PVA hydrogel substrate

REFERENCES

- [1] Khutoryanskiy, V.V., "Advances in Mucoadhesion and Mucoadhesive Polymers", *Macromolecular Bioscience* **11.**, 748–764, (2011).
- [2] Gyarmati, B.; Stankovits, G.; Szilágyi, B.Á.; Galata, D.L.; Gordon, P.; Szilágyi, A. "A robust mucin-containing poly(vinyl alcohol) hydrogel model for the *in vitro* characterization of mucoadhesion of solid dosage forms", *Colloids and Surfaces B: Biointerfaces* **213.**, 112406, (2022).

Formulation of Lipases into Polymer Nanofibers for Pancreatin Replacement Therapies

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ABSTRACT

Chronic Pancreatitis is part of the group of lysosomal storage diseases that includes about 50 inherited diseases. These are caused by a lack of enzymes in the body, which can lead to the formation and accumulation of toxic substances through altered metabolic processes, causing many different symptoms [1]. Solutions for the external replacement of the missing enzymes have appeared in literature since the 1960s, but their actual therapeutic application has only been in place since the 1990s [2]. By enzyme replacement therapies, the symptoms of the aforementioned metabolic diseases can be treated remarkably well.

The aim of our research is to produce a lipase-containing nanofibrous formulation that may be suitable for the treatment of *Chronic Pancreatitis* during enzyme replacement therapy [3]. In this study, aqueous precursor solutions of commercially available polyvinyl alcohol and polyvinylpyrrolidone with varying molecular weights and concentrations were characterized, nanofibers prepared from them using electrostatic fiber formation. Precursors were optimized for electrospinning then used for the entrapment of lipase from *Porcine pancreas* into polymer nanofibers. In our experiments, we aimed to optimize the fiber formation process and to determine the most suitable polymer type and precursor composition by examining the activity of the enzymes entrapped in the formulations. We also aimed to investigate the bioimprinting effect of substrate like additives during the enzyme entrapment process. In the presence of suitable additives, the enzyme assumes its active conformation, which is preserved during the immobilization process, resulting in increased enzyme activity [4].

The rheological properties of the different precursors were examined with a rotary viscometer. Scanning electron microscopy was used to examine the morphology of the nanofiber matrices and Raman microscopy was applied for structural analysis. The activity of the nanofibrous lipase formulations were investigated in the hydrolysis of 1-octyl acetate.

REFERENCES

- [1] Vellodi, A., "Lysosomal storage disorders." *British journal of haematology* **128**(4), 413-431, (2005).
- [2] Beutler, E.; Kay, A.; Saven, A.; Garver, P.; Thurston, D.; Dawson, A.; Rosenbloom, B., "Enzyme replacement therapy for Gaucher disease" *Blood* **78**(5), 1183-1189, (1991).
- [3] Tóth, G.D.; Kazsoki, A.; Gyarmati, B.; Szilágyi, A.; Vasvári, G.; Katona, G.; Szente, L.; Zelkó, R.; Poppe, L.; Balogh-Weiser, D.; Balogh, G.T., "Nanofibrous Formulation of Cyclodextrin Stabilized Lipases for Efficient Pancreatin Replacement Therapies." *Pharmaceutics*, **13**(7), 972, (2021).
- [4] Weiser, D.; Sóti, P.L.; Bánóczy, G.; Bódai, V.; Kiss, B.; Gellért, Á.; Nagy, Z.K.; Koczka, B.; Szilágyi, A.; Marosi, G.; Poppe, L., "Bioimprinted lipases in PVA nanofibers as efficient immobilized biocatalysts." *Tetrahedron* **72**(46), 7335-7342, (2016).

Solvent specific evaporation from CNT buckypapers with different functionalization

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ABSTRACT

Recent developments in nanotechnology have highlighted the importance of the classical topics of wetting, droplet spreading and evaporation due to their pronounced effect in technological applications. Carbon nanotubes (CNTs) can be transformed by filtration into a self-supporting, porous, paper-like film (buckypaper). Besides offering a convenient alternative to handle CNTs macroscopically, buckypaper is an interesting porous material on its own right [1]. The main goal of this work was to obtain a more detailed picture of the surface properties (namely, wetting and vaporization) of the buckypapers prepared from non-functionalized CNT (nf-CNT), –COOH functionalized CNT (f-CNT), and their mixtures. The evaporation of sessile droplets was studied by simultaneous weight monitoring, contact angle measurement, electric resistance measurement and infrared imaging. The characteristic parameters of the wetting and evaporation processes were determined to represent the evaporation profile [2,3]. It was proved, that this method can be used for qualitative and quantitative chemical analysis. The results allow us to presume the possibility of a potential future application in the field of analytics.

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REFERENCES

- [1] Bogya, E.S.; Szilagyi, B.; Kukovecz, Á.: "Surface pinning explains the low heat transfer coefficient between water and a carbon nanotube film", *Carbon* 100., 27-35, (2016).
- [2] Toth, I.Y.; Janovák, L.; Bogya, E.S. ; Deák, Á. ; Dékány, I.; Rawal, A.; Kukovecz, Á.: „Characterization of the solvent specific evaporation from a fluoropolymer surface roughened by layered double oxide (LDO) particles”, *Journal of Molecular Liquids* 305.,112826, (2020)
- [3] Nagy, K.A.; Tóth, I.Y.; Ballai, G.; Varga, Á.T.; Szenti, I.; Sebők, D.; Kopniczky, J.; Hopp, B.; Kukovecz, Á.: „Wetting and evaporation on a carbon cloth type gas diffusion layer for passive direct alcohol fuel cells” *Journal of Molecular Liquids* 304.,112698 (2020)

A scaling parameter for selectivity in the infinitely long nanopore limit: extension to multivalent electrolytes

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ABSTRACT

Scaling of the behavior of a nanodevice means that the device function (selectivity, in this work) is a unique function of a scaling parameter that is an appropriate combination of the input device parameters. Although nanopores facilitate the transport of ions through a membrane of finite length, if the pore is long compared to the pore radius, we deal with an important limiting case, the infinitely long nanopore (nanotube).

In this case, input device parameters are the pore radius, the electrolyte concentration, the surface charge density on the nanopore's wall, and ionic valences. We showed that the Dukhin number is an appropriate scaling parameter in the nanotube limit for 1:1 electrolytes [1], while in this work obtain the Dukhin number from first principles on the basis of the Poisson-Boltzmann (PB) theory and generalize it to electrolytes containing multivalent ions as well. We show that grand canonical Monte Carlo simulations for charged hard spheres in implicit solvent give results that are similar to those obtained from the PB theory with deviations that are the consequences of ionic correlations (including finite size of ions) beyond the mean-field level of the PB theory.

Such a deviation occurs when charge inversion is present, in 2:2 and 3:1 electrolytes, for example. Scaling can be viewed as a phenomenon resulting from analytical solutions to a mean-field theory such as PB. Deviations from scaling indicate the importance of ionic correlations [2].

REFERENCES

- [1] Zs. Sarkadi, D. Fertig, Z. Ható, M. Valiskó, D. Boda, *J. Chem. Phys.*, 2021, 154(15):154704.
- [2] Zs. Sarkadi, D. Fertig, M. Valiskó, D. Boda, *J. Mol. Liq.* 2022, 357:119072.

Preparation, characterization and stability of magnetite nanoflowers

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ABSTRACT

Promising application possibilities of magnetic nanoparticles (MNPs) includes the fields of magnetic storage devices, magnetic resonance imaging (MRI) and hyperthermia. One of the most auspicious types of magnetite nanoparticles for biomedical purposes is the flower form as a result of the aggregation of primary NPs, combined, improved magnetic response in applied magnetic field is expected [1,2].

To achieve the above mentioned character, the so-called “polyol” technique was applied for the preparation of magnetite nanoflowers (MNF), in a mixture of polyethylene glycol (PEG) and *N*-methyl-diethanolamine (NMDEA) solvents and reaction temperature of 220 °C. The properties of the forming magnetite nanoparticles such as morphology and average particle diameter were strongly affected by the preparation conditions whether the reaction was performed in autoclave or round-bottom flask (without or with stirring, respectively). The effect of heating and cooling rate was also significant on the particle size and morphology (**Fig. 1**).

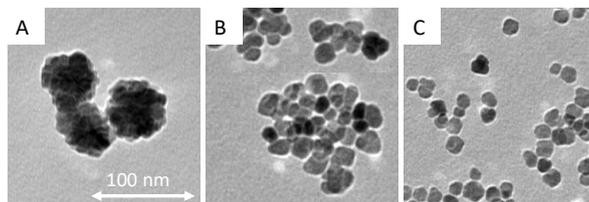


Fig. 1. Magnetite nanoflowers prepared in autoclave with slow (A) and fast cooling (B), or in round-bottom flask (C)

The magnetite structure was verified by X-ray diffraction measurements. Transferring the flower-shaped particles into aqueous phase holds some challenges, however, different carboxylic group-containing stabilizing agents were examined to increase colloid stability for potential biomedical application.

REFERENCES

- [1] Caruntu, D.; Caruntu, G.; Chen, Y.; O'Connor, C.J.; Goloverda, G; Kolesnichenko, L.V., “Synthesis of Variable-Sized Nanocrystals of Fe₃O₄ with High Surface Reactivity”, *Chem. Mater.* **16**, 5527 (2004).
- [2] Socoliuc, V.; Peddis, D.; Petrenko, V.I.; Avdeev, M.V.; Susan-Resiga, D; Szabó, T.; Turcu, R; Tombácz, E; Vékás, L., “Magnetic nanoparticle systems for nanomedicine-a materials science perspective”, *Magnetochemistry* **6**, 1 (2020).

Application differences of liquid and gel alcohol based handrubs formulations

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ABSTRACT

Hand disinfection using alcohol-based handrubs (ABHR, or hand sanitizers) is the cornerstone of hospital hygiene and infection control yet current clinical guidelines do not contain information regarding the hand sanitizer formulation, or application volume. The chemical and rheological differences of ABHRs result in practical differences (spreadability, evaporation rate) during their application, which results in efficiency differences we could impact infection control. In this study, we examined liquid and gel based ABHRs to investigate whether the difference in their physico-chemical parameters results in a significant difference in their successful clinical application and hand hygiene efficiency. In a laboratory setting, we examined handrub density, viscosity and evaporation rate, while in a clinical setting, we investigated spreadability, application time and ABHR dripping. Evaporation rates were times, viscosity was measured by SV-10 Vibrational Viscometer (A&D Co), spreadability was assessed by the Semmelweis Scanner (HandInScan Zrt.), and handrub dripping was evaluated with UV photography. According to our results, ABHR evaporation rates follow a linear pattern, which results in an average loss of 10 % of the initial volume in under 60 seconds. As the gel ABHR being more viscous spills less, and therefore larger volumes can be better handled however, liquid ABHRs can be spread better reaching high spreadability even at lower ABHR volumes. The conclusion is that an optimized handrub protocol would require different volumes for different hand sizes, and ABHR formulation. This research was funded by ÚNKP-21-4-I-SE-33 and ÚNKP-21-4-I-SE-13.

REFERENCE

Voniatis, C., et al. A large-scale investigation of alcohol-based handrub (ABHR) volume: hand coverage correlations utilizing an innovative quantitative evaluation system. *Antimicrob Resist Infect Control* 10, 49 (2021). <https://doi.org/10.1186/s13756-021-00917-8>

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